

# Développement d'équations d'état cubiques adaptées à la représentation de mélanges contenant des molécules polaires (eau, alcools, amines ...) et des hydrocarbures

Yohann Le Guennec

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# THÈSE

Présentée par

**Yohann LE GUENNEC**

Pour obtenir le grade de

DOCTEUR DE L'UNIVERSITÉ DE LORRAINE

Spécialité : Génie des Procédés, des Produits et des Molécules

École doctorale : SIMPPÉ

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# DÉVELOPPEMENT D'ÉQUATIONS D'ÉTAT CUBIQUES ADAPTÉES À LA REPRÉSENTATION DE MÉLANGES CONTENANT DES MOLÉCULES POLAIRES (EAU, ALCOOLS, AMINES ...) ET DES HYDROCARBURES

## MANUSCRIT DE THÈSE

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*"For many practical problems, old theories are sufficient provided that they are used with courage and imagination."*

John M. Prausnitz

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# Liste des abréviations, symboles, indices et exposants

| Abréviation | Signification |
|---|---|
| AC | Association Code |
| EoS | Equation of State |
| FH | Flory-Huggins |
| HV | Huron-Vidal |
| MAPE | Mean Absolute Pourcentage Error |
| MHV-1 | Modified Huron-Vidal with first order approximation |
| NRTL | Non Random Two Liquids |
| PPR78 | Predictive Peng-Robinson 1978 |
| PR | Peng-Robinson |
| RK | Redlich-Kwong |
| SG | Staverman-Guggenheim |
| SRK | Soave-Redlich-Kwong |
| UMR | Universal Mixing Rule |
| VDW | Van der Waals |
| VTPR | Volume Translated Peng-Robinson |

| Symbole latin | Signification | Unité |
|---|---|---|
| $a$ | paramètre énergétique | $Pa.m^6.mol^{-2}$ |
| $a$ | énergie d'Helmholtz molaire | $J.mol^{-1}$ |
| $b$ | covolume | $m^3.mol^{-1}$ |
| $B$ | second coefficient du viriel | $m^3.mol^{-1}$ |
| $c$ | paramètre de translation volumique | $m^3.mol^{-1}$ |
| $C$ | paramètre universel de la règle de mélange de HV | - |
| $c_P$ | capacité calorifique molaire isobare | $J.K^{-1}.mol^{-1}$ |
| $c_v$ | capacité calorifique molaire isochore | $J.K^{-1}.mol^{-1}$ |
| $f$ | fugacité | - |
| $g$ | potentiel chimique | $J.mol^{-1}$ |
| $h$ | enthalpie molaire | $J.mol^{-1}$ |
| $k$ | paramètre d'intération binaire | - |
| $L, M, N$ | paramètres de la fonction α de Twu | - |
| $m$ | paramètre de la fonction α de Soave | - |
| $n$ | nombre de moles | mol |
| $P$ | pression | Pa |
| $q_1$ | paramètre universel de la règle de mélange MHV-1 | - |
| $R$ | constante des gaz parfaits | $J.mol^{-1}.K^{-1}$ |
| $r$ | rayon de Van der Waals | $m^3.mol^{-1}$ |
| $r_1, r_2$ | paramètres universels de l'équation d'état | - |
| $s$ | entropie molaire | $J.K^{-1}.mol^{-1}$ |

| | | |
|---|---|---|
| *s* | paramètre universel de la règle de mélange sur b | - |
| *T* | température | K |
| *u* | énergie interne molaire | $J.mol^{-1}$ |
| *u, w* | paramètres universels de l'équation d'état | - |
| *v* | volume molaire | $m^3.mol^{-1}$ |
| *w* | vitesse du son | $m.s^{-1}$ |
| *x, y, z* | fraction molaire | - |
| *z* | compressibilité | - |

| Symboles grec | Signification | Unité |
|---|---|---|
| $\alpha$ | fonction alpha | - |
| $\alpha$ | coefficient de dilatation isobare | $K^{-1}$ |
| $\gamma$ | coefficient d'activité | - |
| $\Gamma$ | paramètre énergétique réduit | - |
| $\Delta_{vap}H$ | enthalpie de vaporisation | $J.mol^{-1}$ |
| $\eta$ | compacité | - |
| $\theta$ | fraction surfacique | - |
| $\kappa_T$ | coefficient de compressibilité isotherme | $Pa^{-1}$ |
| $\varphi$ | coefficient de fugacité | - |
| $\phi$ | fraction volumique | - |
| $\omega$ | facteur acentrique | - |

| Indice / exposant | Signification |
|---|---|
| 0 | non translaté |
| * | corps pur |
| • | gaz parfait |
| *c* | critique |
| *comb* | combinatoire |
| *E* | excès |
| *éc* | écart |
| *exp* | expérimental |
| *i, j* | indice du composé |
| *id* | idéal |
| *M* | mélange |
| *r* | réduit |
| *rés* | résiduel |
| *sat* | saturation |
| *t* | translaté |

# Introduction

Une connaissance (suffisamment) précise des propriétés thermodynamiques des corps purs et des mélanges est un préalable impérieux à la modélisation des procédés. Les grandeurs thermodynamiques d'intérêt pour l'étude des procédés sont principalement les propriétés d'équilibre entre phases, essentielles à la conception et la simulation des procédés de séparation par exemple, et les propriétés énergétiques (enthalpie, entropie, capacité calorifique) impliquées dans les bilans enthalpiques et exergétiques.

L'information relative au comportement des phases et aux propriétés énergétiques d'un système (corps pur ou mélange) peut être principalement générée de deux manières : soit on effectue des mesures, soit on utilise un modèle adapté pour les prévoir. Les mesures expérimentales présentent l'avantage de fournir une estimation généralement précise des propriétés d'intérêt. Elles présentent néanmoins l'inconvénient de n'être disponibles que pour un nombre discret de conditions expérimentales. Se posent alors les problèmes de l'interpolation et dans une plus large mesure, de l'extrapolation à d'autres conditions opératoires. Les modèles étant imparfaits, l'utilisation d'un modèle thermodynamique induit nécessairement des écarts plus ou moins importants entre les propriétés prédites par le modèle et les valeurs mesurées expérimentalement.

Les modèles contiennent fréquemment des paramètres ajustables (leurs valeurs ne sont pas fixées par la théorie) qui sont généralement régressés sur des données expérimentales. On notera par ailleurs que les modèles reposant sur des bases physiques sont généralement plus propices à la pratique de l'extrapolation que les modèles purement corrélatifs ne reposant sur aucun fondement physique.

Actuellement, il n'existe pas de modèle thermodynamique permettant de représenter avec une précision satisfaisante la variété d'équilibres entre phases pouvant exister dans la nature (liquide-vapeur, liquide-liquide, liquide-liquide-vapeur, solide-liquide, solide-vapeur…). Ainsi, le développement de modèles thermodynamiques toujours plus performants et polyvalents est un domaine actif de recherche.

Deux grandes familles de modèles thermodynamiques sont d'un usage courant : les modèles de coefficient d'activité et les équations d'état.

Un modèle de coefficient d'activité caractérise les déviations à l'idéalité des mélanges à l'état liquide. En le combinant à une équation d'état pour la phase gaz, on peut prévoir

des équilibres entre phases. Cette approche est toutefois limitée au domaine des basses pressions.

Les équations d'état sont divisées en deux catégories : elles peuvent être soit explicites en pression, soit explicites en volume. Seules les équations explicites en pression ont la capacité de prévoir des équilibres de phases, y compris ceux impliquant un composé supercritique. Parmi les équations d'état explicites en pression, utilisées dans l'industrie ou en recherche, sont généralement citées les équations d'état cubiques (Soave-Redlich-Kwong, Peng-Robinson …), les équations d'état de type SAFT (PC-SAFT, SOFT-SAFT …) et les équations d'état spécifiques à un constituant ou un mélange (BWR, GERG, Span-Wagner …).

Historiquement, les premières équations d'état cubiques (Van der Waals, Redlich-Kwong …) requéraient la connaissance de 2 paramètres expérimentaux (la température critique et la pression critique) pour décrire un corps pur. Les déviations calculées entre les prédictions de ces modèles et les données expérimentales de pression de vapeur saturante sont souvent très importantes. Pour les minimiser, un troisième paramètre fut introduit par Soave en accord avec la loi des états correspondants à 3 paramètres : le facteur acentrique. D'autres auteurs préconisent l'incorporation de paramètres ajustables dans les équations d'état cubiques en plus de la température critique et de la pression critique expérimentales (notamment à travers la fonction alpha du terme attractif).

Les équations d'état cubiques peuvent également être utilisées afin de modéliser des mélanges. Lorsque la théorie à un fluide est admise, la forme mathématique du modèle pour les mélanges reste la même que celle du modèle pour les corps purs. En revanche, les paramètres du corps pur doivent être remplacés par ceux du mélange. Les expressions de ces derniers sont appelées règles de mélange. Différentes approches existent pour les déterminer. Elles impliquent généralement un certain nombre de paramètres ajustables.

Pour être appliquées aux corps purs, les équations d'état de type SAFT nécessitent la connaissance d'au moins 3 paramètres (et parfois bien plus), ce nombre étant fonction du nombre de sites d'association affecté à chaque corps pur. À la différence des équations d'état cubiques, les équations d'état de type SAFT possèdent dans leur expression mathématique un terme décrivant le phénomène d'association par liaison hydrogène. La description des mélanges nécessite, comme pour les cubiques, l'adoption de règles de mélange et bien souvent, la détermination de paramètres

binaires ajustables. A l'heure actuelle, les équations de type SAFT peinent à tendre vers des versions industrialisées (c'est-à-dire contenant des paramètres de corps purs estimables pour toutes les molécules courantes selon une procédure universelle et robuste, et disposant de banque de données complètes ou de méthodes prédictives pour les paramètres binaires).

Enfin, les équations d'état spécifiques à un constituant ou un mélange reposent souvent sur un développement du viriel ou de l'énergie de Helmholtz et impliquent généralement plusieurs dizaines de paramètres ajustables par corps pur. Par leur flexibilité, ces modèles permettent une excellente représentation des données expérimentales. Cependant, l'ajustement des nombreux paramètres nécessite la connaissance d'un grand nombre de données expérimentales limitant ainsi ce type d'équations à un petit nombre de molécules ayant un intérêt industriel majeur.

Les équations d'état cubiques offrent donc un bon compromis entre universalité (c'est-à-dire la possibilité de les appliquer à tout corps pur et tout mélange) et précision. Par exemple, les versions originales des équations cubiques de Soave-Redlich-Kwong et de Peng-Robinson ont l'avantage d'être applicables à tout constituant pour lequel on dispose de valeurs de température critique, pression critique et facteur acentrique. Ces données sont souvent présentes dans des bases de données.

L'objectif de cette thèse est de définir une nouvelle équation d'état cubique permettant une amélioration significative de la représentation des équilibres entre phases et des propriétés énergétiques des systèmes contenant des molécules apolaires et polaires mais aussi des systèmes dans lesquels le phénomène d'association intervient et dont la modélisation par une équation d'état est classiquement jugée complexe.

**La première partie de ce manuscrit est dédiée à la recherche d'un modèle de type équation d'état cubique, garantissant** une bonne représentation des équilibres entre phases et des propriétés énergétiques des corps purs. Cette étude de la modélisation des corps purs, a mis en lumière l'absolue nécessité d'imposer de multiples contraintes mathématiques à la variation du terme attractif avec la température afin de garantir une extrapolation fiable au domaine supercritique. Deux modèles thermodynamiques induisant une excellente reproduction des propriétés à saturation et des propriétés énergétiques sont alors proposés.

La secon**de partie de ce manuscrit, s'intéresse à la modélisation des propriétés des mélanges. Elle pose l'ensemble des bases nécessaires au**

**développement de nouvelles équations d'état cubiques.** Les règles de mélange pouvant y être intégrées y sont discutées et une base de données de systèmes **binaires (équilibres de phases, enthalpies de mélange, points critiques ...)** permettant la validation et la comparaison des modèles thermodynamiques est proposée.

# Partie 1
# Étude des corps purs

# Chapitre 1. Les équations d'état cubiques appliquées aux corps purs ; bilan des connaissances acquises sur ce sujet depuis les travaux de Van der Waals

L'étude de la modélisation des corps purs par les équations d'état cubiques est un prérequis à l'étude des mélanges. L'approche ici proposée est chronologique et débute avec l'équation d'état de Van der Waals. Ce chapitre est un résumé de l'état de l'art en matière d'équations d'état cubiques au moment où mes travaux de thèse ont débuté. Les apports de ma thèse à ce sujet sont détaillés dans les chapitres suivants.

## 1.1. L'équation d'état de Van der Waals (1873)

L'équation d'état de Van der Waals [1] fut la première équation d'état capable de reproduire avec satisfaction les courbes isothermes expérimentales dans le plan (pression, volume) d'une quantité fixe de dioxyde de carbone mesurées par Andrews [2] quelques années plus tôt. Il existe une température en deçà de laquelle les isothermes dans le plan pression-volume présentent des paliers horizontaux, caractéristiques du domaine d'équilibre liquide-vapeur, et au-dessus de laquelle les isothermes sont strictement décroissantes. À la valeur exacte de cette température caractéristique, la courbe isotherme présente un point d'inflexion à tangente horizontale que l'équation de Van der Waals parvient à reproduire.

L'équation d'état proposée par Van der Waals en 1873 était donc capable de représenter les phénomènes d'équilibre liquide-vapeur des corps purs, ce qu'aucune autre équation d'état ne permettait jusqu'alors. Mieux encore, Van der Waals proposa un paramétrage permettant à son équation d'état de reproduire exactement la valeur expérimentale de cette température limite qui sera connue sous le nom de température critique, classiquement notée $T_c$.

L'équation d'état de Van der Waals des corps purs s'écrit :

$$P(T,v) = \frac{RT}{v-b} - \frac{a_c}{v^2} \tag{1.1}$$

avec $P$ la pression, $T$ la température et $v$ le volume molaire du système. Le paramètre $R$ est la constante des gaz parfaits et vaut 8,3144621 J.mol$^{-1}$.K$^{-1}$. Le paramètre $a_c$ est appelé paramètre attractif, le paramètre $b$ covolume.

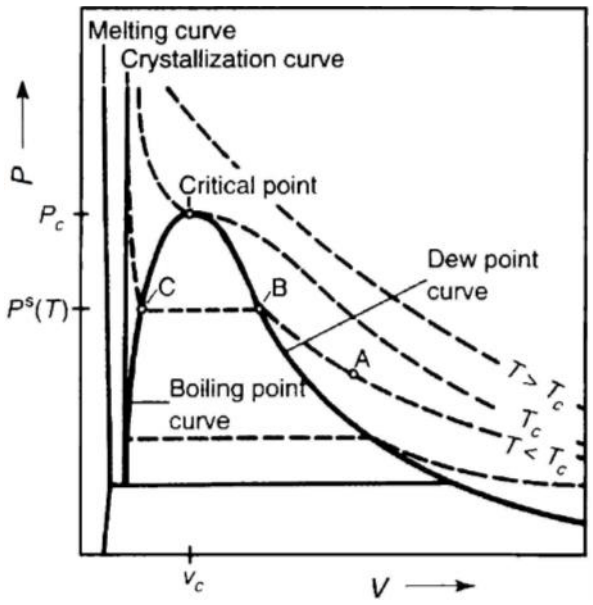



Figure 1.1. Représentation schématique du plan pression-volume d'un corps pur. Les courbes en pointillé sont les isothermes. Le palier horizontal de l'isotherme subcritique est ici représenté par le segment CB [3].

La loi des gaz parfaits ( $Pv = RT$ ), connue dès la fin du XVIIe siècle, qui ne permet pas de modéliser des équilibres liquide-vapeur, est obtenue lorsque l'on pose $b = 0$ et $a_c = 0$. Cette loi suppose que les molécules du système sont ponctuelles, c'est-à-dire que leur volume propre est nul, et qu'aucune force d'interaction ne s'exerce entre les molécules du système.

En comparaison, l'équation d'état de Van der Waals a été construite en considérant que les molécules du système ont toutes un volume propre incompressible et que par conséquent, le fluide possède un volume molaire minimal. Sous pression infinie ce volume molaire est atteint : les molécules sont dans un état de compacité maximale, leur volume molaire ne peut plus être réduit. Ce volume molaire minimal est appelé covolume et noté $b$. Pour un système composé de molécules non sujettes à des forces intermoléculaires, la prise en compte du volume propre des molécules peut être traduite par l'expression suivante, obtenue par modification de la loi des gaz parfaits :

$$P^{\text{répulsif}}(T, v) = \frac{RT}{v - b} \tag{1.2}$$

Ce terme est dit *répulsif*. À ceci, Van der Waals ajoute des interactions énergétiques attractives entre les molécules du système. Physiquement, ces interactions visent à réduire la pression dans le système en permettant à une molécule en mouvement d'être

« freinée » par ses plus proches voisines, diminuant ainsi sa vitesse d'impact sur les parois du système et donc la pression en son sein. Le terme attractif s'écrit alors :

$$P^{\text{attractif}}(T,v) = -\frac{a_c}{v^2} \tag{1.3}$$

Le terme attractif et le terme répulsif ont alors été combinés par Van der Waals pour obtenir son équation d'état. La distinction « terme répulsif », « terme attractif » est encore employée de nos jours afin d'identifier les différents membres des équations d'état cubiques.

L'équation (1.1) est dite « cubique », car elle peut être réécrite sous la forme d'une équation polynomiale de degré 3 du volume molaire $v$ :

$$v^3 - \left(1 + \frac{RT}{Pb}\right) b \times v^2 + \frac{a_c}{P} \times v - \frac{a_c b}{P} = 0 \tag{1.4}$$

Ainsi, l'équation d'état de Van der Waals permet, pour une valeur de la température et une valeur de la pression fixées, de déterminer le volume molaire du corps pur par recherche des racines du polynôme (1.4).

L'équation d'état de Van der Waals n'est cependant pas utilisée en pratique, car si elle décrit qualitativement les phénomènes de transition de phases fluides, elle ne permet pas de reproduire quantitativement les comportements expérimentaux. Les déviations entre les propriétés calculées par le modèle thermodynamique et les données expérimentales restent élevées. Ainsi, de nombreux modèles thermodynamiques dérivant du modèle de Van der Waals ont été proposés dans la littérature avec pour objectif d'améliorer la représentation des données expérimentales.

### 1.2. L'équation d'état cubique généralisée appliquée aux corps purs et son paramétrage par application des spécifications critiques

Toutes les équations d'état dérivant du modèle de Van der Waals admettent la forme générale suivante (si l'on exclut les équations d'état « translatées » qui seront discutées par la suite) :

$$P(T,v) = \frac{RT}{v-b} - \frac{a_c \times \alpha(T_r)}{(v - r_1 b)(v - r_2 b)} \tag{1.5}$$

En comparaison avec l'équation (1.1), de nouveaux termes sont apparus :

- La fonction $\alpha$ , propre au corps pur, qui introduit une dépendance en température dans le terme attractif de l'équation d'état. $T_r$ , la température réduite du corps pur, est définie comme le rapport de la température du système divisée par la température critique $T_c$ du composé.
- Les paramètres $r_1$ et $r_2$ , généralement indépendants du corps pur étudié. Le cas échéant, ces paramètres sont dits *universels*.

Une écriture alternative de l'équation (1.5) pouvant être rencontrée dans la littérature [4] fait intervenir des coefficients $u$ et $w$ plutôt que $r_1$ et $r_2$ :

$$P(T,v)=\frac{RT}{v-b}-\frac{a_c\times\alpha(T_r)}{v^2+ubv+wb^2} \tag{1.6}$$

Comme illustré dans le Tableau 1.1, si l'on choisit certaines valeurs spécifiques de $r_1$ et $r_2$ (ou respectivement $u$ et $w$ ) ainsi qu'une certaine expression de la fonction $\alpha$ , on retrouve des équations d'état cubiques couramment utilisées.

D'après Valderamma [5], plusieurs centaines d'équations d'état cubiques différentes ont été développées durant le siècle qui suivit la proposition de Van der Waals. Les quatre équations d'état reportées dans le Tableau 1.1 ne sont donc pas les seules équations ayant été reportées dans la littérature. Cependant, ce sont celles ayant connu les plus grands succès auprès de la communauté des thermodynamiciens des fluides, mais aussi des acteurs du monde industriel, notamment ceux du domaine pétrolier, au cours du 20e siècle.

| Équation **d'état** | Année | $r_1$ | $r_2$ | $u$ | $w$ | $\alpha$ |
|---|---|---|---|---|---|---|
| Van der Waals [1] | 1873 | 0 | 0 | 0 | 0 | 1 |
| Redlich-Kwong [6] | 1949 | $-1$ | 0 | 1 | 0 | $\frac{1}{\sqrt{T_r}}$ |
| Soave-Redlich-Kwong [7] | 1972 | $-1$ | 0 | 1 | 0 | $\begin{cases}\alpha=\left[1+m(\omega)\left(1-\sqrt{T_r}\right)\right]^2\\ m=0.480+1.574\omega\\ \quad -0.176\omega^2\end{cases}$ |
| Peng-Robinson [8] | 1976 | $-1-\sqrt{2}$ | $-1+\sqrt{2}$ | 2 | -1 | $\begin{cases}\alpha=\left[1+m(\omega)\left(1-\sqrt{T_r}\right)\right]^2\\ m=0.37464+1.54226\omega\\ \quad -0.26992\omega^2\end{cases}$ |

Tableau 1.1. Quelques équations d'état couramment utilisées ou rencontrées dans la littérature

### 1.2.1. Paramétrage par application des spécifications critiques

Les paramètres $a_c$ et $b$ sont traditionnellement déterminés par application des spécifications critiques, des spécifications qui traduisent mathématiquement la présence d'un point d'inflexion à tangente horizontale sur l'isotherme critique du composé étudié (comme observé sur la Figure 1.1) :

$$\begin{cases} P\left(T_c^{\exp}, v_c^{eos}\right) = P_c^{\exp} \\ \left(\frac{\partial P}{\partial v}\right)_T \left(T_c^{\exp}, v_c^{eos}\right) = 0 \\ \left(\frac{\partial^2 P}{\partial v^2}\right)_T \left(T_c^{\exp}, v_c^{eos}\right) = 0 \end{cases} \tag{1.7}$$

Les inconnues de ce système sont le volume molaire critique calculé par l'équation d'état $v_c^{eos}$ (*eos* étant l'abréviation de « Equation of State », le terme anglais pour « Équation d'état ») ainsi que les paramètres $a_c$ et $b$. La température critique expérimentale $T_c^{\exp}$ et la pression critique expérimentale $P_c^{\exp}$ du composé sont donc nécessaires pour résoudre l'équation (1.7). Ces grandeurs ont été mesurées pour de nombreux corps purs et certaines sont librement accessibles (site du NIST par exemple : https://webbook.nist.gov/chemistry/). On notera que le volume molaire

critique expérimental n'est pas utilisé pour effectuer le paramétrage par application des spécifications critiques.

Les expressions de $a_c$, $b$ et $v_c^{eos}$ obtenues par résolution du système d'équations (1.7) peuvent être exprimées en fonction de la compacité critique $\eta_c = b / v_c^{eos}$ qui elle-même ne dépend que de $r_1$ et $r_2$ :

$$\eta_c = \frac{1}{\sqrt[3]{(1-r_1)(1-r_2)^2} + \sqrt[3]{(1-r_2)(1-r_1)^2} + 1} \tag{1.8}$$

$$\begin{cases} a_c = \Omega_a \times \dfrac{\left(RT_c^{\exp}\right)^2}{P_c^{\exp}} \\ \Omega_a = \dfrac{(1-\eta_c r_1)(1-\eta_c r_2)\left[2-\eta_c(r_1+r_2)\right]}{(1-\eta_c)\left[3-\eta_c(1+r_1+r_2)\right]^2} \end{cases} \quad \begin{cases} b = \Omega_b \times \dfrac{RT_c^{\exp}}{P_c^{\exp}} \\ \Omega_b = \dfrac{\eta_c}{3-\eta_c(1+r_1+r_2)} \end{cases} \quad \text{et } v_c^{eos} = \frac{b}{\eta_c} \tag{1.9}$$

Les paramètres $r_1$ et $r_2$ étant universels (c.-à-d., les mêmes pour tous les corps purs), l'équation (1.8) montre que la compacité critique est également prédite universelle. La connaissance des expressions de $a_c$ et $b$ grâce aux équations (1.8) et (1.9) rend possible l'utilisation de l'équation d'état cubique.

Toujours par résolution du système d'équations (1.7), le volume molaire critique du corps pur calculé par l'équation d'état est alors estimé par la relation $v_c^{eos} = b / \eta_c$. Une conséquence directe est que le facteur de compressibilité critique du composé s'écrit :

$$z_c^{eos} = \frac{P_c^{\exp} v_c^{eos}}{RT_c^{\exp}} = \frac{1}{3-\eta_c(1+r_1+r_2)} \tag{1.10}$$

L'équation (1.10) montre que l'expression de $z_c^{eos}$ est la même quel que soit le composé étudié, $r_1$, $r_2$ et $\eta_c$ étant les mêmes pour tous les corps purs. L'équation d'état étant contrainte par application des spécifications critiques à reproduire exactement les valeurs de la température critique expérimentale et de la pression critique expérimentale, une déviation sur le facteur de compressibilité critique de l'équation d'état calculé ne pourra se traduire que par un écart sur le volume molaire critique du composé calculé par l'équation d'état.

Les valeurs de $z_c^{eos}$ des quatre équations d'état issues du Tableau 1.1 sont reportées dans le Tableau 1.2 :

| **Équation d'état** | $z_c^{eos}$ |
|---|---|
| Van der Waals | 0.375 |
| Redlich-Kwong | 0.333 |
| Soave-Redlich-Kwong | |
| Peng-Robinson | 0.3074 |

Tableau 1.2. Valeurs du facteur de compressibilité critique calculé par application des spécifications critiques pour différentes équations d'état

En comparaison, la distribution des facteurs de compressibilité critiques expérimentaux est illustrée sur la Figure 1.2 :

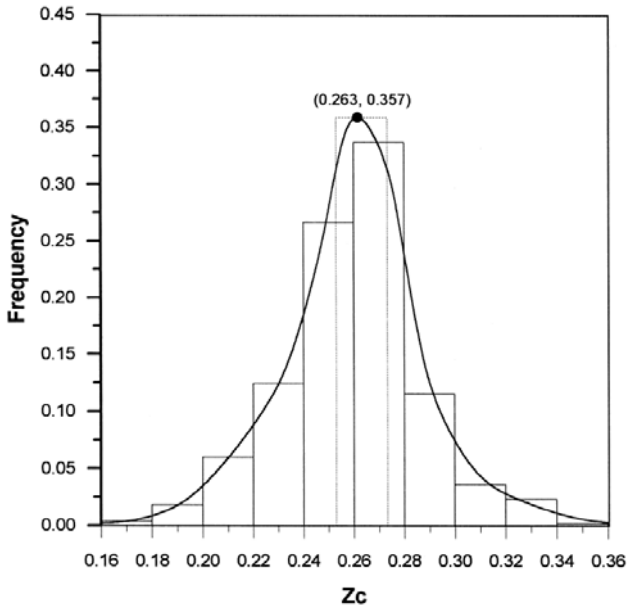



Figure 1.2. Distribution des facteurs de compressibilité critiques (statistiques réalisées pour 555 corps purs) [9]

Une valeur moyenne de 0.263 est obtenue pour le facteur de compressibilité critique, soit une déviation de 42% par rapport à la valeur calculée avec l'équation de Van der Waals qui sera nécessairement égale à la déviation moyenne sur le volume molaire critique. En pratique, on observe que la déviation sur le volume molaire critique causée par l'application des spécifications critiques se propage en partie aux volumes molaires et en particulier à ceux de la phase liquide. Il s'ensuit que les propriétés volumiques de la phase liquide (densité, compressibilité isotherme ...) sont entachées d'une erreur significative.

### 1.2.2. L'équation d'état de Redlich-Kwong (1949)

Dans l'objectif d'améliorer la reproduction des propriétés PVT (pression-volume molaire-température) des corps purs, Redlich et Kwong [6] proposèrent deux modifications de l'équation de Van der Waals :

- D'une part, la modification des valeurs des paramètres $r_1$ et $r_2$ ,
- D'autre part, l'introduction d'une fonction $\alpha$ dépendant de la température.

Ces modifications induisent la diminution de la valeur du facteur de compressibilité critique calculé par l'équation d'état. Ce faisant, un facteur de compressibilité critique de 0.333 est obtenu conduisant à une amélioration de la reproduction de facteur de compressibilité sur l'ensemble du domaine de température et de pression pour les composés considérés par les auteurs comme le méthane, l'éthane, le n-butane (Figure 1.3), l'hydrogène et le dioxyde de carbone.

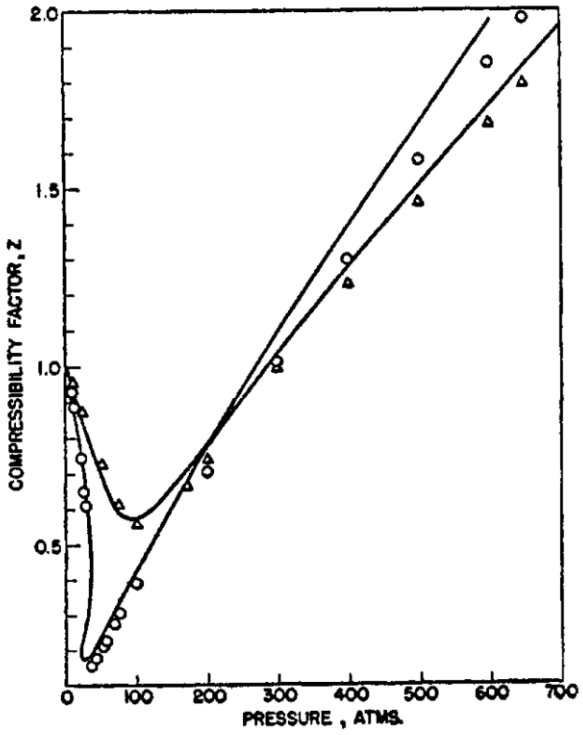



Figure 1.3. Reproduction des facteurs de compressibilité expérimentaux du n-butane par l'équation de Redlich-Kwong à 137.8°C et 237.8°C [6]

Bien que la prédiction des pressions de vapeur saturante soit grandement améliorée par rapport à l'équation de Van der Waals, elle reste insatisfaisante pour un grand nombre de composés.

### 1.2.3. L'équation de Soave-Redlich-Kwong (1972)

Soave [7] a proposé une fonction $\alpha$ différente de celle utilisée par Redlich et Kwong qui a conduit à une nette amélioration de la reproduction des pressions de vapeur saturante des corps purs. L'avantage de la formulation proposée par Soave est que celle-ci est entièrement définie par la valeur du facteur acentrique $\omega$ du corps pur, une quantité introduite par Pitzer [10,11] et révélatrice de la non sphéricité d'une molécule. Les valeurs du facteur acentrique sont disponibles dans la littérature pour un grand nombre de corps purs :

$$\begin{cases} \alpha = \left[1 + m(\omega)\left(1 - \sqrt{T_r}\right)\right]^2 \\ m = 0.480 + 1.574\omega - 0.176\omega^2 \end{cases} \tag{1.11}$$

L'utilisation de cette fonction $\alpha$ permet une excellente reproduction des pressions de vapeur saturante des composés apolaires comme illustré dans le Tableau 1.3 où une déviation inférieure à 5% est toujours obtenue là où des déviations allant jusqu'à 400% sont obtenues avec l'équation de Redlich-Kwong :

| Composé | Redlich-Kwong | Soave-Redlich-Kwong |
|---|---|---|
| Ethylène | 20.1% | 2.0% |
| Propylène | 23.5% | 0.7% |
| Propane | 28.8% | 2.0% |
| Isobutane | 52.4% | 2.4% |
| Cyclopentane | 66.0% | 0.8% |
| Toluène | 129.0% | 0.8% |
| n-hexane | 159.0% | 1.9% |
| n-octane | 268.0% | 2.1% |
| n-decane | 402.0% | 1.0% |

Tableau 1.3. Déviations relatives entre valeurs calculées et expérimentales de la pression de vapeur saturante de 9 corps purs. Les déviations ont été calculées sur une gamme de températures réduites supérieures à 0.4 [7].

Cependant, l'équation d'état de Redlich-Kwong modifiée par Soave (abrégée en SRK) ne permet toujours pas de calculer avec une précision acceptable les volumes molaires du liquide à saturation.

### 1.2.4. L'équation d'état de Peng-Robinson (1976)

Peng et Robinson proposent en 1976 [8] une équation d'état cubique permettant d'améliorer le calcul des volumes molaires liquides. Pour ce faire, ils s'inspirent des modifications proposées par Redlich et Kwong puis Soave en redéterminant les valeurs des paramètres $r_1$ et $r_2$ d'une part, ainsi qu'en développant une nouvelle expression polynomiale du paramètre $m$ de la fonction $\alpha$ de Soave, d'autre part. Une nette amélioration de la reproduction des volumes molaires liquides est atteinte, tant que la température réduite reste inférieure à 0.9 (Figure 1.4) tout en garantissant également une excellente reproduction des pressions de vapeur saturante.

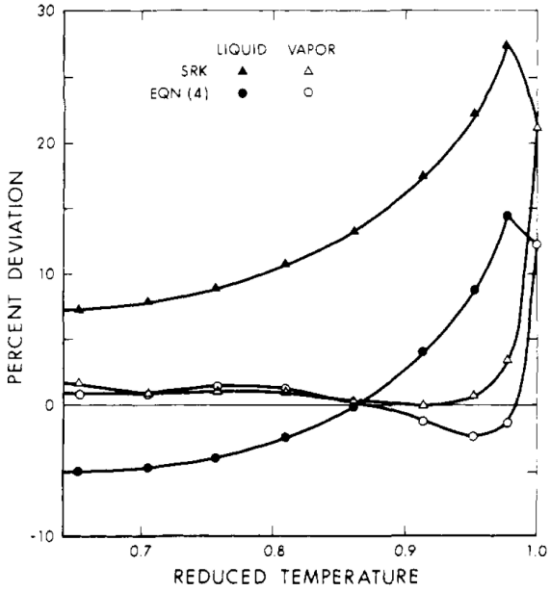



Figure 1.4. Erreurs sur les volumes molaires liquides et gazeux calculés par l'équation d'état de Soave-Redlich-Kwong et de Peng-Robinson [8]

### 1.3. Les voies d'amélioration des équations d'état cubiques explorées

Depuis la proposition initiale de Van der Waals jusqu'aux travaux de Peng et Robinson, deux grandes voies d'amélioration ont été proposées :

- La modification des paramètres $r_1$ et $r_2$, qui permet, entre autres, d'améliorer la reproduction des propriétés volumiques à saturation.
- L'ajout d'une dépendance en température dans le terme attractif de l'équation d'état grâce à la fonction $\alpha$, la plus connue étant celle proposée par Soave, permettant une meilleure représentation des pressions de vapeur saturante.

Ces deux voies d'amélioration ont été grandement poursuivies par les chercheurs à travers le monde, dans l'objectif d'améliorer la reproduction des données expérimentales par les modèles thermodynamiques.

### 1.3.1. Modification des paramètres $r_1$ et $r_2$

Les équations d'état proposées par Redlich et Kwong ainsi que Peng et Robinson considèrent des paramètres $r_1$ et $r_2$ universels.

On rappelle qu'il est équivalent, comme cela est fait dans cette section, car il s'agit de l'approche choisie par les auteurs des publications citées, de parler des paramètres $r_1$ et $r_2$ ou des paramètres $u$ et $w$.

Comme observé par Schmidt et Wenzel [12], les paramètres $u$ et $w$ des équations de Redlich-Kwong, Peng-Robinson et Harmens [13] (une équation d'état spécifique au mélange $N_2$-$O_2$-Ar) respectent la contrainte mathématique suivante :

$$u + w = 1 \tag{1.12}$$

Ces auteurs observent aussi que l'équation d'état de Redlich-Kwong convient mieux aux composés ayant un facteur acentrique de 0 tandis que l'équation de Peng-Robinson permet une meilleure représentation des molécules ayant un facteur acentrique de 0.35. Schmidt et Wenzel décident alors d'imposer la contrainte suivante sur le paramètre $w$ :

$$w = -3\omega \tag{1.13}$$

Ainsi :

$$\underbrace{\begin{cases} w(\omega = 0) = 0 \\ u(\omega = 0) = -1 \end{cases}}_{\substack{\text{Redlich-Kwong} \\ \text{si } \omega = 0}} \text{ et } \underbrace{\begin{cases} w(\omega = 0.35) \approx -1 \\ u(\omega = 0.35) \approx 2 \end{cases}}_{\substack{\text{Peng-Robinson} \\ \text{si } \omega \approx 0.35}} \tag{1.14}$$

Ainsi, l'équation d'état de Schmidt et Wenzel admet des valeurs de $r_1$ et $r_2$ (ou de manière équivalente $u$ et $w$) fonctions du facteur acentrique du corps pur choisi. Ce faisant, les auteurs obtiennent des déviations sur les pressions de saturation très proches de celles calculées avec l'équation de Peng-Robinson (0.90% au lieu de 0.91%), mais une nette amélioration de la représentation des densités liquides à saturation qui passe de 4.74% avec l'équation de Peng-Robinson à 1.80% avec l'équation de Schmidt

et Wenzel pour des composés apolaires ou faiblement polaires loin de leur température critique.

Forts de ce succès, d'autres auteurs ont proposé des équations d'état cubiques considérant des valeurs de $r_1$ et $r_2$ variables : l'équation de Harmens et Knapp [14] la même année que celle de Schmidt et Wenzel ainsi que celle de Patel et Teja [15] deux ans plus tard. Des conclusions similaires à celle de Schmidt et Wenzel sont obtenues.

Bien que cette approche permette une nette amélioration des volumes molaires du liquide à saturation et puisse permettre une légère amélioration du calcul de la pression de saturation, elle n'est pas largement utilisée. En effet, le fait que les paramètres $r_1$ et $r_2$ dépendent du corps pur étudié rend difficile le passage aux mélanges pour lesquels il faut alors déterminer des valeurs de $r_1$ et $r_2$ propres à l'équation d'état du mélange, parfois en introduisant un paramètre supplémentaire à ajuster, rendant l'ajustement des paramètres des mélanges plus complexe.

Une autre méthodologie de modification des équations d'état consiste à jouer sur la fonction $\alpha$ pour améliorer la représentation des pressions de vapeur saturante, et à introduire un paramètre de translation volumique (dont l'intégration dans l'équation d'état des mélanges est plus aisée) afin d'améliorer la représentation des densités liquides.

### 1.3.2. Les fonctions α

Comme montré par Soave, l'ajout de sa fonction $\alpha$ (dépendant de la température) dans l'équation d'état cubique permet une nette amélioration de la représentation des pressions de vapeur saturante et seulement une faible amélioration des volumes molaires liquides.

Les fonctions $\alpha$ peuvent être classées en deux catégories : *généralisées* ou *spécifiques*. En effet, une fonction $\alpha$ dont la détermination de la valeur numérique à une température donnée ne nécessite que la connaissance du facteur acentrique et de la température critique du corps pur est dite *généralisée*. À l'inverse, certaines fonctions $\alpha$ dites *spécifiques* détaillées par la suite utilisent un certain nombre de paramètres spécifiques au constituant considéré qui doivent être préalablement ajustés sur des données expérimentales, permettant ainsi une meilleure reproduction desdites données expérimentales. En contrepartie, ces fonctions $\alpha$ ne sont donc pas utilisables s'il n'existe pas de données expérimentales, à l'inverse des fonctions $\alpha$ généralisées.

### 1.3.3. Procédure d'ajustement des fonctions α

Que ce soit afin d'ajuster les paramètres propres au corps pur dans le cas d'une fonction $\alpha$ spécifique ou ses paramètres universels dans le cas d'une fonction $\alpha$ généralisée, il est nécessaire de définir quelles sont les propriétés thermodynamiques dont on cherche à améliorer la reproduction. Pour des raisons pratiques, les pressions de vapeur saturante sont généralement les seules propriétés sur lesquelles sont ajustées les fonctions $\alpha$. En effet, on sait qu'il est primordial pour une équation d'état cubique de bien représenter cette propriété si l'on souhaite modéliser avec précision les équilibres liquide-vapeur des systèmes multiconstituants. De plus, il existe de nombreuses données de pression de vapeur saturante dans la littérature, certaines ayant été utilisées pour ajuster les paramètres de la loi d'Antoine, permettant ainsi de générer une grande quantité de pseudo-points expérimentaux à partir de ceux préalablement mesurés.

Comme étudié par Neau et al. [16,17], les fonctions $\alpha$ généralisées existant dans la littérature permettent une représentation satisfaisante de propriétés à saturation autres que la pression de vapeur saturante alors qu'elles n'ont pas été ajustées dessus : l'enthalpie de vaporisation ainsi que la capacité calorifique du liquide à saturation. Des résultats satisfaisants sont aussi obtenus pour l'enthalpie et la capacité calorifique dans le domaine supercritique.

Privat et al. [18] ont cependant réalisé l'ajustement des paramètres des fonctions $\alpha$ non généralisées sur les propriétés suivantes : pression de saturation, enthalpie de vaporisation et capacité calorifique du liquide à saturation. Des déviations très faibles entre le modèle et les données expérimentales sont obtenues, validant l'intérêt d'utiliser des propriétés supplémentaires aux pressions de vapeur saturante pour l'ajustement des paramètres de fonctions $\alpha$ non généralisées. Cependant, il existe des corps purs pour lesquels les données d'enthalpie de vaporisation ou de capacité calorifique du liquide à saturation sont indisponibles. Cette observation amène la question : quelles propriétés doivent être a minima incluses dans la **procédure de régression des paramètres de la fonction α afin d'obtenir des** résultats satisfaisants ?

De plus, cette procédure d'ajustement des paramètres de la fonction $\alpha$ se base uniquement sur des données subcritiques (les grandeurs à saturation) alors que la fonction $\alpha$ doit pouvoir être utilisée dans le domaine supercritique, c'est-à-dire en extrapolation. À cause du grand nombre de paramètres pouvant être présents dans ces

fonctions $\alpha$ non généralisées, il existe un risque important que l'extrapolation de ces fonctions à haute température n'ait aucun sens physique. Notons qu'une mauvaise représentation des propriétés supercritiques des corps purs se répercuterait nécessairement sur la modélisation des systèmes multiconstituants. La question suivante peut alors être posée : les paramètres des fonctions $\alpha$ spécifiques, ajustés sur des données **d'équilibre liquide**-vapeur, peuvent-ils être utilisés en extrapolation pour estimer des propriétés supercritiques ? Comme nous allons le voir par la suite, il existe un nombre limité de contraintes théoriques que doivent respecter les fonctions $\alpha$ ; aucune d'elles ne permet d'apporter une réponse au questionnement précédent (indiqué en gras).

Dans un premier temps, un état des lieux de ces contraintes est effectué puis quelques fonctions $\alpha$ de la littérature sont passées en revue. Les réponses aux questions posées dans cette section ainsi que les suivantes trouveront leurs réponses dans les articles accompagnant ce manuscrit.

#### 1.3.3.1. Contraintes sur les fonctions α

Par construction, on impose à toutes les fonctions $\alpha$ d'être unitaires à la température critique :

$$\alpha(T_r = 1) = 1 \tag{1.15}$$

Le numérateur du terme attractif s'écrivant $a(T_r) = a_c \times \alpha(T_r)$, la fonction $\alpha$ peut donc être considérée comme une correction à apporter au terme attractif en dehors du point critique, ce dernier étant parfaitement représenté lorsque les paramètres $a_c$ et $b$ sont déterminés par application des spécifications critiques et ne nécessitent donc pas de correction.

Si la fonction $\alpha$ venait à être négative pour certaines valeurs de température, le terme attractif de l'équation d'état jouerait le rôle du terme répulsif, augmentant ainsi la pression du système. Un tel résultat irait à l'encontre de la théorie de Van der Waals pour qui les forces attractives diminuent la pression du système. La fonction $\alpha$ doit donc être positive.

Si les dérivées successives de la fonction $\alpha$ par rapport à la température présentent des discontinuités, les propriétés thermodynamiques dérivées telles que l'enthalpie et les capacités calorifiques présenteront également des discontinuités qui ne sont pas observées expérimentalement. Ces propriétés dépendant respectivement des dérivées

premières et secondes de la fonction $\alpha$, la fonction $\alpha$, sa dérivée première et sa dérivée seconde doivent donc être des fonctions continues de la température [16,17].

Enfin, il est observé en pratique que la fonction $\alpha$ doit être décroissante afin d'améliorer la reproduction des données expérimentales par l'équation d'état.

En conclusion, avant le début de cette thèse, les fonctions $\alpha$ devaient respecter l'ensemble des contraintes suivantes :

$$\begin{cases} \alpha\left(T_r = 1\right) = 1 \\ \alpha > 0 \\ \dfrac{d\alpha}{dT_r} < 0 \\ \alpha\left(T_r\right) \in C^2 \end{cases} \tag{1.16}$$

D'autres conditions empiriques ont été proposées par Twu [19] :

- La fonction $\alpha$ doit tendre vers o lorsque la température tend vers l'infini.
  Il est en effet commun de supposer que les forces d'interaction énergétiques, c'est-à-dire le terme attractif de l'équation d'état, sont nulles entre les molécules du système à haute température et que seules les forces répulsives gouvernent la physique du système. Cependant, il n'existe pas de démonstration mathématique permettant de valider cette hypothèse.
- La fonction $\alpha$ doit pouvoir présenter un maximum afin d'être en mesure de représenter les fluides quantiques (des molécules ayant un comportement particulier à basse température) tels que l'hélium et l'hydrogène.
  Ces molécules sont des cas particuliers qui ne s'insèrent pas dans la théorie de Van der Waals généralisée dont une conséquence est la stricte décroissance de la fonction $\alpha$, interdisant la présence d'un maximum. La fonction $\alpha$ est donc utilisée pour compenser un défaut théorique de l'équation d'état cubique quant à la représentation des fluides quantiques.
- La fonction $\alpha$ doit pouvoir représenter les pressions de vapeur saturante des composés depuis le point triple jusqu'au point critique.
  L'utilisation de fonctions $\alpha$ ayant des paramètres ajustables plutôt que des fonctions $\alpha$ généralisées peut permettre d'accroître la précision des équations d'état cubiques en matière de pressions de vapeur saturante.

Dans l'article [20] présenté dans le chapitre qui suit, nous nous sommes intéressés en détail aux contraintes à imposer aux fonctions $\alpha$. Cette étude a abouti à l'établissement d'une liste de contraintes augmentée par rapport à celle présentée ci-dessus.

Il est désormais possible de lister les fonctions $\alpha$ couramment utilisées, que ce soit dans des publications scientifiques ou dans des simulateurs de procédés, et de vérifier si celles-ci respectent les contraintes précédemment énoncées.

#### 1.3.3.2. Les fonctions α polynomiales

Les fonctions $\alpha$ pouvant se réécrire sous la forme d'un polynôme de la racine carrée de la température réduite sont dites polynomiales. À titre d'exemple, la fonction $\alpha$ de Soave se réécrit :

$$\alpha(T_r)=\left[1+m\left(1-\sqrt{T_r}\right)\right]^2 \Rightarrow \alpha(X)=(1+m)^2-2m(1+m)X+m^2X^2 \qquad (1.17)$$

avec $X=\sqrt{T_r}$. Une telle forme polynomiale impose à la fonction $\alpha$ de diverger vers $+\infty$ lorsque la température tend vers $+\infty$, imposant nécessairement à la fonction $\alpha$ d'être croissante à haute température, ce qui va à l'encontre des contraintes sur les fonctions $\alpha$. Heureusement, cette divergence de la fonction $\alpha$ polynomiale ne se manifeste que pour des températures réduites très élevées pour lesquelles il n'y a pas ou peu de procédés industriels développés, limitant ainsi le problème en pratique.

La première fonction $\alpha$ polynomiale proposée a été celle de Soave. Très utilisée en raison de ses excellentes performances et de son caractère généralisé, elle présente néanmoins quelques défauts mis en évidence dans la littérature [15,19,21]:

- Mauvaise reproduction des pressions de vapeur saturante des composés lourds à basse température
- Mauvaise reproduction des pressions de vapeur saturante des molécules polaires à toute température, sauf au voisinage du point critique

Les fonctions $\alpha$ présentées ci-dessous sont des propositions visant à combler ces lacunes en modifiant la fonction $\alpha$ de Soave tout en conservant une expression relativement similaire à la sienne.

La fonction généralisée $\alpha$ développée par Peng et Robinson en 1978 [22] considère différentes expressions de $m$ en fonction de la valeur du facteur acentrique dans la fonction $\alpha$ de Soave :

$$\begin{cases} \alpha(T_r) = \left[1 + \kappa\left(1 - \sqrt{T_r}\right)\right]^2 \\ \kappa(\omega \le 0.491) = 0.37464 + 1.54226\omega - 0.26992\omega^2 \\ \kappa(\omega > 0.491) = 0.379642 + 1.48503\omega - 0.164423\omega^2 + 0.016666\omega^3 \end{cases} \quad (1.18)$$

Alors que la fonction $\alpha$ de Soave avait été ajustée uniquement sur des composés ayant un facteur acentrique inférieur ou égal à 0.5, les coefficients polynomiaux de cette fonction $\alpha$ pour les composés dont le facteur acentrique est supérieur à 0.491 ont été ajustés sur les pressions de vapeur saturante de molécules ayant un facteur acentrique compris entre 0.2 et 2.0, évitant ainsi d'utiliser la fonction $\alpha$ en extrapolation.

Cette fonction $\alpha$ est utilisée dans les modèles PPR78 [23,24] pour l'ensemble des composés ainsi que NRTL-PR [25] pour les hydrocarbures et les composés non associés.

La fonction spécifique $\alpha$ de Mathias-Copeman [26] vise à améliorer la représentation des composés polaires en introduisant 3 paramètres ajustables $c_1$, $c_2$ et $c_3$ par corps pur :

$$\alpha(T_r) = \left[1 + c_1\left(1 - \sqrt{T_r}\right) + c_2\left(1 - \sqrt{T_r}\right)^2 + c_3\left(1 - \sqrt{T_r}\right)^3\right]^2 \quad (1.19)$$

En effet, il a été observé qu'il est nécessaire d'utiliser jusqu'à 3 paramètres par corps pur afin d'obtenir une bonne représentation des composés polaires et associés alors qu'un seul paramètre est suffisant pour les autres molécules. Grâce à sa flexibilité, cette fonction $\alpha$ est utilisée dans de nombreux modèles dont PSRK [27] et dans une version modifiée d'UNIFAC [28]. Dans le cas où $c_2 = c_3 = 0$ et $c_1 = m$, la fonction $\alpha$ de Soave est obtenue. En pratique cette fonction $\alpha$ est souvent découpée en deux parties : dans le domaine subcritique, l'équation (1.19) est utilisée tandis que dans le domaine supercritique, l'équation (1.19) avec $c_2 = c_3 = 0$ est utilisée, créant ainsi une discontinuité des propriétés dérivées au point critique [16,17].

Les fonctions $\alpha$ de Stryjek-Vera des modèles PRSV [29] et PRSV2 [30] visent à améliorer la reproduction des pressions de saturation à basse température en ajoutant une dépendance en température dans le paramètre $m$ de la fonction de Soave. La fonction $\alpha$ du modèle PRSV2 s'écrit alors :

$$\begin{cases} \alpha(T_r) = \left[1 + \kappa\left(1 - \sqrt{T_r}\right)\right]^2 \\ \kappa = \kappa_0 + \left[\kappa_1 + \kappa_2\left(\kappa_3 - T_r\right)\left(1 - \sqrt{T_r}\right)\right]\left(1 + \sqrt{T_r}\right)\left(0.7 - T_r\right) \\ \kappa_0 = 0.378893 + 1.4897153\omega - 0.17131848\omega^2 + 0.0196544\omega^3 \end{cases} \quad (1.20)$$

Les paramètres $\kappa_1$, $\kappa_2$ et $\kappa_3$ sont des paramètres ajustables. Si $\kappa_2 = 0$ la fonction $\alpha$ du modèle PSRV est obtenue. Cette fonction $\alpha$ montre bien la nécessité d'introduire une dépendance en température plus complexe que celle initialement proposée par Soave pour reproduire les systèmes à basse température, mais également l'ajout de nombreux paramètres ajustables.

On notera enfin les propositions successives faites par Soave ayant pour objectif d'obtenir une fonction $\alpha$ comblant les lacunes de sa fonction $\alpha$ de 1972. Bien que permettant en effet une amélioration de la représentation des propriétés thermodynamiques, les fonctions $\alpha$ proposées sont spécifiques et nécessitent donc des paramètres ajustables pour chaque corps pur. Aucune de ces fonctions $\alpha$ ne connut la gloire de sa fonction de 1972.

#### 1.3.3.3. Les fonctions *α* exponentielles

Les fonctions $\alpha$ exponentielles ont été introduites par Heyen [34] puis popularisées par Twu et al. [19,35]. Ces fonctions, apparues à la fin des années 1980, ont pour principal intérêt de ne pas diverger à haute température, contrairement aux fonctions $\alpha$ polynomiales.

La fonction $\alpha$ proposée par Heyen a la forme suivante :

$$\alpha(T_r) = \exp\left[k\left(1 - T_r^n\right)\right] \quad (1.21)$$

Les paramètres *k* et *n* sont corrélables au facteur acentrique des corps purs, mais les corrélations données par Heyen ne sont pas applicables aux équations de Soave-Redlich-Kwong ou de Peng-Robinson. Elles conviennent pour une autre équation non détaillée dans le présent manuscrit.

Twu et al. ont alors proposé une expression à 2 [35] puis 3 [19] paramètres ajustables pour plus de flexibilité :

$$\alpha(T_r) = T_r^{N(M-1)} \exp\left[L\left(1 - T_r^{MN}\right)\right] \quad (1.22)$$

La fonction de Heyen est obtenue si $M=1$. La fonction de Twu à 3 paramètres présente l'avantage d'être flexible et de permettre une excellente représentation des pressions de vapeur saturante sur tout le domaine de température pour des molécules apolaires et polaires. Cependant, l'ajustement des 3 paramètres requiert un nombre important de données expérimentales. Pour pallier le manque éventuel de données, Twu et al. ont alors proposé une version généralisée de leur fonction $\alpha$ [36,37] qui dépend linéairement du facteur acentrique :

$$\begin{cases} \alpha = \alpha^{(0)} + \omega\left[\alpha^{(1)} - \alpha^{(0)}\right] \\ \alpha^{(0)} = T_r^{N^{(0)}\left[M^{(0)}-1\right]} \exp\left[L^{(0)}\left(1 - T_r^{M^{(0)}N^{(0)}}\right)\right] \\ \alpha^{(1)} = T_r^{N^{(1)}\left[M^{(1)}-1\right]} \exp\left[L^{(1)}\left(1 - T_r^{M^{(1)}N^{(1)}}\right)\right] \end{cases} \quad (1.23)$$

Les valeurs des paramètres sont données dans le Tableau 1.4.

| | | $T_r \leq 1$ | | $T_r > 1$ | |
|---|---|---|---|---|---|
| | | $\alpha^{(0)}$ | $\alpha^{(1)}$ | $\alpha^{(0)}$ | $\alpha^{(1)}$ |
| Redlich-Kwong | L | 0.141599 | 0.500315 | 0.441411 | 0.032580 |
| | M | 0.919422 | 0.799457 | 6.500018 | 1.289098 |
| | N | 2.496441 | 3.291790 | -0.200000 | -8.000000 |
| Peng-Robinson | L | 0.125283 | 0.511614 | 0.401219 | 0.024955 |
| | M | 0.911807 | 0.784054 | 4.963070 | 1.248089 |
| | N | 1.948150 | 2.812520 | -0.200000 | -8.000000 |

Tableau 1.4. Paramètres universels de la fonction α de Twu généralisée

La fonction $\alpha$ de Twu généralisée est découpée en deux parties : l'une applicable au domaine subcritique de température et l'autre applicable au domaine supercritique de température. Pour le domaine subcritique, les paramètres ont été ajustés sur les données de pression de vapeur saturante d'hydrocarbures. Dans le domaine supercritique, certains paramètres ont été ajustés afin que les dérivées premières et secondes des fonctions $\alpha$ soient continues au point critique afin d'éviter que certaines propriétés physiques calculées soient discontinues tandis que d'autres ont été ajustés afin de reproduire des données de solubilité de l'hydrogène dans des hydrocarbures.

Cette fonction $\alpha$ permet une meilleure reproduction des pressions de vapeur saturante à basse température que les fonctions $\alpha$ de Soave et de Stryjeck-Vera. Cependant, à cause de l'absence de paramètres ajustables, son utilisation se limite principalement aux systèmes apolaires.

#### 1.3.3.4. Comment générer des fonctions α exponentielles à partir de fonctions α polynomiales ?

Mahmoodi et Sedigh [38] ont proposé une méthode permettant de convertir une fonction polynomiale en une fonction exponentielle grâce à l'utilisation de développements limités autour du point critique du corps pur. Cette méthode est peu utilisée ; elle a pour principal intérêt d'éviter le problème de divergence des fonctions $\alpha$ polynomiales à haute température. Comme évoqué précédemment, ce problème de divergence est toutefois négligeable en pratique. À titre d'exemple, le développement limité à l'ordre 1 du logarithme de la fonction $\alpha$ de Soave autour du point critique est :

$$\ln(\alpha) = 2m\left(1-\sqrt{T_r}\right) \tag{1.24}$$

La fonction $\alpha$ résultante est alors :

$$\alpha = \exp\left[2m\left(1-\sqrt{T_r}\right)\right] \tag{1.25}$$

qui n'est autre que la fonction $\alpha$ de Heyen avec $k = 2m$ et $n = 0.5$. Cependant, pour que des résultats précis soient obtenus, les paramètres du polynôme donnant les variations de $m(\omega)$ doivent être réajustés avant toute utilisation de la fonction $\alpha$ exponentielle.

#### 1.3.3.5. Conclusions sur les fonctions α

Un nombre limité de fonctions $\alpha$ a été présenté dans ce manuscrit ; les fonctions décrites précédemment sont jugées représentatives des évolutions majeures qui ont pu être apportées aux fonctions $\alpha$. La représentation des pressions de vapeur saturante à basse température pour des composés lourds et polaires peut être correctement effectuée si une fonction $\alpha$ avec au moins 3 paramètres ajustables est utilisée. Pour les molécules apolaires pour lesquelles aucune donnée expérimentale ne serait disponible afin de réaliser l'ajustement des paramètres, l'utilisation d'une fonction $\alpha$ généralisée, telle que celle de Twu, est à privilégier.

Les fonctions $\alpha$ ne permettent cependant pas une amélioration des volumes molaires des corps purs alors qu'il s'agit là de leur principal point faible. Comme montré

précédemment, la l'ajustement des paramètres $r_1$ et $r_2$ de l'équation d'état pour chaque corps pur (équation de Patel-Teja par exemple) permet une nette amélioration de la restitution des volumes molaires, mais peut difficilement être appliquée à des mélanges, car il devient alors nécessaire de corréler les paramètres $r_1$ et $r_2$ du mélange à ceux des corps purs. La méthode de translation volumique vise à apporter une réponse alternative tout aussi efficace et plus aisément transposable aux mélanges.

### 1.3.4. La méthode de translation volumique proposée par Péneloux

La translation volumique est un concept qui fut développé et popularisé par Péneloux et al. [39] afin d'améliorer la reproduction des volumes molaires du liquide à saturation calculé par l'équation d'état cubique. Comme détaillé dans le paragraphe précédent traitant des fonctions $\alpha$ , les propriétés thermodynamiques d'équilibre liquide-vapeur sont correctement représentées si une fonction $\alpha$ assez flexible est utilisée dans le modèle. Ce n'est pas le cas des propriétés volumiques peu impactées par le choix de la fonction, $\alpha$ mais qui seront grandement modifiées par l'utilisation de la méthode de translation volumique.

La méthode est dite de translation volumique, car elle se traduit, à une température et une pression fixées, par une translation des volumes molaires d'une quantité fixe. Dans le plan (P,v), elle se matérialise par une translation de l'isotherme selon l'axe des volumes molaires (Figure 1.5).

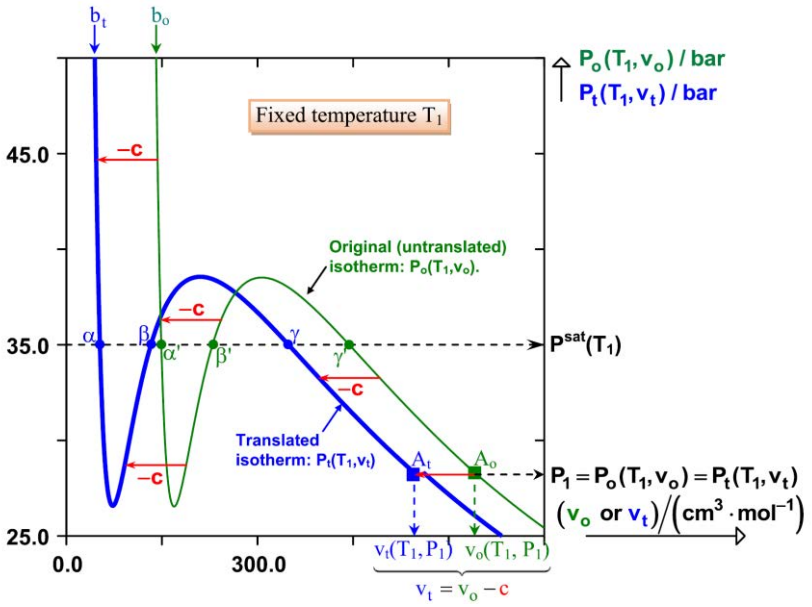



Figure 1.5. Illustration de la méthode de translation volumique [40]

Mathématiquement, il suffit de remplacer dans l'expression de l'équation d'état tous les $v$ par la quantité $v+c$.

$$P(T,v)=\frac{RT}{v-b}-\frac{a_c\times\alpha(T_r)}{(v-r_1b)(v-r_2b)}$$
$$\text{translation}\Downarrow\text{volumique} \qquad (1.26)$$
$$P^t(T,v)=\frac{RT}{v+c-b}-\frac{a_c\times\alpha(T_r)}{(v+c-r_1b)(v+c-r_2b)}$$

Où l'exposant $t$ désigne une quantité translatée – ici l'équation d'état. Le paramètre $c$ est ici supposé constant.

En réalisant ce changement, tous les volumes molaires calculés avec l'équation d'état translatée seront diminués d'une quantité $c$ par rapport au volume molaire calculé avec l'équation d'état non translatée. Le paramètre $c$ peut donc être ajusté afin de reproduire exactement la valeur du volume molaire du liquide à saturation à la température souhaitée par l'utilisateur de l'équation.

Le paramètre de translation volumique a été corrélé par Péneloux et al. à un paramètre relatif au corps pur, ici au facteur de compressibilité de Rackett $z_{RA}$ [41] afin de reproduire la valeur du volume molaire du liquide à saturation à une température réduite de 0.7 :

$$\begin{cases} c_{SRK}=\dfrac{RT_c}{P_c}(0.1156-0.4077z_{RA}) \\ c_{PR}=\dfrac{RT_c}{P_c}(0.1154-0.4406z_{RA}) \end{cases} \qquad (1.27)$$

Le facteur $z_{RA}$ a été recalculé pour chaque corps pur par les auteurs afin que l'équation d'état cubique permette de reproduire à une température réduite de 0.7 la valeur du volume molaire du liquide à saturation obtenu par application de la corrélation de Rackett [42] :

$$v_{liq}^{sat}(T_r=0.7)=\frac{RT_c}{P_c}\times z_{RA}^{1+1(1-T_r)^{2/7}} \qquad (1.28)$$

Les déviations calculées par Péneloux pour différentes familles chimiques de corps purs sont reportées dans le Tableau 1.5.

| Famille chimique | Soave-Redlich-Kwong | Peng-Robinson | Soave-Redlich-Kwong translatée |
|---|---|---|---|
| Alcanes | 10.86% | 4.47% | 1.47% |
| alcènes | 10.04% | 3.14% | 0.90% |
| Cycloalcanes | 8.06% | 5.80% | 2.11% |
| Composés aromatiques | 14.52% | 5.28% | 1.12% |
| Chloroalcanes | 10.16% | 5.51% | 2.08% |
| Amines | 9.70% | 3.68% | 1.74% |
| Aldéhydes, cétones, esters, éthers | 13.68% | 4.56% | 1.52% |
| Alcools | 10.93% | 4.25% | 3.80% |
| Composés inorganiques | 6.98% | 10.79% | 2.68% |
| Moyenne | 10.55% | 5.28% | 1.94% |

Tableau 1.5. Déviations relatives moyennes calculées pour trois équations d'état dont une translatée [39]

Une déviation d'environ 2% en moyenne est obtenue avec la méthode de translation volumique, soit 5 fois moins que la déviation obtenue avec l'équation de Soave-Redlich-Kwong et 2.5 fois moins qu'avec l'équation d'état Peng-Robinson. Pour rappel, la déviation moyenne obtenue avec l'équation de Schmidt et Wenzel, calculée sur un nombre de composés différent, est de 1.80%.

Comme montré par Péneloux, la méthode de translation volumique présente l'avantage de ne pas modifier la valeur de la pression de vapeur saturante calculée par l'équation d'état. Ainsi, les paramètres de la fonction $\alpha$ déterminés afin de reproduire au mieux la pression de saturation n'ont pas à être recalculés lorsque le paramètre $c$ est introduit dans l'équation d'état. Il est ainsi possible de découpler la reproduction de la pression de vapeur saturante des corps purs de celle des volumes molaires du liquide à saturation.

Cependant, comme évoqué précédemment, lorsque les données sont disponibles, il est préférable d'ajuster les paramètres des fonctions $\alpha$ sur les données de pression de saturation, mais aussi sur celles d'enthalpie de vaporisation ainsi que de capacité calorifique du liquide à saturation. Or, s'il est bien connu que la pression de vapeur

saturante est invariante par application d'une translation volumique, l'effet d'une telle transformation sur les autres propriétés utilisables dans l'ajustement des paramètres des fonctions $\alpha$ est mal connu.

Si l'enthalpie de vaporisation et la capacité calorifique du liquide à saturation sont invariantes par translation volumique, le découplage des procédures d'ajustement des paramètres de la fonction $\alpha$ et du paramètre $c$ pourra être maintenu. Sinon il sera nécessaire d'effectuer un ajustement simultané de ces paramètres sur l'ensemble de ces propriétés. Cette question est traitée dans l'article [40] présenté par la suite.

### 1.3.5. L'ajout d'une dépendance en température dans le terme de translation volumique

Lorsque le paramètre de translation volumique est choisi constant comme c'est le cas dans l'article de Péneloux et al. [39], il est possible d'améliorer grandement la reproduction des volumes molaires du liquide à saturation tant que la température réduite du corps pur reste approximativement inférieure à 0.9. Au-delà il est nécessaire d'introduire une dépendance en température du paramètre $c$ afin de reproduire les données expérimentales. Citons par exemple les propositions de Watson [43], Soreide [44], Magoulas et Tassios [45], Ungerer et Batut [46], Ji et Lempe [47], Tsai et Chen [48] et de Miqueu et al. [49] permettant effectivement d'obtenir une excellente représentation des volumes molaires liquides pour tout le domaine de température subcritique.

Cependant, il a été très tôt démontré que l'introduction d'une dépendance en température dans le paramètre de translation volumique est nécessairement accompagnée d'incohérences thermodynamiques :

- Pfohl [50] montre qu'une translation volumique dépendant de la température induit un croisement d'isothermes dans le plan pression-volume molaire, phénomène non conforme à la réalité expérimentale. Le croisement d'isothermes intervient par ailleurs à des niveaux de pressions compatibles avec ceux rencontrés dans des procédés industriels (Figure 1.6).

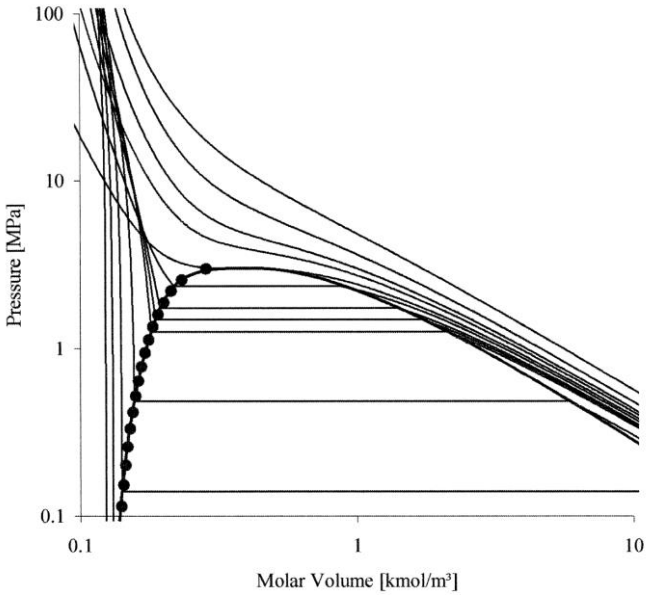



Figure 1.6. Croisements d'isothermes pouvant être observés lorsque le paramètre de translation volumique est une fonction de la température [50]

- Salim et Trebble [51] montrent que, quelle que soit la dépendance en température du paramètre $c$, des capacités calorifiques isochores négatives – ce qui est théoriquement interdit – seront calculées à haute pression et que seul un paramètre $c$ constant permet de s'affranchir d'une telle incohérence.

Jusqu'à peu, le domaine de validité des méthodes de translation volumiques dépendant de la température était méconnu et il était risqué de les appliquer. Les travaux récents de Shi et al. [52,53] proposent une méthode permettant de déterminer si un croisement d'isotherme peut être observé dans le domaine d'application de l'équation d'état. Cela permet donc de définir un domaine de confiance des équations d'état incluant un paramètre de translation volumique dépendant de la température. Néanmoins, cette approche étant fondamentalement incohérente, elle n'a pas été retenue dans le cadre de cette thèse.

### 1.4. Équations d'état cubiques récentes applicables aux corps purs

Comme discuté précédemment, la modification des fonctions $\alpha$ et l'utilisation d'une méthode de translation volumique constituent des voies d'amélioration de la modélisation des corps purs par les équations d'état cubiques. Certains auteurs ont proposé des équations d'état de type Soave-Redlich-Kwong et Peng-Robinson intégrant ce type de modifications.

Ici, l'attention est portée à des modèles thermodynamiques qui ont généralement été développés dans le but de modéliser des mélanges, mais pour lesquels les auteurs ont

dû porter une attention particulière à la bonne représentation des corps purs, une étape préalable à la bonne représentation des mélanges. Leur application aux mélanges est discutée dans un autre chapitre. Une présentation chronologique est ici proposée.

On notera que tous les modèles utilisent les valeurs de $r_1$ et $r_2$ de l'équation de Peng-Robinson.

### 1.4.1. Le modèle VTPR (2001)

La fonction $\alpha$ de Twu à 3 paramètres ajustables est utilisée. La fonction de Mathias-Copeman était initialement utilisée, mais a finalement été supprimée à cause de la discontinuité de la fonction $\alpha$ au point critique. Un paramètre de translation volumique indépendant de la température est utilisé dans l'équation d'état. Le paramètre $c$ est ajusté afin de reproduire le volume molaire du liquide à saturation expérimental à une température réduite de 0.7.

### 1.4.2. Le modèle UMR-PR (1990) [45,57]

Pour les composés apolaires, la fonction $\alpha$ de Soave est utilisée, mais l'expression de $m$ est calculée par le polynôme de degré 4 suivant :

$$m(\omega) = 0.384401 + 1.52276\omega - 0.213808\omega^2 + 0.034616\omega^3 - 0.001976\omega^4 \quad (1.29)$$

Pour les composés polaires, la fonction $\alpha$ de Mathias-Copeman est utilisée dans le domaine subcritique tandis que la fonction $\alpha$ de Soave est utilisée dans le domaine supercritique. Dans les premières versions, un paramètre de translation volumique fonction de la température était utilisé mais a finalement été remplacé par un paramètre $c$ constant à cause des incohérences causées par ce choix. Cette équation d'état a été utilisée pour le développement de l'équation d'état des mélanges UMR-PRU [57] quelques années plus tard.

### 1.4.3. Le modèle PPR78 (2004) [23,24]

La fonction $\alpha$ de Peng et Robinson de 1978 est utilisée. Aucun paramètre de translation volumique n'est utilisé, car leur reproduction n'est pas considérée par les auteurs.

### 1.4.4. Le modèle NRTL-PR (2006) [25]

Pour les composés non associés, la fonction $\alpha$ de Peng et Robinson de 1978 est utilisée. Pour les composés associés, une fonction $\alpha$ de Soave modifiée, où les paramètres $m$ et $\gamma$ doivent être ajustés pour chaque corps pur, est utilisée :

$$\alpha(T_r) = \left[1 + m\left(1 - T_r^{\gamma}\right)\right]^2 \tag{1.30}$$

Aucun paramètre de translation volumique n'est utilisé, car la reproduction des propriétés volumiques n'est pas étudiée.

Parmi les modèles cités, aucun ne permet un calcul prédictif des propriétés thermodynamiques et volumiques des corps purs, c'est-à-dire combinant une fonction $\alpha$ généralisée ne présentant pas de défaut théorique (excluant ainsi les fonctions $\alpha$ polynomiales, donc celle de Soave) et un paramètre $C$ constant calculé de manière prédictive.

Plus de détails concernant la diversité des équations d'état cubiques proposées au cours de ces 150 dernières années (depuis la proposition de Van der Waals) peuvent être trouvés dans les travaux de Valderrama [5] et, plus récemment, de Lopez-Echeverry et al. [58], eux-mêmes faisant références à de nombreuses autres études bibliographiques.

### 1.5. Conclusion

L'amélioration de la reproduction des propriétés d'équilibre liquide-vapeur et volumiques des corps purs par une équation d'état cubique est un enjeu majeur pour la modélisation des mélanges. Cette amélioration peut passer par la modification de la fonction, $\alpha$ mais aussi par l'introduction d'un paramètre de translation volumique constant.

Parmi toutes les fonctions $\alpha$ disponibles dans la littérature, les fonctions de type exponentiel sont à préférer aux fonctions de type polynomial pour des raisons de comportement à haute température [21]. Cependant, le choix des propriétés à régresser ainsi que la méthodologie à adopter pour la détermination des paramètres des fonctions $\alpha$ restent des questions ouvertes. Ainsi, les questions suivantes restent en suspens :

- Est-il possible de dériver des contraintes supplémentaires sur les fonctions $\alpha$ par une approche plus théorique dont il faudrait tenir compte au moment de l'ajustement des paramètres ?
- Les paramètres des fonctions $\alpha$ non généralisées ajustés sur des données de pression de vapeur saturante, d'enthalpies de vaporisation et de capacité calorifique des liquides peuvent-ils être utilisés en extrapolation pour estimer des propriétés supercritiques ?

- Est-il prudent d'ajuster les paramètres des fonctions $\alpha$ sans données de pression de saturation ?

De plus, l'ajout d'un paramètre de translation volumique nécessairement constant pour des raisons de cohérence thermodynamiques nécessite de déterminer quelles propriétés utilisées dans l'ajustement des paramètres des fonctions $\alpha$ sont invariantes par rapport au paramètre $c$.

Une fois les réponses aux questions précédentes établies, un nouveau modèle thermodynamique pour les corps purs pourra être proposé puis développé.

Les articles faisant suite à ce chapitre visent à répondre aux questions soulevées dans ce chapitre :

- *J.-N. Jaubert, R. Privat, Y. Le Guennec, L. Coniglio, Note on the properties altered by application of a Péneloux–type volume translation to an equation of state, Fluid Phase Equilibria. 419 (2016) 88–95. doi:10.1016/j.fluid.2016.03.012.* [40]

  Il est démontré que les propriétés suivantes : pression de vapeur saturante, enthalpie de vaporisation et capacité calorifique liquide, utilisées pour l'ajustement des paramètres des fonctions $\alpha$, sont invariantes par effet du paramètre de translation volumique s'il est choisi indépendant de la température. Plus généralement, une liste exhaustive des propriétés invariantes par translation volumique est établie. On démontre alors qu'il est possible de décorréler l'ajustement des propriétés thermodynamiques (pression de vapeur saturante, enthalpie de vaporisation, capacité calorifique liquide) par la fonction $\alpha$ de celui des volumes molaires par le paramètre de translation volumique.

- *Y. Le Guennec, S. Lasala, R. Privat, J.-N. Jaubert, A consistency test for α-functions of cubic equations of state, Fluid Phase Equilibria. 427 (2016) 513–538. doi:10.1016/j.fluid.2016.07.026.* [20]

  Il est démontré formellement qu'une fonction $\alpha$ doit être convexe (de dérivée seconde positive) sur tout le domaine de température. Il est montré qu'une fonction $\alpha$ spécifique mal paramétrée, c'est-à-dire paramétrée sur des données subcritiques qui ne vérifierait pas cette contrainte, peut induire des difficultés majeures à représenter des comportements d'équilibre liquide-vapeur de systèmes binaires. Par ailleurs, il est observé qu'imposer que la dérivée

troisième de la fonction α soit négative permet une nette amélioration de la reproduction des propriétés supercritiques : enthalpie et capacité calorifique, sans dégrader la reproduction des propriétés subcritiques, ni des comportements de phases des systèmes binaires. Une fonction $\alpha$ respectant l'intégralité des contraintes établies (dérivée seconde positive et dérivée troisième négative) est alors dite cohérente ou de façon équivalente, on dit qu'elle passe le test de cohérence des fonctions $\alpha$ . La confrontation des fonctions $\alpha$ de la littérature à notre test de cohérence montre qu'aucune d'elles n'est cohérente. Il est prouvé que certaines fonctions spécifiques peuvent être rendues cohérentes sous réserve que les paramètres ajustables soient contraints. Les contraintes explicites que doivent respecter les paramètres d'une dizaine de fonctions $\alpha$ sont données en annexe de l'article.

- *Y. Le Guennec, R. Privat, S. Lasala, J.-N. Jaubert, On the imperative need to use a consistent α-function for the prediction of pure-compound supercritical properties with a cubic equation of state, Fluid Phase Equilibria. 445 (2017) 45–53. doi:10.1016/j.fluid.2017.04.015.* [59]

  Cet article compare les capacités à prédire des propriétés supercritiques d'une fonction $\alpha$ de Twu (à 3 paramètres) cohérente avec celles d'une fonction $\alpha$ non cohérente. Les propriétés supercritiques considérées sont l'enthalpie résiduelle ainsi que la capacité calorifique résiduelle à pression constante. L'étude est réalisée sur 9 composés pour lesquels le logiciel REFPROP peut fournir des données pseudo-expérimentales précises. En comparaison avec une fonction $\alpha$ incohérente, on observe une division de l'erreur par 10 lorsqu'une fonction $\alpha$ cohérente est utilisée, démontrant ainsi les capacités d'extrapolation des fonctions $\alpha$ cohérentes.

- *Y. Le Guennec, R. Privat, J.-N. Jaubert, Development of the translated-consistent tc-PR and tc-RK cubic equations of state for a safe and accurate prediction of volumetric, energetic and saturation properties of pure compounds in the sub- and super-critical domains, Fluid Phase Equilibria. 429 (2016) 301–312. doi:10.1016/j.fluid.2016.09.003.* [60]

  Les trois précédents articles ont pu mettre en évidence la possibilité de décorréler l'ajustement des propriétés thermodynamiques et volumiques ainsi que le besoin d'utiliser une fonction $\alpha$ cohérente. Dans le cadre du

développement des modèles tc-PR et tc-RK, une fonction $\alpha$ de Twu à 3 paramètres ajustés sur des données de pression de vapeur saturante, enthalpie de vaporisation et capacité calorifique du liquide à saturation a été utilisée. La cohérence de la fonction $\alpha$ a été imposée. De plus un paramètre de translation volumique, reproduisant le volume molaire du liquide à saturation expérimental à une température réduite de 0.8 a été intégré au modèle. Des qualités de modélisation élevées sont obtenues pour les plus de 900 composés considérés issus de la base de données de la DIPPR. Les valeurs des paramètres de la fonction $\alpha$ de Twu ainsi que celles du paramètre de translation volumique sont données en annexe de l'article pour chacun de ces composés. Des versions généralisées des modèles tc-PR et tc-RK ont également été développées, conduisant à des déviations plus faibles sur les propriétés (pression de vapeur saturante, enthalpie de vaporisation, capacité calorifique liquide, densité liquide) que celles obtenues avec les modèles de Peng-Robinson et de Redlich-Kwong munis de la fonction de Soave.

- *A. Pina-Martinez, Y. Le Guennec, R. Privat, J.-N. Jaubert, P.M. Mathias, Analysis of the Combinations of Property Data That Are Suitable for a Safe Estimation of Consistent Twu α-Function Parameters: Updated Parameter Values for the Translated-Consistent tc -PR and tc -RK Cubic Equations of State, Journal of Chemical & Engineering Data. (2018). doi:10.1021/acs.jced.8b00640. [61]*

  Grâce à la réévaluation des erreurs sur les corrélations fournies par la banque de données de la DIPPR, une mise à jour des modèles tc-PR et tc-RK a été réalisée, incluant les paramètres de la fonction $\alpha$ de Twu ainsi que la valeur du paramètre de translation volumique pour respectivement 1721 et 1489 molécules (contre respectivement 1116 et 997 molécules auparavant). Il a également été établi que les paramètres de la fonction $\alpha$ doivent être a minima ajustés sur des données de pression de vapeur saturante. Si des données d'enthalpie de vaporisation ou de capacité calorifique à saturation sont disponibles, il est alors recommandé de les ajouter à la procédure d'ajustement. Les versions généralisées des modèles tc-PR et tc-RK ont été mises à jour à la lumière de nos nouveaux résultats (cf. Annexes A-1 et A-2).

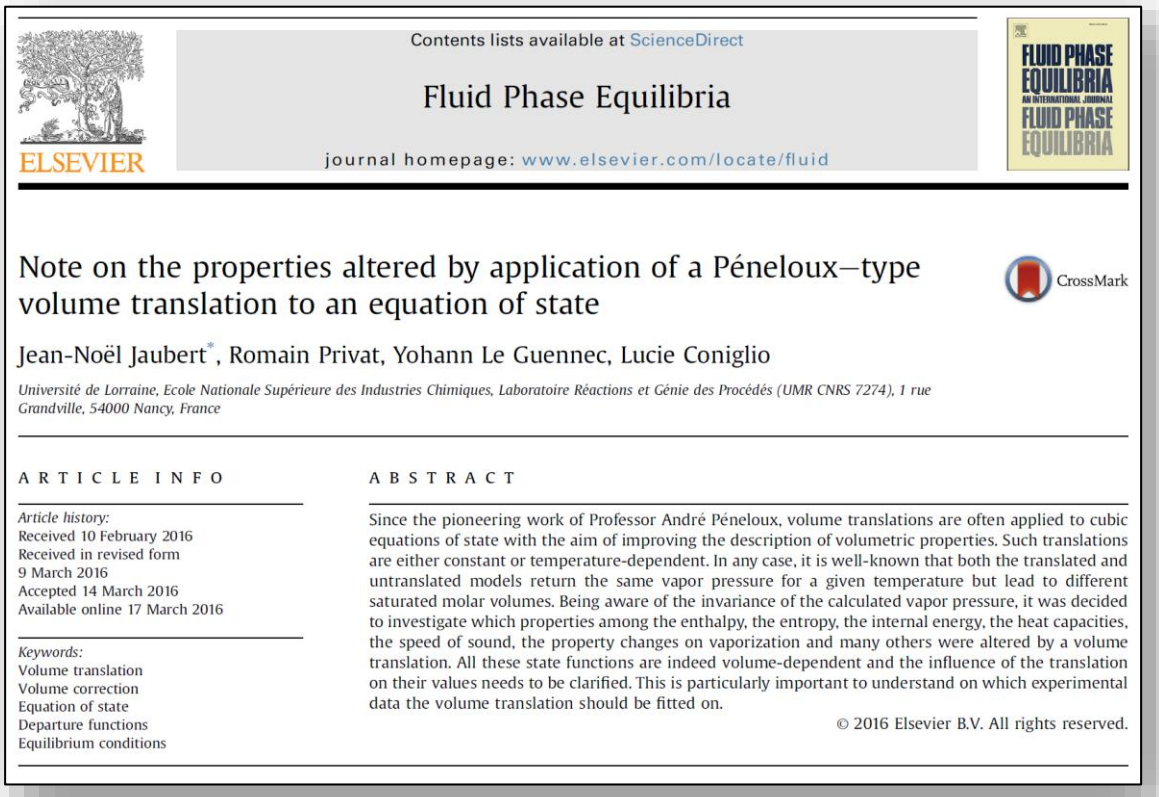
# Chapitre 2. Article “Note on the properties altered by application of a Péneloux–type volume translation to an equation of state”

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ABSTRACT

Since the pioneering work of Professor André Péneloux, volume translations are often applied to cubic equations of state with the aim of improving the description of volumetric properties. Such translations are either constant or temperature-dependent. In any case, it is well-known that both the translated and untranslated models return the same vapor pressure for a given temperature but lead to different saturated molar volumes. Being aware of the invariance of the calculated vapor pressure, it was decided to investigate which properties among the enthalpy, the entropy, the internal energy, the heat capacities, the speed of sound, the property changes on vaporization and many others were altered by a volume translation. All these state functions are indeed volume-dependent and the influence of the translation on their values needs to be clarified. This is particularly important to understand on which experimental data the volume translation should be fitted on.

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**Abstract**

Since the pioneering work of Professor André Péneloux, volume translations are often applied to cubic equations of state with the aim of improving the description of volumetric properties. Such translations are either constant or temperature-dependent. In any case, it is well-known that both the translated and untranslated models return the same vapor pressure for a given temperature but lead to different saturated molar volumes. Being aware of the invariance of the calculated vapor pressure, it was decided to investigate which properties among the enthalpy, the entropy, the internal energy, the heat capacities, the speed of sound, the property changes on vaporization and many others were altered by a volume translation. All these state functions are indeed volume-dependent and the influence of the translation on their values needs to be clarified. This is particularly important to understand on which experimental data the volume translation should be fitted on.

**Keywords**

volume translation, volume correction, equation of state, departure functions, equilibrium conditions.

## 2.1. Introduction

Equations of state (EoS), routinely used in process and product design are pressure explicit functions which quantify the relationship between the pressure, molar volume and temperature of a pure component. In the crowd of the proposed models, the most popular ones are certainly the SAFT-type and cubic EoS. It is however well-known that cubic EoS provide inaccurate liquid densities. To fix the ideas, the Soave-Redlich-Kwong (SRK) [7] and the Peng-Robinson (PR) [8] EoS predict the saturated-liquid volumes with an average deviation of about 16 % and 8 % respectively [18]. One method to overcome this shortcoming is the so-called volume translation proposed by Péneloux et al. in 1982 [39]. This technique is widely applied in process and product design where an EoS is used to estimate densities and other thermodynamic properties. For a given component, the saturated-liquid volume calculated at a given temperature is usually notably different from the experimental value but the difference between the calculated and the experimental volume is more or less constant when varying the temperature out of the critical region. Consequently, a temperature-independent volume translation (all the calculated molar volumes are translated by a constant amount c) significantly improves the description of the saturated liquid densities in the low temperature range ( $T_R < 0.8$ ). To overcome the failure of this principle near the critical temperature, many authors [45,54,57,62–66] adopted a temperature-dependent volume correction *c(T)*. It is however well-established that temperature-dependent volume translations are thermodynamically inconsistent since they lead to the crossing of isotherms in a (pressure, volume) plane and to negative heat capacities [50,67,68].

In his pioneering paper, Péneloux explains that both the translated and untranslated models return the same vapor pressure for a given temperature but lead to different saturated molar volumes. Being aware of this result, it was decided to investigate which properties among the enthalpy, the entropy, the internal energy, the heat capacities, the speed of sound, the property changes on vaporization and many others were altered by a volume translation. Returned from a pressure-explicit EoS, all these state functions are temperature and volume dependent and the influence of the translation on their values needs to be clarified. This is particularly important to understand on which experimental data the volume translation should be fitted. Indeed:

1) if neither the experimental VLE data (vapor pressures, property changes on vaporization) nor the other thermodynamic properties (enthalpy, entropy, etc.) are

affected by a volume translation, the problem of reproducing liquid densities with an EoS can be disconnected from the problem of predicting other thermodynamic properties. In such a case, the volume translation would have to be fitted on density data while the other EoS parameters (e.g. those involved in the cohesive parameter of cubic EoS) should be fitted on all the other experimental data. Therefore, the volume translation should be only applied to the molar volume returned by the EoS when a density value is required. Such a correction would thus be a kind of external procedure taking place once the EoS is solved.

2) if the volume correction alters both the experimental VLE data and all the other thermodynamic properties (enthalpy, heat capacity, etc.), it is no more possible to uncouple the problem of reproducing liquid densities from the problem of predicting other properties. In such case, the volume translation and the other EoS parameters should be fitted simultaneously on all the available experimental data.

Another objective of this note is to compare the influence of both a temperature-independent and a temperature-dependent volume translation on the properties computable by an EoS.

The results presented in this paper are general and could be applied to any pressure-explicit EoS, e.g., SAFT-type or cubic EoS. We however do not see a real need to apply a volume translation to a SAFT-type EoS since such equations are parameterized to provide satisfactory estimation of liquid densities.

To close this introduction, we wanted to state that in a somewhat abstruse paper published in 1993, working specifically on cubic EoS, Leibovici [69] was able to identify a series of properties not influenced by a temperature-independent volume translation, but however did not realize that his conclusions did not depend on the mathematical expression of the EoS and never discussed the case of a temperature-dependent volume translation.

## 2.2. Effect of a Péneloux–type volume translation along the volume axis

In this section, we want to establish the list of the properties which are affected and the list of the properties which are unaltered by a Péneloux-type volume translation. Two cases are considered depending whether the volume translation is taken constant or temperature-dependent.

Following Zabaloy and Brignole [70], we decided to avoid the concept of pseudo-volume ($\tilde{v}$), pseudo-covolume ($\tilde{b}$) and pseudo equation of state introduced by Péneloux. We indeed believe that such concepts have brought confusion explaining why some researchers applied the volume translation approach without using the original formalism.

### 2.2.1. The concept of volume translation as introduced by André Péneloux.

By solving a Van der Waals (VdW)-type EoS (SRK, PR ...) at given T and P, the calculated molar volume, noted $v_o$, is generally notably different from the corresponding experimental value. As a first example, we know by experience that the volumes returned by the SRK EoS are generally too large and they thus need to be reduced by a quantity c (the volume correction) in order to get a new volume $v_t$ closer to the experimental value than $v_o$. The subscripts *o* and *t* refer to *original* (i.e. untranslated) and to *translated* equations of state, respectively. As a second example, depending on the studied component, molar volumes returned by the PR EoS are either too large or too small: they thus need to be either reduced or enlarged and the volume correction c is either positive or negative.

By definition of the volume translation *c*, the original and translated molar volumes are linked by:

$$v_t = v_o - c \tag{2.1}$$

Consequently, we can assert that obtaining a consistent translated EoS from an original untranslated equation just consists in replacing $v_o$ by ($v_t + c$) within the untranslated expression.

Mathematically speaking, this translation is thus defined by the following equation:

$$\underbrace{P_t(T, v_t)}_{\substack{\text{mathematical} \\ \text{expression of} \\ \text{the translated EoS}}} = P_o(T, v_t + c) \tag{2.2}$$

Since the original and translated states of the considered pure fluid have the same pressure and temperature (the two states only differ by the value of the molar volume), one has:

$$\begin{cases} P = \underbrace{P_t(T,v_t)}_{\substack{\text{value of the pressure returned by the translated EoS (the temperature is T and the molar volume } v_t)}} = \underbrace{P_o(T,v_o)}_{\substack{\text{value of the pressure returned by the original EoS (the temperature is T and the molar volume } v_o)}} \\ v_t = v_o - c \end{cases} \tag{2.3}$$

Let us take as an example, the Van der Waals EoS. The original equation writes:

$$P_o(T,v_o) = \frac{RT}{v_o - b_o} - \frac{a}{v_o^2} \tag{2.4}$$

(the reason for which subscript o has been added to the covolume *b* is discussed below).

Consequently, the translated form is:

$$P_t(T,v_t) = \frac{RT}{(v_t + c) - b_o} - \frac{a}{(v_t + c)^2} \tag{2.5}$$

According to Equ. (2.3) and as illustrated in Figure 2.1, the Péneloux–type volume correction corresponds to a translation of the whole original P-v isotherm (of the amount –*c*) along the volume axis.

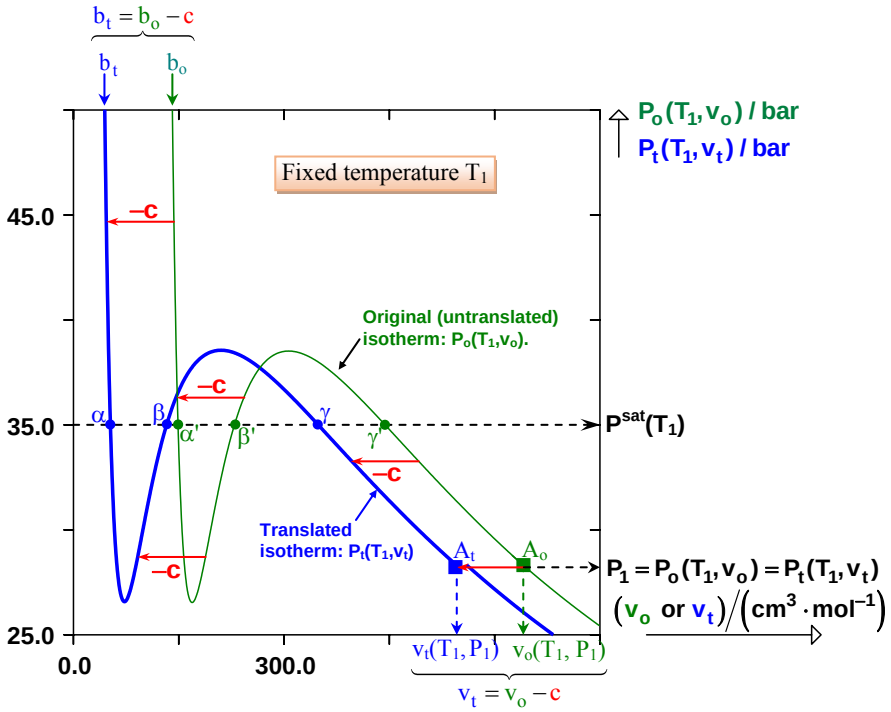



Figure 2.1. Graphical illustration of the Péneloux-type volume translation concept.

In Van der Waals's theory, the covolume *b* has a physical meaning: it is the molar volume when the pressure tends to infinity. Since the volume correction translates the whole isotherm (see Figure 2.1), the covolume (which is a particular molar volume) automatically undergoes the same translation so that the translated covolume verifies: $b_t = b_o - c$. The same result can equivalently be obtained from Equ. (2.5): when the pressure tends to infinity, the molar volume $v_t$ goes to $(b_o - c)$ which is, by definition, the covolume of the translated equation. Equ. (2.5), i.e. the translated form of the VdW EoS can be alternatively written:

$$P_t(T, v_t) = \frac{RT}{v_t - b_t} - \frac{a}{(v_t + c)^2} \tag{2.6}$$

It is noticeable that by applying a volume translation to the VdW EoS, the Clausius [71] equation [Equ. (2.6)] is obtained. Consequently, the volume translation induced a change of EoS. Although Equ. (2.6) and Equ. (2.5) are strictly equivalent, we recommend to use Equ. (2.6) since it contains the true covolume. Comparison of Equs. (2.4) and (2.6) makes it possible to conclude that the volume translation does not alter the mathematical expression of the repulsive term. In both cases, it writes: $RT/(v-b)$ where *b* is the EoS covolume.

In conclusion, Péneloux's concept can be summarized as follows:

1) Starting with a non-translated EoS: $P_o(T, v_o)$, the mathematical expression of the translated equation is obtained by replacing $v_o$ by ( $v_t + c$ ) so that $P_t(T, v_t) = P_o(T, v_t + c)$.

2) In order to make appear the translated covolume (the true covolume of the translated equation), $b_o$ must be replaced by ($b_t + c$).

We can thus assert that a translated EoS can be obtained from an original untranslated equation by replacing in the untranslated expression:

$$\begin{cases} v_o \ by \ (v_t + c) \\ b_o \ by \ (b_t + c) \end{cases} \tag{2.7}$$

### 2.2.2. Application of the volume translation concept to Van der Waals-type equations of state

In the present section, results of the previous section are applied to the special case of Van der Waals-type equations of state. For pure species, original (untranslated) cubic EoS have the following general form:

$$P_o(T,v_o)=\frac{RT}{v_o-b_o}-\frac{a_{c,o}\cdot\alpha(T)}{(v_o-r_1b_o)(v_o-r_2b_o)} \qquad (2.8)$$

$r_1$ and $r_2$ are two universal constants of the EoS (not depending on the nature of the studied fluid). For illustration, the values of these constants associated with classical cubic EoS are reported in Table 1. $b_o$ is the *covolume* (value taken by the molar volume when the pressure tends to infinity). The cohesive parameter, $a_o(T)=a_{c,o}\cdot\alpha(T)$, accounts for molecular attraction: $a_{c,o}$ is the value of $a_o$ at the critical temperature and $\alpha(T)$ is the so-called α function which is temperature dependent (except for the Van der Waals EoS for which $\alpha=1$). Due to its definition, this function is equal to one at the critical temperature: $\alpha(T_c)=1$.

| EoS | $r_1$ | $r_2$ |
|---|---|---|
| Van der Waals (VdW) | 0 | 0 |
| Soave-Redlich-Kwong (SRK) | –1 | 0 |
| Peng-Robinson (PR) | $-1-\sqrt{2}$ | $-1+\sqrt{2}$ |

Table 2.1. Parameters for three different cubic EoS

The values of $a_{c,o}$, $b_o$ and $z_{c,o}$ (the critical compressibility factor) are usually expressed with respect to the experimental values of the critical temperature $T_{c,\exp}$ and critical pressure $P_{c,\exp}$ by imposing the critical constraints recalled in Equ. (2.9):

$$\begin{cases} P_{c,\exp} - P_{EoS}(T_{c,\exp}, v_c) = 0 \\ \left(\frac{\partial P_{EoS}}{\partial v}\right)_T \Big|_{\substack{T=T_{c,\exp} \\ v=v_c}} = 0 \\ \left(\frac{\partial^2 P_{EoS}}{\partial v^2}\right)_T \Big|_{\substack{T=T_{c,\exp} \\ v=v_c}} = 0 \end{cases} \quad (2.9)$$

By applying these constraints to Equ. (2.8), one obtains:

$$\begin{cases} z_{c,o} = \dfrac{1}{3-\eta_{c,o}(1+r_1+r_2)} \text{ with } \eta_{c,o} = \dfrac{b_o}{v_{c,o}} = \dfrac{1}{\sqrt[3]{(1-r_1)(1-r_2)^2} + \sqrt[3]{(1-r_2)(1-r_1)^2} + 1} \\ a_{c,o} = \Omega_{a,o} \cdot \dfrac{R^2 T_{c,\exp}^2}{P_{c,\exp}} \text{ with } \Omega_{a,o} = \dfrac{(1-\eta_{c,o}\cdot r_1)(1-\eta_{c,o}\cdot r_2)\cdot\left[2-\eta_{c,o}(r_1+r_2)\right]}{(1-\eta_{c,o})\left[3-\eta_{c,o}(1+r_1+r_2)\right]^2} \\ b_o = \Omega_{b,o} \cdot \dfrac{RT_{c,\exp}}{P_{c,\exp}} \text{ with } \Omega_{b,o} = \dfrac{\eta_{c,o}}{3-\eta_{c,o}(1+r_1+r_2)} \end{cases}$$

(2.10)

The expression of the translated EoS is obtained by replacing in Equ. (2.8) $v_o$ by $(v_t + c)$ and $b_o$ by $(b_t + c)$. We thus get:

$$P_t(T, v_t) = \frac{RT}{(v_t + c) - (b_t + c)} - \frac{a_{c,t} \cdot \alpha(T)}{\left[(v_t + c) - r_1(b_t + c)\right]\left[(v_t + c) - r_2(b_t + c)\right]} \quad (2.11)$$

that is:

$$P_t(T, v_t) = \frac{RT}{v_t - b_t} - \frac{a_{c,t} \cdot \alpha(T)}{\left[v_t - r_1 b_t + c(1-r_1)\right]\left[v_t - r_2 b_t + c(1-r_2)\right]} \quad (2.12)$$

By applying the critical constraints to Equ. (2.12), one obtains:

$$\begin{cases} z_{c,t} = z_{c,o} - \dfrac{P_{c,\exp} \cdot c}{RT_{c,\exp}} \\ a_{c,t} = a_{c,o} \\ b_t = b_o - c \end{cases} \quad (2.13)$$

It is thus noticeable that unlike $z_{c,o}$, $z_{c,t}$ is not a universal constant anymore: for a given EoS (i.e., for given values of $r_1$ and $r_2$) $z_{c,t}$ becomes component-dependent (this is a simple consequence of the critical volume translation). The volume translation

however does not alter $a_c$ ($a_{c,t} = a_{c,o}$) and as previously mentioned modifies the true covolume ($b_t = b_o - c$).

To conclude this section, the translated and untranslated forms of the most industrially used cubic EoS (i.e., the SRK and PR EoS) are provided. For the sake of simplicity and clarity, the subscripts t (for translated) and o (for original) are removed.

The original SRK EoS [7,72] writes:

$$P(T,v) = \frac{RT}{v-b} - \frac{a_c \cdot \alpha(T)}{v(v+b)} \text{ with } \begin{cases} z_c = \frac{1}{3} \\ a_c = \frac{1}{9\left(\sqrt[3]{2}-1\right)} \frac{R^2 T_{c,\exp}^2}{P_{c,\exp}} \\ b = \frac{\sqrt[3]{2}-1}{3} \frac{RT_{c,\exp}}{P_{c,\exp}} \end{cases} . \tag{2.14}$$

so that, the expression of the translated SRK EoS is:

$$P(T,v) = \frac{RT}{v-b} - \frac{a_c \cdot \alpha(T)}{(v+c)(v+b+2c)} \text{ with } \begin{cases} z_c = \frac{1}{3} - \frac{P_{c,\exp} \cdot c}{RT_{c,\exp}} \\ a_c = \frac{1}{9\left(\sqrt[3]{2}-1\right)} \frac{R^2 T_{c,\exp}^2}{P_{c,\exp}} \\ b = \frac{\sqrt[3]{2}-1}{3} \frac{RT_{c,\exp}}{P_{c,\exp}} - c \end{cases} \tag{2.15}$$

For the SRK EoS, Péneloux [39] recommends using:

$$c_{SRK} = \frac{RT_c}{P_c}\left(0.1156 - 0.4077 \cdot z_{RA}\right) \tag{2.16}$$

where $z_{RA}$ is the Rackett compressibility factor [41].

In a similar way, the original PR EoS [8], widely used for mixtures [23,54,57,73,74], writes:

$$P(T,v)=\frac{RT}{v-b}-\frac{a_c\cdot\alpha(T)}{v(v+b)+b(v-b)} \quad \text{with} \quad \begin{cases} \eta_c=\left[1+\sqrt[3]{4-2\sqrt{2}}+\sqrt[3]{4+2\sqrt{2}}\right]^{-1}\approx 0.25308 \\ z_c=\dfrac{1}{\eta_c+3}\approx 0.30740 \\ a_c=\dfrac{40\eta_c+8}{49-37\eta_c}\dfrac{R^2T_{c,\exp}^2}{P_{c,\exp}}\approx 0.45724\dfrac{R^2T_{c,\exp}^2}{P_{c,\exp}} \\ b=\dfrac{\eta_c}{\eta_c+3}\dfrac{RT_{c,\exp}}{P_{c,\exp}}\approx 0.07780\dfrac{RT_{c,\exp}}{P_{c,\exp}} \end{cases}$$

(2.17)

Consequently, the translated PR EoS is:

$$P(T,v)=\frac{RT}{v-b}-\frac{a_c\cdot\alpha(T)}{(v+c)(v+b+2c)+(b+c)(v-b)} \text{ with } \begin{cases} z_c\approx 0.30740-\dfrac{P_{c,\exp}\cdot c}{RT_{c,\exp}} \\ a_c\approx 0.45724\dfrac{R^2T_{c,\exp}^2}{P_{c,\exp}} \\ b\approx 0.07780\dfrac{RT_{c,\exp}}{P_{c,\exp}}-c \end{cases} \quad (2.18)$$

For the PR EoS, Péneloux recommends using [75] the never published following relation:

$$c_{PR}=\frac{RT_c}{P_c}\left(0.1154-0.4406\cdot z_{RA}\right) \quad (2.19)$$

### 2.2.3. Properties altered by application of a Péneloux-type volume translation to an equation of state

The previous section has highlighted that a volume translation is equivalent to a change of EoS; this is particularly visible when comparing Equs. (2.8) and (2.12). We thus want to study the relations between the thermodynamic functions (enthalpy, entropy ...) calculated from the original and the translated EoS. To do that, let us consider a pure component at temperature $T_1$ and pressure $P_1$ modelled by an original (untranslated) EoS. Its molar volume is $v_o(T_1,P_1)$ and the state of this fluid is identified by point $A_o$ in Fig. 1. At the same temperature $T_1$ and pressure $P_1$, let us now consider the same pure component modelled by the translated EoS. Its molar volume is thus $v_t(T_1,P_1)$ and the state of this fluid corresponds to point $A_t$ in Fig. 1.

We basically know that:

$$\Delta v = v_t(T,P) - v_o(T,P) = -c \tag{2.20}$$

Let us address some other thermodynamic functions.

### 2.2.3.1. Chemical potential change

By noting $g(T,P)$ , the real fluid chemical potential (molar Gibbs energy) and $g^{\bullet}(T,P)$ the perfect gas state chemical potential at the same temperature and pressure as the real fluid, one has from classical thermodynamics:

$$g(T,P) = g^{\bullet}(T,P) + \int_0^P \left[ v(T,P) - \frac{RT}{P} \right] dP \tag{2.21}$$

Where $v(T,P)$ is the real fluid molar volume at selected *T* and *P*.

The chemical potential estimated from the original EoS (point $A_o$) satisfies:

$$g_o(T,P) = g^{\bullet}(T,P) + \int_0^P \left[ v_o(T,P) - \frac{RT}{P} \right] dP \tag{2.22}$$

Similarly, the chemical potential estimated from the translated EoS (point $A_t$) verifies:

$$g_t(T,P) = g^{\bullet}(T,P) + \int_0^P \left[ v_t(T,P) - \frac{RT}{P} \right] dP \tag{2.23}$$

By replacing $v_t(T,P)$ by $\left[ v_o(T,P) - c \right]$ in Equ. (2.23), one has:

$$\begin{aligned} g_t(T,P) &= g^{\bullet}(T,P) + \int_0^P \left[ v_o(T,P) - c - \frac{RT}{P} \right] dP \\ &= \underbrace{g^{\bullet}(T,P) + \int_0^P \left[ v_o(T,P) - \frac{RT}{P} \right] dP}_{g_o(T,P)} - Pc \end{aligned} \tag{2.24}$$

We thus get:

$$\Delta g = g_t(T,P) - g_o(T,P) = -Pc \tag{2.25}$$

As a conclusion, the translated and untranslated models predict different chemical potentials.

By definition of the fugacity coefficient, one has:

$$\ln \varphi(T,P) = \frac{g(T,P) - g^{\bullet}(T,P)}{RT} \tag{2.26}$$

So that:

$$\Delta \ln \varphi = \ln \varphi_t(T,P) - \ln \varphi_o(T,P) = -\frac{Pc}{RT} \tag{2.27}$$

The fugacity is defined by: $f = P\varphi$, so that:

$$\Delta \ln f = \ln f_t(T,P) - \ln f_o(T,P) = -\frac{Pc}{RT} \tag{2.28}$$

### 2.2.3.2. Entropy change

Entropy $s(T,P)$ can be derived from $g(T,P)$ by: $S = -\left(\partial g/\partial T\right)_P$. Derivation of Equ. (2.25) gives:

$$\Delta s = s_t(T,P) - s_o(T,P) = P \cdot c' \tag{2.29}$$

where $c' = dc/dT$ is the derivative of the volume translation with respect to the temperature. From Equ. (2.29), it is obvious that both EoS give the same entropy if a temperature-independent volume translation is applied. On the other hand, different molar entropies are obtained by using a temperature-dependent volume translation.

To sum up, we can state that to obtain the numerical value of the molar entropy with the translated EoS, i.e., $s_t(T,P)$, at set temperature *T* and pressure *P*, the following steps have to be followed:

1) At the set *T* and *P*, solve the original EoS in order to get the original molar volume ($v_o$).

2) Knowing *T* and $v_o$, compute the molar entropy for the original EoS, i.e., $s_o(T,P)$.

3) At the set temperature, compute the volume translation *c* and its derivative with respect to temperature, i.e., $c'(T)$.

4) Calculate $s_t(T,P)$ with Equ. (2.29), i.e., $s_t(T,P) = s_o(T,P) + P \cdot c'(T)$.

### 2.2.3.3. Enthalpy change

$$\Delta h = \Delta g + T\Delta s \tag{2.30}$$

By combining Equs. (2.25) and (2.29), one has:

$$\Delta h = h_t(T,P) - h_o(T,P) = P(Tc' - c) \tag{2.31}$$

Regardless of the volume-translation type (constant or temperature-dependent), the two EoS generally predict different molar enthalpies. In the particular case where c is a linear function of T, i.e., $c = kT$, we get $Tc' = c$ so that, following Equ. (2.31), the two EoS predict identical molar enthalpies.

#### 2.2.3.4. Internal energy change

$$\Delta u = \Delta h - P\Delta v \tag{2.32}$$

By combining Equs. (2.31) and (2.20), one has:

$$\Delta u = u_t(T,P) - u_o(T,P) = TPc' \tag{2.33}$$

We can thus conclude that both EoS return the same internal energy if a temperature-independent volume translation is applied. On the other hand, different internal energies are obtained if using a temperature-dependent volume translation.

#### 2.2.3.5. Helmholtz energy change

$$\Delta a = \Delta u - T\Delta s \tag{2.34}$$

By combining Equs. (2.33) and (2.29), we get:

$$\Delta a = a_t(T,P) - a_0(T,P) = 0 \tag{2.35}$$

and both EoS always give the same Helmholtz energy.

#### 2.2.3.6. Constant pressure heat capacity change

Constant pressure heat capacity $c_P(T,P)$ can be calculated from $h(T,P)$ by: $c_P = \left(\partial h/\partial T\right)_P$. The derivation of Equ. (2.31) gives:

$$\Delta c_P = c_{P,t}(T,P) - c_{P,o}(T,P) = TPc'' \tag{2.36}$$

where $c'' = d^2c / dT^2$ is the second derivative of the volume translation with respect to the temperature. The translated and untranslated EoS thus give the same $c_P$ if a temperature-independent volume translation is applied.

#### 2.2.3.7. Isothermal compressibility ( $\kappa_T$ ) and volume expansivity ($\alpha$) change

By definition the isothermal compressibility is $\kappa_T = -\frac{1}{v}\left(\frac{\partial v}{\partial P}\right)_T$ , so that $\left(\kappa_T \cdot v\right) = -\left[\left(\frac{\partial P}{\partial v}\right)_T\right]^{-1}$.

Starting from:
$$\begin{cases} P_t(T,v_t) = P_0(T,v_0) \\ v_0 = v_t + c \end{cases} \tag{2.37}$$

The chain rule gives:
$$\left(\frac{\partial P_t}{\partial v_t}\right)_T = \left(\frac{\partial P_o}{\partial v_o}\right)_T \times \underbrace{\left(\frac{\partial v_o}{\partial v_t}\right)_T}_{=1} = \left(\frac{\partial P_o}{\partial v_o}\right)_T \tag{2.38}$$

Consequently: $$\Delta(\kappa_T \cdot v) = (\kappa_T \cdot v)_t - (\kappa_T \cdot v)_o = 0 \quad (2.39)$$

Such a result could have been deduced from Fig. 1 which highlights that: $\left[\frac{\partial P_o(T,v_o)}{\partial v_o}\right]_T\Big|_{v_{A_o}} = \left[\frac{\partial P_t(T,v_t)}{\partial v_t}\right]_T\Big|_{v_{A_t}}$.

By definition, the volume expansivity is $\alpha = \frac{1}{v}\left(\frac{\partial v}{\partial T}\right)_P$, so that $\alpha v = \left(\frac{\partial v}{\partial T}\right)_P$.

Since: $v_t = v_o - c$, one has: $(\alpha v)_t = \left(\frac{\partial v_t}{\partial T}\right)_P = \left[\frac{\partial (v_o - c)}{\partial T}\right]_P = (\alpha v)_o - c'$ (2.40)

Consequently: $$\Delta(\alpha \cdot v) = (\alpha \cdot v)_t - (\alpha \cdot v)_o = -c' \quad (2.41)$$

### 2.2.3.8. Constant volume heat capacity change

We know from classical thermodynamics that: $c_v = c_P - T\frac{(\alpha v)^2}{(\kappa_T v)}$ (2.42)

From Equs. (2.36), (2.39) and (2.41) one gets:

$$\begin{aligned}
\Delta c_v &= \Delta c_P - \frac{T}{(\kappa_T v)}\left[(\alpha v)_t^2 - (\alpha v)_o^2\right] \\
&= \Delta c_P - \frac{T}{(\kappa_T v)}\left[\left[(\alpha v)_o - c'\right]^2 - (\alpha v)_o^2\right] \\
&= \Delta c_P - \frac{T}{(\kappa_T v)}\left[-2c'(\alpha v)_o + c'^2\right] \\
&= TPc'' + \frac{Tc'}{(\kappa_T v)}\left[2(\alpha v)_o - c'\right]
\end{aligned} \quad (2.43)$$

Similarly to $c_P$, the two EoS return the same $c_v$ if a temperature-independent volume translation is applied.

### 2.2.3.9. Speed of sound

The speed of sound, denoted *w*, is defined by:

$$w^2 = \left(\frac{\partial P}{\partial \rho}\right)_{\bar{S}} \quad (2.44)$$

where $\rho$ is the density and $\bar{S}$ the specific entropy.

By introducing, $\gamma = \frac{\bar{C}_P}{\bar{C}_v}$ where $\bar{C}_P$ and $\bar{C}_v$ are the specific heat capacities and the molar weight M, starting from:

$$d\bar{S} = \frac{\bar{C}_v \cdot \kappa_T}{\alpha T} dP - \frac{\bar{C}_P \bar{V}}{\alpha T} d\rho \tag{2.45}$$

one gets:

$$w = v\sqrt{\frac{\gamma}{M(\kappa_T v)}} \tag{2.46}$$

$\Delta(\kappa_T \cdot v) = 0$ and $\gamma$ will be the same for the two EoS if a temperature-independent volume translation is used. Even so, the two EoS always lead to different values of the speed of sound.

#### 2.2.3.10. Second virial coefficient

The virial EoS [76] writes:

$$z(T,v) = \frac{Pv}{RT} = 1 + \frac{B(T)}{v} + \frac{C(T)}{v^2} + \frac{D(T)}{v^3} + \ldots \tag{2.47}$$

The second virial coefficient *B(T)* thus verifies:

$$B(T) = \lim_{v \to +\infty} v(z-1) \tag{2.48}$$

We have:

$$\begin{aligned} \Delta[v(z-1)] &= [v(z-1)]_t - [v(z-1)]_o \\ &= v_t(z_t - 1) - v_o(z_o - 1) \end{aligned} \tag{2.49}$$

Since:

$$z_t = \frac{Pv_t}{RT} = \frac{P(v_o - c)}{RT} = z_o - \frac{Pc}{RT} \tag{2.50}$$

one has:

$$\begin{aligned} \Delta[v(z-1)] &= v_t\left(z_o - \frac{Pc}{RT} - 1\right) - v_o(z_o - 1) \\ &= \underbrace{(v_t - v_o)}_{-c}(z_o - 1) - z_t c \end{aligned} \tag{2.51}$$

By the end:

$$\begin{aligned}\Delta B &= B_t(T,P) - B_o(T,P) \\ &= \lim_{\substack{v_o \to +\infty \\ v_t \to +\infty}} \Delta\left[v(z-1)\right] \\ &= \lim_{\substack{z_o \to 1 \\ z_t \to 1}} \left[-c(z_o - 1) - z_t c\right] \\ &= -c\end{aligned} \tag{2.52}$$

This result was expected because the second virial coefficient has the feature of a volume.

### 2.2.3.11. Vapor-liquid equilibrium condition

#### a) Vapor pressure

The original and the translated EoS lead exactly to the same vapor pressures. This is an intuitive result if one refers to Maxwell's equal area rule. According to this rule, the $P = P^{sat}$ line cuts the p-v isotherm in such a way that the areas between the line and the curve above and below the line are equal. Fig. 1 highlights that the areas are kept during a translation of the whole isotherm so that the vapor pressure is not modified (area $\alpha\beta\gamma$ = area $\alpha'\beta'\gamma'$). It is alternatively possible to reach this conclusion by starting from the uniformity of the pure-component chemical potential in the liquid and vapor phases. At a given temperature, the vapor pressure ($P_0^{sat}$) calculated by the original EoS satisfies:

$$g_{o,liq}(T, P_o^{sat}) = g_{o,gas}(T, P_o^{sat}) \tag{2.53}$$

In the same way, the vapor pressure calculated by the translated EoS ($P_t^{sat}$) must satisfy:

$$g_{t,liq}(T, P_t^{sat}) = g_{t,gas}(T, P_t^{sat}) \tag{2.54}$$

By sending Equ. (2.25) in Equ. (2.54), one has:

$$g_{o,liq}(T, P_t^{sat}) - P_t^{sat} c_{liq} = g_{o,gas}(T, P_t^{sat}) - P_t^{sat} c_{gas} \tag{2.55}$$

Let us here recall that $c$ is a component-specific parameter which, at the most, is temperature-dependent (its value is not influenced by the pure-component aggregation state). At equilibrium, the liquid and gas phases have the same temperature so that $c_{liq} = c_{gas}$ even when the volume translation is temperature-dependent. Equ. (2.55) thus writes:

$$g_{o,liq}(T, P_t^{sat}) = g_{o,gas}(T, P_t^{sat}) \tag{2.56}$$

Solving Equ. (2.53) for $P_0^{sat}$ and Equ. (2.56) for $P_t^{sat}$ leads to:

$$P_t^{sat} = P_0^{sat} \tag{2.57}$$

At this step, let us recall [39] that for mixtures a linear dependence with respect to mole fractions of the volume translation ($c_{mixture} = \sum x_i c_i$) is the only one mixing rule which leaves the phase equilibrium conditions unchanged.

**b) Property change on vaporization**

A property change on vaporization (e.g. entropy of vaporization) is the difference between the molar property in the gas ($m_{gas}$) and liquid ($m_{liq}$) phases when a pure component is in vapor-liquid equilibrium. If M designates a property, one has:

$$\Delta_{vap} M(T, P^{sat}) = m_{gas}(T, P^{sat}) - m_{liq}(T, P^{sat}) \tag{2.58}$$

By using the same notations as previous, one obtains:

$$\begin{aligned} \Delta_{vap} M_t(T, P^{sat}) - \Delta_{vap} M_o(T, P^{sat}) &= \left[ m_{t,gas}(T, P^{sat}) - m_{t,liq}(T, P^{sat}) \right] \\ &\quad - \left[ m_{o,gas}(T, P^{sat}) - m_{o,liq}(T, P^{sat}) \right] \\ &= \Delta m_{gas}(T, P^{sat}) - \Delta m_{liq}(T, P^{sat}) \end{aligned} \tag{2.59}$$

As an example, the use of Equ. (2.31) makes it possible to establish that the difference between the enthalpies of vaporization calculated by the original and the translated equations of state is:

$$\Delta_{vap} H_t - \Delta_{vap} H_o = P^{sat} \left[ T \left( c'_{gas} - c'_{liq} \right) + c_{liq} - c_{gas} \right] = 0 \tag{2.60}$$

The obtained value is zero because in both phases the temperature is the same and consequently $c_{liq} = c_{gas}$ and $c'_{gas} = c'_{liq}$.

By having a look at Equs. (2.20), (2.29), (2.33), (2.35) and (2.36), we can assert that $\Delta v$, $\Delta s$, $\Delta u$, $\Delta a$ and $\Delta c_P$ are either constant, temperature-dependent or both pressure and temperature-dependent. Consequently, these quantities have the same values in the liquid and gas phases and both EoS return the same values for: $\Delta_{vap} V$, $\Delta_{vap} S$, $\Delta_{vap} U$, $\Delta_{vap} A$ and $\Delta_{vap} C_P$. Equ. (2.43) shows that $\Delta c_v = 0$ when a temperature-independent volume translation is used so that in such a case, the original and translated EoS return the same $\Delta_{vap} C_v$. On the other hand, when a temperature-

dependent volume translation is used, the quantity $\Delta c_{v,gas}(T,P^{sat})$ is different from $\Delta c_{v,liq}(T,P^{sat})$. This is because in Equ. (2.43), the values of $(\kappa_T v)$ and $(\alpha v)$ are different in the liquid and gas phases. In other words, $\Delta_{vap}C_{v,t} \neq \Delta_{vap}C_{v,o}$ and the two EoS do not return a unique value for $\Delta_{vap}C_v$.

*Remark:* as discussed by Zabaloy and Brignole [70], the use of the Clapeyron equation:

$$\frac{dP^{sat}}{dT} = \frac{\Delta_{vap}H}{T\left(v_{gas} - v_{liq}\right)} \quad \Leftrightarrow \quad \Delta_{vap}H(T) = T\left(\frac{dP^{sat}}{dT}\right)\left(v_{gas} - v_{liq}\right) \qquad (2.61)$$

makes it possible to immediately conclude that the heat of vaporization is unaffected by the volume translation. This is because both the translated and untranslated models return the same saturation pressure and hence, the same derivative of the saturation pressure with respect to the temperature. They return different saturated molar volumes but the difference between the saturated vapor and liquid volumes is independent of *c*. Consequently, $\Delta_{vap}S = \Delta_{vap}H/T$, $\Delta_{vap}U = T\Delta_{vap}S - P^{sat}\left(v_{gas} - v_{liq}\right)$ and $\Delta_{vap}A = -P^{sat}\left(v_{gas} - v_{liq}\right)$ are also unaffected by a volume translation.

### 2.3. Conclusion

This note highlights that working with pure components, the application of a temperature-independent volume translation on a given equation of state ...

| **...** leaves unaffected, the calculated: | **...** affects, the calculated: |
|---|---|
| • Entropy: *s*<br>• Internal energy: *u*<br>• Helmholtz energy: *a*<br>• Constant pressure heat capacity: $c_P$<br>• $\left(\kappa_T \cdot v\right) = -\left(\frac{\partial v}{\partial P}\right)_T$<br>• $\alpha v = \left(\frac{\partial v}{\partial T}\right)_P$<br>• Constant volume heat capacity: $c_v$<br>• Vapor pressure: $P^{sat}$<br>• ALL the property changes on vaporization: $\Delta_{vap}V$ , $\Delta_{vap}H$ , $\Delta_{vap}S$ , $\Delta_{vap}U$ , $\Delta_{vap}A$ , $\Delta_{vap}C_v$ and $\Delta_{vap}C_P$ | • Volume<br>• Chemical potential: *g*<br>• Fugacity coefficient: $\varphi$<br>• Fugacity: *f*<br>• Enthalpy: *h*<br>• Speed of sound: *w*<br>• Second virial coefficient: *B* |

Vapor pressures, property changes on vaporization, but also many thermodynamic properties like the heat capacities are not altered by a temperature-independent volume translation. It is thus clear that the problem of reproducing both experimental phase equilibrium and experimental thermodynamic properties can be separated from the problem of reproducing experimental liquid densities. Working with cubic EoS, it is advised to determine the parameters of the alpha function on many diversified experimental data except densities (vapor pressure, heat of vaporization, heat capacities) and in a second step to determine the value of the volume translation on liquid densities and possibly speed of sound experimental data.

The use of speed of sound data is however subject to discussion. If it is only desired to improve the modelling of liquid molar volumes, it is necessary to fit the volume-translation value (*c*) on experimental saturated liquid densities, classically available from small temperatures to the critical point. At this step, it could be argued that speed

of sound data could be used as volumetric properties at supercritical temperatures. It is however impossible to guarantee that a better prediction of the high temperature speed of sound (*w*) data, improves the accuracy of the calculated supercritical molar volumes. Indeed, w not only depends on v but is also a function of $\gamma$ and $\kappa_T v$ which are often misestimated by cubic EoS. A very interesting discussion on the ability of cubic EoS to predict the sound velocities in liquids can be found in a paper by Polishuk [77]. Such a paper demonstrates that working with cubic EoS, the covolumes are too big and consequently the sound velocities are poorly predicted.

On the other hand, the application of a temperature-dependent volume translation on a given equation of state ...

| **... leaves unaffected**, the calculated: | **... affects,** the calculated: |
|---|---|
| • Helmholtz energy: *a*<br>• $(\kappa_T \cdot v) = -\left(\frac{\partial v}{\partial P}\right)_T$<br>• Vapor pressure: $P^{sat}$<br>• Most of the property changes on vaporization: $\Delta_{vap}V$, $\Delta_{vap}H$, $\Delta_{vap}S$, $\Delta_{vap}U$, $\Delta_{vap}A$ and $\Delta_{vap}C_P$. | • Volume<br>• Chemical potential: *g*<br>• Fugacity coefficient: φ<br>• Fugacity: *f*<br>• Entropy: *s*<br>• Enthalpy: *h*<br>• Internal energy: *u*<br>• Constant pressure heat capacity: $C_P$<br>• $\alpha v = \left(\frac{\partial v}{\partial T}\right)_P$<br>• Constant volume heat capacity: $C_V$<br>• Speed of sound: *w*<br>• Second virial coefficient: *B*<br>• $\Delta_{vap}C_v$ |

Once again, vapor pressures and property changes on vaporization (except $\Delta_{vap}C_v$) are not altered by a temperature-dependent volume translation. On the other hand, most of the thermodynamic properties like the heat capacities are now affected by the volume correction. It is thus no more possible to uncouple the problem of reproducing liquid densities from the problem of predicting other properties. Working with cubic

EoS, it is advised to simultaneously determine the parameters of the alpha function and those of the volume translation, *c(T)*, on all the available experimental data.

The use of a temperature-dependent volume translation is however not advised since it is a non-consistent thermodynamic approach [50,67,68].

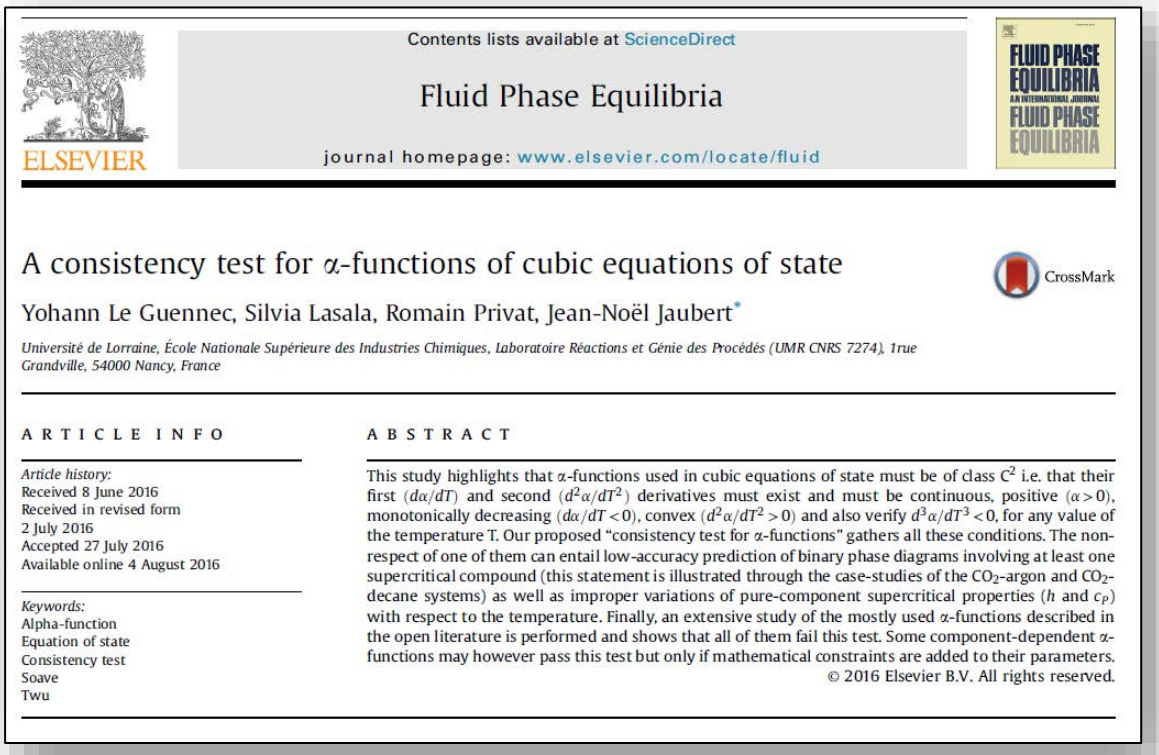
# Chapitre 3. Article “A consistency test for α-functions of cubic equations of state”

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A consistency test for α-functions of cubic equations of state

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ABSTRACT

This study highlights that α-functions used in cubic equations of state must be of class $C^2$ i.e. that their first $(d\alpha/dT)$ and second $(d^2\alpha/dT^2)$ derivatives must exist and must be continuous, positive $(\alpha > 0)$, monotonically decreasing $(d\alpha/dT < 0)$, convex $(d^2\alpha/dT^2 > 0)$ and also verify $d^3\alpha/dT^3 < 0$, for any value of the temperature T. Our proposed “consistency test for α-functions” gathers all these conditions. The non-respect of one of them can entail low-accuracy prediction of binary phase diagrams involving at least one supercritical compound (this statement is illustrated through the case-studies of the $CO_2$-argon and $CO_2$-decane systems) as well as improper variations of pure-component supercritical properties ($h$ and $c_P$) with respect to the temperature. Finally, an extensive study of the mostly used α-functions described in the open literature is performed and shows that all of them fail this test. Some component-dependent α-functions may however pass this test but only if mathematical constraints are added to their parameters.

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**Highlights**

1) A *consistency test* for α-functions is derived.
2) α-functions must be positive, decreasing, convex with negative third derivative.
3) VLE data solely shape the α-function in the subcritical domain, not beyond.
4) α-functions should pass this test to safely extrapolate to the supercritical domain.
5) No α-function from the literature passes the proposed consistency test.

**Abstract**

This study highlights that α-functions used in cubic equations of state must be of class $C^2$ i.e. that their first $(d\alpha/dT)$ and second $\left(d^2\alpha/dT^2\right)$ derivatives must exist and must be continuous, positive $(\alpha>0)$, monotonically decreasing $(d\alpha/dT<0)$, convex $\left(d^2\alpha/dT^2>0\right)$ and also verify $d^3\alpha/dT^3<0$, for any value of the temperature T. Our proposed "consistency test for α-functions" gathers all these conditions. The non-respect of one of them can entail low-accuracy prediction of binary phase diagrams involving at least one supercritical compound (this statement is illustrated through the case-studies of the $CO_2$-argon and $CO_2$-decane systems) as well as improper variations of pure-component supercritical properties ( $h$ and $c_P$ ) with respect to the temperature. Finally, an extensive study of the mostly used α-functions described in the open literature is performed and shows that all of them fail this test. Some component-dependent α-functions may however pass this test but only if mathematical constraints are added to their parameters.

**Keywords**

Alpha-function; Equation of state; Consistency test; Soave; Twu

### 3.1. Introduction

Numerous modifications to the Van der Waals cubic equation of state (CEoS) have been presented over the years [5], with the aim of representing with increasingly accuracy the properties of complex systems. As a matter of facts, most of these improvements do not incorporate a substantial difference in the functional combination of attractive and repulsive forces, with respect to the original formulation introduced by Van der Waals. As a rare exception, let us mention the Cubic-Plus-Association model (CPA) [78], which combines the Soave-Redlich-Kwong attractive and repulsive terms [7] with an association term introduced by Wertheim [79]. Indeed, analogously to the Van der Waals expression of the pressure equation [1], a generic CEoS may be written as the sum of a repulsive and an attractive term:

$$P = P_{rep} + P_{att} \tag{3.1}$$

Although the analytical expressions of the repulsive and attractive terms proposed in literature do not correctly quantify the actual repulsive and attractive contributions to pressure, their sum results in a quantitative representation of fluid properties being sufficiently accurate to make their combination the "cornerstone of the generalized Van der Waals theory" [80].

Since the Van der Waals proposal, even the most successful two-parameter CEoS still expresses their attractive and repulsive terms by introducing a parameter $a$ which is a measure of the attractive forces ("energy parameter") between molecules, and a parameter $b$ which is a measure of the size ("intrinsic volume" or "co-volume") of the molecules. It results the general formulation of a two-parameter CEoS:

$$P(T,v) = \frac{RT}{v-b} + \frac{-a(T)}{(v-r_1 b)(v-r_2 b)} \tag{3.2}$$

where $r_1$ and $r_2$ are two universal constants which depend on the selected CEoS.

The most successful theoretically-based modification to the Van der Waals CEoS consisted in the recognition by Clausius in 1879 [71] of the temperature-dependency of the energy parameter. In 1949, Redlich and Kwong [6] proposed the first temperature-dependent formulation which resulted to be sufficiently accurate to gain popularity in the industry. Starting from this outcome, many researches have been focused on the improvement of the functional form of this term, which soon proved to strongly affect the modelling capability of a CEoS in fluid equilibrium calculations. The attractive term of any CEoS can be written as:

$$a(T) = a_c \cdot \alpha(T) \tag{3.3}$$

i.e. as the product of the value of the attractive term at the critical temperature $(a_c)$ multiplied by a so-called *α-function*. Such α-functions have a strong impact on the accuracy of CEoS and must be selected with caution. Not only the properties of pure compounds in the supercritical region are highly affected by the mathematical expression of the α-function but also the vapor-liquid equilibrium calculations of multicomponent systems. From our experience, when applied to mixtures, the accuracy of CEoS is equally affected by the choice of the mixing rules and by the expression of the α-function.

The first aim of this paper is thus to present the requirements that an α-function should absolutely fulfil in order to guarantee safe predictions of the vapor-liquid equilibrium and of derived thermodynamic properties at all temperatures. Emphasis will be made on the incapacity of α-functions regressed on subcritical properties to correctly extrapolate in the supercritical temperature domain without addition of supplementary constraints during the regression procedure. Such constraints ensure, among others, the proper curvature of the α-function. Similarly to the consistency tests developed to certify the quality of experimental vapor-liquid equilibrium data, it is proposed to develop a consistency test for α-functions, i.e., to derive a list of *consistent* constraints applicable to any α-function. Such a test aims at identifying which α-functions are (or not) thermodynamically consistent and should (or not) be used. In this paper, this consistency test will be applied to twelve α-functions issued from the literature.

### 3.2. Definition, historical background and general classification of the α-functions

#### 3.2.1. Definition of the α-function

As for the original Van der Waals equation of state, the critical attractive parameter ( $a_c$ ), the covolume $(b)$ and the critical molar volume $(v_c)$ of any CEoS can be determined by applying the so-called critical constraints:

$$\begin{cases} P\left(T_c^{\exp}, v_c^{EoS}\right) = P_c^{\exp} \\ \left(\frac{\partial P}{\partial v}\right)_T \Big|_{\substack{T=T_c^{\exp} \\ v=v_c^{EoS}}} = 0 \\ \left(\frac{\partial^2 P}{\partial v^2}\right)_T \Big|_{\substack{T=T_c^{\exp} \\ v=v_c^{EoS}}} = 0 \end{cases} \tag{3.4}$$

where $T_c^{\exp}$ and $P_c^{\exp}$ are the experimental critical temperature and pressure and where the critical molar volume $\left(v_c^{EoS}\right)$ is calculated by solving the CEoS under the conditions $T = T_c^{\exp}$ and $P = P_c^{\exp}$. The resulting critical energy parameter $(a_c)$ and covolume $(b)$ are usually expressed in terms of the CEoS-dependent coefficients $\Omega_a$ and $\Omega_b$:

$$\begin{cases} a_c = \Omega_a \dfrac{R^2\left(T_c^{\exp}\right)^2}{P_c^{\exp}} \\ b = \Omega_b \dfrac{RT_c^{\exp}}{P_c^{\exp}} \end{cases} \tag{3.5}$$

While a covolume is necessarily temperature-independent [68], the energy parameter $a(T)$ is written as the product of its value at the critical point, $a_c$, and of a temperature-dependent α-function:

$$a(T) = a_c \cdot \alpha(T) \tag{3.6}$$

Doing so, it follows that $\alpha(T)$ is a non-dimensional factor which becomes unity at the critical temperature

$$\alpha(T_c) = 1 \tag{3.7}$$

Therefore, α-function should be considered as a deviation factor of the energy parameter of a CEoS to its value at the critical temperature.

### 3.2.2. Historical background and general classification of the α-functions

One of the most influential contributions in the prediction of vapor pressures of non-polar and slightly polar pure compounds has been the introduction in 1972 of the Soave α-function [7]. Over the years, further modifications have been introduced to this

functional form, mainly aimed at improving the correlation of vapor pressures. Higher accuracy was achieved by the addition of more parameters [26,29] but as stated by Poling et al. [81], most of the α-functions presented in literature have been developed without evaluating their predictive capability in the supercritical domain. Indeed, the Soave α-function diverges at very high temperature, leading to unrealistic calculations of thermodynamic properties. Therefore, α-functions inspired by the Soave formulation, called *polynomial α-functions* as they are polynomials of the square-root of the reduced temperature, should not be used at high reduced temperature. To overcome this limitation, some authors proposed *exponential α-functions* [19,35–37,82] which are positive and decreasing functions on the whole temperature range.

Aware of the benefits of using a *polynomial α-function* in the subcritical temperature domain and using an *exponential α-function* in the supercritical temperature domain, some authors proposed *piecewise α-functions* with different mathematical expressions for the α-function depending on whether the temperature is above or below the critical temperature, leading to possible discontinuities of the α-function derivatives at the critical temperature. Although this approach seems to be a good compromise between the complexity of the α-function expression and the accuracy of results, it was objected by Coquelet et al. [83] that continuity of the first and second derivatives of the α-function at the critical temperature must be enforced. If not, calculated residual enthalpies and heat capacities show discontinuities at the critical temperature. This abnormal behavior of the *piecewise α-functions* was also highlighted by Boston et al. [84], Twu et al. [36,37] when they respectively proposed their own α-functions and deeply analyzed by Neau et al. [16,17].

As reported by Valderrama [5], numerous α-functions can be found in the literature and are compared in some recent papers [85,86]. Enumerating all the existing *α-functions* is not of practical interest as only a dozen of them are used in the commercial process simulation software. Therefore, a general classification of the α-functions based on their mathematical form (polynomial or exponential) and on the unicity of their formulation (T-overall formulation or piecewise) is presented in Table 3.1. Moreover, we found desirable to distinguish two kinds of α-functions: *component-dependent* α-functions and *generalized* ones. Parameters of component dependent α-functions have to be regressed, component by component, on experimental data while coefficients of generalized α-functions are determined with correlations needing the acentric factor $(\omega)$ as input parameter. Therefore, generalized α-functions can be

applied to pure compounds for which no experimental vapor-liquid equilibrium data, except $\omega$, are known. This advantage is counterbalanced by a less accurate prediction of the thermodynamic properties.

In the rest of the article, emphasis will be made on two α-functions having a T-overall formulation: the model proposed by Soave (1972) (from now on, called Soave) and the one introduced by Twu (1991) (from now on, called Twu91). Their expressions are reported below.

- The Soave α-function [7]

$$\begin{cases} \alpha(T_r) = \left[1 + m(\omega)\left(1 - \sqrt{T_r}\right)\right]^2 \\ m(\omega) = 0.480 + 1.574\omega - 0.176\omega^2 & \text{for the Redlich-Kwong CEoS} \\ m(\omega) = 0.37464 + 1.54226\omega - 0.26992\omega^2 & \text{for the Peng-Robinson CEoS} \end{cases} \quad (3.8)$$

This α-function is polynomial, generalized and it has a T-overall formulation. Having regard to its simplicity and to the accuracy of results obtained by using it, this α-function should be regarded as a reference before deriving any new α-function. These reasons justify, in fact, its widespread popularity.

- The Twu91 α-function [19]

$$\alpha(T_r) = T_r^{N(M-1)} \exp\left[L\left(1 - T_r^{MN}\right)\right] \quad (3.9)$$

This α-function is exponential, component-specific and it has a T-overall formulation. Parameters L, M and N have to be optimized, component by component, over experimental data so that better accuracy is expected in comparison to the Soave α-function.

| | Component-**dependent α**-functions | |
|---|---|---|
| | T-overall formulation<br>(unique temperature formulation) | Piecewise |
| Polynomial | Soave (1984) [32]<br>$\alpha = 1 + (1 - T_r)\left(a + \frac{b}{T_r}\right)$ | Stryjek-Vera [29]<br>$\alpha = \left[1 + \kappa\left(1 - \sqrt{T_r}\right)\right]^2$<br>$\kappa = \kappa_0 + \kappa_1\left(1 + \sqrt{T_r}\right)(0.7 - T_r)$<br>$\kappa_0 = 0.378893 + 1.4897153\omega - 0.17131848\omega^2 + 0.0196554\omega^3$<br>$\begin{cases} \kappa_1(T \le 0.7T_c) \ne 0 \\ \kappa_1(T > 0.7T_c) = 0 \end{cases}$ |
| | Gibbons-Laughton [87]<br>$\alpha = 1 + X(T_r - 1) + Y\left(\sqrt{T_r} - 1\right)$ | Mathias-Copeman [26]<br>$\alpha_{SUB} = \alpha(T_r \le 1) = \left[\begin{array}{l} 1 + c_1\left(1 - \sqrt{T_r}\right) + c_2\left(1 - \sqrt{T_r}\right)^2 \\ + c_3\left(1 - \sqrt{T_r}\right)^3 \end{array}\right]^2$<br>$\alpha_{SUP} = \alpha(T_r \ge 1) = \left[1 + m\left(1 - \sqrt{T_r}\right)\right]^2$ |
| Exponential | Twu (1988) [35]<br>$\alpha = T_r^{2(M-1)} \exp\left[L\left(1 - T_r^{2M}\right)\right]$ | – Not any – |

| | | |
|---|---|---|
| | Twu (1991) [19]<br>$\alpha = T_r^{\delta} \exp\left[ L\left(1 - T_r^{\gamma}\right)\right]$<br>Trebble-Bishnoi [88]<br>$\alpha = \exp\left[ L\left(1 - T_r\right)\right]$ | |
| Polynomial & Exponential | Melhem-Saini-Goodwin [89]<br>$\alpha = \exp\begin{bmatrix} m\left(1 - T_r\right) \\ +n\left(1 - \sqrt{T_r}\right)^2 \end{bmatrix}$ | Boston-Mathias [84]<br>$\begin{cases} \alpha_{SUB} = \alpha\left(T_r \le 1\right) = \alpha_{SOAVE} = \left[1 + m\left(1 - \sqrt{T_r}\right)\right]^2 \\ \alpha_{SUP} = \alpha\left(T_r > 1\right) = \exp\left[ L\left(1 - T_r^{\gamma}\right)\right] \end{cases}$<br>with $\begin{cases} L = \dfrac{2m}{1+m} \\ \gamma = 1 + \dfrac{m}{2} \end{cases}$ |

Mathias [90]

$$\begin{cases} \alpha_{SUB} = \alpha\left(T_r \le 1\right) = \left[1 + m(\omega)\left(1 - \sqrt{T_r}\right) - p\left(1 - T_r\right)\left(0.7 - T_r\right)\right]^2 \\ \alpha_{SUP} = \alpha\left(T_r > 1\right) = \left[\exp\left[L\left(1 - T_r^{\gamma}\right)\right]\right]^2 \end{cases}$$

with $\begin{cases} L = 1 + \dfrac{m}{2} + 0.3p \\ \gamma = \dfrac{L-1}{L} \end{cases}$

**Generalized α-functions**

| | T-overall formulation (unique temperature formulation) | Piecewise |
|---|---|---|
| Polynomial | Soave (1972) [7]<br>$\begin{cases} \alpha = \left[1 + m(\omega)\left(1 - \sqrt{T_r}\right)\right]^2 \\ m_{RK}(\omega) = 0.480 + 1.574\omega - 0.176\omega^2 \\ m_{PR}(\omega) = 0.37464 + 1.54226\omega - 0.26992\omega^2 \end{cases}$ | – Not any – |
| Exponential | Trebble-Bishnoi [91] | Twu (1995) [36,37] |

| | |
|---|---|
| $\alpha = \exp\left[L\left(1-T_r\right)\right]$<br>For alkanes, water and carbon dioxide:<br>if $\omega \le 0.4$: $L = 0.418 + 1.58\omega - 0.580\omega^2$<br>if $\omega \ge 0.4$: $L = 0.212 + 2.20\omega - 0.831\omega^2$ | $\begin{cases} \alpha = \alpha^{(0)} + \omega\left[\alpha^{(1)} - \alpha^{(0)}\right] \\ \alpha^{(0)} = T_r^{N^{(0)}\left[M^{(0)}-1\right]} \exp\left[L^{(0)}\left(1-T_r^{M^{(0)}N^{(0)}}\right)\right] \\ \alpha^{(1)} = T_r^{N^{(1)}\left[M^{(1)}-1\right]} \exp\left[L^{(1)}\left(1-T_r^{M^{(1)}N^{(1)}}\right)\right] \end{cases}$<br>(see appendix C for more details) |

Table 3.1. Classification of α-functions commonly found in process simulation software.

Component-dependent α-functions are usually parameterized over vapor-liquid equilibrium data, which are also the most reported data in the literature. Therefore, most of the α-functions will have a similar behavior in the subcritical temperature domain. However, the literature lacks of specific, theoretically-based guidelines to derive an α-function that could guarantee consistent predictions, also in the supercritical temperature domain, of thermodynamic properties related to the α-function itself and to its derivatives. With that respect, the purpose of the next section is to present requirements that a proper α-function should fulfil.

### 3.3. Requirements for a consistent α-function

Firstly, to avoid non-physical positive values of the attractive term, α-functions should be positive and thus lead to a decrease of the pressure of the system when the attraction between molecules increases. As stated by Deiters [92], a negative α-function "only results from compensating an insufficient repulsion term" and should be regarded as a consequence of a maladjusted model but not as a theoretical valid behavior.

Secondly, α-functions should be constant at the infinite temperature limit. This constant can be positive or zero. Colina et al. [93] give proof that the limiting value of α at the infinite temperature limit would be equal to zero, by assuming that (i) "at infinite temperature, the cubic EoS reduces to a hard-body EoS, with residual internal energy identically zero at all densities" and (ii) the Van der Waals repulsive term $RT/(v-b)$ correctly represents hard-body repulsions. However, Abbott and Prausnitz [94] and Sandler [95] leave some uncertainty on whether the α-function at infinite temperature should assume a zero rather than a positive finite value. Since no unquestionable theoretical evidences have been found on this issue, we do not conclude about the constant value of the α-function at infinite temperature.

Thirdly, as temperature decreases, the average molecular kinetic energy is reduced, resulting in a system where molecules are particularly prone to interacting, upon collision. This explains why the CEoS energy parameter should become increasingly important when temperature decreases. In other words, α has to be a decreasing function of temperature, its first derivative has not only to be negative but has also to cancel out at the infinite temperature limit to ensure a finite α-value. It should be noticed that, if an α-function is both positive and decreasing, it will automatically admit a finite value at the infinite temperature limit.

The last point is that not only the α-function but also its first and second derivatives with respect to the temperature have to be continuous functions of temperature in order to avoid discontinuities in the calculated state functions. As highlighted in Eq.(3.10), α indeed appears in the mathematical expression of the fugacity and the residual molar enthalpy, the first derivative of α appears in the mathematical expression of the residual molar enthalpy and entropy and the second derivative of α appears in the mathematical expression of the residual heat capacity at constant volume.

$$\begin{cases} \ln f(T,v) = v\left[\dfrac{1}{v-b} - \dfrac{a_c \boldsymbol{\alpha(T)}}{RT(v-r_1 b)(v-r_2 b)}\right] - 1 - \ln\left(\dfrac{v-b}{RT}\right) \\ \qquad\qquad + \dfrac{a_c \boldsymbol{\alpha(T)}}{RTb(r_1-r_2)} \ln\left(\dfrac{v-r_1 b}{v-r_2 b}\right) \\ s^{res}(T,v) = R\ln\left(\dfrac{v-b}{v}\right) - \dfrac{a_c}{b(r_1-r_2)} \dfrac{\boldsymbol{d\alpha(T)}}{\boldsymbol{dT}} \ln\left(\dfrac{v-r_1 b}{v-r_2 b}\right) \\ h^{res}(T,v) = \dfrac{RTb}{v-b} - \dfrac{a_c \boldsymbol{\alpha(T)} v}{(v-r_1 b)(v-r_2 b)} + \dfrac{a_c}{b(r_1-r_2)}\left[\boldsymbol{\alpha(T)} - T\dfrac{\boldsymbol{d\alpha(T)}}{\boldsymbol{dT}}\right] \ln\left(\dfrac{v-r_1 b}{v-r_2 b}\right) \\ c_v^{res}(T,v) = \dfrac{-Ta_c}{b(r_1-r_2)} \dfrac{\boldsymbol{d^2\alpha(T)}}{\boldsymbol{dT^2}} \ln\left(\dfrac{v-r_1 b}{v-r_2 b}\right) \end{cases} \tag{3.10}$$

We can summarize our observations by:

$$\text{For all T: } \begin{cases} \alpha(T) \geq 0 \text{ and continuous} \\ \dfrac{d\alpha}{dT} \leq 0 \text{ and continuous} \\ \dfrac{d^2\alpha}{dT^2} \text{ continuous} \end{cases} \tag{3.11}$$

These conditions are often cited in the literature as sufficient conditions for consistent predictions of thermodynamic properties but: are they really sufficient? In the next section, we are going to answer this key question through a case study: the calculation of the isothermal phase diagram of the system $CO_2$-argon at 253.1 K, with the Peng-Robinson CEoS, associated with two α functions that satisfy criteria in (3.11). Before presenting calculation results over this system, it is worth pointing out that it is a complex mixture to be modelled since it exhibits a type III phase behavior in the classification scheme of Van Konynenburg and Scott [96].

### 3.4. Case-study: prediction of the $CO_2$-argon binary phase diagram

The $CO_2$-argon binary system is considered as a key system for $CO_2$-Capture and Storage (CCS) applications [97]. It is desired to predict the phase diagram of this system at 253.1 K with the Peng-Robinson CEoS and highly efficient mixing rules which combine the expression by Huron and Vidal [98] with the residual part of the Wilson activity-coefficient model [99]. The two parameters of the Wilson model were regressed in order to minimize the following objective function which takes into account the deviations between calculated and experimental molar fractions of $CO_2$ in the liquid (x) and gas (y) phases:

$$F_{obj,1} = \sum_{i=1}^{N_{exp}} \left( \frac{x_i^{\exp} - x_i^{calc}}{\sigma_{x_i}^{\exp}} \right)^2 + \sum_{i=1}^{N_{exp}} \left( \frac{y_i^{\exp} - y_i^{calc}}{\sigma_{y_i}^{\exp}} \right)^2 \tag{3.12}$$

where $\sigma_{\Gamma_i}^{\exp}$ is the experimental standard deviation associated to the $i^{th}$ data point of property $\Gamma$.

In order to test the influence of the selected α-function on the resulting calculations, two different α-functions, that are the Soave and the Twu91 α-functions, were successively considered for both pure carbon dioxide and argon. The m-parameter of the Soave α-function was calculated by applying Eq. (3.8), while the three parameters L, M and N of the Twu91 α-function were determined by minimizing the objective function expressed by Eq. (3.13), which takes into account the deviations between calculated and pseudo-experimental vapor pressures ($P^{sat}$), enthalpies of vaporization $\left(\Delta_{vap}H\right)$ and saturated liquid heat capacities ($c_{P,L}^{sat}$):

$$F_{obj,2} = \sum_{i=1}^{50} \left| \frac{P_{EoS}^{sat}(\mathrm{P},T_i) - P_{DIPPR}^{sat}(T_i)}{P_{DIPPR}^{sat}(T_i)} \right| + \sum_{i=1}^{50} \left| \frac{\Delta_{vap}H_{EoS}(\mathrm{P},T_i) - \Delta_{vap}H_{DIPPR}(T_i)}{\Delta_{vap}H_{DIPPR}(T_i)} \right| + \sum_{i=1}^{50} \left| \frac{c_{P,L,EoS}^{sat}(\mathrm{P},T_i) - c_{P,L,DIPPR}^{sat}(T_i)}{c_{P,L,DIPPR}^{sat}(T_i)} \right| \tag{3.13}$$

The pseudo-experimental $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$ data were extracted from the correlations available in the DIPPR database: for each property, 50 equidistant data points were generated in the temperature validity range of the correlations. Following this regression procedure, optimal parameters have been obtained for the Twu91 α-function. Those are reported in Table 3.2.

| | $CO_2$ | Argon |
|---|---|---|
| L | 0.040 | 0.027 |
| M | 0.943 | 0.968 |
| N | 8.538 | 8.213 |

Table 3.2. Twu91 α-function parameters of $CO_2$ and argon obtained by minimizing Eq. (3.13).

A significant difference between the two calculated phase diagrams of the $CO_2$-argon system is observable in Figure 3.1. To better analyze the cause of such a difference, it is worth recalling that the two phase diagrams were modeled using the same CEoS and the same mixing rules; they thus only differ in the choice of the α-function.

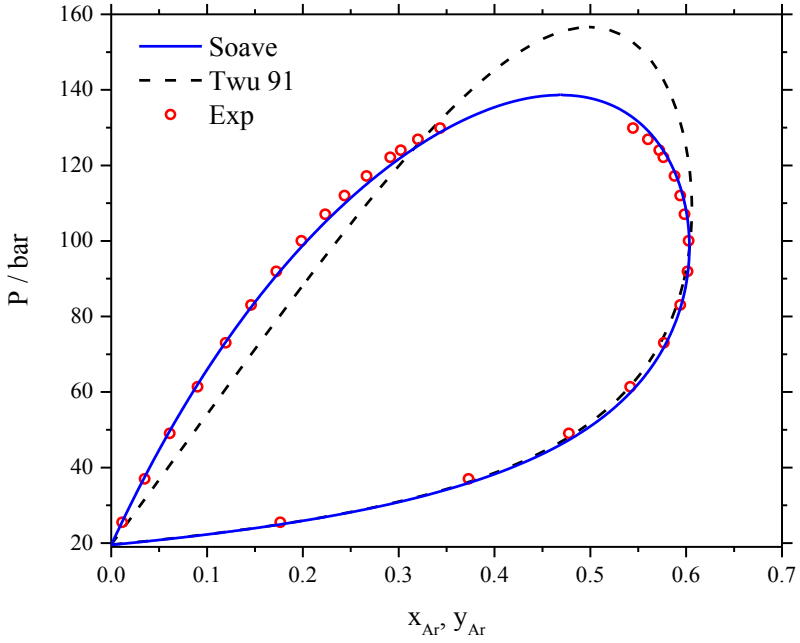



Figure 3.1. Binary phase diagram of the $CO_2$-Ar system at 253.1 K calculated with the Peng-Robinson CEoS and two different α-functions parameterized on subcritical vapor-liquid equilibrium data.

When the Soave α-function is used for both compounds, a nearly perfect prediction of the phase diagram is achieved (the continuous curve is extremely close to the experimental data points). On the other hand, very poor results are obtained with the Twu91 α-function. By having a look at the dashed curve in Figure 3.1, it could be erroneously concluded that the Peng-Robinson EoS is totally unable to correlate the $CO_2$-argon system and that it over predicts the binary critical pressure and the

solubility of argon in $CO_2$. It is undeniably surprising to observe that the generalized Soave α-function, which does not contain any adjustable parameter, performs better than the component-dependent Twu91 α-function that involves three adjustable parameters per component. In order to better understand the origin of the significant difference between the two calculated phase diagrams, it is necessary to analyze more closely each of the two α-functions (Soave and Twu91) which were designed to accurately reproduce pure component vapor-liquid equilibrium data. To this aim, α-curves of $CO_2$ and argon are reported in Figure 3.2 and Figure 3.3. The two figures highlight that, in the temperature range where the parameters were fitted (let us say between $0.4T_c$ and $T_c$), the Soave and Twu 91 α-functions are superimposed for both pure components.

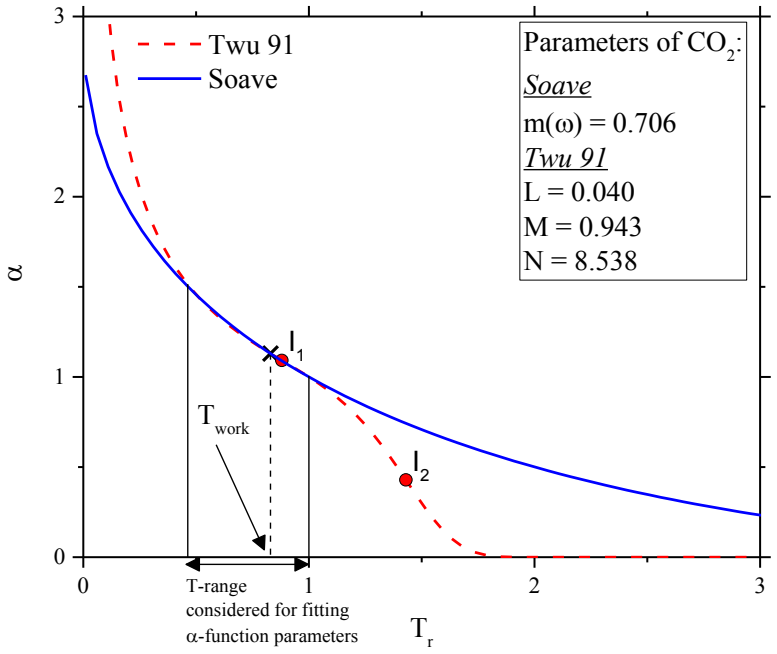



Figure 3.2. α-curves of $CO_2$ parameterized on subcritical vapor-liquid equilibrium data.

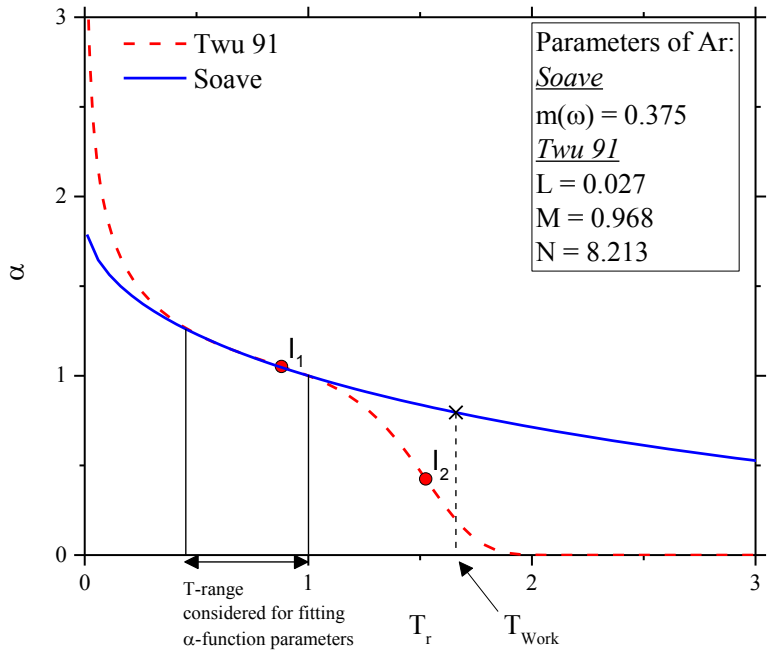



Figure 3.3. α-curves of argon parameterized on subcritical vapor-liquid equilibrium data.

At the working temperature of 253.1 K, pure $CO_2$ is subcritical ($T_c$ = 304.21 K) while pure argon is supercritical ($T_c$ = 150.86 K). Since for $CO_2$ the working temperature is in the range where the parameters were fitted, it is not surprising to observe (see x symbol in Figure 3.2) that, at this temperature, the two α-functions return the same value. On the other hand, at 253.1 K, argon is supercritical ($T_r$ = 1.7), that is at a temperature completely outside the range where the parameters were fitted. At this temperature, the two α-functions take totally different values ($\alpha_{Soave} \approx 0.8$ and $\alpha_{Twu} \approx 0.2$), as shown in Figure 3.3. At this step it is thus possible to conclude that the mismatch in α-values for argon is the unique responsible for the poor correlation of the $CO_2$-argon vapor-liquid equilibrium data with the Twu91 α-function at 253.1 K. Such a difference between α-function values in the supercritical domain, for both $CO_2$ and argon, appears to be caused by the presence of two inflection points along the Twu91 α-curve. As highlighted by Figure 3.2 and Figure 3.3, Twu91 α-functions of argon and $CO_2$ go from convex to concave to convex with a steep and quick decrease in the concave part of the α-curve. On the other hand, the Soave α-function is strictly convex on the whole temperature range with a significantly slower decrease in the supercritical domain. Figure 3.2 and Figure 3.3 thus give rise to two questions which are addressed in the next section: are the two inflection points observed on the Twu91 α-curve the actual responsible for the poor correlation of the binary vapor-liquid

equilibrium data and, above all, are such inflection points thermodynamically consistent?

### 3.5. Are inflection points on α-curves thermodynamically consistent?

To begin, let us recall that at an inflection point, the curvature of a function changes sign and hence its second derivative vanishes:

$$\left.\frac{d^2\alpha}{dT_r^2}\right|_{T_r,\text{inflection point}} = 0 \tag{3.14}$$

Among all the thermodynamic properties that can be derived from a CEoS, the residual heat capacity at constant volume is directly proportional to the second derivative of the α-function:

$$c_v^{res}(T,v) = \frac{Ta_c}{b(r_1-r_2)}\frac{d^2\alpha}{dT^2}\ln\left(\frac{v-r_2b}{v-r_1b}\right) \tag{3.15}$$

The $c_v$ coefficient is given by:

$$c_v(T,v) = c_v^{\bullet}(T) + c_v^{res}(T,v) \tag{3.16}$$

with $c_v^{\bullet}$ the heat capacity at constant volume of the perfect gas. As a direct consequence, if an α-curve exhibits an inflection points at temperature $T^*$, the second derivative of α with respect to the temperature vanishes (see Eq.(3.14)) at $T^*$, $c_v^{res}$ cancels out and, thus, $c_v$ takes the value of that of the perfect gas, $c_v^{\bullet}$ (see Eq.(16)), uniquely dependent on temperature. It is thus possible to write that, at $T^*$:

$$c_v(T^*,v) = c_v^{\bullet}(T^*) \tag{3.17}$$

and whatever the molar volume is (i.e. irrespectively of the pressure), $c_v$ is the same (that of the perfect gas). Since, at the temperature $T^*$, $c_v$ results to be pressure independent, all the isobaric curves in a $c_v$-$T$ plane are going to intersect at such a temperature. For illustration purpose, the change of $c_v$ with respect to $T$, calculated for pure $CO_2$ with the Twu91 α-function (see Table 3.2 for values of L, M and N), is shown in Figure 3.4 within the pressure range 50-150 bar. As expected, at the two reduced temperatures ($T_{r,1}^*$ and $T_{r,2}^*$) where the α-curve exhibits an inflection point

(i.e. where the second derivative vanishes) all the isobars (P / bar = 50, 100, 150) in the ($c_V$, $T$) plane intersect. Experimental evidences about this peculiar behavior have never been observed and therefore we are convinced of its unphysical foundation. Consequently, the presence of inflection points on α-curves should be regarded as thermodynamically inconsistent and should, thus, be avoided. In other words, the second derivative of α-functions should never cancel out.

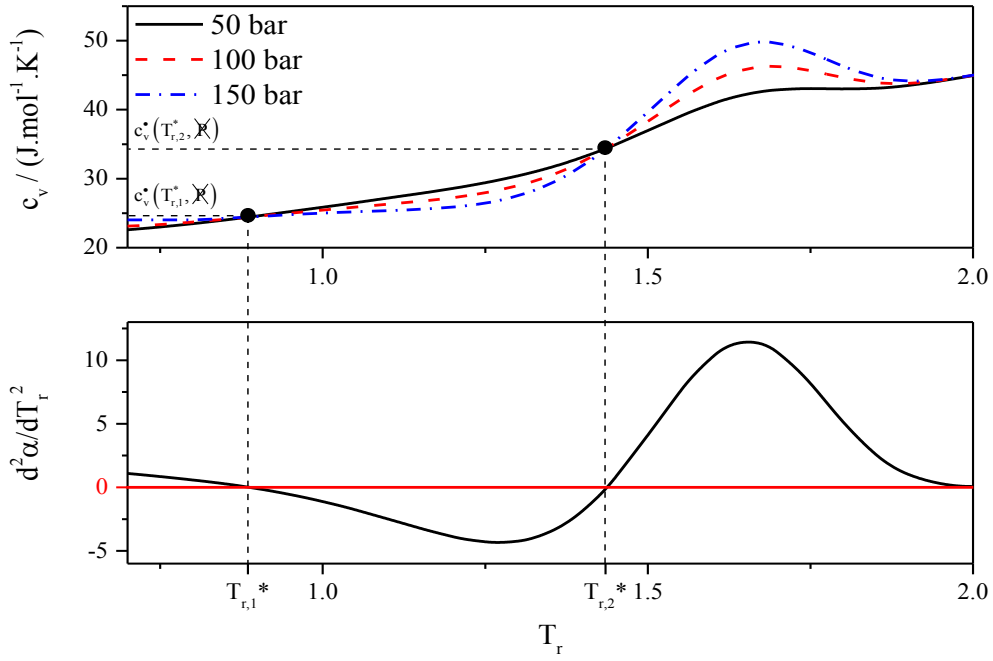



Figure 3.4. Illustration of the unphysical isobars crossing when the second derivative of an α-function cancels – case of $CO_2$.

To avoid inconsistent inflection points on the α-curve we must impose the convexity of the α-function, for any temperature value:

$$\frac{d^2\alpha}{dT^2} \geq 0 \text{ for all T} \tag{3.18}$$

That being said, parameters of the Twu91 α-function of $CO_2$ and argon have thus been re-regressed in this section by imposing the constraint $d^2\alpha/dT^2 > 0$ on the second derivative (the mathematical aspects are derived in Appendix A). Corresponding values for the L, M and N parameters are reported in Table 3.3.

| | $CO_2$ | Argon |
|---|---|---|
| L | 0.091 | 0.072 |
| M | 0.890 | 0.919 |
| N | 3.805 | 2.667 |

Table 3.3. Parameters regressed for the Twu91 α-function when convexity of the α-curve is enforced.

α-curves obtained with and without the imposition of the convexity of the corresponding α-function (Eq. (3.18)), are reported in Figure 3.5 and Figure 3.6. The second derivative of the convex α-function is also reported, to enable the reader to attest that, as imposed, it is always positive.

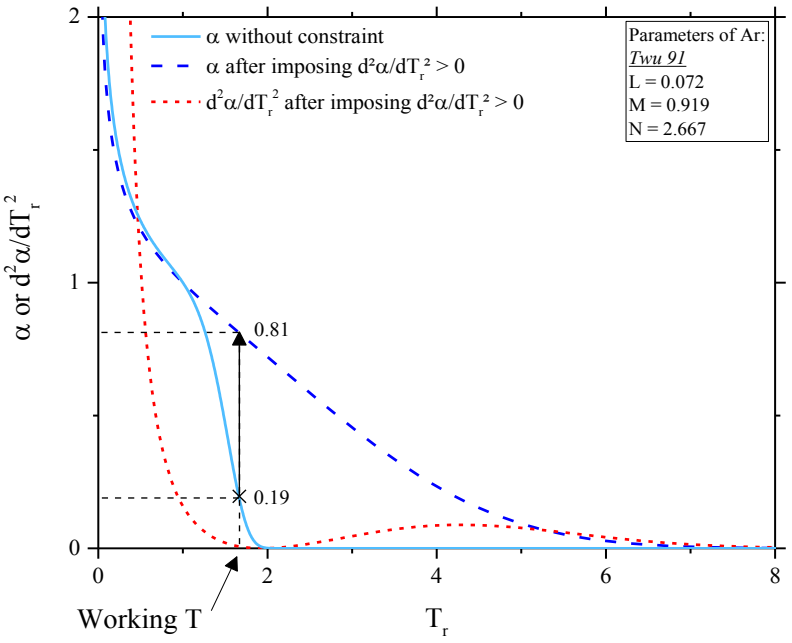



Figure 3.5. α-function of pure argon and its second derivative when the convexity constraint is enforced.

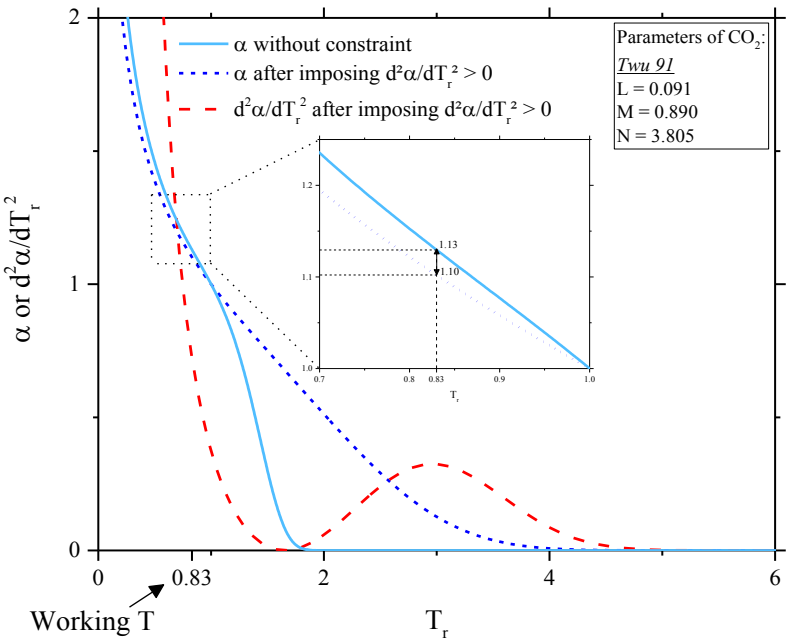



Figure 3.6. α-function of pure $CO_2$ and its second derivative when the convexity constraint is enforced.

As highlighted by Figure 3.5 at the working temperature of 253.1 K, the value of the non-convex α-function of argon (being *supercritical* in this condition) is 0.19. Differently, Twu91 L, M and N parameters optimized under the imposition of the convexity constraint lead to an α-function value of 0.81, at the same temperature of 253.1 K. On the other hand, at 253.1 K α-value of $CO_2$, (being *subcritical* at that temperature), is only slightly affected by the addition of the convexity constraint (see Figure 3.6); it raises from 1.10 to 1.13.

Moreover, it should be noticed, from both Figure 3.5 and Figure 3.6, that major changes on α-curves, deriving from the imposition of constraint in Eq. (3.18), lie in the *supercritical* domain, leaving almost unchanged the *subcritical* part of it. This is a straightforward consequence of the fact that, as mentioned above, only subcritical data were used in the optimization procedure. It is also possible to conclude that different sets of parameters leading to the same objective function value, i.e. leading to the same α-function values in the subcritical domain, are obtained when Eq. (3.13) is minimized. Such sets of parameters however lead to totally different behaviors in the supercritical region.

Furthermore, Figure 3.7 reports the comparison between experimental VLE data and phase diagrams calculated by means of the PR-EoS either combined with the Soave α-function (as previously shown in Figure 3.1) or with the re-parameterized Twu91 model

(L, M, N parameters collected in Table 3.3). Comparing Figure 3.1 and Figure 3.7, that only differ in the VLE calculations performed with the Twu91 model, it is possible to attest that the imposition of the condition $d^2\alpha/dT^2 > 0$ to Twu91 parameters (Figure 3.7) results in a spectacular improvement of the accuracy of such a model. Figure 3.7 also highlights that a similar accuracy of prediction is achieved using either the Twu91 α-function with the convexity constraint or the Soave α-function.

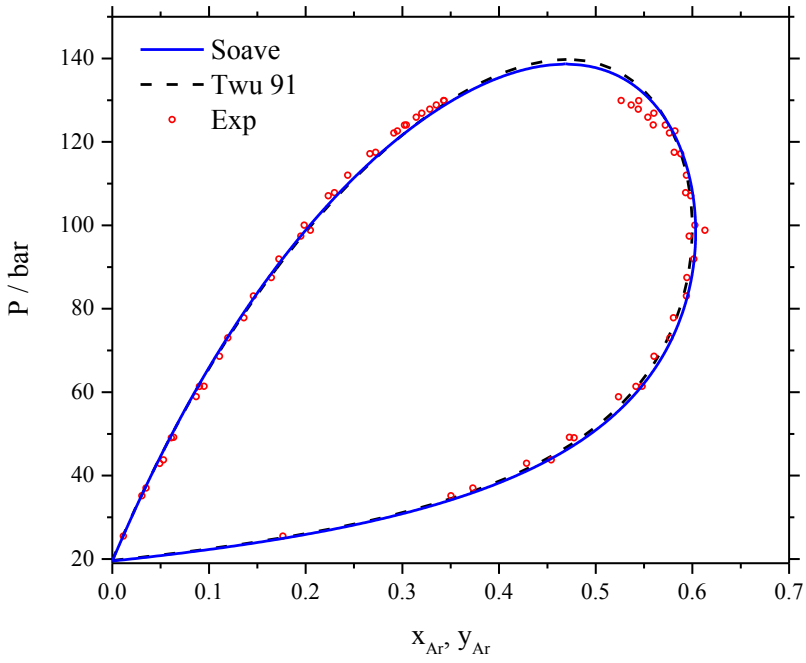



Figure 3.7. Binary phase diagram of the $CO_2$-Ar system at 253.1 K when the convexity constraint is enforced ($d^2\alpha/dT^2 > 0$).A satisfactory prediction of the binary phase diagram being now achieved by the imposition of $d^2\alpha/dT^2 > 0$, our following priority concern is the investigation of the necessity of adding new constraints to properly predict state functions, such as enthalpies and heat capacities, also in the supercritical domain.

### 3.6. Relevance of the parameters obtained by imposing $d^2\alpha/dT^2 > 0$ to predict state functions in the supercritical domain

Pseudo-experimental enthalpy ($h$) and heat capacity ($C_P$) were generated for pure $CO_2$ and pure argon in the supercritical domain, in particular for reduced temperatures ranging from 1.2 to 5. The reference Span-Wagner equation [100] was used in this work to estimate properties of $CO_2$ at 10, 59.7, 109, 159 and 209 bar, while the Tegeler-Span-

Wagner reference equation [101] was used for argon at 10, 42, 74, 106 and 138 bar. Figure 3.8 shows the comparison between properties calculated with these reference models and their values determined with the Peng-Robinson EoS combined with the Twu91 $\alpha$-function (see Table 3.3 for values of L, M, and N). As it can be seen from Figure 3.8c and Figure 3.8d, molar enthalpies ( $h$ ) are well represented by the newly regressed $\alpha$-functions for both $CO_2$ and Ar: not only the numerical values are accurately predicted but also the change of $h$ with respect to the temperature is properly reproduced. Totally different conclusions apply for the $c_P$ . The Peng-Robinson EoS with the currently evaluated $\alpha$-function predicts a "wave shape" while the application of reference equations results in a weak change of the $c_P$ with respect to temperature (a minimum is only observed). Such unexpected behavior is particularly visible in Figure 3.8b, relative to $CO_2$. By comparing Figure 3.6 and Figure 3.8b, it is noticeable that both $d^2\alpha/dT^2$ and $c_P$ curves exhibit the same "wave shape" in a similar temperature range. It is thus expected that the $c_P$ curve would exhibit a more realistic trend by removing the "wave shape" on the $d^2\alpha/dT^2$ curve. To do that, it is enough to eliminate (see Figure 3.6) the increasing part of such a function. In other words, it is expected that the imposition of condition $d^3\alpha/dT^3 < 0$ would result in $c_P$ variations with temperature, calculated with the PR EoS, being similar to those obtained with the reference equations.

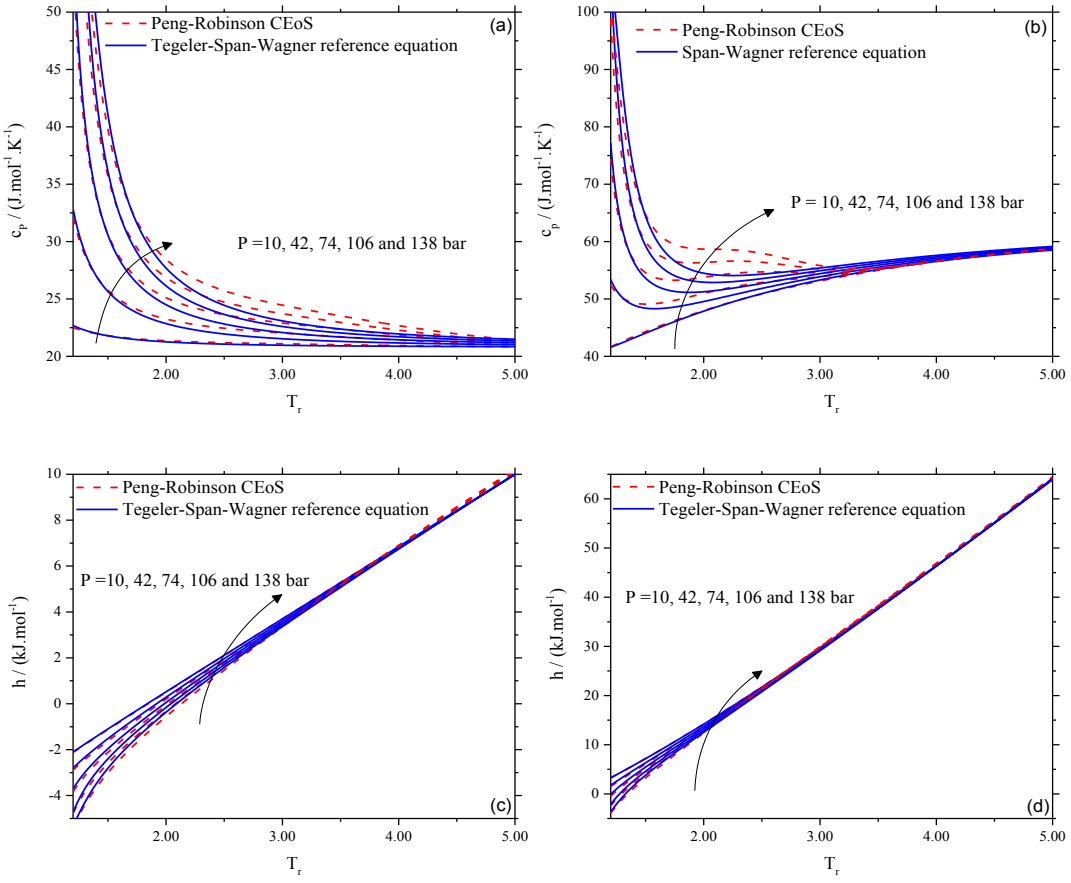



Figure 3.8. Prediction of supercritical $c_P$ of argon (a) and $CO_2$ (b) and prediction of supercritical $h$ of argon (c) and $CO_2$ (d) when convexity constraint ($d^2\alpha/dT^2 > 0$) only is applied.

To check this hypothesis, the parameters of the Twu91 α-function of $CO_2$ and argon have been thus re-optimized under the simultaneous imposition of $d^2\alpha/dT^2 > 0$ and $d^3\alpha/dT^3 < 0$. Optimal values of parameters are reported in Table 3.4.

| | $CO_2$ | Argon |
|---|---|---|
| L | 0.091 | 0.072 |
| M | 0.890 | 0.919 |
| N | 3.805 | 2.667 |

Table 3.4. Parameters regressed for the Twu91 α-function when both the convexity of the α-curve $\left(d^2\alpha/dT^2 > 0\right)$ and the negativity of the third derivative of the α-function $\left(d^3\alpha/dT^3 < 0\right)$ are enforced.

α-functions that result from the use of these parameters (Table 3.4) are represented in Figure 3.9 and Figure 3.10. These figures also report the second derivatives, calculated with respect to temperature, relative to these α-functions. A major change in the shape of the α-curve which results from the use of this new set of constraints concerns the rate at which α-functions decrease to zero. It can be seen that the use of parameters reported in Table 3.3 (optimized over the unique constraint $d^2\alpha/dT^2 > 0$) results in α-functions that equal zero at a reduced temperature $T_r \sim 4$, while the application of parameters optimized under the simultaneous imposition of $d^2\alpha/dT^2 > 0$ and $d^3\alpha/dT^3 < 0$ generates α-functions that equal zero at higher reduced temperatures, $T_r > 8$. Therefore, for such functions, the attractive term of the CEoS used for the calculations still plays a relevant role at high temperature.

Supercritical $h$ and $c_P$ of $CO_2$ and argon are represented in Figure 3.11. For both compounds, the quality of prediction of $h$ is similar to the one previously obtained when the third derivative of the α-functions could be positive. On the other hand, this new set of parameters not only guarantees more accurate $c_P$ values but also correct trends of $c_P$ -variations with temperature, with respect to results obtained from reference models.

It is legitimate now to wonder what was the prize to pay to get such a large improvement of the state functions in the supercritical domain. Were subcritical properties damaged? To answer this question, deviations on $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$ for both compounds have been calculated and reported in Table 3.5. The content of this table enables the comparison between results obtained with the addition of the

constraint on the third derivative of the α-function to the results obtained when only the convexity constraint was enforced. As highlighted by Table 3.5, this huge improvement on the prediction of the supercritical properties is marginally counterbalanced by a small accuracy decrease of $c_{P,L}^{sat}$ of $CO_2$ and argon. Moreover, it is worth noting that $P^{sat}$ of $CO_2$ is better predicted when the negativity constraint on the third derivative of the α-function is set and that $\Delta_{vap}H$ is calculated with the same accuracy in both cases.

Finally, the $CO_2$-argon binary phase diagram is represented in Figure 3.12. Impressive results are obtained by the application of the full set of constraints ($d^2\alpha/dT^2 > 0$ and $d^3\alpha/dT^3 < 0$), even slightly better than when only the convexity constraint is enforced. As shown by Figure 3.12, the resulting optimal Twu91 formulation is characterized by an accuracy similar to that of the Soave α-function.

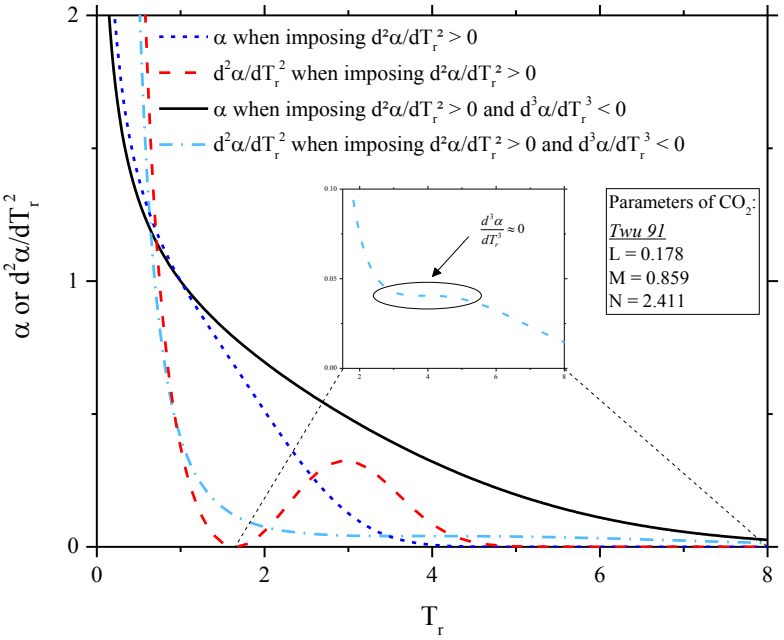



Figure 3.9. α-function of $CO_2$ and it second derivative when constraints $d^2\alpha/dT^2 > 0$ and $d^3\alpha/dT^3 < 0$ are simultaneously applied.

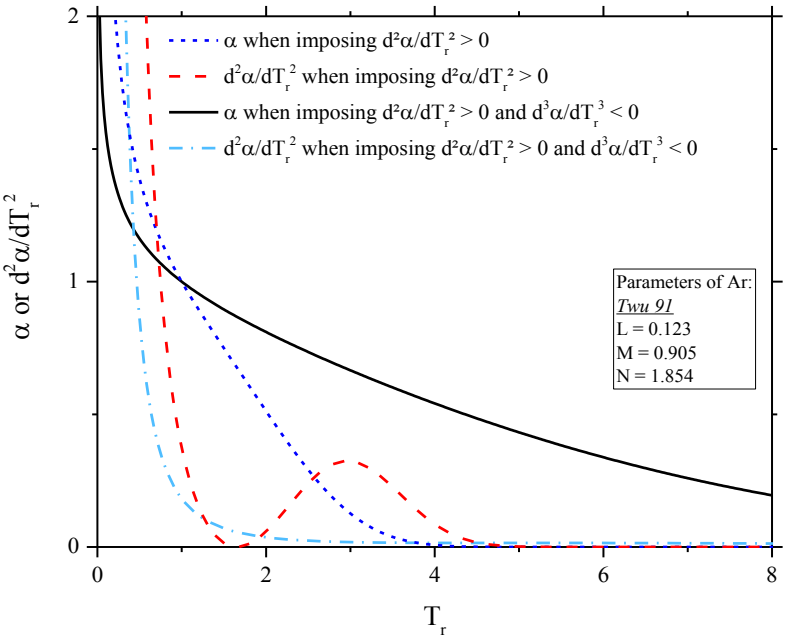



Figure 3.10. α-function of argon and it second derivative when constraints $d^2\alpha/dT^2 > 0$ and $d^3\alpha/dT^3 < 0$ are simultaneously applied.

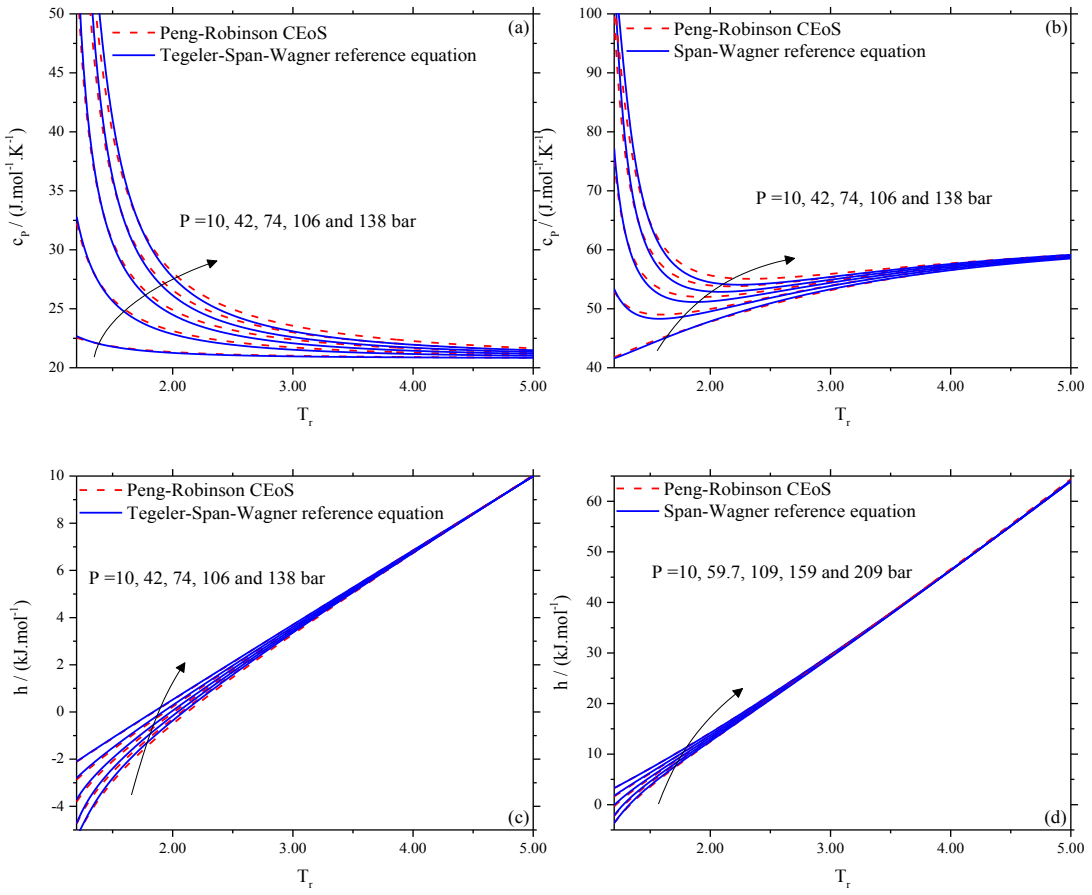



Figure 3.11. Prediction of supercritical $c_P$ of argon (a) and $CO_2$ (b) and prediction of supercritical $h$ of argon (c) and $CO_2$ (d) when constraints $d^2\alpha/dT^2 > 0$ and $d^3\alpha/dT^3 < 0$ are both applied.

| | Constraints applied | Error $P^{sat}$ | Error $\Delta_{vap}H$ | Error $c_{p,L}^{sat}$ |
|---|---|---|---|---|
| Argon | $\frac{d^2\alpha}{dT_r^2} \geq 0$ | 0.27% | 2.16% | 3.95% |
| | $\frac{d^2\alpha}{dT_r^2} \geq 0$ and $\frac{d^3\alpha}{dT_r^3} \leq 0$ | 0.28% | 2.30% | 4.74% |
| $CO_2$ | $\frac{d^2\alpha}{dT_r^2} \geq 0$ | 0.56% | 0.92% | 5.52% |
| | $\frac{d^2\alpha}{dT_r^2} \geq 0$ and $\frac{d^3\alpha}{dT_r^3} \leq 0$ | 0.29% | 1.01% | 6.99% |

Table 3.5. Comparison of the errors calculated on subcritical properties for $CO_2$ and argon when only a constraint on the second derivative of the α-function is applied and when the constraint on the third derivative is added to the previous one.

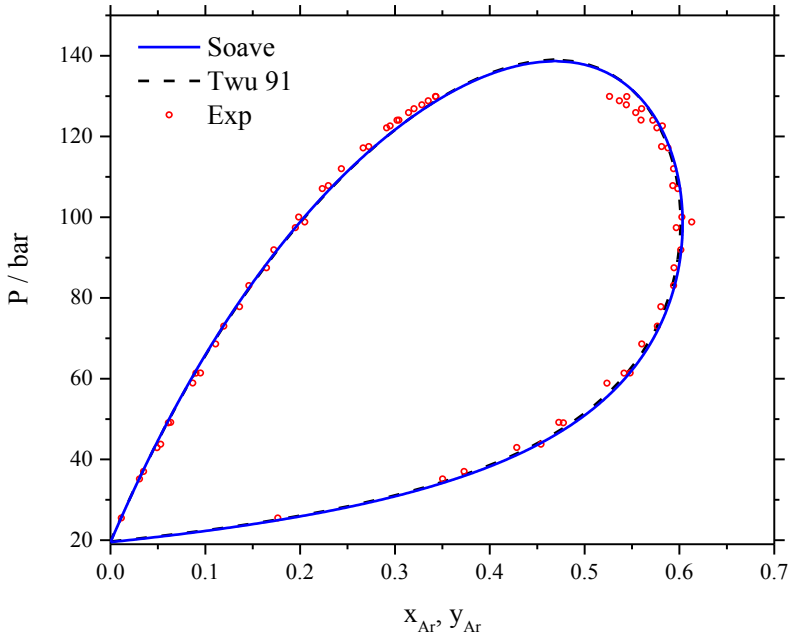



Figure 3.12. Binary phase diagram of the $CO_2$-argon system at 253.1 K when constraints $d^2\alpha/dT^2 > 0$ and $d^3\alpha/dT^3 < 0$ are simultaneously applied.

In conclusion, the addition of a new negativity constraint on the third derivative of the α-function (i) leads to a thermodynamically consistent α-function on the whole temperature range, avoiding non-physical $c_P$ changes with respect to temperature, (ii) allows for a good prediction of subcritical properties used in the regression procedure and (iii) correctly extrapolates to the supercritical domain. We can thus claim that a proper α-function must satisfy all the following constraints:

$$\text{For all T:} \begin{cases} \alpha \geq 0 & \text{and} \quad \alpha(T) \text{ continuous} \\ \dfrac{d\alpha}{dT_r} \leq 0 & \text{and} \quad \dfrac{d\alpha}{dT_r} \text{ continuous} \\ \dfrac{d^2\alpha}{dT_r^2} \geq 0 & \text{and} \quad \dfrac{d^2\alpha}{dT_r^2} \text{ continuous} \\ \dfrac{d^3\alpha}{dT_r^3} \leq 0 \end{cases} \tag{3.19}$$

The set of conditions reported in Eq. (3.19) establishes what we decided to call a "*consistency test for an α-function*". In other words, if one of these constraints is not satisfied, the EoS will possibly return – depending on the temperature and pressure domain – inaccurate or unexpected values.

At this step, it could be argued that our derivations rely on the unique analysis of the Ar + $CO_2$ binary system which contains two molecules having the same size. In order to convince the reader that our conclusions are general, the size-asymmetric $CO_2$ + n-decane system is studied in the next section.

### 3.7. Study of a size-asymmetric binary mixture with classical mixing-rules: case of the $CO_2$ + n-$C_{10}$ system

In this section, our objective is to test the influence of the selected $\alpha$-function on the correlation of the properties of the $CO_2$ + n-decane size-asymmetric binary system with the PR EoS. As was previously made, three $\alpha$-functions will be compared: the soave $\alpha$-function, an inconsistent Twu91 $\alpha$-function (which fails the proposed consistency test) and a consistent-Twu91 $\alpha$-function (which passes the proposed consistency test). To treat this system, classical mixing rules are preferred over complex mixing rules for two reasons: (i) excellent accuracy of prediction is achieved for this system by only regressing a $k_{ij}$ over experimental phase equilibrium data and (ii) discussion will be facilitated when it will come to compare different optimal $k_{ij}$ values. Their expressions are reported below:

$$\begin{cases} a(T,x) = \sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j \sqrt{a_i(T)a_j(T)}\left(1-k_{ij}\right) \\ b(x) = \sum_{i=1}^{N} x_i b_i \end{cases} \tag{3.20}$$

In a first step, the isothermal (*P,x,y*) phase diagram was calculated at 520 K with the 3 different $\alpha$-functions. For $CO_2$, the parameters are those determined in the previous sections (see Table 3.2 and Table 3.4) and the plots of the inconsistent and consistent Twu91 $\alpha$-functions are shown in Figure 3.2 and Figure 3.9 respectively. For n-$C_{10}$, the three parameters of the Twu91 $\alpha$-function are those which minimize Eq. (3.13). They were determined twice: (i) without any specific constraints and (ii) by simultaneously imposing $d^2\alpha/dT^2 > 0$ and $d^3\alpha/dT^3 < 0$ in order to get a consistent $\alpha$-function. At 520 K, $CO_2$ is supercritical $\left(T_{r,CO_2} = 1.71\right)$ and as highlighted by Figure 3.2 and Figure 3.9, at such a temperature, the inconsistent and consistent Twu91 $\alpha$-functions have very different values. On the other hand, n-$C_{10}$ is subcritical $\left(T_{r,n-C_{10}} = 0.84\right)$ so that the two Twu91 $\alpha$-functions, the parameters of which were fitted in this temperature

range, have very similar values. Calculations of the phase diagrams at 520 K are reported in Figure 3.13. In this figure, no difference can be seen between the red full curve (Soave α-function) and the blue dashed curve (consistent Twu91 α-function): they are superimposed even in the vicinity of the critical pressure. Fitted $k_{ij}$ values to be used with the Soave and the consistent Twu91 α-functions are also very close with respective values of 0.14 and 0.11 which correspond to expected values of this parameter. Figure 3.13 also highlights that the green dashed curve corresponding to the inconsistent Twu91 α-function does not correlate badly the experimental data points although it over predicts the critical pressure. However, the major drawback with the use of this inconsistent α-function is the value of the optimal $k_{ij}$ which was found to be equal to –2.43, far beyond an acceptable value. This abnormal $k_{ij}$ value can be explained by the role this parameter plays when the inconsistent Twu91 α-function is used. Indeed, in this case, the $k_{ij}$ endorses the role of a corrective term which restores the quality of prediction of the CEoS by counterbalancing the wrongly estimated α-value of $CO_2$ at 520 K. At this step, one could believe that it is not necessary to regress the α-function parameters by imposing the constraints listed in Eq. (3.19) as long as the $k_{ij}$, or any other parameter from any mixing rule, can compensate the defects of the α-function. This reasoning is however not admissible because, as previously demonstrated, heat capacities and enthalpies of $CO_2$ at 520 K will be extremely poorly predicted if the α-function does not pass the proposed consistency test. Therefore, a too large $k_{ij}$ value is not only an unordinary value but also a warning against poorly regressed α-function parameters that might lead to inaccurate predictions of supercritical properties of pure compounds.

In the next few lines, in order to convince the reader of the absolute necessity of using a consistent α-function in their calculations, the mixing enthalpies ($h^M$) of the $CO_2$ + n-$C_{10}$ system are predicted with the three considered α-functions (Soave, consistent and inconsistent Twu91). Calculations are performed at 125 bar and at 470.11 K and 573.11 K and the results are reported in Figure 3.14 and Figure 3.15. At 470.11 K and 125 bar (Figure 3.14), the inconsistent Twu91 α-function (that corresponds to $k_{ij} = -2.43$) over predicts by a factor 100 the experimental mixing enthalpies and wrongly predicts a one-phase system whatever the composition is. On the other hand, coupling a $k_{ij}$ of 0.11 with the consistent Twu91 α-function or a $k_{ij}$ of 0.14 with the

Soave α-function leads to an accurate prediction of $h^M$. It is believed that the consistent Twu91 α-function performs better than the Soave α-function (see Figure 3.14b) because its parameters were not only regressed on vapor pressures but also on vaporization enthalpies and heat capacities (Soave solely parameterized his α-function with the objective of reproducing the experimental vapor pressures). At 573.11 K and 125 bar (Figure 3.15) a non–existing VLE is predicted and poor results are obtained for the mixing enthalpies when a $k_{ij}$ of −2.34 is coupled with the inconsistent Twu91 α-function while the two others α-functions allow for an excellent adequacy between the experimental points and the predicted curves.

In conclusion, we can state that the constraints defined by Eq. (3.19) apply whatever the binary system. This section also pointed out that the classical Van der Waals mixing rules, involving a $k_{ij}$, do not permit to overcome the limitations of a poorly regressed α-function. Indeed, when a very large $k_{ij}$ is calculated to balance the deficiencies of a non-consistent α-function, not so bad VLE correlation can be achieved but extremely poor predictions of the derived properties (here illustrated with the mixing enthalpies) is performed.

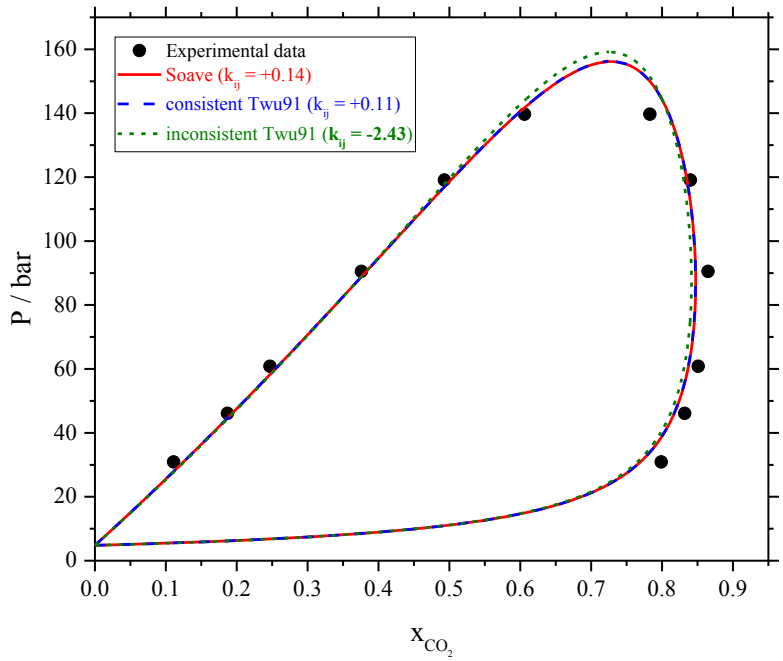



Figure 3.13. Prediction of the $CO_2$–n-$C_{10}$ phase diagram at 520 K with different α-functions and classical mixing rules. Red full curve is calculated with the Soave α-function while blue and green dashed curves are calculated with the Twu91 α-function. Parameters of the α-function used to calculate the green curve do not satisfy the consistency test while parameters of the blue curve do.

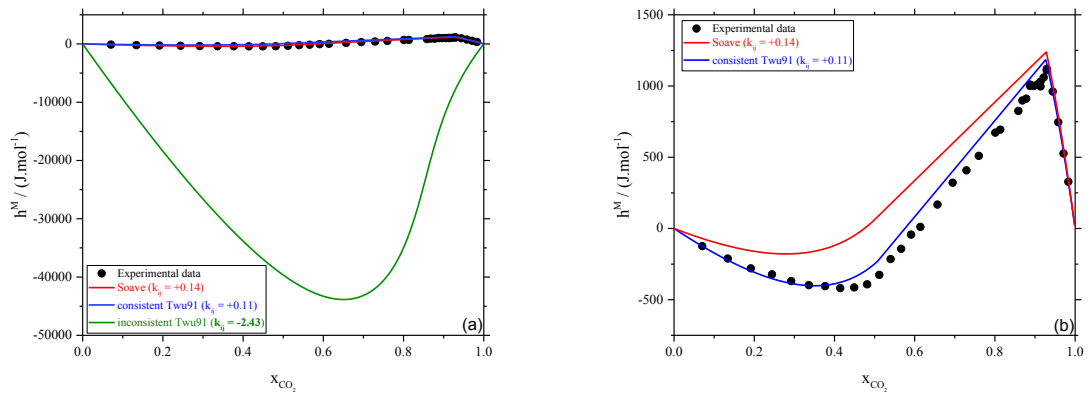



Figure 3.14. Calculation of the mixing enthalpies of the $CO_2$–n-$C_{10}$ system at 470.11 K and 125 bar.

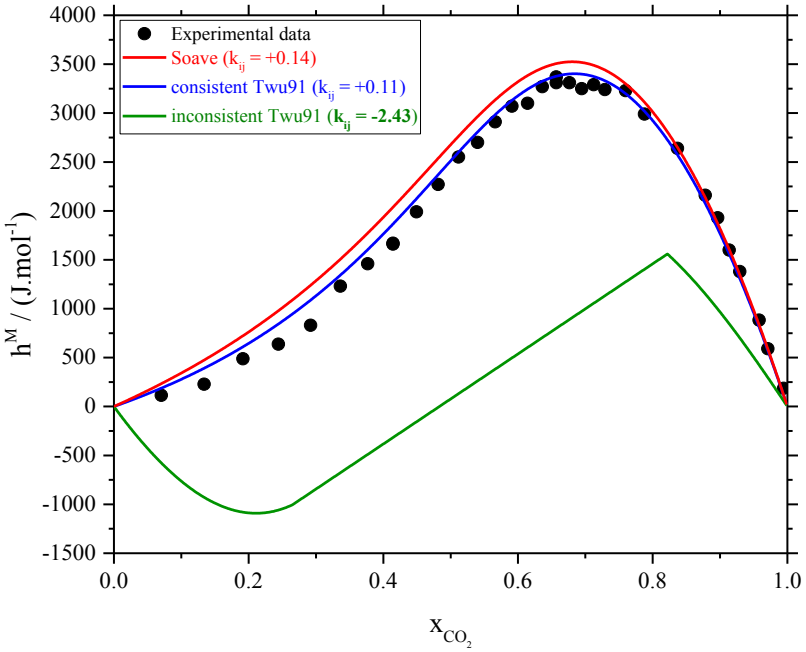



Figure 3.15. Calculation of the mixing enthalpies of the $CO_2$–n-$C_{10}$ system at 573.11 K and 125 bar.

Although it is claimed that the consistency test developed in this paper apply whatever the component, a special attention should be paid to the so-called "quantic fluids" like He and $H_2$. This is the aim of the next section.

### 3.8. The special case of quantic fluids ($H_2$ and He)

$H_e$ and $H_2$, the critical temperatures of which are 5.20 K and 33.15 K respectively, are qualified of *quantic fluids* as their low temperature physical behaviors can only be represented if quantum effects are taken into account in the modelling procedure. Consequently, they must be treated apart from other *classical* fluids. As an example,

Gasem et al. [102] and Mahmoodi et al. [85] noticed that when α-functions of $H_2$ and He are both regressed on vapor pressures, they exhibit an increasing $(d\alpha / dT > 0)$ and concave portion $\left(d^2\alpha / dT^2 < 0\right)$ followed, at least for $H_2$, by a decreasing $(d\alpha / dT < 0)$ and convex portion $\left(d^2\alpha / dT^2 > 0\right)$ in the supercritical domain.

Working with quantic fluids and in order to determine the proper shape (convex or concave) of α-functions in the subcritical temperature range, let us recall that $c_v^{res}$ and the second derivative of the α-function have always the same sign. We indeed can write:

$$c_v^{res}(T,v) = \underbrace{\frac{Ta_c}{b(r_1-r_2)}\ln\left(\frac{v-r_2 b}{v-r_1 b}\right)}_{>0} \times \underbrace{\frac{d^2\alpha}{dT^2}}_{\substack{phase \\ independant}} \tag{3.21}$$

Along the vaporization curve, i.e. when the pure component is in VLE, the 2 phases have the same temperature i.e. the same $d^2\alpha / dT^2$ value and both the liquid and vapor phases $c_v^{res}$ calculated from a CEoS have the same sign (the sign of the second derivative of the α-function). Extracted from the NIST database, the quantity $c_v^{res}$ of He and $H_2$ for both the liquid and vapor phases are shown in Figure 3.16 and Figure 3.17.

One can see that for $H_2$ at a temperature lower than 28.5 K, experimental $c_v^{res}$ of the liquid phase is negative while it is positive for the vapor phase. Therefore, at these low temperatures, where fluids are quantic, the second derivative of the α-function should be both positive and negative. This contradiction leads us to affirm that the same α-function cannot represent simultaneously the liquid and vapor phases. In other words, these fluids do not follow the 3-parameter law of corresponding states in the low temperature range. It is also possible to conclude that $c_v^{res}$ data in the subcritical temperature range are not relevant data to fit the parameters of α-functions.

Although the quantum effects cannot be described by a 2-parameter CEoS, it would be valuable to accurately represent the behavior of He and $H_2$ in some specific temperature ranges due to their use in some chemical process plants. First, it must be noticed that in most applications, the operating temperature is far above the respective critical temperatures of these two compounds. Therefore, focusing on the subcritical

temperature range is not relevant. Secondly, it is expected that at reasonably high temperatures the α-function of each of these pure compounds behaves like a classical fluid, i.e. it satisfies, all the criteria defined by Eq.(3.19).

In order to verify whether or not α-functions of He and $H_2$ at sufficiently high temperatures behave conventionally, a regression of the Twu91 parameters was performed on both subcritical [ $P^{sat}(T)$ and $\Delta_{vap}H(T)$ ] and supercritical [ $c_v^{res}(T,P)$ and $h^{res}(T,P)$ ] data. The same weight was given to all the properties. Subcritical $c_v^{res}$ were excluded from the regression procedure since values for the liquid and vapor phases are conflicting. The supercritical experimental data were generated using the NIST database at pressures of 10, 100 and 1000 bar, for temperatures varying between 150 and 750 K with a step of 50 K. For comparison purpose, regression of the α-function parameters was also performed on (i) only subcritical data and (ii) only supercritical data. Results of these calculations are reported in Figure 3.18 and Figure 3.19 and numerical values of the MAPE are reported in Table 3.6.

Results shown in Figure 3.18 and Figure 3.19 are in accordance with previous literature studies as almost all α-functions are increasing functions of temperature in the low temperature range. The single exception is the α-curve of $H_2$ with parameters regressed on supercritical data which is a monotonically decreasing, convex function of temperature. This result is highly reassuring as at temperatures above 150 K (the smallest temperature of the experimental supercritical data) we expect the fluid not to behave as a "quantic fluid" anymore, i.e. to respect the constraints defined by Eq. (3.19). The following conclusions can be drawn from Table 3.6, Figure 3.18 and Figure 3.19:

- When the L, M and N parameters are only regressed on subcritical data, excellent representation of the subcritical properties is achieved although an increasing α-function is calculated on this temperature range, demonstrating the unusual behavior of fluids in "quantic state". Meanwhile, supercritical properties are poorly represented (see Table 3.6). As seen in Figure 3.18, in the case of He, the α-function goes to zero at a temperature of 40 K (red dashed curve) and, thus, is unable to accurately extrapolate at higher temperatures making this α-function unsuitable for most of the actual processes involving this molecule.
- When the α-function parameters are regressed on both subcritical and supercritical properties, a slight accuracy decrease of prediction is observed for the subcritical properties while supercritical ones are largely improved. This enhancement is

caused by the shape of the α-function at high temperature, which is adjusted to represent the residual heat capacities and enthalpies. This improvement is obvious when attention is paid to the change of the He α-function with respect to the case when only subcritical data were regressed. Now the α-function is very different from zero at temperatures above 150 K, dividing by two the error over heat capacities while leaving almost unchanged the other properties. An excellent improvement of the supercritical properties is also achieved when considering $H_2$.

- Finally, regression on solely supercritical properties is not desirable as errors on saturated pressures and vaporization enthalpies skyrocket while the benefit on the prediction accuracy of supercritical properties is not significant. More generally, one can observe that on the temperature range for which experimental data were generated and used in the regression procedure, the α-function is a strictly decreasing, convex function of temperature. A graphical representation of the third derivative would show that it is negative. This confirms that molecules which behave as "quantic fluids" in the low temperature range do not keep this unusual tendency at higher temperature and that the consistency test, defined by Eq.(3.19), is satisfied.

In conclusion, α-functions of quantic fluids:

- Exhibit a *bell* shape (increasing and concave functions) below 40 – 50 K.
- Become decreasing, convex and with a negative third derivative at temperatures higher than 50 K (i.e. they satisfy Eq. (3.19)).
- Should be regressed on both subcritical and supercritical data to achieve satisfying representation accuracy of the thermodynamic properties on the whole temperature range.

| | | MAPE (%) | | | |
|---|---|---|---|---|---|
| | Type of data used in the regression procedure | $P^{sat}$ | $\Delta_{vap}H$ | Supercritical $h^{res}$ | Supercritical $c_v^{res}$ |
| He | Subcritical | 0.001 | 3.68 | 20.79 | 100.00 |
| | Supercritical | 141.44 | 78.29 | 21.30 | 24.17 |
| | Both | 1.75 | 7.00 | 18.09 | 42.77 |
| $H_2$ | Subcritical | 0.02 | 3.17 | 54.52 | 58.91 |
| | Supercritical | 38.23 | 50.23 | 4.90 | 44.22 |
| | Both | 2.16 | 4.66 | 6.08 | 56.27 |

Table 3.6. MAPE calculated for He and $H_2$ with respect to the type of data used in the regression procedure of the Twu91 α-function parameters (subcritical, supercritical or both).

After this debate on the particular behavior of quantic fluids, the next section aims at discussing which α-functions, published in the open literature, pass the proposed consistency test (see Eq. (3.19)).

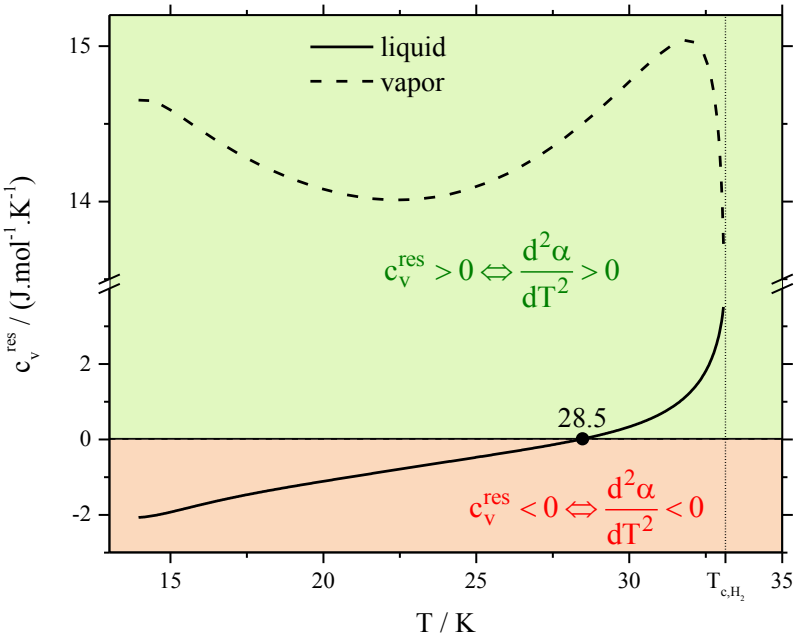



Figure 3.16. Residual heat capacities of vapor and liquid phases of saturated $H_2$.

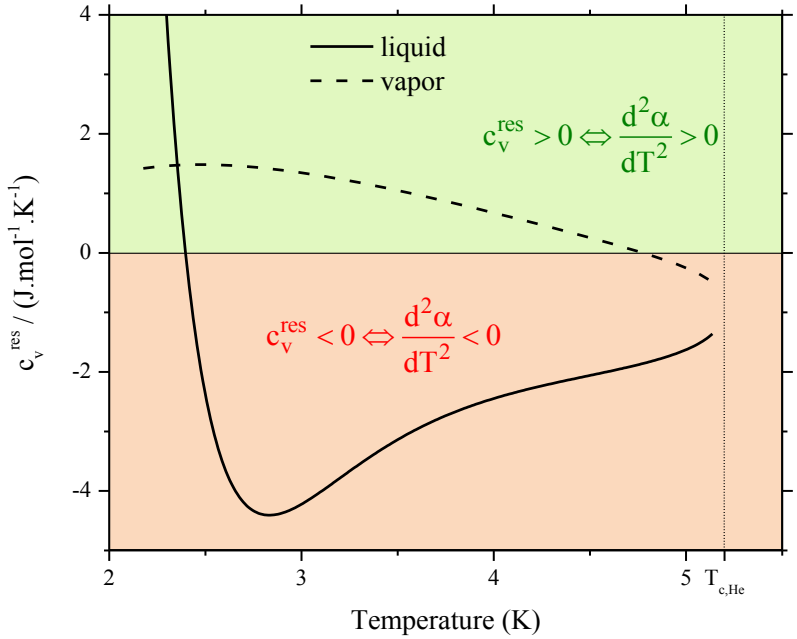



Figure 3.17. Residual heat capacities of vapor and liquid phases of saturated He.

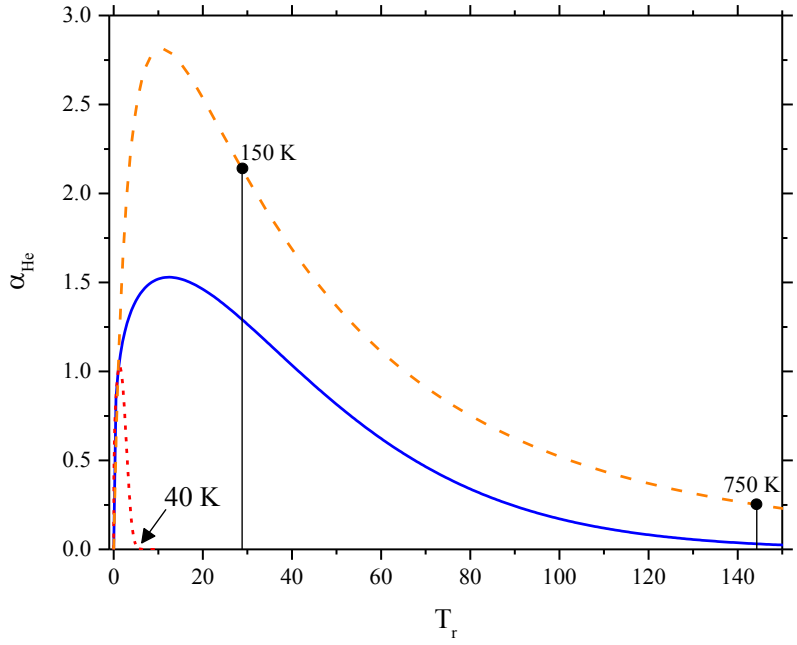



Figure 3.18. Optimized α-functions of He. Small dashed curve is regressed on subcritical data, large dashed curve is regressed on supercritical data, full curve is regressed on both subcritical and supercritical data.

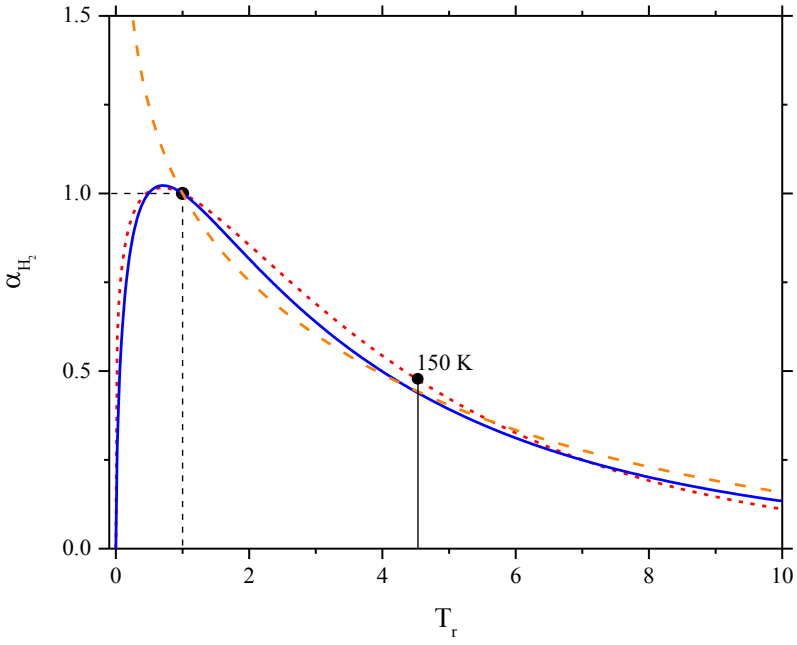



Figure 3.19. Optimized α-functions of $H_2$. Small dashed curve is regressed on subcritical data, large dashed curve is regressed on supercritical data, full curve is regressed on both subcritical and supercritical data.

### 3.9. Do current α-functions available in the open literature pass the proposed consistency test?

Mathematical conditions on the α-function and its successive derivatives aimed at ensuring consistent and accurate calculations of thermodynamic properties in both subcritical and supercritical domains have been identified along the previous part of this paper (see Eq. (3.19)). This section evaluates which of the mostly used α-functions of the literature fulfil all these conditions. Mathematical derivations are detailed in Appendices A to L and only main results are reported in Table 3.7.

The twelve selected α-functions are those which are generally available in process simulation software. We selected:

1- Soave 1972
2- Soave 1984
3- Gibbons-Laughton
4- Stryjek-Vera
5- Mathias-Copeman
6- Mathias
7- Twu 1995
8- Boston-Mathias
9- Trebble-Bishnoi
10- Melhem-Saini-Goodwin
11- Twu 1988
12- Twu 1991

As highlighted in Table 3.7, eight over twelve of these well-known α-functions (Soave 1972, Soave 1984, Gibbons-Laughton, Stryjek-Vera, Boston-Mathias, Mathias-Copeman, Mathias, Twu 1995) fail the proposed consistency test whatever the values of the parameters are. The four remaining α-functions (Trebble-Bishnoi, Melhem-Saini-Goodwin, Twu 1988, Twu 1991) pass the test but only if constraints (sometimes drastic) are added to the parameters.

We can thus conclude that, presently, it is impossible to find an α-function which passes our consistency test for any values of the parameters.

From a practical point of view:

1- All α-functions which derive from the Soave α-function, the so-called "polynomial α-functions", are not monotonically decreasing functions of temperature; therefore, special caution should be taken when those are applied to light supercritical compounds at reduced temperatures above the temperature at which the minimum of these α-functions occurs.

2- The higher the number of adjustable parameters in α-functions, the harder the optimization procedure will be since more constraints on the parameters will have to be added, to ensure that the function passes the consistency test. Two-parameter α-functions appear as a good trade-off between complexity and flexibility of the α-function formulation.

3- Piecewise α-functions should at least have 2 parameters in the subcritical and supercritical temperature domains. Application of the continuity constraint of the first and second derivatives of an α-function permits to establish relations between subcritical and supercritical parameters. As a consequence, thermodynamic properties, such as $h$ and $c_v$, would be kept continuous at the critical temperature.

4- It should be noticed that, among the two generalized α-functions studied in this paper (Soave and Twu 1995), none of them satisfies all the constraints of the proposed consistency test. For molecules with an acentric factor out of the range $[0;1]$ or for the prediction of heat capacities just above the critical temperature, the Soave α-function should be preferred.

### 3.10. Conclusion

- The main conclusion of this article is that α-functions must:
  1. Be of class C², i.e., their first $(d\alpha/dT)$ and second $\left(d^2\alpha/dT^2\right)$ derivatives must exist and must be continuous for any temperature value,
  2. Be positive for any temperature value $(\alpha(T)\geq 0)$,
  3. Be monotonically decreasing for any temperature value $(d\alpha/dT\leq 0)$,
  4. Be convex for any temperature value $\left(d^2\alpha/dT^2\geq 0\right)$,
  5. Also verify $d^3\alpha/dT^3\leq 0$ for any temperature value.

All these requirements are absolutely necessary to get accurate and physically meaningful behaviors in both the subcritical and supercritical domains. Other key conclusions follow.

- The role of the α-function is at least as important as the role of mixing rules. As highlighted with the $CO_2$-argon binary system, even with the most elaborated mixing rules, an inconsistent α-function will always lead to poor results if at least one component is supercritical. The reverse is also true: a consistent α-function coupled with unsuitable mixing rules cannot lead to accurate results.
- When the parameters of component-specific α-functions are fitted in order to pass our consistency test [Eq. (19)], pure component properties in the supercritical region are highly improved without deteriorating the accuracy of the calculated subcritical properties.
- The parameter-optimization procedure, aimed at determining the parameters of a given α-function by minimizing the deviations between calculated and experimental vapor-liquid equilibrium data, can generate many sets of parameters leading to similar objective function values (meaning that the same behavior is observed when temperature is below the critical temperature of the pure compound) but inducing totally different behaviors in the supercritical domain. The constraints proposed in this paper make it possible to select the best set of parameters. It is believed that similar constraints should be developed for SAFT-type EoS [103]. It is indeed well-known that the fitting of the three parameters $m$, $\sigma$ and $\epsilon$ on saturation pressures and liquid densities leads to many triplets of solutions for which the objective function is the same.
- None of the α-functions currently published in the open literature passes the proposed consistency test. Researches in this area thus need to be intensified.

**Acknowledgment**

The French Petroleum Company TOTAL and more particularly Dr. Pierre DUCHET–SUCHAUX, Dr. Laurent AVAULLÉE and Freddy GARCIA (experts in thermodynamics) are gratefully acknowledged for sponsoring this research.

| | α-function | Class $C^2$(*) | $\alpha \geq 0$ | $\frac{d\alpha}{dT_r} \leq 0$ | $\frac{d^2\alpha}{dT_r^2} \geq 0$ | $\frac{d^3\alpha}{dT_r^3} \leq 0$ | Condition(s) |
|---|---|---|---|---|---|---|---|
| Soave (1972) [7] | $\begin{cases} \alpha = \left[1 + m(\omega)\left(1 - \sqrt{T_r}\right)\right]^2 \\ m_{RK}(\omega) = 0.480 + 1.574\omega - 0.176\omega^2 \\ m_{PR}(\omega) = 0.37464 + 1.54226\omega - 0.26992\omega^2 \end{cases}$ | ☑ | ☑ | ☒ | ☑ | ☑ | $m(1+m) \geq 0$ |
| Soave (1984) [32] | $\alpha = 1 + (1 - T_r)\left(a + \frac{b}{T_r}\right)$ | ☑ | a ≥ 0: ☒ / ☑<br>a ≤ 0: ☑ / ☒ | | ☑ | ☑ | $b > 0$ |
| Gibbons-Laughton [87] | $\alpha = 1 + X(T_r - 1) + Y\left(\sqrt{T_r} - 1\right)$ | ☑ | ☑ | ☒ | ☑ | ☑ | $\begin{cases} X \geq 0 \\ -2X - 2\sqrt{X} \leq Y \\ Y \leq \min\left(0; -2X + 2\sqrt{X}\right) \end{cases}$ |
| Stryjek-Vera [29] | $\alpha = \left[1 + \kappa\left(1 - \sqrt{T_r}\right)\right]^2$<br>$\kappa = \kappa_0 + \kappa_1\left(1 + \sqrt{T_r}\right)(0.7 - T_r)$<br>$\kappa_0 = 0.378893 + 1.4897153\omega - 0.17131848\omega^2$<br>$+0.0196554\omega^3$<br>$\begin{cases} \kappa_1(T \leq 0.7T_c) \neq 0 \\ \kappa_1(T > 0.7T_c) = 0 \end{cases}$ | ☒ | ☑ | ☒ | ☑ | ☑ | $\kappa(1+\kappa) \geq 0$ |
| Mathias-Copeman [26] | $\alpha_{SUB} = \alpha(T_r \leq 1) = \left[1 + c_1\left(1 - \sqrt{T_r}\right) + c_2\left(1 - \sqrt{T_r}\right)^2 + c_3\left(1 - \sqrt{T_r}\right)^3\right]^2$<br>$\alpha_{SUP} = \alpha(T_r > 1) = \left[1 + m(\omega)\left(1 - \sqrt{T_r}\right)\right]^2$ | ☒ | ☑ | ☒ | ☑ | ☑ | |

| α-function | Class $C^2$(*) | $\alpha \geq 0$ | $\frac{d\alpha}{dT_r} \leq 0$ | $\frac{d^2\alpha}{dT_r^2} \geq 0$ | $\frac{d^3\alpha}{dT_r^3} \leq 0$ | Condition(s) |
|---|---|---|---|---|---|---|
| Mathias [90]<br>$\alpha_{SUB} = \alpha(T_r \leq 1) = \left[1 + m(\omega)\left(1 - \sqrt{T_r}\right) - p\left(1 - T_r\right)\left(0.7 - T_r\right)\right]^2$<br>$\begin{cases} \alpha_{SUP} = \alpha(T_r > 1) = \left[\exp\left[L\left(1 - T_r^{\gamma}\right)\right]\right]^2 \\ L = 1 + \frac{m}{2} + 0.3p \\ \gamma = \frac{L-1}{L} \end{cases}$ | ☒ | ☑ | | | | |
| Twu (1995) [36,37]<br>$\begin{cases} \alpha = \alpha^{(0)} + \omega\left[\alpha^{(1)} - \alpha^{(0)}\right] \\ \alpha^{(0)} = T_r^{N^{(0)}\left[M^{(0)}-1\right]} \exp\left[L^{(0)}\left(1 - T_r^{M^{(0)}N^{(0)}}\right)\right] \\ \alpha^{(1)} = T_r^{N^{(1)}\left[M^{(1)}-1\right]} \exp\left[L^{(1)}\left(1 - T_r^{M^{(1)}N^{(1)}}\right)\right] \end{cases}$<br>(see coefficients in Appendix C) | ☑ | ☑ | ☑ | ☑ | ☒ | $\omega \in [0;1]$ |
| Boston-Mathias [84]<br>$\alpha_{SUB} = \alpha(T_r \leq 1) = \alpha_{SOAVE} = \left[1 + m(\omega)\left(1 - \sqrt{T_r}\right)\right]^2$<br>$\alpha_{SUP} = \alpha(T_r \geq 1) = \exp\left[L\left(1 - T_r^{\gamma}\right)\right]$<br>$\begin{cases} L = \frac{2m}{1+m} \\ \gamma = \frac{1+m}{2} \end{cases}$ | ☒ | ☑ | | | | $0 \leq m \leq 3$ |
| Trebble-Bishnoi [88]<br>$\alpha = \exp\left[L\left(1 - T_r\right)\right]$ | ☑ | ☑ | ☑ | ☑ | ☑ | $L \geq 0$ |
| Melhem-Saini- | ☑ | ☑ | ☑ | ☑ | ☑ | $m \geq n \geq 0$ |

| | α-function | Class $C^2$(*) | $\alpha \geq 0$ | $\frac{d\alpha}{dT_r} \leq 0$ | $\frac{d^2\alpha}{dT_r^2} \geq 0$ | $\frac{d^3\alpha}{dT_r^3} \leq 0$ | Condition(s) |
|---|---|---|---|---|---|---|---|
| Goodwin [89] | | | | | | | |
| Twu (1988) [35] | $\alpha = T_r^{2(M-1)} \exp\left[L\left(1-T_r^{2M}\right)\right]$ | ☑ | ☑ | ☑ | ☑ | ☑ | $\begin{cases} LM \geq 0 \\ M \leq 0.8909 \end{cases}$ |
| Twu (1991) [19] | $\alpha = T_r^{\delta} \exp\left[L\left(1-T_r^{\gamma}\right)\right]$ | ☑ | ☑ | ☑ | ☑ | ☑ | $\begin{cases} \delta \leq 0 \\ L\gamma \geq 0 \\ \gamma \leq 1-\delta \end{cases}$ or $\begin{cases} \delta \leq 0 \\ L\gamma \geq 0 \\ \gamma \leq 1-2\delta+2\sqrt{\delta(\delta-1)} \\ 4Y^3+4ZX^3+27Z^2 \\ \quad -18XYZ-X^2Y^2 \geq 0 \end{cases}$ with $\begin{cases} X=-3(\gamma+\delta-1) \\ Y=\gamma^2+3\delta\gamma-3\gamma+3\delta^2-6\delta+2 \\ Z=-\delta\left(\delta^2-3\delta+2\right) \end{cases}$ |

Table 3.7. Mathematical analysis of the mostly used α-functions.

(*) α function is said to be of class $C^2$ if the function, its first derivative and its second derivative are all continuous.

## 3.11. Appendices

### 3.11.1. Appendix A: mathematical study of the Twu91 α-function [19]

Although classically expressed by introducing 3 adjustable parameters denoted L, M and N (see Eq. (3.22)), the Twu91 α-function can be alternatively written under a simpler form involving three different adjustable parameters denoted L, $\delta$ and $\gamma$ (this form appears more convenient to perform a mathematical analysis of the function and its derivatives):

$$\alpha(T_r) = T_r^{N(M-1)} \exp\left[ L\left(1 - T_r^{MN}\right)\right] \tag{3.22}$$

$$\alpha(T_r) = T_r^{\delta} \exp\left[ L\left(1 - T_r^{\gamma}\right)\right] \tag{3.23}$$

where $\delta$ and $\gamma$ are related to M and N following:

$$\begin{cases} \delta = N(M-1) \\ \gamma = NM \end{cases} \Leftrightarrow \begin{cases} N = \gamma - \delta \\ M = \dfrac{\gamma}{\gamma - \delta} \end{cases} \tag{3.24}$$

- **Is the α-function of class C²?** Yes.

It is recalled that a given function is said to be of class $C^2$ if its first and second derivatives exist and are continuous.

- **Is the α-function always positive?** Yes.
- **Is the first derivative of the α-function always negative?**

The first derivative of this α-function is

$$\begin{cases} \dfrac{d\alpha}{dT_r}(T_r) = -\dfrac{\alpha(T_r)}{T_r} P(T_r) \\ P(T_r) = -\delta + L\gamma T_r^{\gamma} \end{cases} \tag{3.25}$$

The quantity $\dfrac{d\alpha}{dT_r}(T_r)$ is positive provided $P(T_r)$ is positive itself.

Study of the sign of $P(T_r)$ (reported in Table 3.8): $T_r$ is positive so P is a monotonic function of $T_r$. Therefore, $P(T_r)$ is positive for any value of $T_r > 0$ if the limits of P are both positive when $T_r$ tends to 0 or to $+\infty$.

$$\gamma > 0 \Rightarrow \begin{cases} \lim_{T_r \to 0} T_r^{\gamma} = 0 \\ \lim_{T_r \to +\infty} T_r^{\gamma} = +\infty \end{cases} \qquad \gamma < 0 \Rightarrow \begin{cases} \lim_{T_r \to 0} T_r^{\gamma} = +\infty \\ \lim_{T_r \to +\infty} T_r^{\gamma} = 0 \end{cases}$$

| | $L > 0$ | $L < 0$ | $L > 0$ | $L < 0$ |
|---|---|---|---|---|
| $\lim_{T_r \to 0} P(T_r)$ | $-\delta$ | $-\delta$ | $-\infty$ | $+\infty$ |
| $\lim_{T_r \to +\infty} P(T_r)$ | $+\infty$ | $-\infty$ | $-\delta$ | $-\delta$ |
| Acceptable solution? | Yes, if $\delta < 0$ | No | No | Yes, if $\delta < 0$ |

Table 3.8. Limit of P at the infinite temperature limit with respect to the signs of L and γ.

Summary: $P(T_r)$ is positive for any positive value of $T_r$ if:

$$\begin{cases} L\gamma > 0 \\ \delta < 0 \end{cases} \tag{3.26}$$

- **Is the second derivative of the α-function always positive?**

Following Eq. (3.26), it is now assumed that $L\gamma > 0$ and $\delta < 0$. The second derivative of the Twu91 α-function writes

$$\begin{cases} \dfrac{d^2\alpha}{dT_r^2}(T_r) = \dfrac{\alpha(T_r)}{T_r^2} Q(\theta) \\ Q(\theta) = \theta^2 - (2\delta + \gamma - 1)\theta + \delta(\delta - 1) \\ \theta = L\gamma T_r^{\gamma} \end{cases} \tag{3.27}$$

$T_r$ and $L\gamma$ being positive, the variable $\theta$ is also positive. Polynomial $Q(\theta)$ is positive if [104]:

$$\begin{cases} -(2\delta + \gamma - 1) > -2\sqrt{\delta(\delta - 1)} \\ \textit{and} \\ \delta(\delta - 1) > 0 \end{cases} \tag{3.28}$$

Since $\delta < 0$, the second condition of Eq. (3.28) is already true and can be left aside. Finally, Eq. (3.28) leads to a single inequality:

$$\gamma < 1 - 2\delta + 2\sqrt{\delta(\delta - 1)} \tag{3.29}$$

- Is the third derivative of **the α**-function always negative?

Inequalities (3.26) and (3.29) are now assumed to be true. The third derivative of the Twu91 α-function is:

$$\begin{cases} \dfrac{d^3\alpha}{dT_r^3}(T_r) = -\dfrac{\alpha(T_r)}{T_r^3} R(\theta) \\ R(\theta) = \theta^3 - 3(\gamma + \delta - 1)\theta^2 + \left(\gamma^2 + 3\delta\gamma - 3\gamma + 3\delta^2 - 6\delta + 2\right)\theta - \delta\left(\delta^2 - 3\delta + 2\right) \\ \theta = L\gamma T_r^{\gamma} \end{cases} \tag{3.30}$$

with $\theta > 0$. The quantities X, Y and Z are defined as

$$\begin{cases} X = -3(\gamma + \delta - 1) \\ Y = \gamma^2 + 3\delta\gamma - 3\gamma + 3\delta^2 - 6\delta + 2 \\ Z = -\delta\left(\delta^2 - 3\delta + 2\right) = -\delta(\delta - 1)(\delta - 2) \end{cases} \tag{3.31}$$

Polynomial $R(\theta)$ is positive if [104]:

$$\begin{cases} X > 0 \\ Y > 0 \\ Z > 0 \end{cases} \text{ or } \begin{cases} Z > 0 \\ H = 4Y^3 + 4ZX^3 + 27Z^2 - 18XYZ - X^2Y^2 > 0 \end{cases} \tag{3.32}$$

Since $\delta < 0$ (see Eq. (3.26)), the condition $Z > 0$ (where $Z$ is defined by Eq. (3.31)) is always verified. According to Eqs. (3.30) and (3.32), it can be concluded that $\dfrac{d^3\alpha}{dT_r^3}(T_r)$ is negative provided:

$$\begin{cases} X > 0 \\ Y > 0 \end{cases} \text{ or } \quad H = 4Y^3 + 4ZX^3 + 27Z^2 - 18XYZ - X^2Y^2 > 0 \tag{3.33}$$

A graphical representation of the constraints $Y < 0$ (red area) and $X < 0$ (yellow area) is proposed in Figure 3.20.

Colored areas are forbidden to parameters γ and δ, only the white area is permitted. The concavity constraint of the α-function is also represented (the blue area is an area wherein the condition $\dfrac{d^2\alpha}{dT_r^2}(T_r) \geq 0$ is not satisfied). An analysis of the graphic shows

that if the constraint $X > 0$ is satisfied then the convexity constraint and the $Y > 0$ constraint are automatically satisfied.

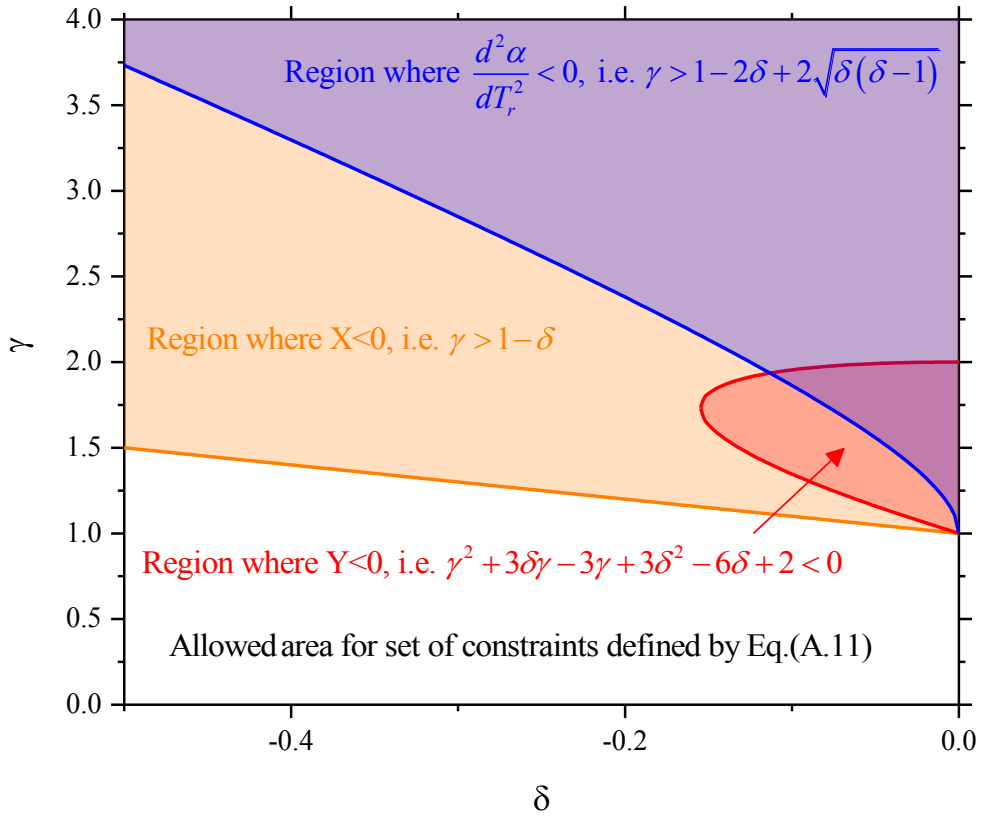



Figure 3.20. Representation of the set of constraints defined by Eq. (3.32).

- Conclusion:

Therefore, the Twu91 α-function is a positive decreasing convex function of temperature with a negative third derivative if one of the two following sets of constraints is verified

$$\begin{cases} \delta < 0 \\ L\gamma > 0 \\ \gamma < 1 - \delta \end{cases} \text{ or } \begin{cases} \delta < 0 \\ L\gamma > 0 \\ \gamma < 1 - 2\delta + 2\sqrt{\delta(\delta - 1)} \\ 4Y^3 + 4ZX^3 + 27Z^2 - 18XYZ - X^2Y^2 > 0 \end{cases} \tag{3.34}$$

Where the quantities X, Y and Z are defined by Eq. (3.31).

### 3.11.2. Appendix B: mathematical study of the Twu88 α-function [35]

This α-function writes

$$\alpha(T_r) = T_r^{2(M-1)} \exp\left[ L\left(1 - T_r^{2M}\right) \right] \tag{3.35}$$

This α-function is a particular case of the Twu91 α-function with N set to 2. Therefore, results derived in Appendix A for the Twu91 α-function can be used to determine the conditions on the L and M parameters that lead to a consistent Twu88 α-function.

For this α-function, the relations between parameters M, N and δ, γ are

$$\begin{cases} \delta = 2(M-1) \\ \gamma = 2M \\ N = 2 \end{cases} \tag{3.36}$$

- **Is the α-function of class C²?** Yes.
- **Is the α-function always positive?** Yes.
- **Is the first derivative of the α-function always negative?**

By combining Eqs. (3.26) and (3.36), one obtains:

$$\begin{cases} L\gamma > 0 \\ \delta < 0 \end{cases} \Leftrightarrow \begin{cases} M < 1 \\ LM > 0 \end{cases} \tag{3.37}$$

- **Is the second derivative of the α-function always positive?**

It is now assumed that $M < 1$ and $LM > 0$. By combining Eqs. (3.29) and (3.36), one obtains:

$$\gamma < 1 - 2\delta + 2\sqrt{\delta(\delta-1)} \;\Leftrightarrow\; 6M - 5 < 2\sqrt{2(M-1)(2M-3)} \tag{3.38}$$

A mathematical study of inequality (3.38) makes it possible to demonstrate that the only acceptable values of M are such that:

$$M \le \frac{1}{2} + \frac{1}{\sqrt{5}} \approx 0.947 \tag{3.39}$$

Note that the combination of inequalities $M < 1$ and (3.39) results in the single inequality (3.39).

- **Is the third derivative of the α-function always negative?**

One assumes that $LM > 0$ and $M \le \frac{1}{2} + \frac{1}{\sqrt{5}}$. According to Eqs. (3.31), (3.33) and (3.36), two possible sets of conditions ensure the negativity of $\frac{d^3\alpha}{dT_r^3}(T_r)$:

1. Either $X > 0$ *and* $Y > 0$:

As for the Twu91 α-function, the constraint $X > 0$ entails the convexity of the Twu88 α-function and the inequality $Y > 0$.

$$X > 0 \;\Leftrightarrow\; \gamma < 1-\delta \;\Leftrightarrow\; M < 0.75 \tag{3.40}$$

2. Or $H = 4Y^3 + 4ZX^3 + 27Z^2 - 18XYZ - X^2Y^2 > 0$:

   In the case of the Twu88 α-function, this inequality writes:

$$-16448M^6 + 55296M^5 - 64416M^4 - 29376M^3 - 4020M^2 + 216M - 4 \geq 0 \tag{3.41}$$

   By solving numerically this inequality, one obtains:

$$M \in [0.0448, 0.8909] \cup [1, 1.2902] \tag{3.42}$$

   Combining inequalities (3.39) and (3.42) leads to:

$$M \in [0.0448, 0.8909] \tag{3.43}$$

   As previous, it can be proved that choosing the M parameter in this range ensures also the convexity of the Twu88 α-function.

Finally, according to Eqs. (3.40) and (3.43), one deduces that the third derivative of the Twu88 α-function is negative provided:

$$M < 0.8909 \tag{3.44}$$

- Conclusion:

To summarize, the Twu88 α-function is a positive decreasing convex function of temperature with a negative third derivative if the following set of constraints is verified (resulting from the combination of Eqs. (3.37) and (3.44)):

$$\begin{cases} LM > 0 \\ M < 0.8909 \end{cases} \tag{3.45}$$

### 3.11.3. Appendix C: mathematical analysis of the Twu95 α-function [36,37]

This α-function is said generalized since it does not involve adjustable parameters. The sole knowledge of an experimental value of the acentric factor ($\omega$) makes it possible to evaluate $\alpha(T_r)$.

$$\begin{cases} \alpha(T_r) = \alpha^{(0)}(T_r) + \omega\left[\alpha^{(1)}(T_r) - \alpha^{(0)}(T_r)\right] \\ \alpha^{(0)}(T_r) = T_r^{N^{(0)}\left[M^{(0)}-1\right]} \exp\left[L^{(0)}\left(1 - T_r^{M^{(0)}N^{(0)}}\right)\right] \\ \alpha^{(1)}(T_r) = T_r^{N^{(1)}\left[M^{(1)}-1\right]} \exp\left[L^{(1)}\left(1 - T_r^{M^{(1)}N^{(1)}}\right)\right] \end{cases} \quad (3.46)$$

The universal parameters ($L^{(k)}$, $M^{(k)}$, $N^{(k)}$ for $k = 0$ and $k = 1$) involved in this α-function are reported in Table 3.9.

| | | $T_r \leq 1$ | | $T_r > 1$ | |
|---|---|---|---|---|---|
| | | $\alpha^{(0)}$ | $\alpha^{(1)}$ | $\alpha^{(0)}$ | $\alpha^{(1)}$ |
| Redlich-Kwong | L | 0.141599 | 0.500315 | 0.441411 | 0.032580 |
| | M | 0.919422 | 0.799457 | 6.500018 | 1.289098 |
| | N | 2.496441 | 3.291790 | -0.200000 | -8.000000 |
| Peng-Robinson | L | 0.125283 | 0.511614 | 0.401219 | 0.024955 |
| | M | 0.911807 | 0.784054 | 4.963070 | 1.248089 |
| | N | 1.948150 | 2.812520 | -0.200000 | -8.000000 |

Table 3.9. Universal parameters regressed for the Twu95 α-function.

Different sets of parameters are used in the subcritical and supercritical domains. These parameters were regressed to obtain an α-function of class $C^2$.

- **Is the α-function of class $C^2$?** Yes, due to the addition of this constraint during the regression procedure of the universal parameters (see Figure 3.21)

The presence of salient points on the second derivative curves of this α-function can however be noticed (which is the consequence of a non-continuous third derivative of the α-function).

- **Is the α-function always positive?** No (see α-function curves plotted for negative or high positive values of ω in Figure 3.21(a)).
- **Is the first derivative of the α-function always negative?** No (see Figure 3.21(b)).
- **Is the second derivative of the α-function always positive?** No (see Figure 3.21(c)).

- **Is the third derivative of the α-function always negative?** No (see Figure 3.21(d)).
- Conclusion:

To conclude, Figure 3.21 shows that the consistency test proposed in this article (see Eq.(3.19)) is passed by molecules having an acentric factor ranging between 0 and 1. For molecules having a higher acentric factor, the first and second derivatives of the Twu95 α-function fail the proposed consistency test (this is for instance the case of n-alkanes heavier than n-$C_{22}$).

Let us note also that regardless of the ω-value, the sign of the third derivative of the Twu95 α-function is not constant on the whole temperature range (see Figure 3.21(d)). Inevitably, poor predictions of heat capacities are obtained in the temperature domain where the third derivative of the α-function is positive. For all molecules, this temperature domain is located in the vicinity of the critical temperature, i.e., it can be reached in many practical cases. Predictions of heat capacities with the Twu95 α-function could thus be less accurate than those calculated with other simpler α-functions.

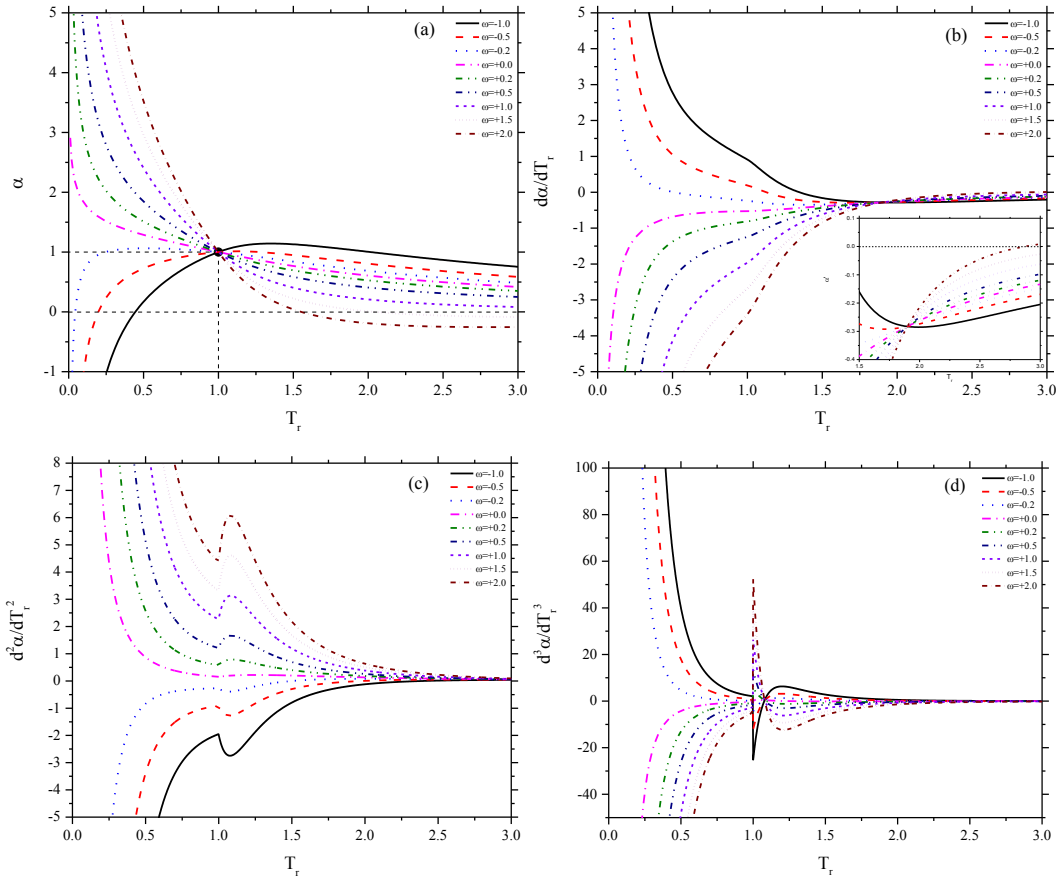



Figure 3.21. The Twu95 α-function (a) and its first (b), second (c) and third derivatives (d) (case of the RK EoS).

### 3.11.4. Appendix D: mathematical study of the Trebble and Bishnoi α-function [88]

This α-function contains only one adjustable parameter (L):

$$\alpha(T_r) = \exp\left[L\left(1 - T_r\right)\right] \tag{3.47}$$

This α-function can be seen as a particular case of the Twu91 α-function with N set to 1 and M set to 1.

- **Is the α-function of class C²?** Yes.
- **Is the α-function always positive?** Yes.
- **Is the first derivative of the α-function always negative?**

The first derivative of this α-function writes

$$\frac{d\alpha}{dT_r}(T_r) = -L \cdot \alpha(T_r) \tag{3.48}$$

As a consequence, $d\alpha/dT_r$ is negative provided L is positive.

- **Is the second derivative of the α-function always positive?** Yes.

The second derivative of this α-function indeed writes

$$\frac{d^2\alpha}{dT_r^2}(T_r) = L^2 \cdot \alpha(T_r) \tag{3.49}$$

- **Is the third derivative of the α-function always negative?**

The third derivative of the Trebble-Bishnoi α-function is:

$$\frac{d^3\alpha}{dT_r^3}(T_r) = -L^3 \cdot \alpha(T_r) \tag{3.50}$$

It is assumed that $L > 0$. Doing so, $\alpha > 0$ and $\frac{d^3\alpha}{dT_r^3}(T_r) < 0$.

- Conclusion:

To conclude, the Trebble and Bishnoi α-function passes the proposed consistency test provided $L > 0$.

### 3.11.5. Appendix E: mathematical study of the Melhem-Saini-Goodwin α-function [89]

This α-function involves 2 adjustable parameters (m and n):

$$\alpha(T_r)=\exp\left[m\left(1-T_r\right)+n\left(1-\sqrt{T_r}\right)^2\right] \tag{3.51}$$

- **Is the α-function of class C²?** Yes.
- **Is the α-function always positive?** Yes.
- **Is the first derivative of the α-function always negative?**

The first derivative of the α-function is:

$$\begin{cases}\dfrac{d\alpha}{dT_r}(T_r)=-\dfrac{\alpha(T_r)}{\sqrt{T_r}}P\left(T_r\right)\\ P\left(T_r\right)=(m-n)\sqrt{T_r}+n\end{cases} \tag{3.52}$$

The quantity $P\left(T_r\right)$ is positive if:

$$\begin{cases}m-n\geq 0\\ n\geq 0\end{cases}\Leftrightarrow m\geq n\geq 0 \tag{3.53}$$

- **Is the second derivative of the α-function always positive?** Yes.

The second derivative of the Melhem-Saini-Goodwin α-function is:

$$\begin{cases}\dfrac{d^2\alpha}{dT_r^2}(T_r)=\dfrac{\alpha(T_r)}{2T_r^{3/2}}Q\left(\sqrt{T_r}\right)\\ Q\left(\sqrt{T_r}\right)=\underbrace{2(m-n)^2}_{>0}\left(\sqrt{T_r}\right)^3+\underbrace{4n(m-n)}_{>0}\left(\sqrt{T_r}\right)^2+\underbrace{2n^2}_{>0}\left(\sqrt{T_r}\right)+\underbrace{n}_{>0}\end{cases} \tag{3.54}$$

Under assumption (3.53), all the coefficients of the polynomial Q are positive, therefore, Q is always positive.

- **Is the third derivative of the α-function always negative?**

The third derivative of this α-function is:

$$\begin{cases}\dfrac{d^3\alpha}{dT_r^3}(T_r)=-\dfrac{\alpha(T_r)}{4T_r^{5/2}}R\left(\sqrt{T_r}\right)\\ R\left(\sqrt{T_r}\right)=\underbrace{4(m-n)^3}_{>0}\left(\sqrt{T_r}\right)^5+\underbrace{12n(m-n)^2}_{>0}\left(\sqrt{T_r}\right)^4+\underbrace{12n^2(m-n)}_{>0}\left(\sqrt{T_r}\right)^3\\ \qquad\qquad+\left(4n^3+6mn-6n^2\right)\left(\sqrt{T_r}\right)^2+\underbrace{6n^2}_{>0}\left(\sqrt{T_r}\right)+\underbrace{3n}_{>0}\end{cases} \tag{3.55}$$

By noting that:

$$m > n > 0 \Rightarrow 6mn > 6n^2 \Rightarrow 4n^3 + (6mn - 6n^2) > 0 \qquad (3.56)$$

it can be claimed that under assumption (3.53), all the coefficients of the polynomial R are positive and thus $R\left(\sqrt{T_r}\right) \geq 0$. Consequently, the third derivative of the Melhem-Saini-Goodwin $\alpha$-function is always negative.

- Conclusion:

The Melhem-Saini-Goodwin $\alpha$-function is consistent (i.e., positive, decreasing, convex with a negative third derivative) provided $m \geq n \geq 0$.

### 3.11.6. Appendix F: mathematical study of the Soave72 α-function [32]

The Soave72 α-function involved a generalized parameter (m) correlated to the acentric factor ($\omega$):

$$\begin{cases} \alpha(T_r) = \left[1 + m(\omega)\left(1 - \sqrt{T_r}\right)\right]^2 \\ m(\omega) = 0.480 + 1.574\omega - 0.176\omega^2 \quad \text{for the RK EoS} \\ m(\omega) = 0.37464 + 1.54226\omega - 0.26992\omega^2 \quad \text{for the PR EoS} \end{cases} \tag{3.57}$$

The Soave72 function is certainly the most employed α-function in the oil and gas industries. It is in particular used in the PPR78 [23,73,74] and PR2SRK predictive models [72].

- **Is the α-function of class C²?** Yes.
- **Is the α-function always positive?** Yes.
- **Is the first derivative of the α-function always negative?**

The first derivative of the Soave72 α-function is:

$$\frac{d\alpha}{dT_r}(T_r) = -\frac{m(\omega)}{\sqrt{T_r}}\left[1 + m(\omega)\left(1 - \sqrt{T_r}\right)\right] = -m(\omega)\sqrt{\frac{\alpha(T_r)}{T_r}} \tag{3.58}$$

The limit of the first derivative of the α-function when the temperature tends to $+\infty$ is:

$$\lim_{T_r \to +\infty} \frac{d\alpha}{dT_r}(T_r) = \left[m(\omega)\right]^2 > 0 \tag{3.59}$$

It appears that the first derivative of the Soave72 α-function is not always negative.

Due to its polynomial expression in $\sqrt{T_r}$, the Soave72 α-function can only exhibit two types of behavior, depending on the $\omega$-value:

- either the function is decreasing then increasing for increasing values of $T_r$,
- or, the function is monotonically increasing.

To discriminate between these two scenarios, the limit of the first derivative of the α-function when the temperature tends to 0 is now studied:

$$\lim_{T_r \to 0} \frac{d\alpha}{dT_r}(T_r) = -sign\left[m(1+m)\right]\infty \tag{3.60}$$

*Case 1:* $m(1+m) > 0$

If $m(1+m)$ is positive (what is the case for more than 99% of the compounds), one has $\lim_{T_r \to 0} \frac{d\alpha}{dT_r}(T_r) = -\infty$ and the Soave72 α-function exhibits a minimum at a reduced temperature denoted $T_{r,\min}$. For $T_r \in \left\lfloor 0 ; T_{r,\min} \right\rfloor$, α is a decreasing function while it is an increasing function for $T_r > T_{r,\min}$. Such a behavior is observed for the following values of the acentric factor:

$$\omega \in ]-1;-0.8580] \cup ]-0.2952;9.2384[ \cup [9.8012;+\infty[ \qquad \textit{for} \text{ the RK EoS} \quad (3.61)$$

$$\omega \in ]-1;-0.7838] \cup ]-0.2334;5.9472[ \cup [6.4976;+\infty[ \qquad \text{for the PR EoS} \quad (3.62)$$

To understand whether the irregular behavior of the Soave72 α-function (i.e., increasing of α for $T_r > T_{r,\min}$) may affect practical applications, the relation between $T_{r,\min}$ and ω is now investigated. $T_{r,\min}$ is obtained by solving:

$$\begin{aligned} & \frac{d\alpha}{dT_r}(T_{r,\min}) = 0 \\ \Leftrightarrow\ & m(\omega)\left[1 + m(\omega)\left(1 - \sqrt{T_{r,\min}}\right)\right] = 0 \\ \Leftrightarrow\ & T_{r,\min} = \left[\frac{1+m(\omega)}{m(\omega)}\right]^2 \end{aligned} \qquad (3.63)$$

Note that at $T_{r,\min}$, the Soave72 α-function cancels: $\alpha\left(T_{r,\min}\right) = 0$.

The evolution of $T_{r,\min}$ with respect to the acentric factor is reported in Figure 3.22.

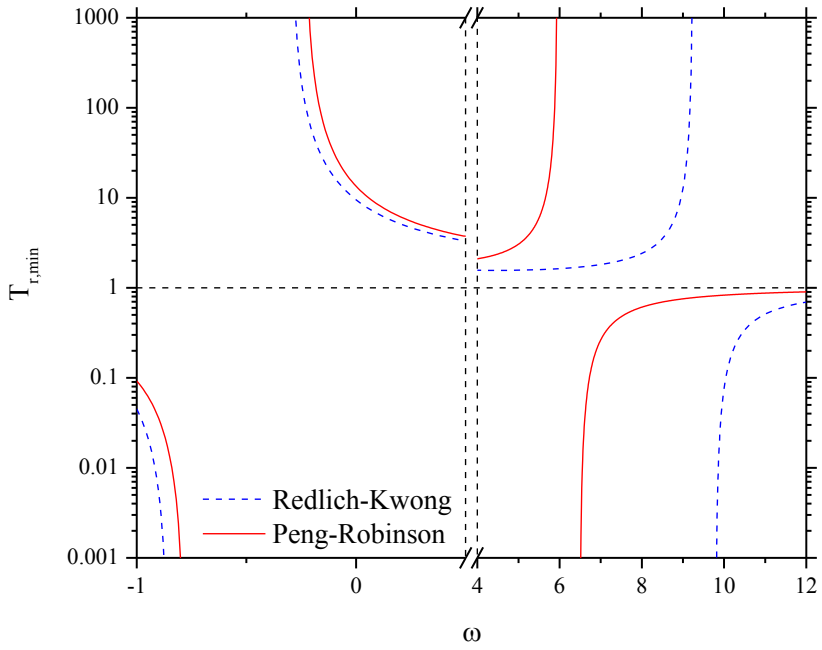



Figure 3.22. $T_{r,\min}$ as a function of ω.

To complete the analysis, some values of $T_{r,\min}$ and $T_{\min}$ are reported in Table 3.10 for a series of real compounds of various sizes (i.e., a large range of acentric-factor values is covered). It is observed that in practice, $T_{\min}$ is often higher than 1500 K, largely above common temperatures encountered in practical applications.

| Component | Acentric factor ω | $T_c$ / K | RK CEoS | | PR CEoS | |
|---|---|---|---|---|---|---|
| | | | $T_{r,min}$ | $T_{min}$/K | $T_{r,min}$ | $T_{min}$/K |
| Methane | 0.012 | 190.564 | 9.045 | 1723.566 | 12.591 | 2399.325 |
| n-decane | 0.492 | 617.700 | 3.330 | 2057.108 | 3.748 | 2314.913 |
| n-eicosane | 0.907 | 768.000 | 2.456 | 1886.582 | 2.705 | 2077.277 |
| n-triacontane | 1.307 | 844.000 | 2.094 | 1767.355 | 2.305 | 1945.584 |
| Water | 0.345 | 647.096 | 3.992 | 2583.530 | 4.595 | 2973.520 |
| $CO_2$ | 0.224 | 304.21 | 4.905 | 1492.258 | 5.839 | 1776.253 |
| Argon | 0.000 | 150.860 | 9.507 | 1434.218 | 13.463 | 2031.065 |
| Ethanol | 0.644 | 514.000 | 2.904 | 1492.795 | 3.228 | 1659.020 |
| Ammonia | 0.253 | 405.650 | 4.641 | 1882.512 | 5.469 | 2218.676 |

Table 3.10. Values of $T_{min}$ for some chemical compounds using either the PR or RK CEoS

*Case 2:* $m(1+m)<0$

This case is observed for the following values of the acentric factor:

$$\omega \in ]-0.8580;-0.2952] \cup ]9.2384;9.8012[ \quad \text{for the RK EoS} \quad (3.64)$$

$$\omega \in ]-0.7838;-0.2334] \cup ]5.9472;6.4976[ \quad \text{for the PR EoS} \quad (3.65)$$

In practice, this instance arises for molecules having negative acentric factors (e.g., helium, aluminum and arsenic). In such a case: $\lim_{T_r \to 0} \frac{d\alpha}{dT_r}(T_r) = +\infty$ and the Soave72 α-function is an increasing function of temperature for any positive value of $T_r$. This behavior is not desirable and therefore, the Soave72 α-function should be used only for molecules having an acentric factor ω in the ranges defined by Eq.(3.61) or Eq.(3.62).

- **Is the second derivative of the α-function always positive?**

It is now assumed that $m(1+m)>0$ (which is obtained for acentric factor values lying in the ranges defined by Eq.(3.61) or Eq.(3.62)). The second derivative of the Soave72 α-function is:

$$\frac{d^2\alpha}{dT_r^2}(T_r)=\frac{m(\omega)\left[m(\omega)+1\right]}{2T_r^{3/2}} \tag{3.66}$$

Since $m(1+m)>0$, the convexity constraint is verified.

- Is the third derivat**ive of the α**-function always negative?

The third derivative of the Soave72 α-function is:

$$\frac{d^3\alpha}{dT_r^3}(T_r)=-\frac{3}{4}\frac{m(\omega)\left[m(\omega)+1\right]}{T_r^{5/2}} \tag{3.67}$$

As previous, assuming $m(1+m)>0$, the negativity of the third derivative is ensured.

- Conclusion:

When the quantity $m(1+m)$ is positive (i.e., for acentric-factor values lying in the ranges defined by Eq.(3.61) or Eq.(3.62), which is verified in practice for more than 99% of real components), the Soave α-function is consistent up to the temperature defined by Eq.(3.63), which is generally higher than 1500 K (it can thus be claimed that the Soave 72 α-function is consistent on temperature ranges of practical interest).

Such an α-function can thus be considered as fully consistent in most cases explaining why it has achieved great success in the industry.

### 3.11.7. Appendix G: mathematical study of the Soave84 α-function [32]

This α-function involves two adjustable parameters a and b:

$$\alpha(T_r) = 1 + (1 - T_r)\left(a + \frac{b}{T_r}\right) \tag{3.68}$$

- **Is the α-function of class C²?** Yes.
- **Is the α-function always positive?** Yes.

The Soave84 α-function can be written as a second order polynomial of the reduced temperature

$$\begin{cases} \alpha(T_r) = \dfrac{1}{T_r} F(T_r) \\ F(T_r) = -aT_r^{\,2} + T_r(1 + a - b) + b \end{cases} \tag{3.69}$$

Polynomial $F(T_r)$ is positive provided [104]:

$$\begin{cases} a \le 0 \\ b \ge 0 \\ 1 + a - b \ge -2\sqrt{-ab} \end{cases} \tag{3.70}$$

- **Is the first derivative of the α-function always negative?**

The first derivative of the Soave84 α-function is:

$$\begin{cases} \dfrac{d\alpha}{dT_r}(T_r) = -\dfrac{P(T_r)}{T_r^{\,2}} \\ P(T_r) = aT_r^{\,2} + b \end{cases} \tag{3.71}$$

Polynomial $P(T_r)$ is positive provided:

$$\begin{cases} a \ge 0 \\ b \ge 0 \\ 0 \ge -2\sqrt{ab} \end{cases} \tag{3.72}$$

Note that the last condition is automatically satisfied. It appears that constraints (3.70) and (3.72) are contradictory and cannot be satisfied simultaneously.

Therefore, if a is positive:

- $\alpha(T_r)$ is negative, at least, on a certain temperature range
- $\dfrac{d\alpha}{dT_r}(T_r)$ is negative for any (positive) temperature value

On the other hand, if a is negative:

- $\alpha(T_r)$ is positive for any (positive) temperature value
- $\frac{d\alpha}{dT_r}(T_r)$ is positive, at least, on a certain temperature range

- **Is the second derivative of the α-function always positive?**

The second derivative of the Soave84 α-function is:

$$\frac{d^2\alpha}{dT_r^2}(T_r) = \frac{2b}{T_r^3} \tag{3.73}$$

It appears that $\frac{d^2\alpha}{dT_r^2}(T_r)$ is positive provided b is positive.

- **Is the third derivative of the α-function always negative?**

The third derivative of the α-function writes

$$\frac{d^3\alpha}{dT_r^3}(T_r) = -\frac{6b}{T_r^4} \tag{3.74}$$

It appears that $\frac{d^3\alpha}{dT_r^3}(T_r)$ is negative provided b is positive.

- Conclusion:

The only possibility for satisfying both the positivity condition for the Soave84 α-function and the negativity condition for its first derivative would be to set:

$$a = 0 \tag{3.75}$$

This would lead to modify the mathematical expression of the Soave84 α-function. As a conclusion, the Soave84 α-function cannot pass the proposed consistency test.

### 3.11.8. Appendix H: mathematical analysis of the Stryjek-Vera α-function [29]

The Stryjek-Vera α-function involves one adjustable parameter ($\kappa_1$) and one universal parameter ($\kappa_0(\omega)$):

$$\begin{aligned}
&\alpha(T_r) = \left[1 + \kappa(T_r)\cdot\left(1 - \sqrt{T_r}\right)\right]^2 \\
&\kappa(T_r) = \kappa_0(\omega) + \kappa_1\left(1 + \sqrt{T_r}\right)\left(0.7 - T_r\right) \\
&\kappa_0(\omega) = 0.378893 + 1.4897153\omega - 0.17131848\omega^2 + 0.0196554\omega^3 \\
&\begin{cases} \kappa_1\left(T_r \le 0.7\right) \ne 0 \\ \kappa_1\left(T_r > 0.7\right) = 0 \end{cases}
\end{aligned} \tag{3.76}$$

The Stryjek-Vera α-function is identical to the Soave α-function for reduced temperatures above 0.7. Therefore, it suffers from all the identified defects of the Soave α-function described in Appendix F. In addition, the Stryjek-Vera α-function exhibits a discontinuous behavior in $T_r = 0.7$ which is prejudicial to all derived EoS-properties (enthalpy, entropy, heat capacity etc.).

### 3.11.9. Appendix I: mathematical study of the Mathias-Copeman α-function [26]

This α-function uses two different expressions depending on the temperature domain considered (sub- or super-critical) and involves three adjustable parameters ($c_1$, $c_2$, $c_3$)

$$\alpha(T_r)=\begin{cases} if\ T_r\le 1: & \alpha_{SUB}(T_r)=\left[\begin{array}{l}1+c_1\left(1-\sqrt{T_r}\right)+c_2\left(1-\sqrt{T_r}\right)^2\\+c_3\left(1-\sqrt{T_r}\right)^3\end{array}\right]^2 \\ if\ T_r>1: & \alpha_{SUP}(T_r)=\left[1+c_1\left(1-\sqrt{T_r}\right)\right]^2 \end{cases} \quad (3.77)$$

- **Is the α-function of class C²?**

  The first derivatives of the Mathias-Copeman α-function are:

$$\frac{d\alpha}{dT_r}(T_r)=\begin{cases} if\ T_r\le 1: & \frac{d\alpha_{SUB}}{dT_r}(T_r)=-\sqrt{\frac{\alpha_{SUB}(T_r)}{T_r}}\left[\begin{array}{l}c_1+2c_2\left(1-\sqrt{T_r}\right)\\+3c_3\left(1+T_r-2\sqrt{T_r}\right)\end{array}\right] \\ if\ T_r>1: & \frac{d\alpha_{SUP}}{dT_r}(T_r)=-c_1\sqrt{\frac{\alpha_{SUP}(T_r)}{T_r}} \end{cases} \quad (3.78)$$

  It appears that:

$$\frac{d\alpha_{SUB}}{dT_r}(T_r=1)=\frac{d\alpha_{SUP}}{dT_r}(T_r=1)=-c_1 \quad (3.79)$$

  The Mathias-Copeman α-function is thus at least of class C¹.

  The second derivatives of the Mathias-Copeman α-function are:

$$\frac{d^2\alpha}{dT_r^2}(T_r)=\begin{cases} if\ T_r\le 1: & \frac{d^2\alpha_{SUB}}{dT_r^2}(T_r)=\frac{P(T_r)}{2T_r^{3/2}} \\ & P(T_r)=12c_3^2T_r^{5/2}-15c_3\left(c_2+3c_3\right)T_r^2 \\ & \quad +4T_r^{3/2}\left(2c_1c_3+10c_2c_3+c_2^2+15c_3^2\right) \\ & \quad -3T_r\left(4c_1c_3+c_1c_2+c_3+2c_2^2+10c_3^2+10c_2c_3\right) \\ & \quad +3c_3^2+2c_2^2+c_1^2+3c_3+c_1+3c_1c_2+5c_2c_3 \\ & \quad +4c_1c_3+2c_2 \\ if\ T_r>1: & \frac{d^2\alpha_{SUP}}{dT_r^2}(T_r)=\frac{c_1\left(1+c_1\right)}{2T_r^{3/2}} \end{cases}$$

(3.80)

Therefore, one has:

$$\begin{cases} \dfrac{d^2\alpha_{SUB}}{dT_r^2}(T_r=1)=\dfrac{c_1(1+c_1)}{2} \\ \dfrac{d^2\alpha_{SUP}}{dT_r^2}(T_r=1)=\dfrac{c_1(1+c_1)+2c_2}{2} \end{cases} \tag{3.81}$$

As a consequence, the Mathias-Copeman α-function is of class $C^2$ provided $c_2$ is set equal to 0. Doing so, this α-function would loose one of its three adjustable parameters.

- Conclusion:

At this step, there is no need to pursue the study: it is obvious that the Mathias-Copeman α-function cannot pass the consistency test since the $C^2$-class condition requires to annihilate coefficient $c_2$ and consequently to modify the α-function expression.

In addition, it is remarkable that the Mathias-Copeman α-function is similar to the Soave 72 α-function for $T_r > 1$ except that the universal $m(\omega)$ parameter of the Soave function is replaced by an adjustable parameter $c_1$.

If, as often seen in practice, the parameter $c_1$ is set to $m(\omega)$, the Mathias-Copeman α-function would loose a second adjustable parameter ($c_1$). It would result that the Mathias-Copeman α-function would only contain one adjustable parameter ($c_3$).

Furthermore, similarly to the Soave 72 α-function, the Mathias-Copeman α-function exhibits an unphysical behavior at infinite temperature:

$$\lim_{T_r \to +\infty} \alpha(T_r) = \lim_{T_r \to +\infty} \alpha_{SUP}(T_r) = +\infty \tag{3.82}$$

### 3.11.10. Appendix J: mathematical study of the Boston-Mathias α-function [84]

The Boston-Mathias α-function contains one universal parameter $m(\omega)$ :

$$\alpha(T_r)=\begin{cases} if\ T_r\le 1: & \alpha_{SUB}(T_r)=\alpha_{SOAVE}(T_r)=\left[1+m(\omega)\cdot\left(1-\sqrt{T_r}\right)\right]^2 \\ if\ T_r>1: & \alpha_{SUP}(T_r)=\exp\left[L\left(1-T_r^{\gamma}\right)\right] \\ \text{with}: & L=\dfrac{m(\omega)}{\gamma}\ \ and\ \ \gamma=1+\dfrac{m(\omega)}{2} \end{cases} \tag{3.83}$$

The relations between parameters L, γ and $m(\omega)$ were derived by Boston and Mathias assuming that

- The first derivatives of $\sqrt{\alpha_{SUB}}$ and $\sqrt{\alpha_{SUP}}$ are equal at the critical temperature,
- The second derivative of $\sqrt{\alpha_{SUP}}$ has to be equal to zero at the critical temperature.

A priori, these assumptions do not guaranty for the function to be of class $C^2$ and more generally, to pass the proposed consistency test for α-functions.

- **Is the α-function of class $C^2$?**

The first derivatives of the Boston-Mathias α-function are:

$$\frac{d\alpha}{dT_r}(T_r)=\begin{cases} if\ T_r\le 1: & \dfrac{d\alpha_{SUB}}{dT_r}(T_r)=-m(\omega)\sqrt{\dfrac{\alpha_{SUB}(T_r)}{T_r}} \\ if\ T_r>1: & \dfrac{d\alpha_{SUP}}{dT_r}(T_r)=-L\gamma T_r^{\gamma-1}\alpha_{SUP}(T_r) \end{cases} \tag{3.84}$$

At $T_r=1$, one has:

$$\begin{cases} \dfrac{d\alpha_{SUB}}{dT_r}(T_r=1)=-m(\omega) \\ \dfrac{d\alpha_{SUP}}{dT_r}(T_r=1)=-L\gamma=-\dfrac{m(\omega)}{\gamma}\gamma=-m(\omega) \end{cases} \tag{3.85}$$

This proves that the Boston-Mathias α-function is at least of class $C^1$.

The second derivatives of the Boston-Mathias α-function are:

$$\frac{d^2\alpha}{dT_r^2}(T_r)=\begin{cases} if\ T_r \le 1: & \dfrac{d^2\alpha_{SUB}}{dT_r^2}(T_r)=\dfrac{1}{2}\dfrac{m(\omega)\left[m(\omega)+1\right]}{T_r^{3/2}} \\ if\ T_r > 1: & \dfrac{d^2\alpha_{SUP}}{dT_r^2}(T_r)=L\gamma T_r^{\gamma-2}\left[L\gamma T_r^{\gamma}-\gamma+1\right]\alpha_{SUP}(T_r) \end{cases} \quad (3.86)$$

At $T_r=1$, one has:

$$\begin{cases} \dfrac{d^2\alpha_{SUB}}{dT_r^2}(T_r=1)=\dfrac{m(\omega)\left[m(\omega)+1\right]}{2} \\ \dfrac{d^2\alpha_{SUP}}{dT_r^2}(T_r=1)=L\gamma\left[L\gamma-\gamma+1\right]=m(\omega)\left[m(\omega)-1-\dfrac{m(\omega)}{2}+1\right]=\dfrac{\left[m(\omega)\right]^2}{2} \end{cases} \quad (3.87)$$

Since $\frac{d^2\alpha_{SUB}}{dT_r^2}(T_r=1) \neq \frac{d^2\alpha_{SUP}}{dT_r^2}(T_r=1)$, the Boston-Mathias α-function is thus not of class $C^2$.

- Conclusion:

At this step, there is no need to pursue the study. Not being of class $C^2$, the Boston-Mathias α-function does not pass the proposed consistency test.

### 3.11.11. Appendix K: mathematical study of the Mathias α-function [90]

The Mathias α-function contains one universal parameter ( $m(\omega)$ ) and one (component-dependent) adjustable parameter (p).

$$\alpha(T_r)=\begin{cases} if\ T_r\le 1: & \alpha_{SUB}(T_r)=\left[1+m(\omega)\left(1-\sqrt{T_r}\right)-p\left(1-T_r\right)\left(0.7-T_r\right)\right]^2 \\ if\ T_r>1: & \alpha_{SUP}(T_r)=\left[\exp\left[L\left(1-T_r^{\gamma}\right)\right]\right]^2 \\ \text{with}: & L=1+\dfrac{m(\omega)}{2}+0.3p \quad and \quad \gamma=\dfrac{L-1}{L} \end{cases} \tag{3.88}$$

The expressions of parameters L and γ were derived by Mathias by assuming that:

- The first derivatives of $\sqrt{\alpha_{SUB}}$ and $\sqrt{\alpha_{SUP}}$ are equal at the critical temperature,
- The second derivative of $\sqrt{\alpha_{SUP}}$ is equal to zero at the critical temperature.

A priori, these assumptions do not guaranty for the function to be of class $C^2$ and more generally, to pass the proposed consistency test for α-functions.

- **Is the α-function of class $C^2$?**

The first derivatives of the Mathias α-function are:

$$\frac{d\alpha}{dT_r}(T_r)=\begin{cases} if\ T_r\le 1: & \dfrac{d\alpha_{SUB}}{dT_r}(T_r)=-2\sqrt{\alpha_{SUB}(T_r)}\left[\dfrac{m(\omega)}{2\sqrt{T_r}}+p\left(2T_r-1.7\right)\right] \\ if\ T_r>1: & \dfrac{d\alpha_{SUP}}{dT_r}(T_r)=-2L\gamma T_r^{\gamma-1}\alpha_{SUP}(T_r) \end{cases} \tag{3.89}$$

At $T_r=1$:

$$\begin{cases} \dfrac{d\alpha_{SUB}}{dT_r}(T_r=1)=-2\left[\dfrac{m(\omega)}{2}+p\left(1.7-2\right)\right]=-2\left[\dfrac{m(\omega)}{2}+0.3p\right] \\ \dfrac{d\alpha_{SUP}}{dT_r}(T_r=1)=-2L\gamma=-2\left[\dfrac{m(\omega)}{2}+0.3p\right] \end{cases} \tag{3.90}$$

This proves that the Mathias α-function is at least of class $C^1$.

The second derivatives of the Mathias α-function are:

$$\frac{d^2\alpha}{dT_r^2}(T_r)=\begin{cases} if\ T_r\le 1: & \dfrac{d^2\alpha_{SUB}}{dT_r^2}(T_r)=2\left[\dfrac{m(\omega)}{2\sqrt{T_r}}+p\left(2T_r-1.7\right)\right]^2 \\ & \qquad +2\sqrt{\alpha_{SUB}(T_r)}\left(\dfrac{m(\omega)}{4T_r^{3/2}}-2p\right) \\ if\ T_r>1: & \dfrac{d^2\alpha_{SUP}}{dT_r^2}(T_r)=2L\gamma T_r^{\gamma-2}\left[2L\gamma T_r^{\gamma}-\gamma+1\right]\alpha_{SUP}(T_r) \end{cases} \tag{3.91}$$

At $T_r=1$, one has:

$$\begin{cases} \dfrac{d^2\alpha_{SUB}}{dT_r^2}(T_r=1)=0.5m^2+0.6mp++0.18p^2+0.5m-4p \\ \dfrac{d^2\alpha_{SUP}}{dT_r^2}(T_r=1) \qquad =2L\gamma\left[2L\gamma-\gamma+1\right] \\ \qquad\qquad =\dfrac{10m^2+12mp+5m^3+9m^2p+5.4mp^2+10m+3.6p^2+1.08p^3+6p}{10+5m+3p} \end{cases}$$

(3.92)

Since $\frac{d^2\alpha_{SUB}}{dT_r^2}(T_r=1) \neq \frac{d^2\alpha_{SUP}}{dT_r^2}(T_r=1)$, the Boston-Mathias α-function is thus not of class $C^2$.

- Conclusion:

At this step, there is no need to pursue the study. Not being of class $C^2$, the Mathias α-function does not pass the proposed consistency test.

### 3.11.12. Appendix L: mathematical study of the Gibbons and Laughton α-function [87]

The α-function involved two adjustable parameters denoted X and Y:

$$\alpha(T_r) = 1 + X\left(T_r - 1\right) + Y\left(\sqrt{T_r} - 1\right) \tag{3.93}$$

- **Is the α-function of class C²?** Yes.
- **Is the α-function always positive?**

Eq.(3.93) can be alternatively written :

$$\alpha(T_r) = X\left(\sqrt{T_r}\right)^2 + Y\sqrt{T_r} + (1 - X - Y) \tag{3.94}$$

Which is a second-order polynomial of the square root of the reduced temperature. Therefore, this polynomial is positive if [104]

$$\begin{cases} X \geq 0 \\ Y \leq 1 - X \\ Y \geq -2\sqrt{X(1 - X - Y)} \end{cases} \tag{3.95}$$

As will be shown below, the parameter $Y$ is necessarily negative to ensure that the α-function is decreasing at low temperature. The third inequality of Eq. (3.95) can be squared, both sides of the equation being negative, in order to solve this inequality with respect to Y. The resolution of the inequality provides the following existence interval for parameter Y

$$-2X - 2\sqrt{X} \leq Y \leq -2X + 2\sqrt{X} \tag{3.96}$$

One can demonstrate that $-2X + 2\sqrt{X} \leq 1 - X$ . Therefore, positivity condition of the α-function is, reminding that Y has to be negative:

$$\begin{cases} X \geq 0 \\ -2X - 2\sqrt{X} \leq Y \leq \min\left(0; -2X + 2\sqrt{X}\right) \end{cases} \tag{3.97}$$

- **Is the first derivative of the α-function always negative?**

The first derivative of the Gibbons and Laughton α-function is:

$$\frac{d\alpha}{dT_r}(T_r) = X + \frac{Y}{2\sqrt{T_r}} \tag{3.98}$$

When $T_r$ tends to 0, the limit of Eq.(3.98) is:

$$\lim_{T_r \to 0} \frac{d\alpha}{dT_r}(T_r) = \begin{cases} -\infty & \text{if Y<0} \\ +\infty & \text{if Y>0} \end{cases} \tag{3.99}$$

Therefore, Y has to be negative

When $T_r$ tends to $+\infty$, the limit of Eq.(3.98) is:

$$\lim_{T_r \to +\infty} \frac{d\alpha}{dT_r}(T_r) = X \tag{3.100}$$

Therefore, X has to be negative. This condition is contradictory with condition (3.95). The reason of this contradiction is that the Gibbons and Laughton α-function exhibits a minimum when $\begin{cases} X \geq 0 \\ Y \leq 0 \end{cases}$ (this behavior is similar to the one of the Soave 72 α-function). As a conclusion, the Gibbons and Laughton α-function can only be decreasing on a limited temperature range $\left] 0 ; T_{r,\min} \right]$. As illustrated in Figure 3.23, the minimum of the α-function is found at

$$\sqrt{T_{r,\min}} = \frac{-Y}{2X} \tag{3.101}$$

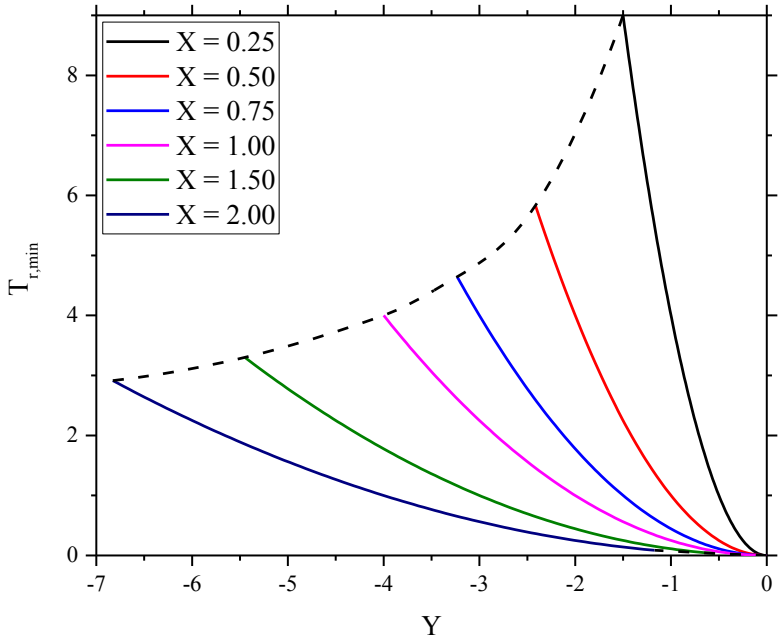



Figure 3.23. Changes of $T_{r,min}$ with respect to the change of $Y$ for different values of $X$.

Note that the value of the α-function at $T_{r,\min}$ is not equal to zero.

$$\alpha(T_{r,\min}) = \frac{-Y^2}{4X} + 1 - X - Y \tag{3.102}$$

- **Is the second derivative of the α-function always positive?**

The second derivative of the Gibbons and Laughton α-function is:

$$\frac{d^2\alpha}{dT_r^2}(T_r) = -\frac{1}{4}\frac{Y}{T_r^{3/2}} \tag{3.103}$$

As a consequence, $\frac{d^2\alpha}{dT_r^2}(T_r)$ is positive provided Y is negative.

- **Is the third derivative of the α-function always negative?**

The third derivative of the Gibbons and Laughton α-function is:

$$\frac{d^3\alpha}{dT_r^3}(T_r) = \frac{3}{8}\frac{Y}{T_r^{5/2}} \tag{3.104}$$

As a consequence, $\frac{d^3\alpha}{dT_r^3}(T_r)$ is negative provided Y is negative.

- Conclusion:

The Gibbons and Laughton α-function behaves as a consistent α-function, up to a certain reduced temperature $T_{r,min}$ defined by Eq.(3.101) if

$$\begin{cases} X \geq 0 \\ -2X - 2\sqrt{X} \leq Y \leq \min\left(0; -2X + 2\sqrt{X}\right) \end{cases} \tag{3.105}$$

# Chapitre 4. Article “On the imperative need to use a consistent α-function for the prediction of pure-compound supercritical properties with a cubic equation of state”

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On the imperative need to use a consistent α-function for the prediction of pure-compound supercritical properties with a cubic equation of state

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ABSTRACT

Since Van der Waals, the attractive term $a(T)$ of any cubic equation of state is expressed as the product of its value at the critical temperature ($a_c$) by the so-called alpha function. Our recent investigations made it however possible to conclude that to get accurate and physically meaningful behaviors in both the subcritical and supercritical domains, it was necessary to work with a *consistent* α-function, i.e., with an α-function which is positive, decreasing, convex and with a negative third derivative. This paper aims at quantifying the gain of accuracy resulting from the use of a consistent α-function when a cubic equation of state is used to calculate the properties of a pure compound in the supercritical region. As a key conclusion, embedding a consistent α-function in a cubic equation of state instead of an inconsistent one entails a division by a factor 9 of the deviations between calculated and experimental data.

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## Highlights

1) α-functions must be positive, decreasing, convex with negative third derivative.
2) Gain of accuracy resulting from the use of a consistent α-function is quantified.
3) Working with a consistent α-function increases by a factor 9 the accuracy.

## Abstract

Since Van der Waals, the attractive term $a(T)$ of any cubic equation of state is expressed as the product of its value at the critical temperature ($a_c$) by the so-called alpha function. Our recent investigations made it however possible to conclude that to get accurate and physically meaningful behaviors in both the subcritical and supercritical domains, it was necessary to work with a *consistent* α-function, i.e., with an α-function which is positive, decreasing, convex and with a negative third derivative. This paper aims at quantifying the gain of accuracy resulting from the use of a consistent α-function when a cubic equation of state is used to calculate the properties of a pure compound in the supercritical region. As a key conclusion, embedding a consistent α-function in a cubic equation of state instead of an inconsistent one entails a division by a factor 9 of the deviations between calculated and experimental data.

## Keywords

Alpha function; Cubic equation of state; Consistency test; Supercritical properties

### 4.1. Introduction

Since the Van der Waals proposal, two-parameter cubic equations of state (CEoS) express their attractive and repulsive terms by introducing a parameter $a$ which is a measure of the attractive forces ("energy parameter") between molecules, and a parameter $b$ which is a measure of the size ("intrinsic volume" or "co-volume") of the molecules. It results the general formulation of a two-parameter CEoS:

$$P(T,v)=\frac{RT}{v-b}+\frac{-a(T)}{(v-r_1b)(v-r_2b)} \tag{4.1}$$

where $r_1$ and $r_2$ are two universal constants depending on the selected CEoS. To make the application of the critical constraints easier, it is convenient to write:

$$a(T)=a_c\times\alpha(T) \tag{4.2}$$

i.e. to express the attractive term as the product of its value at the critical temperature ($a_c$) by the so-called alpha function. Doing so, it follows that the dimensionless, temperature-dependent $\alpha$-function becomes unity at the critical temperature. In a previous paper [20], we demonstrated that not only the $\alpha$-function but also its first, second [86] and third derivatives should satisfy the following constraints over the whole temperature domain:

$$\text{For all T:}\begin{cases}\text{The } \alpha\text{-function must be:} & \begin{cases}\text{- positive } [\alpha(T)>0]\\ \text{- continuous}\end{cases}\\ \text{The first derivative of the } \alpha\text{-function } \dfrac{d\alpha}{dT} \text{ must be:} & \begin{cases}\rightarrow \text{ negative}\\ \textit{(in order to get a decrasing } \alpha\textit{- function)}\\ \rightarrow \text{ continuous}\end{cases}\\ \text{The second derivative of the } \alpha\text{-function } \dfrac{d^2\alpha}{dT^2} \text{ must be:} & \begin{cases}\rightarrow \text{ positive}\\ \textit{(in order to guarantee a convex } \alpha\textit{- function)}\\ \rightarrow \text{ continuous}\end{cases}\\ \text{The third derivative of the } \alpha\text{-function } \dfrac{d^3\alpha}{dT^3} \text{ must be:} & \{\quad \rightarrow \text{ negative}\end{cases} \tag{4.3}$$

An $\alpha$-function which simultaneously satisfies all these criteria is labeled *consistent* and the set of constraints reported in Eq. (4.3) was called *consistency test for an $\alpha$-function*. In other words, a consistent $\alpha$-function is simply an $\alpha$-function that passes the so-called consistency test. In case of test failure, i.e., if one of these constraints is not satisfied, the $\alpha$-function is declared inconsistent. Our previous paper [20] and another one by Peyman and Sedigh [38] made it possible to conclude that to get accurate and

physically-meaningful behaviors in both the subcritical and supercritical domains, it was absolutely necessary to work with a consistent $\alpha$-function. Such a paper [20] also highlighted that none of the $\alpha$-functions classically available in process simulator software (Soave 1972 [7], Soave 1984 [32], Gibbons-Laughton [87], Stryjek-Vera [29], Boston-Mathias [84], Mathias-Copeman [26], Mathias [90], Twu 1995 [36,37], Trebble-Bishnoi [88], Melhem-Saini-Goodwin [89], Twu 1988 [35], Twu 1991 [19]) passes the consistency test for any values of their parameters. This latter conclusion scared many researchers or companies that commercialize process simulator software and we were asked to quantify the loss of accuracy resulting from the use of an inconsistent $\alpha$-function to calculate the properties of a pure compound in the supercritical region. This is thus the aim of this note. While our first article [20] was mostly devoted to the influence of the $\alpha$-function on the reproduction of binary-system phase diagrams, the present paper focuses on the impact of the alpha-function consistency on the modeling of pure-component supercritical properties. The strategy adopted in this article is as follows: 9 pure compounds, for which an EoS developed by the National Institute of Standards and Technology (NIST) was both available and certified accurate in the supercritical domain are selected. For each of them, the Peng-Robinson [8] EoS combined with the Twu 91 $\alpha$-function [19] is also applied. The 3 parameters of such an $\alpha$-function [19] are then regressed twice (respectively without and with the imposition of consistency constraints) in order to accurately reproduce subcritical data including vapor pressures $\left(P^{sat}\right)$, enthalpies of vaporization $\left(\Delta_{vap}H\right)$ and saturated liquid heat capacities $\left(c_{P,L}^{sat}\right)$. More specifically: the first set of parameters is obtained without imposing any constraint during the fitting procedure and the resulting $\alpha$-function is found to be inconsistent; the second set of parameters results from a fitting procedure that ensures to get a consistent $\alpha$-function. The two sets of parameters are used thereafter to estimate residual enthalpies ($h^{res}$) and residual constant-pressure heat capacities ($c_P^{res}$) in the supercritical domain. Results obtained with each set of parameters are compared each other and with the pseudo-experimental data (the adjective *pseudo-experimental* designates here the property values calculated by using a NIST reference EoS considered as accurate as experimental data).

### 4.2. Reasoning for CEoS and α-function choices

The *volume-translated* Peng-Robinson EoS combined with the three-parameter Twu91 α-function [19] is considered in this study. We indeed gave proof during the development of the *translated-consistent* Peng-Robinson (*tc*-PR) EoS [60] of the efficient coupling of such a CEoS with such an α-function. For a pure component, the *volume-translated* Peng-Robinson EoS is:

$$P(T,v) = \frac{RT}{v-b} - \frac{a_c \times \alpha(T_r)}{(v+c)(v+b+2c)+(b+c)(v-b)}$$

with (4.4)

$$\begin{cases} \eta_c = \left[1+\sqrt[3]{4-2\sqrt{2}}+\sqrt[3]{4+2\sqrt{2}}\right]^{-1} \approx 0.25308 \\ a_c = \dfrac{40\eta_c+8}{49-37\eta_c}\dfrac{R^2T_{c,exp}^2}{P_{c,exp}} \approx 0.45724\dfrac{R^2T_{c,\exp}^2}{P_{c,\exp}} \\ b = \dfrac{\eta_c}{\eta_c+3}\dfrac{RT_{c,exp}}{P_{c,exp}} - c \approx 0.07780\dfrac{RT_{c,\exp}}{P_{c,\exp}} - c \end{cases}$$

$T_{c,exp}$ and $P_{c,exp}$ are the experimental critical temperature and critical pressure, respectively. The volume translation $c$ is selected in order to exactly reproduce the experimental value of the saturated liquid molar volume at a reduced temperature of 0.8. The Twu91 α-function, judged to exhibit the best compromise between complexity and flexibility, writes:

$$\alpha(T_r) = T_r^{N(M-1)} \exp\left[L\left(1-T_r^{MN}\right)\right] \quad (4.5)$$

$T_r$ is the reduced temperature and $L$, $M$ and $N$ are the three component-specific adjustable parameters.

### 4.3. Regression procedure of Twu α-function parameters over subcritical data

The three parameters of the Twu91 α-function were determined by minimizing an objective function which takes into account the deviations between calculated and experimental $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$ data. The considered experimental data are in fact pseudo-experimental data that are generated with the help of the DIPPR database that supplies temperature-dependent correlations for $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$. The following rules were applied for the generation of data:

1) 50 equidistant pseudo-experimental data points were generated on their temperature range of validity $[T_{min};T_{max}]$. In the case $T_{max}$ exceeds $0.98T_c$, it was decided to set: $T_{max} = 0.98T_c$.
2) At some occasions, the minimum of the temperature range of validity of $P^{sat}$ was modified in order to ensure that $P^{sat}(T_{min}) > 0.1bar$ (considering that most industrial processes operate at higher pressure values).
3) If, for a given property and a specific pure compound, the relative error reported by the DIPPR between correlated and experimental value was higher than 5 %, the property of the compound under consideration was no longer considered (pseudo-experimental data were not generated). In this paper, in particular, that was the case for the saturated-liquid heat capacities ($c_{P,L}^{sat}$) of Kr and Xe.

In the end, the objective function is:

$$OF = \overbrace{\frac{100}{50}\sum_{i=1}^{50}\left|\frac{P^{sat,DIPPR}\left(T_i^{P^{sat}}\right) - P^{sat,EoS}\left(T_i^{P^{sat}}\right)}{P^{sat,DIPPR}\left(T_i^{P^{sat}}\right)}\right|}^{MAPE\ on\ P^{sat}} + \overbrace{\frac{100}{50}\sum_{i=1}^{50}\left|\frac{\Delta_{vap}H^{DIPPR}\left(T_i^{\Delta_{vap}H}\right) - \Delta_{vap}H^{EoS}\left(T_i^{\Delta_{vap}H}\right)}{\Delta_{vap}H^{DIPPR}\left(T_i^{\Delta_{vap}H}\right)}\right|}^{MAPE\ on\ \Delta_{vap}H} + \underbrace{\frac{100}{50}\sum_{i=1}^{50}\left|\frac{c_{P,L}^{sat,DIPPR}\left(T_i^{c_{P,L}^{sat}}\right) - c_{P,L}^{sat,EoS}\left(T_i^{c_{P,L}^{sat}}\right)}{c_{P,L}^{sat,DIPPR}\left(T_i^{c_{P,L}^{sat}}\right)}\right|}_{MAPE\ on\ c_{P,L}^{sat}} \quad (4.6)$$

As previously mentioned, for each of the 9 pure compounds considered in this study (see next section to get more information on how they were selected), the 3 parameters of the Twu α-function were regressed twice. The first set of parameters was obtained without imposing any constraint during the fitting procedure. For such molecules the resulting α-function was found to be inconsistent and the corresponding parameters are reported in Table 4.1 in the columns headed "*Twu α-function parameters*". The second set of parameters results from a fitting procedure that ensures to get a consistent α-function i.e. an α-function that satisfies the constraints defined in Eq.

(4.3). To reach this goal, Le Guennec et al. [20] established that the 3 ($L$, $M$, $N$) parameters should verify:

$$\begin{cases} \delta < 0 \\ L\gamma > 0 \\ \gamma < 1-\delta \end{cases} \quad \text{or} \quad \begin{cases} \delta < 0 \\ L\gamma > 0 \\ \gamma < 1-2\delta+2\sqrt{\delta(\delta-1)} \\ 4Y^3+4ZX^3+27Z^2-18XYZ-X^2Y^2 > 0 \end{cases}$$

$$\text{with:} \begin{cases} \delta = N(M-1) \\ \gamma = MN \\ X = -3(\gamma+\delta-1) \\ Y = \gamma^2+3\delta\gamma-3\gamma+3\delta^2-6\delta+2 \\ Z = -\delta\left(\delta^2-3\delta+2\right) \end{cases} \tag{4.7}$$

Such consistent parameters are also recorded in Table 4.1 and representations of both consistent and inconsistent α-functions are visible in Table 4.1 for the nine selected compounds. It is noticeable that in the subcritical temperature range where experimental data were used to fit the parameters, the consistent and inconsistent α-functions are very close (they are more or less superimposed) regardless of the component. On the other hand, out of this domain, the two α-functions take totally different values and exhibit very different shapes. We can thus anticipate totally different calculated properties with each of these 2 $\alpha$-functions. At this step, it is legitimate to wonder what was the prize to pay to get a consistent $\alpha$-function. As highlighted in Table 4.1 (see column headed "*O.F.*"), and as expected, consistency is always counterbalanced by an increase of the objective function value defined by Eq. (4.6). Such an increase is however extremely moderate and Table 4.1 (see columns headed "*MAPE on* $P^{sat}$, $\Delta_{vap}H$, $c_{P,L}^{sat}$) stresses that the consistent parameters solely entail a lower accuracy of $c_{P,L}^{sat}$, leave almost unchanged the predictions of $\Delta_{vap}H$ and even improve the predictions of $P^{sat}$. It should be noticed that a modification of Twu α-function parameters modifies the value of the volume translation parameter $c$ (see Table 4.1 column headed "*Volume translation")*. In the next section, residual enthalpies ($h^{res}$) and residual constant-pressure heat capacities ($c_P^{res}$) will be calculated with the two sets of parameters. We thus believe it is important to recall that a volume translation has no influence on the calculated $c_P^{res}$ but impacts the calculated

$h^{res}$. For more information, the reader is referred to our recent papers [19, 20] and to the last section of this paper.

### 4.4. Selection of the 9 test-components and constitution of a database containing supercritical $h^{res}$ and $c_P^{res}$ pseudo-experimental data

Our goal is to demonstrate the imperative need to use a consistent $\alpha$-function for the prediction of pure-compound residual enthalpies and residual heat capacities in the supercritical domain. Since comprehensive sets of experimental enthalpy and heat-capacity data of pure species in the supercritical domain are very rare in open literature and commercial databases, it has been decided to generate pseudo-experimental data by using very accurate equations of state. With this respect, the NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP) contains multi-parameter EoS for 69 non quantic compounds. For these 69 molecules, a regression of the Twu $\alpha$-function parameters was performed over subcritical properties $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$ (generated using the DIPPR database by following the procedure presented in section 3) by minimizing the objective function defined by Eq. (4.6). The regression procedure converged to consistent parameters for 39 components (57 %) meaning that the sets of ($L$, $M$, $N$) parameters were inconsistent for 30 compounds. Among these 30 compounds, 12 have parameters that partially violate the consistency test recalled in Eq. (4.3). It is here meant that for these 12 components, the second derivative of the $\alpha$-function is, as expected, positive regardless of the temperature. On the other hand, we can find temperatures for which the third derivative is positive. All of the 18 remaining components have fully inconsistent ($L$, $M$, $N$) parameters (we can find temperatures for which $d^2\alpha/dT^2 < 0$ and simultaneously $d^3\alpha/dT^3 > 0$). Among them, only 9 have a reference EoS which can be applied up to a reduced temperature of at least 1.7 (EoS showing a lower upper bound of their temperature range of validity are considered as insufficient for this study which focuses on the prediction of supercritical properties). Our goal being to generate pseudo experimental data in the supercritical region, these 9 components were kept as test-components. These are: $CH_4$, $N_2$, CO, $CO_2$, Propane, Ar, $H_2S$, Kr and Xe. As previously explained, for each of these 9 pure components, a second regression procedure with addition of the constraints defined by Eq. (4.7) was performed in order to obtain a consistent set of ($L$, $M$, $N$) parameters.

For each pure compound, pseudo-experimental values of supercritical $h^{res}$ and $c_P^{res}$ were generated by applying the following rules:

1) In a first step, ten equidistant values of temperature were generated between $1.02 \times T_c$ and the maximum temperature at which the NIST EoS can be applied. For $N_2$, $CO_2$ and Ar this maximum temperature leads to calculate an almost null α-function on a large temperature range. As we intend to show the effect of the α-function consistency on the supercritical property prediction, this behavior is not desirable. For these three compounds, it was therefore decided to set the high temperature limit to the temperature at which the consistent α-function value reaches 0.01. The ten values of temperature used to generate pseudo-experimental data of residual enthalpies and residual heat capacities are represented, for each pure component, by vertical lines in Figure 4.1.
2) In a second step, at each of the ten temperatures defined in the first step, ten equidistant pressures were generated between $1.02 \times P_c$ and 600 bar. The upper pressure bound was fixed at 600 bar because most of the chemical processes have a working pressure below this value and because most of reference EoS from the NIST can be applied up to this pressure.

In the end, a total of 100 pseudo-experimental $h^{res}$ and 100 pseudo-experimental $c_P^{res}$ data were generated, for each of the 9 pure compounds in the supercritical region by using the very accurate NIST EoS. A comparison with two versions of the *volume-translated* Peng-Robinson cubic EoS, one using a consistent α-function and the other using an inconsistent α-function, can now be conducted.

### 4.5. Results

This paper aims at showing the effect of the α-function consistency on the quality of prediction of supercritical properties like $h^{res}$ and $c_P^{res}$. To reach this goal, for each of the 9 components previously selected, the mean absolute percentage error (MAPE) between calculated and pseudo-experimental data were calculated for both the residual enthalpies and residual heat capacities and for both the consistent and inconsistent α-function. As previously explained, a total of 200 supercritical experimental data points

(100 $h^{res,exp}$ and 100 $c_P^{res,exp}$) were considered for each component. Such MAPEs are defined as:

$$MAPE \text{ on } h^{res} = \sum_{i=1}^{100} \left| \frac{h^{res,\exp}(T,P) - h^{res,volume\ translated\ PR\ EoS}(T,P)}{h^{res,\exp}(T,P)} \right| \tag{4.8}$$

$$MAPE \text{ on } c_P^{res} = \sum_{i=1}^{100} \left| \frac{c_P^{res,\exp}(T,P) - c_P^{res,volume\ translated\ PR\ EoS}(T,P)}{c_P^{res,\exp}(T,P)} \right| \tag{4.9}$$

Before going further, we believe it is important to bring to the reader's attention that the experimental residual enthalpy may vanish. If this happens, the denominator in Eq. (4.8) becomes zero and for such a data point the corresponding absolute percentage error becomes infinite. As a consequence, and to avoid a bias in the MAPE calculated by Eq. (4.8), we decided not to consider the experimental data points for which the absolute percentage error was higher than $(MAPE + \sigma)$ where $\sigma$ is the standard deviation on the absolute percentage errors.

In a first step, to highlight the huge difference on the calculated $h^{res}$ and $c_P^{res}$ values when a consistent or an inconsistent $\alpha$-function is selected, it was decided to plot for each of the 9 test-components, the absolute percentage error (APE) between calculated and pseudo-experimental data for both the residual enthalpies (see Figure 4.2) and residual heat capacities (see Figure 4.3) and for both the consistent and inconsistent $\alpha$-function. On such plots is also visible the corresponding MAPEs. For a given data point, such APEs are defined as:

$$APE \text{ on } h^{res} = 100 \times \left| \frac{h^{res,\exp}(T,P) - h^{res,volume\ translated\ PR\ EoS}(T,P)}{h^{res,\exp}(T,P)} \right| \tag{4.10}$$

$$APE \text{ on } c_P^{res} = 100 \times \left| \frac{c_P^{res,\exp}(T,P) - c_P^{res,volume\ translated\ PR\ EoS}(T,P)}{c_P^{res,\exp}(T,P)} \right| \tag{4.11}$$

In a second step, in order to better assess the difference between the use of a consistent and an inconsistent $\alpha$-function we decided to define the so-called *degradation factor of a property X*, $\mathcal{DF}_X$, as the ratio of the MAPE obtained with an inconsistent $\alpha$-function by the MAPE obtained with a consistent $\alpha$-function. In other words:

$$\mathcal{DF}_{h^{res}} = \frac{MAPE \text{ on } h^{res} \text{ (inconsistent } \alpha\text{-function)}}{MAPE \text{ on } h^{res} \text{ (consistent } \alpha\text{-function)}} \tag{4.12}$$

$$\mathcal{DF}_{c_P^{res}} = \frac{MAPE \text{ on } c_P^{res} \text{ (inconsistent } \alpha\text{-function)}}{MAPE \text{ on } c_P^{res} \text{ (consistent } \alpha\text{-function)}} \tag{4.13}$$

If the degradation factor, $\mathcal{DF}_X$, is higher than unity then the consistent $\alpha$-function performs better than the inconsistent function in predicting property X, and vice-versa. For each of the nine pure compounds, MAPE on $h^{res}$ and MAPE on $c_P^{res}$ were calculated for both the consistent and inconsistent $\alpha$-function so that $\mathcal{DF}_{h^{res}}$ and $\mathcal{DF}_{c_P^{res}}$ could be estimated. All the numerical values are recorded in Table 4.1 (see the last 4 columns) and we can say that they speak for themselves. The smallest value of $\mathcal{DF}_{h^{res}}$ is 1.8 and it is obtained for $CO_2$. This means that the use of a consistent $\alpha$-function improves by about a factor 2 the average absolute relative deviation on the supercritical residual enthalpies. As a noticeable feature, $\mathcal{DF}_{h^{res}}$ can reach up to 20; this is the case for pure propane. In other words, an average deviation of 100 % on the residual enthalpies is obtained for propane with an inconsistent $\alpha$-function whereas such a deviation is reduced to 5 % with a properly parameterized $\alpha$-function (i.e. a consistent $\alpha$-function). On average, for the 9 test-components, $\mathcal{DF}_{h^{res}} = 10.1$. We thus can claim that the use of a consistent $\alpha$-function makes it possible to improve by approximatively a factor 10 the accuracy on the supercritical residual enthalpy calculations when the *volume-translated* Peng-Robinson CEoS is used. This is a really huge improvement.

Similar conclusions can be conducted for the heat capacities. The smallest value of $\mathcal{DF}_{c_P^{res}}$ is 1.2 and it is obtained for methane. On the other hand, the highest value, close to 25, is obtained for propane. For such a component, the average deviation on supercritical $c_P^{res}$ moves from 150 % to 6 % when an inconsistent $\alpha$-function is replaced by a consistent one. On average, $\mathcal{DF}_{c_P^{res}}$ is close to 8 highlighting once again the imperative need to use a consistent $\alpha$-function to predict pure-component supercritical properties. At this stage, it could be argued that the 9 test-components ($CH_4$, $N_2$, CO, $CO_2$, $C_3H_8$, Ar, $H_2S$, Kr and Xe) are all small, non-polar and non-associating. We however took into account all the compounds for which the

unconstrained fitting procedure lead to fully inconsistent ($L$, $M$, $N$) parameters and for which a reference EoS could be applied in the supercritical domain, i.e., up to a reduced of at least 1.7. In order to convince the reader that our conclusions apply to any component, representations of both consistent and inconsistent $\alpha$-functions for n-decane (a heavy molecule) and n-pentanol (a polar, associated molecule) are visible in Figure 4.4. Such a figure clearly highlights that the plotted $\alpha$-functions have exactly the same trends as the ones depicted in Figure 4.1. Although no pseudo-experimental data are available, we can thus expect similar conclusions than those drawn with the 9 test-components.

### 4.6. A few words on the effect of the volume translation on the calculated $h^{res}$ values

In this paper, all calculations were performed with the *volume-translated* Peng-Robinson EoS. As previously recalled, the volume translation has no influence on the calculated $c_P^{res}$ but impacts the calculated $h^{res}$. Following Jaubert et al. [19], we indeed can write:

$$h^{res,volume\ translated\ PR\ EoS}(T,P) = h^{res,original\ PR\ EoS}(T,P) - cP \qquad (4.14)$$

The goal of this paper is to demonstrate the imperative need to use a consistent $\alpha$-function for the prediction of pure-compound supercritical properties but since many $h^{res}$ calculations were performed in the supercritical region, we can also have a look at the effect of the volume translation on the calculated $h^{res}$ values. We indeed did not find papers addressing this issue in the open literature. By using the consistent Twu $\alpha$-function, it was decided to re-calculate all the $h^{res}$ values (typically 100 values for a given component) by setting $c = 0$. The results are recorded in Table 4.2 for the nine test-components. The temperature and pressure ranges at which calculations were performed are identical to those used to fill Table 4.1 (for each of the 10 ten selected temperatures, ten equidistant pressures were generated between $1.02 \times P_c$ and 600 bar).

In Table 4.2, for each component, the MAPEs between calculated and experimental $h^{res}$ are determined in 3 domains of temperature. In the first domain, the reduced temperature is between 1 and 2 ($1 < T_r < 2$). The second domain corresponds to the case where the reduced temperature is between 2 and 3 ($2 < T_r < 3$) and in the last domain, the reduced temperature is higher than 3. For some components, it was not

possible to perform calculations for reduced temperatures higher than 2 because we were outside the validity range of the reference EoS developed by NIST.

Table 4.2 clearly highlights that for reduced temperatures lower than 3, the volume translation has a strongly positive impact on the calculated $h^{res}$. Increasing again the temperature, the volume translation effect lowers and vanishes at a reduced temperature of about 3.5. At higher reduced temperatures, the volume translation has a negative influence on the calculated $h^{res}$. It is however well-established that the reduced temperature of most of the compounds involved in chemical processes are lower than 3. We can thus assert that the volume translation has two positive effects: it not only strongly increases the accuracy on the calculated liquid density but it also improves the accuracy of the energy balances.

### 4.7. Conclusion

This article leads to conclude about the imperative need to couple a consistent α-function with a cubic EoS so as to accurately reproduce experimental properties in the supercritical domain. This paper focused on supercritical residual enthalpies and heat capacities only but insofar as the two α-functions (consistent and inconsistent) take totally different values and exhibit completely different shapes in the supercritical region (see Figure 4.1), we believe that such conclusions can be extended to any other property. Starting from a database of 69 compounds it was shown that in half cases (43 %) an unconstrained regression of the α-function parameters over subcritical experimental data lead to an inconsistent α-function, demonstrating the necessity of adding mathematical constraints during the regression procedure.

Nine compounds for which the unconstrained regression of the parameters converged to a fully inconsistent α-function (i.e., we can find temperatures for which, inconsistently, $d^2\alpha / dT^2 < 0$ and simultaneously $d^3\alpha / dT^3 > 0$ ) were selected to study the effect of regressing parameters that guarantee the α-function consistency. In particular, deviations between experimental and calculated values of $h^{res}$ and $c_P^{res}$ for temperatures varying between $1.02 \times T_c$ and at least $1.7 \times T_c$ and pressures varying between $1.02 \times P_c$ and 600 bar were calculated with both a consistent and an inconsistent α-function. All calculations done, we can claim that the deviations observed with a CEoS embedding a consistent α-function to predict supercritical

properties will be around 9 times smaller than with a CEoS embedding an inconsistent one.

The imperative need, substantiated throughout this research, of associating to cubic EoS a consistent $\alpha$-function when predicting pure-compound supercritical properties also validates the extensive use of the Soave α-function [7,85], acknowledged to be consistent on a very large temperature range. This explains and justifies a posteriori its widespread application in chemical engineering thermodynamics (e.g. in the PPR78 model [23,24,73,74]), in petroleum applications and its ability to reproduce complex phase behaviors [96].

**Acknowledgment**

The French petroleum company TOTAL and more particularly Dr. Pierre Duchet–Suchaux, Dr. Laurent Avaullée and Freddy Garcia (experts in thermodynamics) are gratefully acknowledged for sponsoring this research.

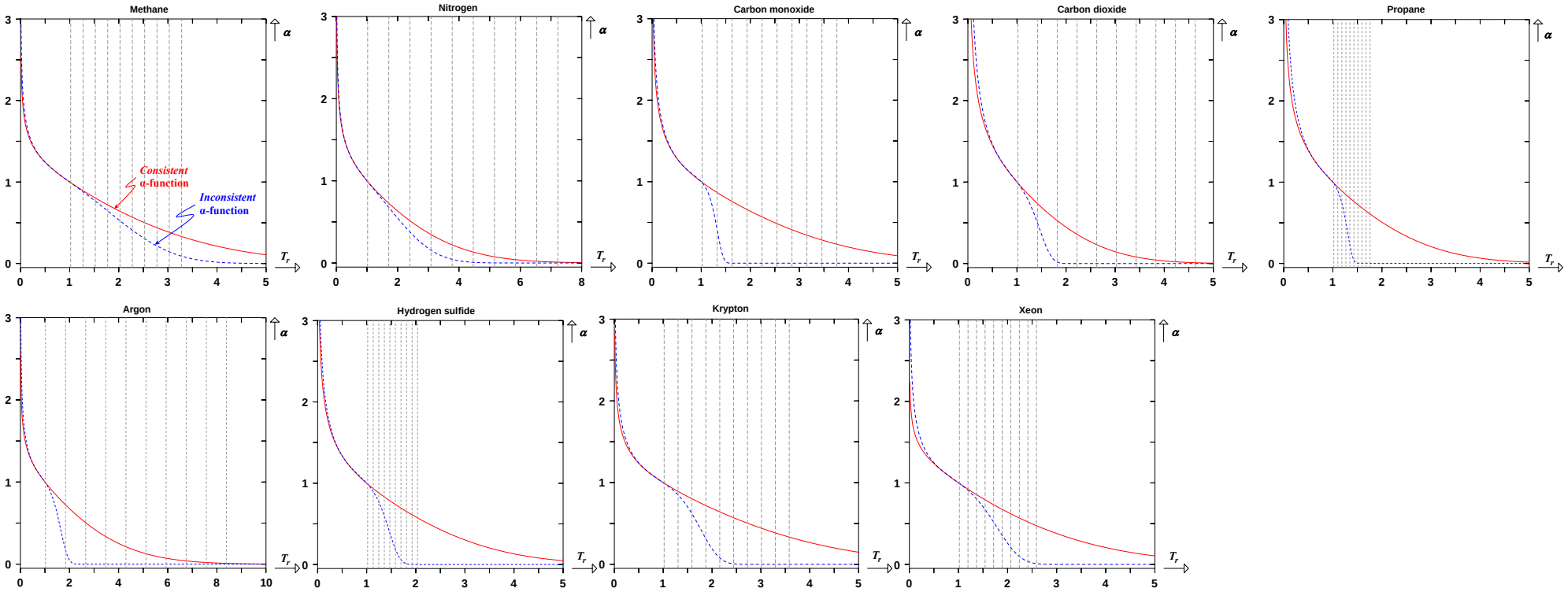



Figure 4.1. Change of Twu α-functions with respect to temperature for the 9 test-components selected in this paper. Solid line: consistent α-function, dashed line: inconsistent α-function. The 10 vertical lines identify the 10 temperatures at which pseudo experimental values of residual enthalpies and residual heat capacities were generated with NIST equations of state.

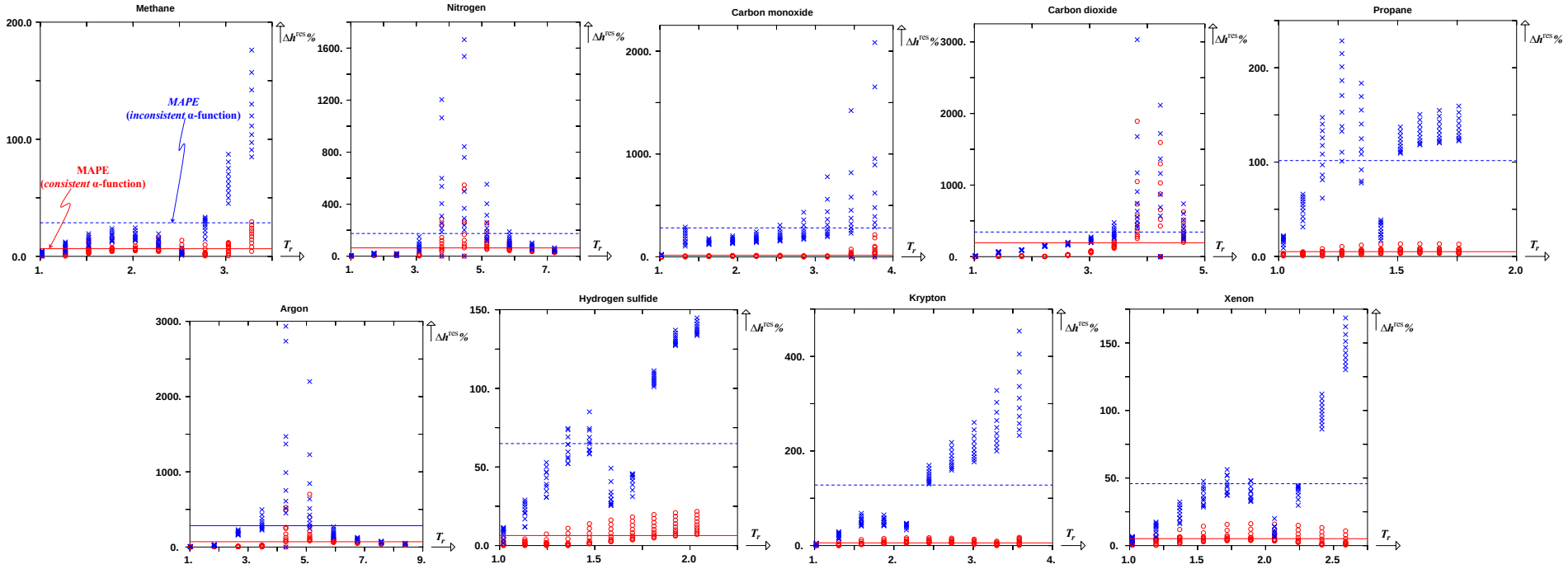



Figure 4.2. Absolute percentage error (APE) between calculated and pseudo-experimental residual enthalpy data [see Eq. (X.10)] for the 9 test-components selected in this paper. (○) consistent α-function, (□) inconsistent α-function. Solid line: MAPE on $h^{res}$ calculated with a consistent α-function, dashed line: MAPE on $h^{res}$ calculated with an inconsistent α-function.

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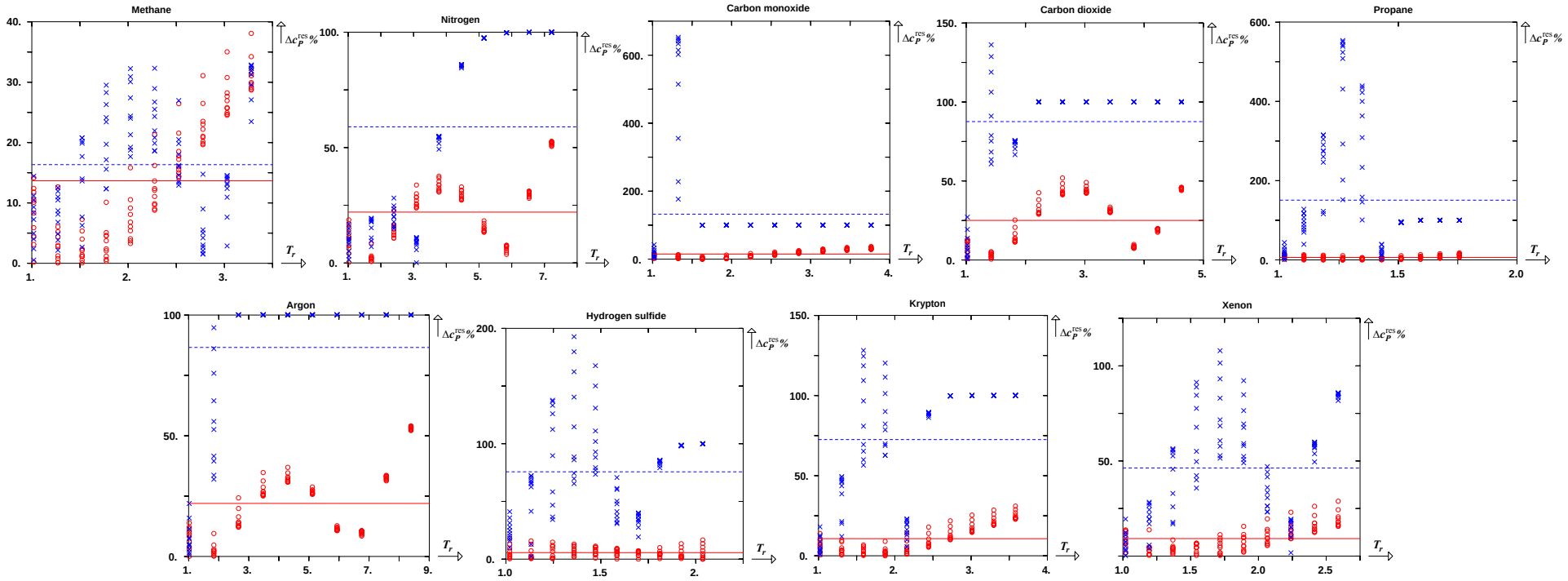



Figure 4.3. Absolute percentage error (APE) between calculated and pseudo-experimental residual heat capacity data [see Eq. (4.11)] for the 9 test-components selected in this paper. (○) consistent α-function, (×) inconsistent α-function. Solid line: MAPE on $c_P^{res}$ calculated with a consistent α-function, dashed line: MAPE on $c_P^{res}$ calculated with an inconsistent α-function.

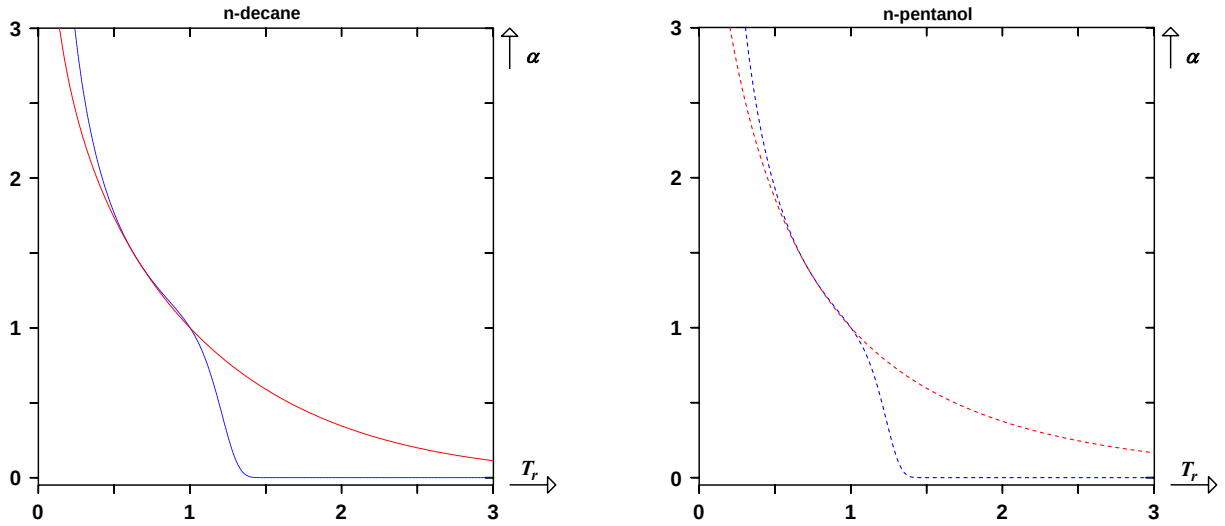



Figure 4.4. Change of Twu α-functions with respect to temperature for a heavy molecule (n-decane) and for a polar and associated molecule (n-pentanol).

| Solid line: consistent α-function, dashed line: inconsistent α-function. **Component** | **Twu α-function type** | **Twu α-function parameters** | | | **Volume translation c ($cm^3.mol^{-1}$)** | **MAPE[(a)] on** | | | **O.F.[(b)] [Eq. (4.6)]** | **MAPE[(a)] on** | | $\mathcal{DF}_{h^{res}}$ **[Eq. (4.12)]** | $\mathcal{DF}_{c_P^{res}}$ **[Eq. (4.13)]** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | **L** | **M** | **N** | | $P^{sat}$ **[Eq. (4.6)]** | $\Delta_{vap}H$ **[Eq. (4.6)]** | $c_{P,L}^{sat}$ **[Eq. (4.6)]** | | $h^{res}$ **[Eq. (4.8)]** | $c_P^{res}$ **[Eq. (4.9)]** | | |
| $CH_4$ | *Consistent* | 0.1471 | 0.9074 | 1.8253 | -3.56 | 0.31% | 1.73% | 7.17% | 9.21% | 6.54% | 13.67% | 4.4 | 1.2 |
| | *Inconsistent* | 0.0777 | 0.9288 | 3.0432 | -3.62 | 0.62% | 1.41% | 6.87% | 8.90% | 28.71% | 16.34% | | |
| $N_2$ | *Consistent* | 0.1240 | 0.8897 | 2.0138 | -3.64 | 0.26% | 1.44% | 3.26% | 4.96% | 62.94% | 22.06% | 2.8 | 2.7 |
| | *Inconsistent* | 0.0760 | 0.9144 | 2.9857 | -3.68 | 0.52% | 1.22% | 2.90% | 4.64% | 173.81% | 58.99% | | |
| CO | *Consistent* | 0.0983 | 0.8777 | 2.1568 | -3.68 | 0.32% | 1.27% | 10.22% | 11.81% | 16.10% | 15.46% | 17.5 | 8.6 |
| | *Inconsistent* | 0.0254 | 0.9740 | 12.6604 | -3.82 | 1.79% | 1.05% | 6.35% | 9.19% | 281.44% | 132.43% | | |
| $CO_2$ | *Consistent* | 0.1783 | 0.8590 | 2.4107 | -1.14 | 0.29% | 1.01% | 6.99% | 8.29% | 194.92% | 25.06% | 1.8 | 3.5 |
| | *Inconsistent* | 0.0406 | 0.9388 | 8.0397 | -1.17 | 0.99% | 0.91% | 1.83% | 3.73% | 342.59% | 87.55% | | |
| $C_3H_8$ | *Consistent* | 0.1596 | 0.8681 | 2.2820 | -3.89 | 0.60% | 1.17% | 12.22% | 13.99% | 5.09% | 6.23% | 20.0 | 24.2 |
| | *Inconsistent* | 0.0265 | 0.9675 | 13.7080 | -3.92 | 1.24% | 5.93% | 3.36% | 10.53% | 101.64% | 150.89% | | |
| Ar | *Consistent* | 0.1228 | 0.9045 | 1.8539 | -3.29 | 0.28% | 2.30% | 4.74% | 7.32% | 71.11% | 21.93% | 4.0 | 3.9 |
| | *Inconsistent* | 0.0272 | 0.9625 | 6.9719 | -3.34 | 0.69% | 1.36% | 3.06% | 5.11% | 284.60% | 86.55% | | |
| $H_2S$ | *Consistent* | 0.1120 | 0.8688 | 2.2735 | -2.51 | 0.58% | 1.44% | 9.75% | 11.77% | 6.40% | 5.64% | 10.1 | 13.4 |
| | *Inconsistent* | 0.0369 | 0.9569 | 8.4609 | -2.70 | 2.08% | 0.96% | 6.79% | 9.83% | 64.88% | 75.72% | | |
| Kr | *Consistent* | 0.1016 | 0.8956 | 1.9487 | -3.33 | 0.17% | 1.59% | N.A. | 1.76% | 6.03% | 10.70% | 21.3 | 6.8 |
| | *Inconsistent* | 0.0230 | 0.9559 | 6.3011 | -3.36 | 0.20% | 1.17% | N.A. | 1.37% | 128.04% | 72.52% | | |
| Xe | *Consistent* | 0.1795 | 0.9203 | 1.7006 | -3.77 | 0.16% | 1.66% | N.A. | 1.82% | 5.15% | 9.23% | 8.9 | 5.0 |
| | *Inconsistent* | 0.0346 | 0.9504 | 5.3899 | -3.78 | 0.46% | 1.12% | N.A. | 1.58% | 45.83% | 46.22% | | |
| **Mean value** | ***Consistent*** | | | | | **0.33%** | **1.51%** | **7.76%** | **7.88%** | **41.59%** | **14.44%** | **10.1** | **7.7** |
| | ***Inconsistent*** | | | | | **0.95%** | **1.68%** | **4.45%** | **6.10%** | **161.28%** | **80.80%** | | |

[(a)] MAPE = *mean absolute percentage error*. [(b)] O.F. = *objective function*.

Table 4.1. Calculated MAPE on $P^{sat}$, $\Delta_{vap}H$, $c_{P,L}^{sat}$ and supercritical $h^{res}$ and $c_P^{res}$ with the *volume-translated* Peng-Robinson EoS and either a consistent or an inconsistent Twu α-function.

| Component | PR EoS type | MAPE[(a)] on $h^{res}$ [Eq. (4.8)] | | |
|---|---|---|---|---|
| | | $1 < T_r < 2$ | $2 < T_r < 3$ | $T_r > 3$ |
| $CH_4$ | *translated* | 4.3% | 5.8% | 12.3% |
| | *non-translated* | 7.4% | 13.7% | 5.8% |
| $N_2$ | *translated* | 4.4% | 8.0% | 88.2% |
| | *non-translated* | 9.1% | 20.3% | 44.5% |
| CO | *translated* | 5.0% | 7.5% | 41.1% |
| | *non-translated* | 10.0% | 22.4% | 23.6% |
| $CO_2$ | *translated* | 5.6% | 13.7% | 392.8% |
| | *non-translated* | 6.4% | 11.7% | 369.7% |
| $C_3H_8$ | *translated* | 5.1% | - | - |
| | *non-translated* | 6.7% | - | - |
| Ar | *translated* | 4.0% | 6.7% | 99.9% |
| | *non-translated* | 7.8% | 19.0% | 44.5% |
| $H_2S$ | *translated* | 5.6% | 13.2% | - |
| | *non-translated* | 7.0% | 16.4% | - |
| Kr | *translated* | 3.9% | 8.8% | 6.1% |
| | *non-translated* | 6.8% | 16.6% | 19.3% |
| Xe | *translated* | 5.1% | 5.2% | - |
| | *non-translated* | 7.6% | 10.6% | - |
| **Mean value** | ***translated*** | **4.8%** | **8.6%** | **106.8%** |
| | ***non-translated*** | **7.6%** | **16.3%** | **84.6%** |

[(a)] MAPE = *mean absolute percentage error*.

Table 4.2. Calculated MAPE on $h^{res}$ with the PR EoS. Effect of the volume translation.

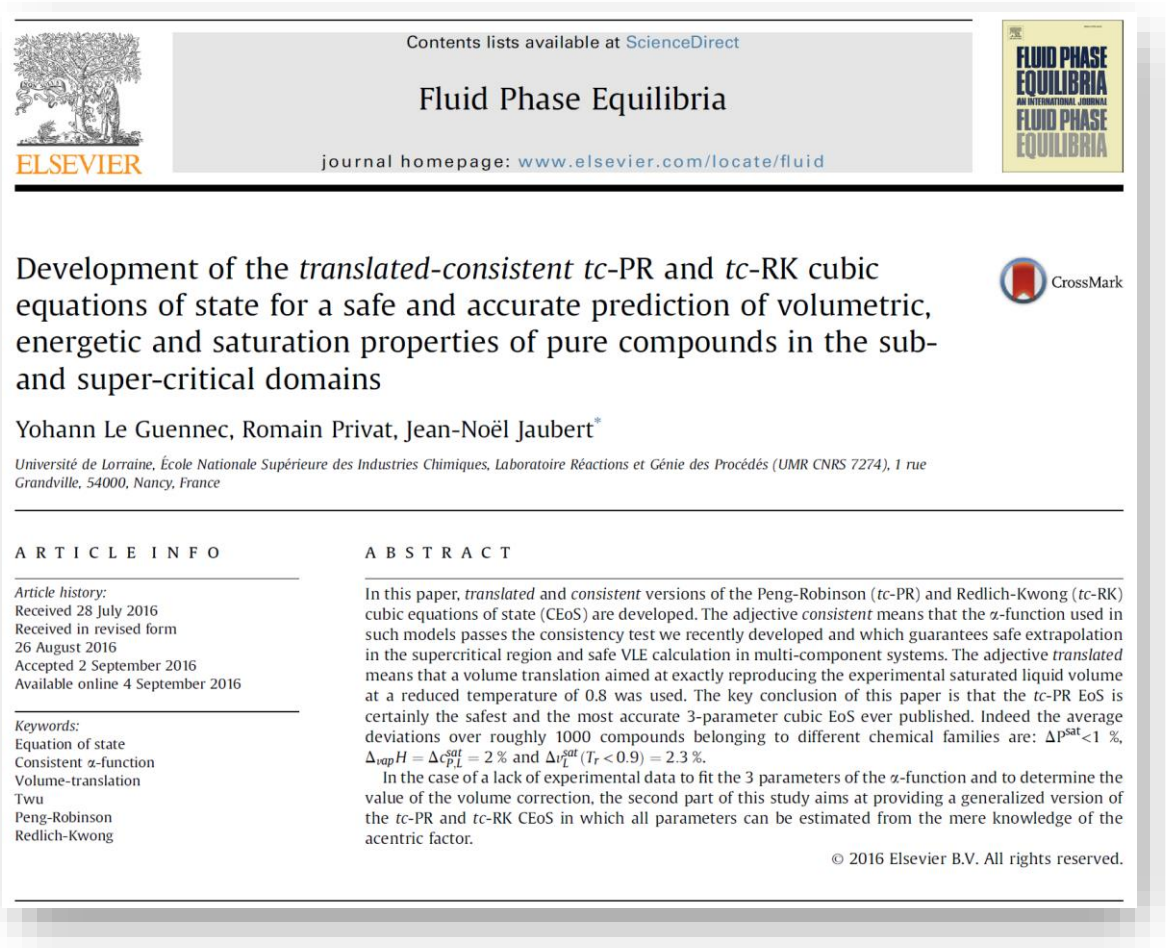
# Chapitre 5. Article "Development of the *translated-consistent* *tc*-PR and *tc*-RK cubic equations of state for a safe and accurate prediction of volumetric, energetic and saturation properties of pure compounds in the sub- and super-critical domains"

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Development of the *translated-consistent* *tc*-PR and *tc*-RK cubic equations of state for a safe and accurate prediction of volumetric, energetic and saturation properties of pure compounds in the sub- and super-critical domains

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ABSTRACT

In this paper, *translated* and *consistent* versions of the Peng-Robinson (*tc*-PR) and Redlich-Kwong (*tc*-RK) cubic equations of state (CEoS) are developed. The adjective *consistent* means that the α-function used in such models passes the consistency test we recently developed and which guarantees safe extrapolation in the supercritical region and safe VLE calculation in multi-component systems. The adjective *translated* means that a volume translation aimed at exactly reproducing the experimental saturated liquid volume at a reduced temperature of 0.8 was used. The key conclusion of this paper is that the *tc*-PR EoS is certainly the safest and the most accurate 3-parameter cubic EoS ever published. Indeed the average deviations over roughly 1000 compounds belonging to different chemical families are: $\Delta P^{sat}<1$ %, $\Delta_{vap}H = \Delta c_{P,L}^{sat} = 2$ % and $\Delta v_L^{sat}(T_r < 0.9) = 2.3$ %.

In the case of a lack of experimental data to fit the 3 parameters of the α-function and to determine the value of the volume correction, the second part of this study aims at providing a generalized version of the *tc*-PR and *tc*-RK CEoS in which all parameters can be estimated from the mere knowledge of the acentric factor.

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**Highlights**

1) *Translated* and *consistent* versions of the PR and RK cubic EoS are developed.
2) *tc*-PR is certainly the safest and the most accurate cubic EoS ever published.
3) Average deviations on vapor pressures are lower than 1 %.
4) Average deviations on enthalpies and heat capacities are about 2 %.
5) Average deviations on saturated liquid volumes are about 2.3 %.

**Abstract**

In this paper, *translated* and *consistent* versions of the Peng-Robinson (*tc*-PR) and Redlich-Kwong (*tc*-RK) cubic equations of state (CEoS) are developed. The adjective *consistent* means that the $\alpha$-function used in such models passes the consistency test we recently developed and which guarantees safe extrapolation in the supercritical region and safe VLE calculation in multi-component systems. The adjective *translated* means that a volume translation aimed at exactly reproducing the experimental saturated liquid volume at a reduced temperature of 0.8 was used. The key conclusion of this paper is that the *tc*-PR EoS is certainly the safest and the most accurate 3-parameter cubic EoS ever published. Indeed the average deviations over roughly 1000 compounds belonging to different chemical families are: $\Delta P^{sat} < 1\,\%$, $\Delta_{vap} H = \Delta c_{P,L}^{sat} = 2\,\%$ and $\Delta v_L^{sat}(T_r < 0.9) = 2.3\,\%$.

In the case of a lack of experimental data to fit the 3 parameters of the $\alpha$-function and to determine the value of the volume correction, the second part of this study aims at providing a generalized version of the *tc*-PR and *tc*-RK CEoS in which all parameters can be estimated from the mere knowledge of the acentric factor.

**Keywords**

Equation of state; Consistent $\alpha$-function; Volume-translation; Twu; Peng-Robinson; Redlich-Kwong

## 5.1. Introduction

As recalled in one of our recent papers [20], numerous modifications to the Van der Waals cubic equation of state (CEoS) [1] have been presented over the years with the aim of representing with increasingly accuracy the properties of complex systems. Despite these modifications, the attractive and repulsive terms of CEoS are still expressed by introducing a parameter *a* which is a measure of the attractive forces between molecules and a parameter *b* which characterizes the size of the molecules. It results the general formulation of a 2-parameter CEoS:

$$P(T,v)=\frac{RT}{v-b}-\frac{a(T)}{(v-r_1 b)(v-r_2 b)} \tag{5.1}$$

where $r_1$ and $r_2$ are two universal constants which depend on the selected EoS. To make easy the application of the critical constraints, it is convenient to write:

$$a(T)=a_c\cdot\alpha(T) \tag{5.2}$$

i.e. to express the attractive term as the product of its value at the critical temperature ($a_c$) by the so-called alpha function. The paper by Le Guennec et al. [20] highlights that such $\alpha$-functions have a strong impact on the accuracy of CEoS and they consequently must be selected with caution. Not only are the properties of pure components in the supercritical region highly affected by the $\alpha$-function but also the vapor liquid equilibrium (VLE) calculation of multi-component systems. It is today acknowledged [20] that when applied to mixtures, the accuracy of CEoS is equally affected by the choice of the mixing rules and by the expression of the $\alpha$-function. A key point of the paper by Le Guennec et al. [20] is the derivation of a list of constraints [see Eq. (5.3)] an $\alpha$-function should absolutely fulfill to guarantee safe predictions at all temperatures:

$$\text{For any reduced temperature } (T_r):\ \begin{cases} \alpha(T_r)\geq 0 & \text{and} \quad \alpha \text{ continuous} \\ \dfrac{d\alpha}{dT_r}(T_r)\leq 0 & \text{and} \quad \dfrac{d\alpha}{dT_r} \text{ continuous} \\ \dfrac{d^2\alpha}{dT_r^2}(T_r)\geq 0 & \text{and} \quad \dfrac{d^2\alpha}{dT_r^2} \text{ continuous} \\ \dfrac{d^3\alpha}{dT_r^3}(T_r)\leq 0 \end{cases} \tag{5.3}$$

This set of conditions has been called "consistency test for an α-function" by analogy to the consistency tests developed to certify the quality of experimental VLE data [105,106]. The paper by Le Guennec et al. [20] also tested whether 12 α-functions, generally available in process simulation software programs, were or not able to pass the proposed consistency test. They concluded that eight over twelve of these well-known α-functions (Soave 1972 [7], Soave 1984 [32], Gibbons-Laughton [87], Stryjek-Vera [29], Boston-Mathias [84], Mathias-Copeman [26], Mathias [90], Twu 1995 [36,37]) failed the proposed consistency test whatever the values of the parameters are. The four remaining α-functions (Trebble-Bishnoi [88], Melhem-Saini-Goodwin [89], Twu 1988 [35], Twu 1991 [19]) pass the test but only if constraints (sometimes drastic) are added to the parameters. Among them, the 3-parameter Twu91 α-function:

$$\alpha(T_r) = T_r^{N(M-1)} \exp\left[ L\left(1 - T_r^{MN}\right)\right] \tag{5.4}$$

was judged to exhibit the best compromise between complexity and flexibility. Twu took inspiration from the previous work of Heyen [34,82], the α-function of which can be recovered by setting M equal to 1. For this reason, the first part of this paper will be devoted to determine a consistent set of (L, M, N) parameters for hundreds of pure components and for both the Peng-Robinson (PR) [8] and the Redlich-Kwong (RK) [6] equations of state which are still both commonly used in process simulation software programs. A *consistent* set means a triplet of parameters ensuring that the α-function is consistent i.e. it satisfies the constraints of Eq. (5.3). Following the procedure proposed by Privat et al. [18], the parameters of the α-function will be determined by minimizing an objective function which takes into account the deviations between calculated and experimental vapor pressures $\left(P^{sat}\right)$, enthalpies of vaporization $\left(\Delta_{vap}H\right)$ and saturated liquid heat capacities $\left(c_{P,L}^{sat}\right)$. In order such consistent CEoS can be used with pure components for which no experimental data is available, a generalized and consistent form of the Twu α-function will be developed in a second step.

It is also well acknowledged that the coupling of the most flexible α-function with any cubic EoS will provide inaccurate liquid densities. Such a property is however extremely important not only in the petroleum industry where the densities of crude oils have to be accurately predicted but also when transport properties calculations are required. Indeed, viscosity and surface tension calculations [107,108] require molar

volumes of the liquid phase as an input parameter. One method to overcome this shortcoming is the so-called volume translation proposed by Péneloux et al. [39] in 1982. For a given component, the saturated-liquid volume calculated at a given temperature is usually notably different from the experimental value but the difference between the calculated and the experimental volume is approximately constant when varying the temperature out of the critical region. Consequently, a temperature-independent volume translation (all the calculated molar volumes are translated by a constant amount) significantly improves the description of the saturated liquid densities as long as the reduced temperature $\left(T_r = T/T_c\right)$ remains lower than 0.9. Moreover, as recently established by Jaubert et al. [40], a temperature-independent volume translation leaves unaffected the calculated vapor pressures, enthalpies of vaporization and saturated liquid heat capacities (the numerical values returned by the translated and untranslated EoS are exactly the same). It is thus clear that the problem of reproducing $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$ data by adjusting the 3 parameters of the $\alpha$-function can be uncoupled from the problem of reproducing experimental liquid-density data. This is why, a section of this paper will be devoted at determining the volume correction for hundreds of compounds and for the two well-established PR and RK EoS. This parameter, noted *c* thereafter, is selected in order to exactly reproduce the experimental saturated liquid volume at a reduced temperature of 0.8 [$v_{L,\text{exp}}^{sat}\left(T_r = 0.8\right)$], that is:

$$c = v_L^{sat,\text{u}-CEoS}\left(T_r = 0.8\right) - v_{L,\text{exp}}^{sat}\left(T_r = 0.8\right) \tag{5.5}$$

where $v_L^{sat,\text{u}-CEoS}\left(T_r = 0.8\right)$ is the molar volume calculated with the original (*untranslated*) CEoS at $T_r = 0.8$.

The coupling of the optimal *c* parameter to the optimal set of L, M, N parameters, makes it possible to define *translated* and *consistent* versions of the PR and RK EoS that we decided to note *tc*-PR and *tc*-RK.

They write:

$$\underline{\underline{\mathrm{tc}-PR:}}$$

$$P(T,v)=\frac{RT}{v-b}-\frac{a_c\cdot\alpha(T_r)}{(v+c)(v+b+2c)+(b+c)(v-b)}$$

with

$$\begin{cases}\alpha(T_r)=T_r^{N(M-1)}\exp\left[L\left(1-T_r^{MN}\right)\right]\\ c=v_L^{sat,\mathrm{u}-PR}(T_r=0.8)-v_{L,\mathrm{exp}}^{sat}(T_r=0.8)\\ \eta_c=\left[1+\sqrt[3]{4-2\sqrt{2}}+\sqrt[3]{4+2\sqrt{2}}\right]^{-1}\approx 0.25308\\ a_c=\dfrac{40\eta_c+8}{49-37\eta_c}\dfrac{R^2T_{c,\mathrm{exp}}^2}{P_{c,\mathrm{exp}}}\approx 0.45724\dfrac{R^2T_{c,\mathrm{exp}}^2}{P_{c,\mathrm{exp}}}\\ b=\dfrac{\eta_c}{\eta_c+3}\dfrac{RT_{c,\mathrm{exp}}}{P_{c,\mathrm{exp}}}-c\approx 0.07780\dfrac{RT_{c,\mathrm{exp}}}{P_{c,\mathrm{exp}}}-c\end{cases}$$

$$\underline{\underline{\mathrm{tc}-RK:}}$$

$$P(T,v)=\frac{RT}{v-b}-\frac{a_c\cdot\alpha(T)}{(v+c)(v+b+2c)}$$

with

$$\begin{cases}\alpha(T_r)=T_r^{N(M-1)}\exp\left[L\left(1-T_r^{MN}\right)\right]\\ c=v_L^{sat,\mathrm{u}-RK}(T_r=0.8)-v_{L,\mathrm{exp}}^{sat}(T_r=0.8)\\ a_c=\dfrac{1}{9\left(\sqrt[3]{2}-1\right)}\dfrac{R^2T_{c,\mathrm{exp}}^2}{P_{c,\mathrm{exp}}}\\ b=\dfrac{\sqrt[3]{2}-1}{3}\dfrac{RT_{c,\mathrm{exp}}}{P_{c,\mathrm{exp}}}-c\end{cases}$$

This paper will conclude that the *tc*-PR is certainly not only the safest but also the most accurate 3-parameter cubic EoS ever published. As a next step, the *tc*-PR EoS will be extended to mixtures through advanced mixing rules which combine the PR EoS with the residual part of the Wilson activity coefficient model. Working on various binary systems ($CO_2$/Ar, $CO_2$/$N_2$, $CO_2$/$O_2$), very encouraging results have already been achieved by Lasala et al. [97] with such mixing rules. The objective of the work presented in this paper i.e. the development of a safe, accurate and translated CEoS is similar to the one expressed, 25 years ago, by Magoulas and Tassios [45] during the development of the well-established *t-m*PR CEoS. Such a version of the PR EoS however suffers from some drawbacks: the *modified* $\alpha$-function is inconsistent and the temperature-dependent volume translation also leads to inconsistent results like the

crossing of isotherms in a (P,v) plane. We were thus convinced that it was time to develop the *tc*-PR CEoS.

### 5.2. Estimation of consistent Twu91 α-function parameters

The mathematical expression of the exponential, component-specific Twu91 α-function is recalled by Eq. (5.4). As explained by Le Guennec et al. [20], the set of (L, M, N) parameters can be labeled *consistent* if the resulting α-function satisfies the constraints defined by Eq. (5.3). To reach this goal, the 3 parameters must fulfill:

$$\begin{cases} \delta < 0 \\ L\gamma > 0 \\ \gamma < 1-\delta \end{cases} \quad \text{or} \quad \begin{cases} \delta < 0 \\ L\gamma > 0 \\ \gamma < 1-2\delta+2\sqrt{\delta(\delta-1)} \\ 4Y^3+4ZX^3+27Z^2-18XYZ-X^2Y^2 > 0 \end{cases}$$

$$\text{with: } \begin{cases} \delta = N(M-1) \\ \gamma = MN \\ X = -3(\gamma+\delta-1) \\ Y = \gamma^2+3\delta\gamma-3\gamma+3\delta^2-6\delta+2 \\ Z = -\delta\left(\delta^2-3\delta+2\right) \end{cases} \tag{5.6}$$

At this step, we want to emphasize that many triplets of (L, M, N) parameters either published by Twu himself [19], by Privat et al. [18] or by Gmehling and coworkers [109,110] during the development of the VTPR universal group contribution EoS do not satisfy such constraints and we strongly advise against their use.

Parameters of α-functions are often fitted to vapor pressure data only; we however do not recommend this practice because it may lead to parameters unsuitable for reproducing heats of vaporization or heat capacities. The reason is that a vapor pressure calculation only involves the α-function itself whereas enthalpy and heat-capacity calculations involve also the first and second derivatives of the α-function respectively. In addition, it has been showed [20] that the use of $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$ data to determine α-function parameters dramatically improves the extrapolability of the EoS in the supercritical domain.

### 5.2.1. Constitution of a pure-compound database

Following the procedure proposed by Privat et al. [18], the consistent parameters of the Twu91 $\alpha$-function were determined by minimizing an objective function which takes into account the deviations between calculated and experimental $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$. The considered experimental data are in fact pseudo-experimental data that are generated with the help of the DIPPR database which provides temperature-dependent correlations for $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$. We decided not to include speeds of sound data in the regression procedure because this property is a function of the isothermal compressibility coefficient which cannot be accurately calculated by any CEoS [40] on a large temperature range.

It is worth noting that the use of a CEoS requires the knowledge of the critical temperature ($T_c$), the critical pressure ($P_c$) and the acentric factor ($\omega$). For each compound and each T-dependent property among $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$, the DIPPR provides a temperature range of validity and a mean relative error between correlated and experimental values. Among the 2130 molecules available in the DIPPR database, only 1197 have:

- the three experimental constants $T_c$, $P_c$ and $\omega$ simultaneously reported,

- and at least one out of the three temperature-dependent properties $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$ estimable with an error lower or equal to 5%.

The following rules were applied for the generation of data:

1) 50 equidistant pseudo-experimental data points were generated on their temperature range of validity $[T_{\min};T_{\max}]$. In the case $T_{\max}$ exceeds $0.98T_c$, it is decided to set: $T_{\max}=0.98T_c$.
2) At some occasions, the minimum of the temperature range of validity of $P^{sat}$ was modified in order to ensure that $P^{sat}(T_{\min})>0.1\,bar$ (considering that most industrial processes operate at higher values of pressure).
3) If for a given property and a given pure compound, the relative error reported by the DIPPR between correlated and experimental value was higher than 5%,

the property of the compound under consideration was no longer considered (pseudo-experimental data were not generated).

4) The properties of some compounds, especially metals or molecules with a negative acentric factor cannot be estimated by a cubic EoS since they do not obey the 3-parameter corresponding states theorem. These 81 molecules were thus removed from our database which at the end contained 1116 compounds. Among the molecules having a negative acentric factor, helium-4, hydrogen and neon were maintained in the final database due to their interest in many industrial applications (see the Supplementary Material section for the whole listing of the 1116 compounds).

After applying these rules, there are 845 compounds (over 1116) for which only one or two out of the three temperature-dependent properties of interest ($P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$) can be accurately estimated (i.e., for which the errors associated to the DIPPR correlations $P^{sat}(T)$, $\Delta_{vap}H(T)$ and $c_{P,L}^{sat}(T)$ are below 5%). The number of compounds for which $P^{sat}$, $\Delta_{vap}H$ or $c_{P,L}^{sat}$ were estimated is reported in Table 5.1.

| Property | Number of compounds for which the property can be accurately generated |
|---|---|
| $P^{sat}$ | 980 |
| $\Delta_{vap}H$ | 805 |
| $c_{P,L}^{sat}$ | 529 |

Table 5.1. Number of compounds for which the properties can be estimated by a DIPPR correlation with an error lower than 5%.

16 families (alkanes, alkenes, alkynes ...) of chemicals were defined. We here want to analyze if the different families have similar occurrences in the complete DIPPR database that contains 2130 compounds and in the sub-database used to fit the Twu91 parameters containing 1116 compounds. For both databases, the numbers of chemical compounds per chemical family are represented in Figure 5.1 whereas relative abundances are reported in Figure 5.2. Note that the proportion of non-associating compounds (alkanes, alkenes, aromatics) increases when passing from the complete database to the sub-database and conversely, the proportion of associating compounds (acids, alcohols...) decreases. Meanwhile, the occurrences of some chemical families such as the aromatics and nitrogen compounds are maintained almost constant in the

two different databases. Therefore, it is concluded that, except for the associating compounds, the final database is representative of the diversity of the chemical compounds that can be found in the complete DIPPR database.

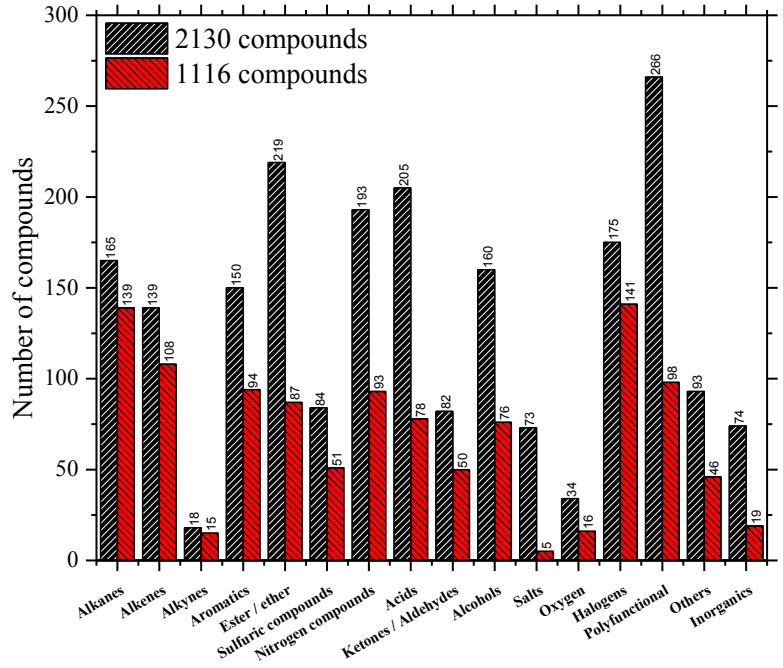



Figure 5.1. Number of compounds in each chemical family for the two different databases.

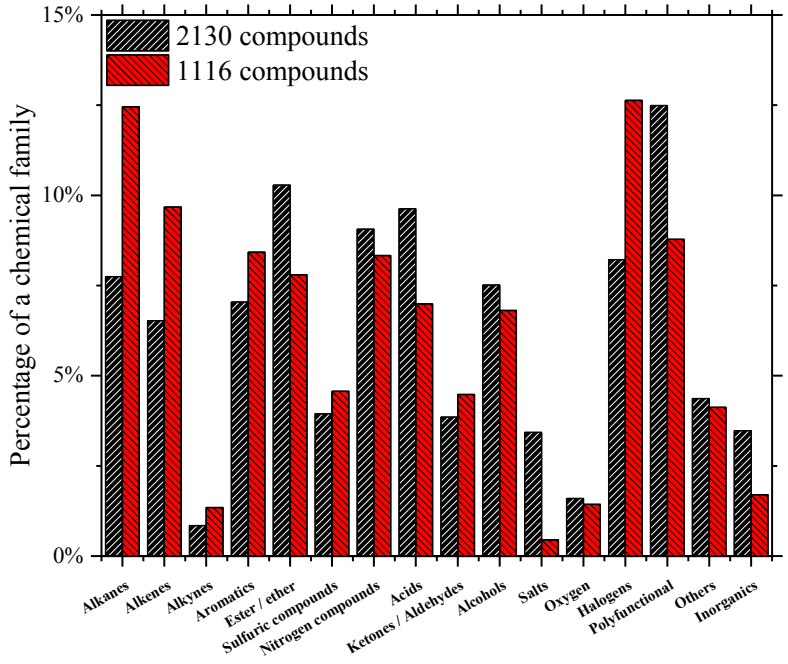



Figure 5.2. Percentage of a given chemical family in a given database.

### 5.2.2. Objective function used in the minimization procedure aimed at identifying optimal (L, M, N) sets

For each component, among the 1116 of our database, the 3 Twu91 $\alpha$-function parameters are those which minimize the objective function depicted in Eq. (5.7). In order to get consistent parameters, the fitting procedure was conducted by imposing the mathematical constraints recalled in Eq. (5.6).

$$OF_{\alpha} = \overbrace{\frac{100}{50}\sum_{i=1}^{50}\left|\frac{P^{sat,DIPPR}\left(T_i^{P^{sat}}\right)-P^{sat,EoS}\left(T_i^{P^{sat}}\right)}{P^{sat,DIPPR}\left(T_i^{P^{sat}}\right)}\right|}^{MAPE\,P^{sat}} + \overbrace{\frac{100}{50}\sum_{i=1}^{50}\left|\frac{\Delta_{vap}H^{DIPPR}\left(T_i^{\Delta_{vap}H}\right)-\Delta_{vap}H^{EoS}\left(T_i^{\Delta_{vap}H}\right)}{\Delta_{vap}H^{DIPPR}\left(T_i^{\Delta_{vap}H}\right)}\right|}^{MAPE\,\Delta_{vap}H} + w\underbrace{\frac{100}{50}\sum_{i=1}^{50}\left|\frac{c_{P,L}^{sat,DIPPR}\left(T_i^{c_{P,L}^{sat}}\right)-c_{P,L}^{sat,EoS}\left(T_i^{c_{P,L}^{sat}}\right)}{c_{P,L}^{sat,DIPPR}\left(T_i^{c_{P,L}^{sat}}\right)}\right|}_{MAPE\,c_{P,L}^{sat}} \quad (5.7)$$

In Eq. (5.7), the choice of the weighing factor w, is not simple. As an example, by setting w to 1, it was observed that for some molecules, the calculated deviation was exaggeratedly small for the heat capacity while inordinately high for the saturation pressure; in such cases, w was determined through a trial and error procedure in order the deviation on the heat capacity is twice as big as the deviation on the saturation pressure. The optimization procedure was performed using a SQP algorithm written in Fortran.

### 5.2.3. Results

Regressed parameters for each of the 1116 compounds considered in this study are reported in the Supplementary material section for both the PR and the RK EoS. Following Le Guennec et al. [20], quantum fluids He and $H_2$ were treated apart from other *classical* fluids. The Mean Absolute Percentage Error (MAPE) on $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$, as defined in Eq. (5.7), are reported in Table 5.2 for both the *consistent*-PR and the *consistent*-RK EoS.

| EoS | MAPE on $P^{sat}$ (980 compounds) | MAPE on $\Delta_{vap}H$ (805 compounds) | MAPE on $c_{P,L}^{sat}$ (529 compounds) |
|---|---|---|---|
| *consistent*-PR | 0.9 % | 2.0 % | 2.0 % |
| *consistent*-RK | 1.1 % | 2.1 % | 2.2 % |

Table 5.2. MAPE on $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$ as predicted by the consistent PR and RK EoS developed in this study.

As a first conclusion, we can state that the coupling of the PR or RK EoS with a consistent Twu91 $\alpha$-function leads to very accurate results: the MAPE on the vapor pressures for roughly 1000 compounds is only 1% whereas the deviations on $\Delta_{vap}H$ and $c_{P,L}^{sat}$ are about 2%. Such results are all the more impressive that our database includes polar and associating compounds. Table 5.2 also makes it possible to conclude that the PR and the RK EoS exhibit very similar accuracy.

It should be emphasized that these enthusiastic results on subcritical properties are obtained with $\alpha$-functions enforced to satisfy the constraints defined by Eq. (5.3). Therefore, with the parameters regressed in this paper, the corresponding Twu91 $\alpha$-functions are intended not only to efficiently represent the saturation properties, but also to safely extrapolate in the supercritical temperature domain. Figure 5.3 makes it possible to analyze the results for each chemical family. It can be observed that the predictions are homogeneous along chemical families. Unsurprisingly, the highest deviations are for the alcohols and the smallest ones for the alkanes.

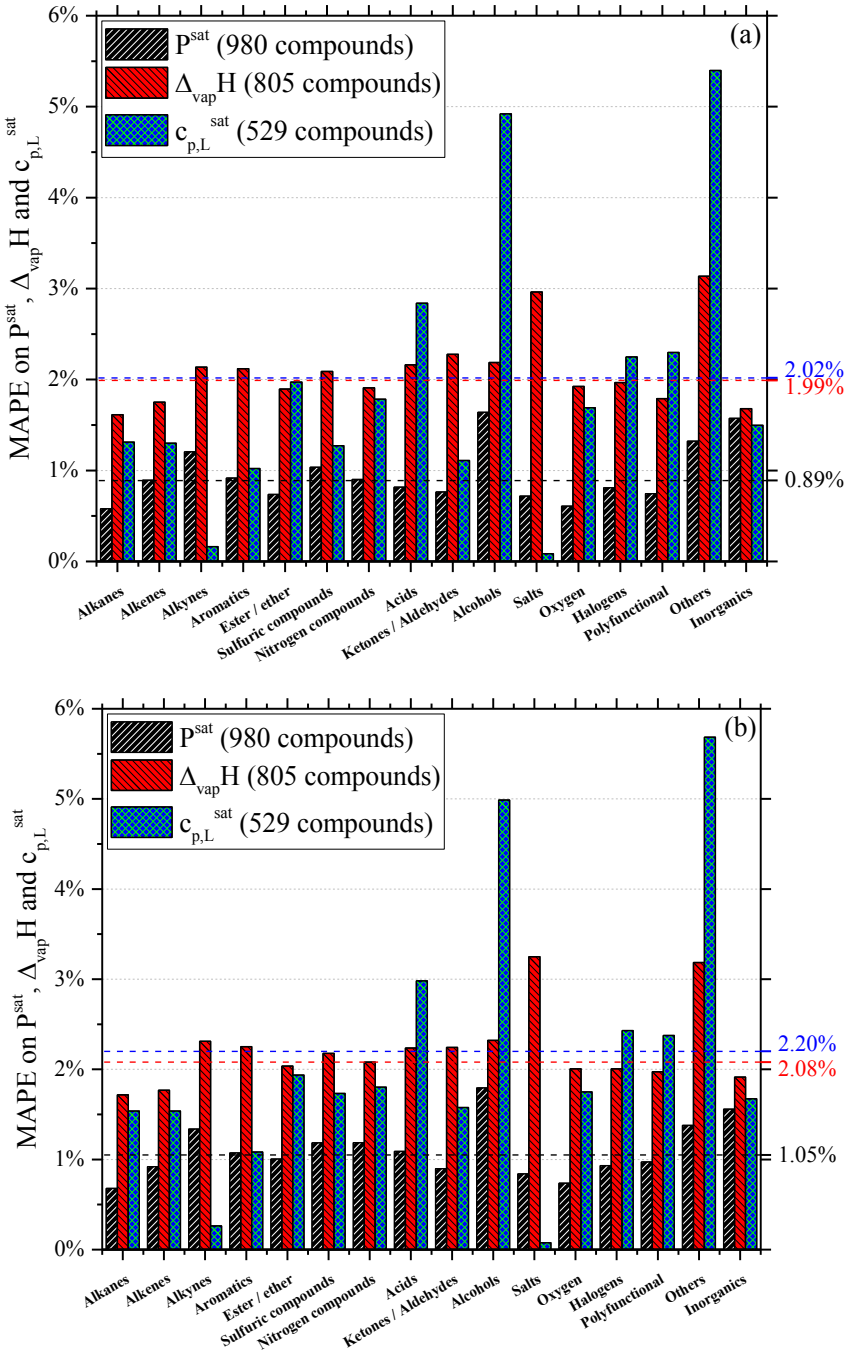



Figure 5.3. MAPE on $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$ for 16 chemical families. Calculations are performed for the database composed of 1116 compounds. (a): consistent-PR, (b): consistent-RK. Average errors for the whole set of compounds are reported for each property in the right axis.

### 5.3. Estimation of volume-translation parameters (c)

As recalled in the introduction, a temperature-independent volume translation significantly improves the description of the saturated liquid densities as long as $T_r < 0.9$ [40]. However regardless of the CEoS, this technique fails near the critical temperature ($0.9 < T_r < 1$) and until now, no consistent solution has been proposed to solve this problem. It is indeed well established that temperature-dependent volume translations, which could lead to accurate liquid densities all along the saturation line and in particular very near to the critical point, are thermodynamically inconsistent since they induce the crossing of isotherms in a (pressure, volume) plane as well as negative heat capacities [50,67,68]. It would be obviously unconceivable to develop inconsistent EoS and consequently, the proposed volume-translation parameter was selected constant.

#### 5.3.1. Choice of a reference temperature to determine the volume-translation parameter

In his paper, Péneloux [39] determined the volume translation parameter c in order to exactly reproduce the experimental saturated liquid volume at a reduced temperature of 0.7. The same choice was made by Gmehling and coworkers [111] during the development of the VTPR group-contribution EoS. In other words, they selected:

$$c = v_L^{sat,\mathrm{u-}CEoS}\left(T_r = 0.7\right) - v_{L,\mathrm{exp}}^{sat}\left(T_r = 0.7\right) \tag{5.8}$$

where $v_L^{sat,\mathrm{u-}CEoS}\left(T_r = 0.7\right)$ is the molar volume calculated with the original (*untranslated*) CEoS at $T_r = 0.7$.

However, neither the pioneering paper by Péneloux nor the paper by Gmehling justifies why a reduced temperature of 0.7 was selected in Eq. (5.8). Our first task was thus to determine the optimal reduced temperature to be used in Eq. (5.8). To do so, it was necessary to constitute a database containing (pseudo-)experimental liquid molar volume data for a large set of pure compounds. Among the 1116 compounds included in the database built in Section 5.2.1, the relative error reported by the DIPPR between correlation and experimental liquid densities was lower than 5% for only 997 chemicals. For each of these 997 compounds, the DIPPR correlation was used to generate 50 equidistant liquid molar volume data points between $T_{r,\mathrm{min}}$ and $T_r = 0.9$. Here $T_{r,\mathrm{min}}$ is the minimum reduced temperature at which $v_L^{sat}$ can be estimated by the

DIPPR correlation whereas $T_r = 0.9$ is, as previously explained, the highest temperature at which the volume-translation concept can be reasonably applied. For each compound, the optimal volume-translation parameter *c* was determined as the one minimizing the following objective function:

$$\begin{aligned} OF_c &= \frac{1}{50}\sum_{i=1}^{50}\left|\frac{v_L^{sat,DIPPR}\left(T_{r,i}\right)-v_L^{sat,t-CEoS}\left(T_{r,i}\right)}{v_L^{sat,DIPPR}\left(T_{r,i}\right)}\right| \\ &= \frac{1}{50}\sum_{i=1}^{50}\left|\frac{v_L^{sat,DIPPR}\left(T_{r,i}\right)-\left[v_L^{sat,\mathrm{u}-CEoS}\left(T_{r,i}\right)-c\right]}{v_L^{sat,DIPPR}\left(T_{r,i}\right)}\right| \end{aligned} \tag{5.9}$$

where $v_L^{sat,t-CEoS}$ is the liquid molar volume calculated from the translated CEoS.

Once the optimal *c* parameter is known, the corresponding optimal reduced temperature ($T_r^*$) is the only one that satisfies exactly the relation:

$$c = v_L^{sat,\mathrm{u}-CEoS}\left(T_r^*\right) - v_L^{sat,DIPPR}\left(T_r^*\right) \tag{5.10}$$

The mean $T_r^*$ value (over the 997 components) was found to be 0.77 for the RK EoS and 0.79 for the PR EoS with a standard deviation of about 0.03. For the sake of simplicity, it was thus decided to select $T_r^* = 0.8$ for both CEoS (RK and PR). In comparison to the previous work of Péneloux who selected $T_r^* = 0.7$, the chosen value ($T_r^* = 0.8$) leads to similar deviations on $v_L^{sat}$ in the low temperature range (below $T_r = 0.7$) but makes it possible to increases the accuracy of the model between $T_r = 0.7$ and $T_r = 0.8$.

To conclude, we advise to calculate the volume translation by:

$$c = v_L^{sat,\mathrm{u}-CEoS}\left(T_r = 0.8\right) - v_{L,\mathrm{exp}}^{sat}\left(T_r = 0.8\right) \tag{5.11}$$

Such a calculation requires the knowledge of the experimental liquid molar volume at $T_r = 0.8$. In the Supplementary material section, instead of reporting $v_{L,\mathrm{exp}}^{sat}\left(T_r = 0.8\right)$ for each of the 997 components of our database, it was preferred to report the corresponding Rackett compressibility factor ($z_{RA}$) appearing in the improvement [42] of the original Rackett equation [41] proposed by Spencer and Danner. The reason

of this choice is that the modified version of the Rackett equation is available in many process simulation software packages making it possible to easily estimate volume translations expressed using a Rackett-type formulation. For clarity, let us recall that the improved Rackett equation [42] writes:

$$v_L^{sat}\left(T_r\right)=\frac{RT_c}{P_c}z_{RA}^{\left[1+(1-T_r)^{2/7}\right]} \tag{5.12}$$

so that $v_L^{sat,EXP}\left(T_r=0.8\right)$ and $z_{RA}$ are linked by:

$$z_{RA}=\left[\frac{P_c\cdot v_L^{sat,EXP}\left(T_r=0.8\right)}{RT_c}\right]^{\left(\frac{1}{1+0.2^{2/7}}\right)} \tag{5.13}$$

Eq. (5.13) was used to fill out the $z_{RA}$ values given in the Supplementary material section. In the same table are also reported the volume translation parameters (*c*) for both the PR and the RK EoS estimated by Eq. (5.11) or equivalently by:

$$c=v_L^{sat,\mathrm{u}-CEoS}\left(T_r=0.8\right)-\frac{RT_c}{P_c}z_{RA}^{\left[1+0.2^{2/7}\right]} \tag{5.14}$$

It is observed that the *c* parameters to be used with the RK EoS are much higher than those suitable for the PR EoS.

### 5.3.2. Results

As was done in the previous section, for the 997 compounds included in our database, 50 equidistant liquid molar volume data points were generated between $T_{r,\min}$ (the minimum reduced temperature at which $v_L^{sat}$ can be estimated from the DIPPR database) and $T_r=0.9$. The MAPE on liquid molar volume, defined as:

$$MAPE=\frac{100}{50}\sum_{i=1}^{50}\left|\frac{v_L^{sat,DIPPR}\left(T_{r,i}\right)-v_L^{sat,CEoS}\left(T_{r,i}\right)}{v_L^{sat,DIPPR}\left(T_{r,i}\right)}\right| \tag{5.15}$$

are reported in Table 5.3 for both the PR and the RK EoS and for both the translated and the original (untranslated) EoS. In all cases, the consistent Twu91 $\alpha$-function developed in this study was used.

| EoS | MAPE on $v_L^{sat}$ (997 compounds) $T_r \leq 0.9$ | |
|---|---|---|
| | Untranslated EoS ($c = 0$) | Translated EoS [c given by Eq. (5.14)] |
| *consistent*-PR | 7.4 % | 2.3 % |
| *consistent*-RK | 17.3 % | 4.0 % |

Table 5.3. MAPE on $v_L^{sat}$ as predicted by the *consistent* PR and RK EoS developed in this study. Effect of the proposed volume translation.

Table 3 highlights the spectacular improvement on the liquid molar volume by using the volume-translation concept. For both CEoS, the ratio between the untranslated and translated MAPE is about 3. As previously explained, such a technique fails in the critical region explaining why in Table 5.3, the deviations are given in a temperature range where $T_r \leq 0.9$. To fairly discuss the accuracy of CEoS, it is thus necessary to give the deviation on the molar critical volume (generally the point where the deviation on the liquid molar volume is the highest). Such results are reported in Table 5.4.

| EoS | MAPE on the molar critical volume, $v_c$. (997 compounds) | |
|---|---|---|
| | Untranslated EoS ($c = 0$) | Translated EoS [c given by Eq. (5.14)] |
| *consistent*-PR | 20 % | 18 % |
| *consistent*-RK | 30 % | 23 % |

Table 5.4. MAPE on $v_c$ as predicted by the *consistent* PR and RK EoS developed in this study. Effect of the proposed volume translation.

As expected, Table 5.4 highlights that critical molar volume are positively impacted by the volume translation technique but not enough to provide a satisfactory representation of the experimental value. Indeed, as shown in Figure 5.4, for almost all chemical families, the MAPE remains above 15% for the PR CEoS and 20% for the RK CEoS. The other results, chemical family by chemical family, detailed in Figure 5.4 make it possible to conclude that homogeneous MAPEs are calculated for all chemical families when a translated CEoS is used. Acids, salts and inorganic compounds, although they show the highest MAPEs after application of the translation method, are greatly improved. Such results demonstrate the validity of the technique for all kind of compounds.

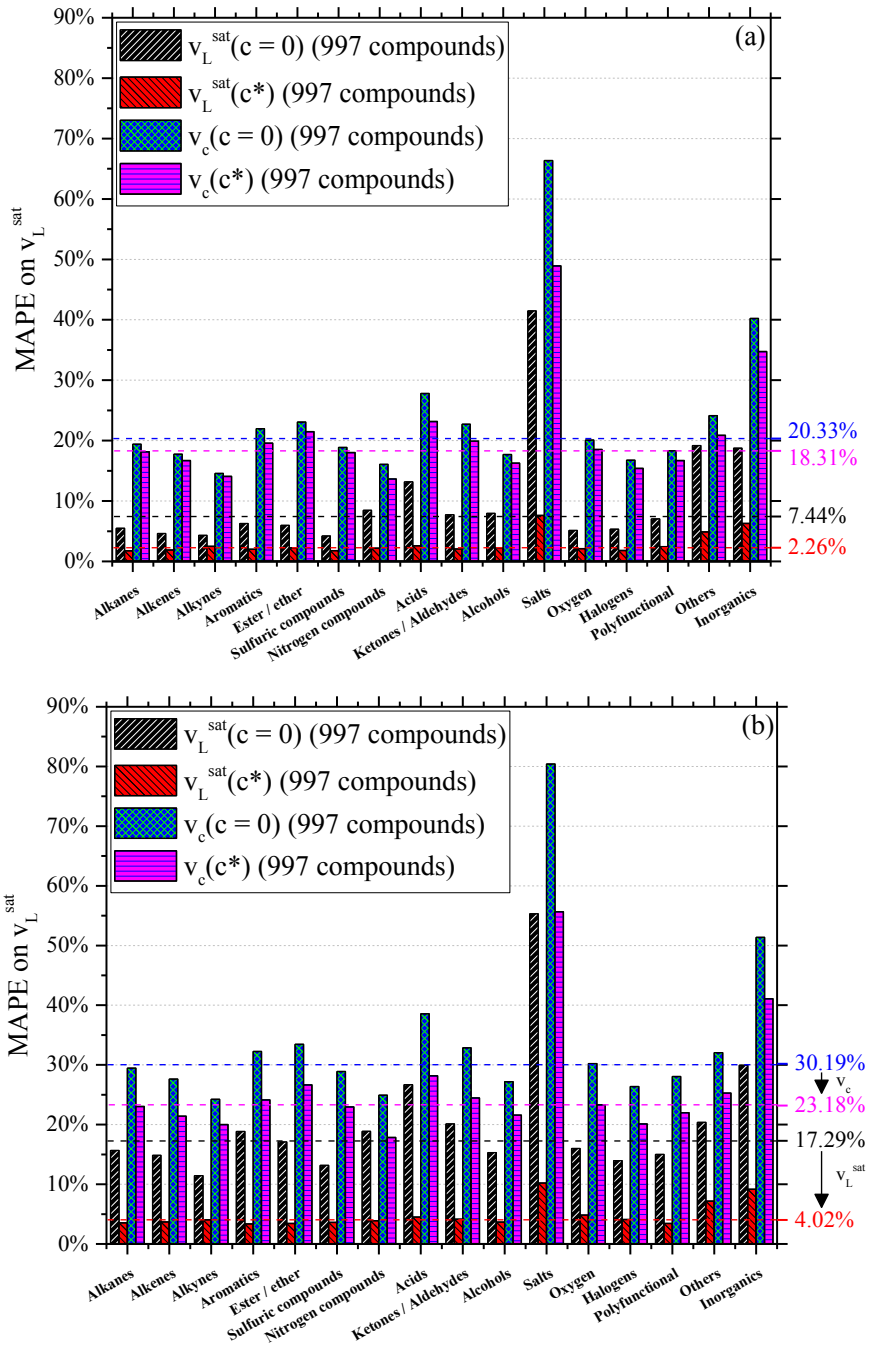



Figure 5.4. MAPE on $v_L^{sat}$ for 16 chemical families. Calculations are performed for a database containing 997 compounds. (a): *consistent*-PR, (b): *consistent*-RK. Average errors for the whole set of compounds are reported for each property in the right axis.

### 5.3.3. Conclusion on the *tc*-PR and *tc*-RK EoS.

The coupling of the consistent Twu91 $\alpha$-function developed in this study with a volume translation calculated in order to reproduce the liquid molar volume at $T_r = 0.8$ makes it possible to define the *translated-consistent tc*-PR and *tc*-RK CEoS, the mathematical expression of which are:

*tc*–PR:

$$P(T,v)=\frac{RT}{v-b}-\frac{a_c\cdot\alpha(T_r)}{(v+c)(v+b+2c)+(b+c)(v-b)}$$

with

$$\begin{cases}\alpha(T_r)=T_r^{N_{PR}(M_{PR}-1)}\exp\left[L_{PR}\left(1-T_r^{M_{PR}N_{PR}}\right)\right]\\ c=v_L^{sat,\mathrm{u}-PR}(T_r=0.8)-\dfrac{RT_{c,\exp}}{P_{c,\exp}}z_{RA}^{\left[1+0.2^{2/7}\right]}\\ \eta_c=\left[1+\sqrt[3]{4-2\sqrt{2}}+\sqrt[3]{4+2\sqrt{2}}\right]^{-1}\approx 0.25308\\ a_c=\dfrac{40\eta_c+8}{49-37\eta_c}\dfrac{R^2T_{c,\exp}^2}{P_{c,\exp}}\approx 0.45724\dfrac{R^2T_{c,\exp}^2}{P_{c,\exp}}\\ b=\dfrac{\eta_c}{\eta_c+3}\dfrac{RT_{c,\exp}}{P_{c,\exp}}-c\approx 0.07780\dfrac{RT_{c,\exp}}{P_{c,\exp}}-c\end{cases}\qquad(5.16)$$

*tc*–RK:

$$P(T,v)=\frac{RT}{v-b}-\frac{a_c\cdot\alpha(T)}{(v+c)(v+b+2c)}$$

with

$$\begin{cases}\alpha(T_r)=T_r^{N_{RK}(M_{RK}-1)}\exp\left[L_{RK}\left(1-T_r^{M_{RK}N_{RK}}\right)\right]\\ c=v_L^{sat,\mathrm{u}-RK}(T_r=0.8)-\dfrac{RT_{c,\exp}}{P_{c,\exp}}z_{RA}^{\left[1+0.2^{2/7}\right]}\\ a_c=\dfrac{1}{9\left(\sqrt[3]{2}-1\right)}\dfrac{R^2T_{c,\exp}^2}{P_{c,\exp}}\\ b=\dfrac{\sqrt[3]{2}-1}{3}\dfrac{RT_{c,\exp}}{P_{c,\exp}}-c\end{cases}\qquad(5.17)$$

The 8 parameters ( $T_{c,\exp}$ , $P_{c,\exp}$ , $L_{PR}$ , $M_{PR}$ , $N_{PR}$ , $L_{RK}$ , $M_{RK}$ and $N_{RK}$ ) are reported for 1116 pure chemicals in the Supplementary material section. Such a section also reports the Rackett compressibility factor ( $z_{RA}$ ) but for only 997 components.

The very accurate results obtained with these two *tc*-CEoS are graphically illustrated in Figure 5.5 and are summarized in Table 5.5. In this table, the MAPEs on the critical temperature and on the critical pressure, which are necessarily zero are reported in order to remember that such errors are not null with EoS that do not satisfy the critical constraints, like e.g. SAFT-type EoS [103]. A proper prediction of pure-component critical coordinates is however a prerequisite to accurately predict global phase

equilibrium diagrams (GPED) of binary systems [96]. In Figure 5.5, we deliberately selected a hydrocarbon (4-methyloctane), i.e. a non-polar and non-associating molecule and an alcohol (meta-cresol) i.e. a polar and associating molecule to highlight that similar deviations are obtained in both cases.

| EoS | MAPE on $P^{sat}$ (980 compounds) | MAPE on $\Delta_{vap}H$ (805 compounds) | MAPE on $c_{P,L}^{sat}$ (529 compounds) | MAPE on $v_L^{sat}$ (997 compounds) $(T_r \leq 0.9)$ | MAPE on $V_c$ (997 compounds) | MAPE on $P_c$ | MAPE on $T_c$ |
|---|---|---|---|---|---|---|---|
| *tc*-PR | 0.9 % | 2.0 % | 2.0 % | 2.3 % | 18 % | 0 % | 0 % |
| *tc*-RK | 1.1 % | 2.1 % | 2.2 % | 4.0 % | 23 % | 0 % | 0 % |

Table 5.5. MAPE on $P^{sat}$, $\Delta_{vap}H$, $c_{P,L}^{sat}$, $v_L^{sat}$, $V_c$, $T_c$ and $P_c$ as predicted by the *tc*-PR and *tc*-RK EoS developed in this study.

At this stage, it could be argued that such CEoS can only be used if sufficient experimental data are known in order to evaluate the parameters $L$, $M$, $N$ and $c$. Therefore, the second part of this article aims at providing a generalized version of the *tc*-PR and *tc*-RK CEoS in order such EoS could be applied to components not included in the DIPPR database or to what petroleum companies call “pseudo-components” (i.e., petroleum cuts).

| 4-methyloctane | m-cresol |
|---|---|

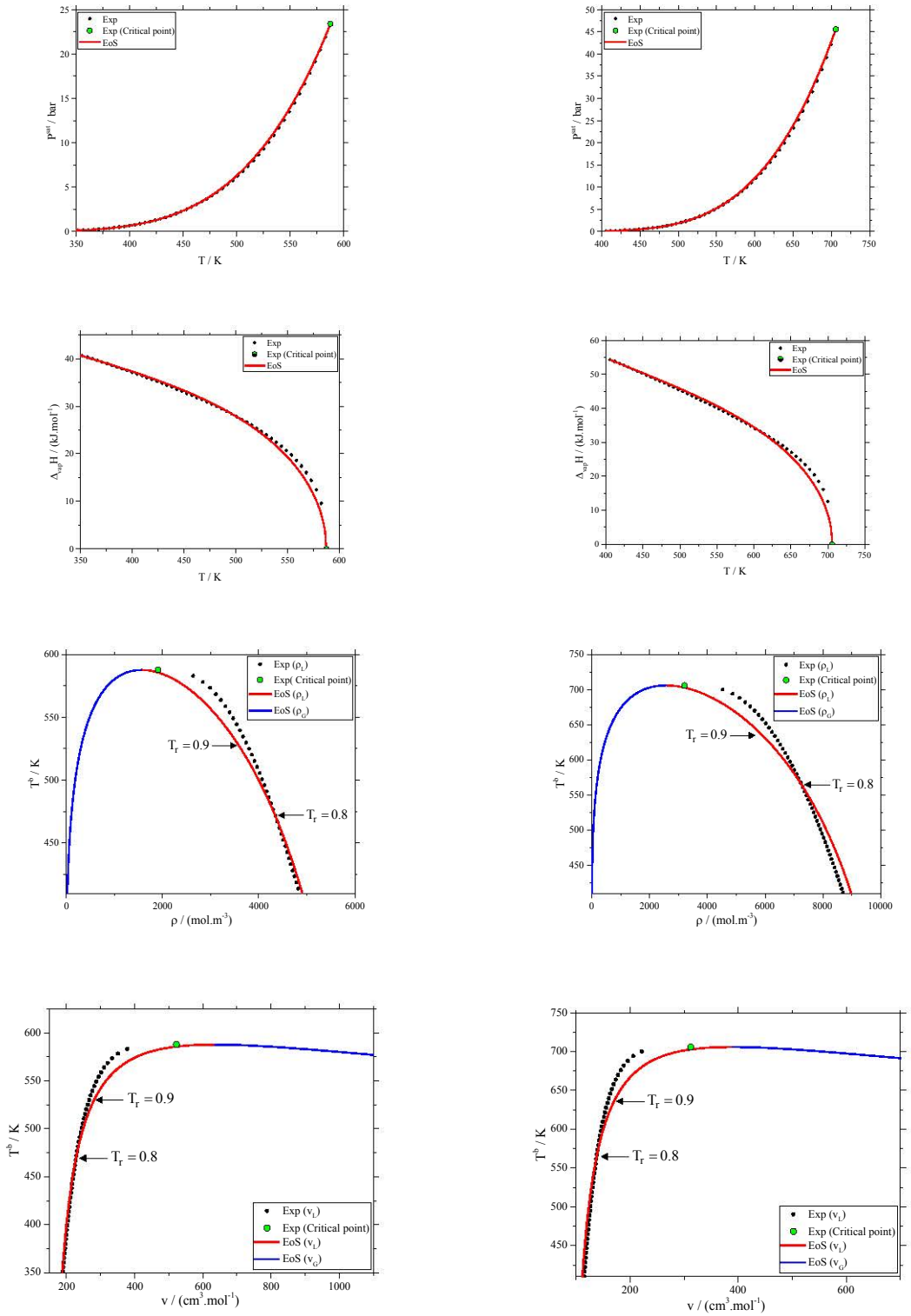



Figure 5.5. Vaporization curve, enthalpy of vaporization with respect to temperature, (temperature, molar density) plane and (temperature, molar volume) plane predicted by the *tc*-PR EoS for pure 4-methyloctane and pure m-cresol.

### 5.4. Toward a generalized CEoS

This section aims at developing a generalized formulation for a consistent Twu-type α-function and at explaining how the volume translation parameter *c* can possibly be generalized.

As discussed by Privat et al. [18], the three parameters L, M and N of the Twu91 α-function are correlated to each other. Consequently, many sets of totally different parameters that however lead to similar values of the objective function defined by Eq. (5.7) can be found. This problem can be solved by fixing one out of the three parameters. Following Twu et al. [35], it was decided to set parameter N to 2 i.e. to generalize the Twu88 α-function. With only 2 parameters, the Twu88 α-function is obviously less flexible than the Twu91 α-function and we can expect less accuracy in the prediction of thermodynamic properties of highly polar compounds. The following formulations which, like for the Soave α-function only require the knowledge of the acentric factor, will be used:

$$\begin{cases} \alpha(T_r) = T_r^{2(M-1)} \exp\left[ L\left(1 - T_r^{2M}\right)\right] \\ L(\omega) = L_1\omega^2 + L_2\omega + L_3 \\ M(\omega) = M_1\omega^2 + M_2\omega + M_3 \end{cases} \tag{5.18}$$

Following Le Guennec et al. [20], the following constraints must be imposed in order to get consistent Twu88 parameters:

$$\begin{cases} L(\omega)\,M(\omega) > 0 \\ M(\omega) < 0.8909 \end{cases} \tag{5.19}$$

#### 5.4.1. A generalized Twu88 α-function

In order to develop a generalized formulation with non-biased optimal parameters ($L_1$, $L_2$, $L_3$, $M_1$, $M_2$, $M_3$), it is essential to work with molecules such that their saturation properties ($P^{sat}$, $\Delta_{vap}H$, $c_{P,L}^{sat}$), their critical parameters ($T_c$, $P_c$) and their acentric factor ($\omega$) are all known with an error lower than 5%. Among the 1197 compounds for which $T_c$, $P_c$ and $\omega$ are reported in the DIPPR database, 261 of them show simultaneously accurate values for $T_c$, $P_c$ and $\omega$ and accurate correlations to estimate $P^{sat}$, $\Delta_{vap}H$ and $c_{P,L}^{sat}$.

Our first task was thus to determine for these 261 chemicals, L and M parameters by minimizing the objective function defined by Eq. (5.7). The obtained L and M parameters are plotted as a function of the acentric factor for 248 pure compounds in Figure 5.6 (13 molecules among the initial package of 261 did not follow the general trend observed for the other chemicals and were discarded).

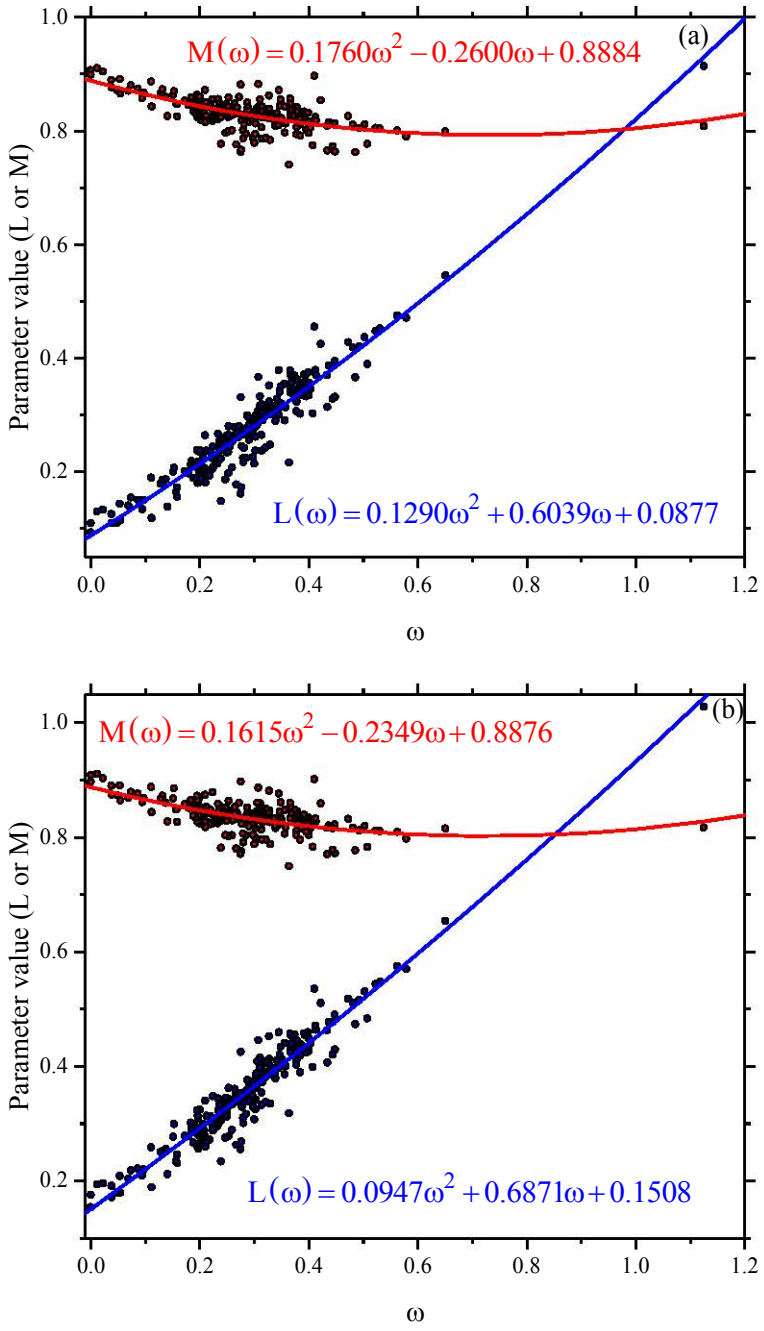



Figure 5.6. *L* and *M* parameters to be used with the generalized Twu88 α-function developed in this work. (a) PR CEoS (b) RK CEoS

The variations of *L* and *M* with respect to $\omega$ were correlated by second order polynomials for both the PR and the RK CEoS. The resulting expressions are:

$$\text{PR CEoS}: \begin{cases} L(\omega) = 0.1290\omega^2 + 0.6039\omega + 0.0877 \\ M(\omega) = 0.1760\omega^2 - 0.2600\omega + 0.8884 \end{cases} \quad (5.20)$$

$$\text{RK CEoS}: \begin{cases} L(\omega) = 0.0947\omega^2 + 0.6871\omega + 0.1508 \\ M(\omega) = 0.1615\omega^2 - 0.2349\omega + 0.8876 \end{cases} \quad (5.21)$$

Such correlations were established from a database in which the acentric factor of the molecules varied between 0 and 1.12. A mathematical study makes it however possible to conclude that such a generalized $\alpha$-function remains consistent (i.e. satisfies $LM > 0$ and $M < 0.8909$) as long as the acentric factor ranges between $-0.01$ and 1.50 (in fact 1.49 for the PR EoS and 1.47 for the RK EoS) what covers most of the possible values for this property. Such results can be graphically rediscovered in Figure 5.7 where stripped areas indicate inconsistent regions for parameters *L* and *M*. Moreover, it is possible to mathematically demonstrate that when $0.8909 < M < 1$, what corresponds to: $\begin{cases} -0.38 < \omega < -0.01 \\ 1.49 < \omega < 1.82 \end{cases}$ for the PR EoS and to $\begin{cases} -0.35 < \omega < -0.01 \\ 1.47 < \omega < 1.83 \end{cases}$ for the RK EoS, (see Figure 5.7), although non-consistent, the $\alpha$-function remains decreasing and can thus be safely used [20] in the subcritical region.

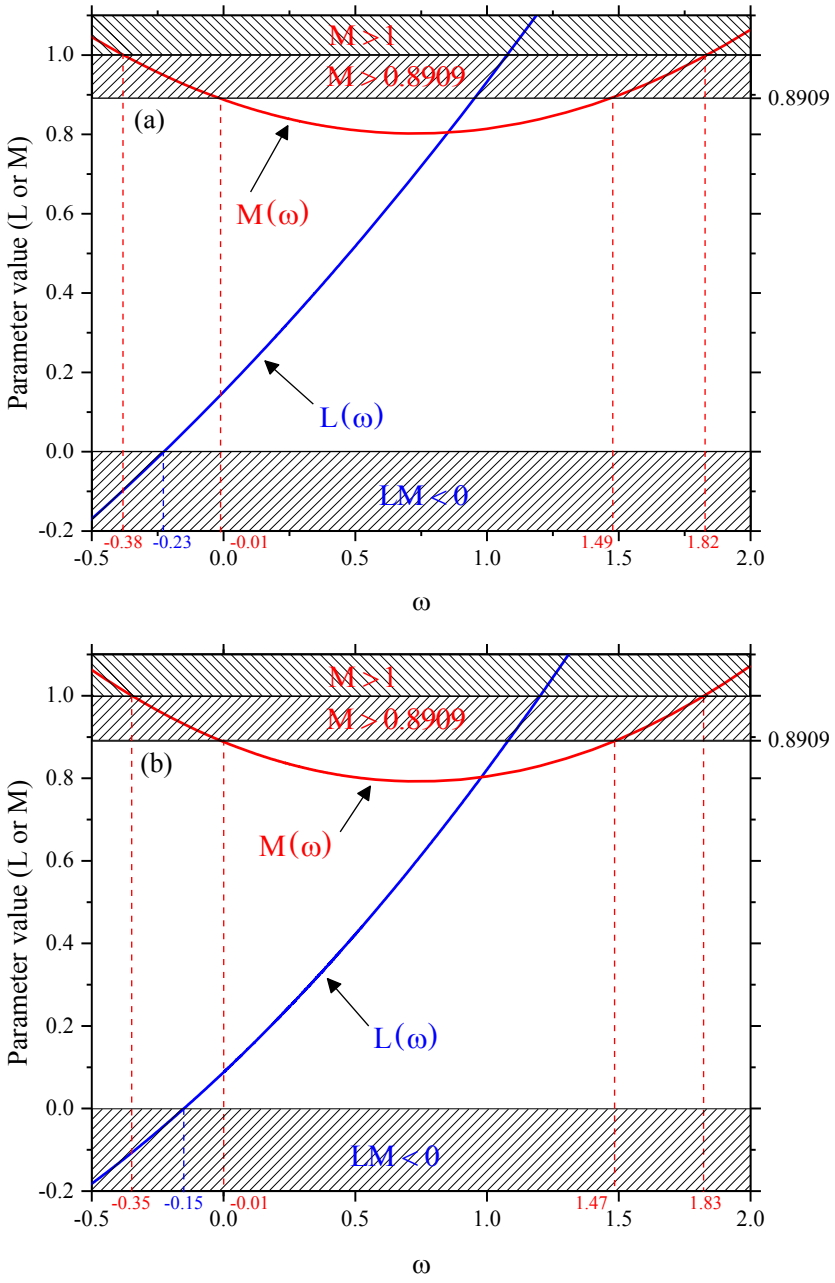



Figure 5.7. Validity ranges of the proposed correlations to estimate *L* and *M* parameters. (a) PR CEoS (b) RK CEoS.

As explained by Le Guennec et al. [20], the 1972 Soave α-function [7] is consistent, i.e. satisfies the constraints given in Eq. (5.3), for 99% of the pure components up to a temperature which is generally higher than 1500 K. This is the reason why the Soave α-function is certainly the most employed α-function in the oil and gas industries: it is in particular used in the PPR78 [23,73,74] and PR2SRK predictive models [72]. Its mathematical expression is:

$$\begin{cases} \alpha(T_r) = \left[1 + m\left(1 - \sqrt{T_r}\right)\right]^2 \\ m(\omega) = 0.37464 + 1.54226\omega - 0.26992\omega^2 \quad \text{for the PR EoS} \\ m(\omega) = 0.480 + 1.574\omega - 0.176\omega^2 \quad \text{for the RK EoS} \end{cases} \tag{5.22}$$

To have a fair overview of the capabilities of these three α-functions:

(i) the component-dependent Twu91 α-function developed in the previous section,

(ii) the generalized Twu88 α-function developed in this section,

(iii) the Soave α-function,

MAPEs on saturation properties can be compared in Table 5.6.

| | Peng-Robinson | | | Redlich-Kwong | | |
|---|---|---|---|---|---|---|
| α-function | Twu91 [Eq. ((5.16))] | gen. Twu88 [Eq. (5.20)] | Soave [Eq. (5.22)] | Twu91 [Eq. (5.17)] | gen. Twu88 [Eq. (5.21)] | Soave [Eq. (5.22)] |
| MAPE on $P^{sat}$ (980 compounds) | 0.9 % | 2.0 % | 2.3 % | 1.1 % | 2.3 % | 2.3 % |
| MAPE on $\Delta_{vap}H$ (805 compounds) | 2.0 % | 2.8 % | 2.9 % | 2.1 % | 3.0 % | 3.1 % |
| MAPE on $c_{P,L}^{sat}$ (529 compounds) | 2.0 % | 6.7 % | 8.5 % | 2.2 % | 6.7 % | 7.0 % |

Table 5.6. Comparison of the MAPEs calculated with the 3-parameter Twu91, the generalized Twu88 and the Soave α-functions for the PR and RK CEoS

Such a table highlights that the 2 generalized α-functions: gen. Twu88 and Soave have similar accuracy with however a small advantage to the first one, especially to predict $c_{P,L}^{sat}$ with the PR EoS. Let us however recall that the proposed gen. Twu88 α-function is fully consistent what ensures a safe extrapolation to the supercritical temperature range. On the other hand, by comparing deviations obtained with the component-dependent Twu91 α-function with those obtained with a generalized α-function, it is noticeable that results are deteriorated. As an example, MAPE on $P^{sat}$ doubled, MAPE on $\Delta_{vap}H$ is multiplied by 1.5 and MAPE on $c_{P,L}^{sat}$ tripled.

In the light of these observations, we can state that we developed a generalized α-function (gen. Twu88), slightly more accurate than the Soave α-function to predict the subcritical properties, that, contrary to the Soave α-function, safely extrapolates to the

supercritical temperature range. However, this generalized α-function should only be used when parameters L, M and N of the component-dependent Twu91 α-function are unknown as much better results can be achieved when using this latter.

### 5.4.2. A generalized volume translation method

As previously stated, it is advised to calculate the volume translation *c* by using the following equation:

$$\begin{aligned} c &= v_L^{sat,\mathrm{u-}CEoS}\left(T_r = 0.8\right) - v_{L,\exp}^{sat}\left(T_r = 0.8\right) \\ &= v_L^{sat,\mathrm{u-}CEoS}\left(T_r = 0.8\right) - \frac{RT_c}{P_c} z_{RA}^{\left[1+0.2^{2/7}\right]} \end{aligned} \tag{5.23}$$

coupled to the $z_{RA}$ values, reported for 997 components in the Supplementary material section. In the case $z_{RA}$ is unknown, we strongly advise to use at least one experimental density available at a reference temperature, $T_r^{ref}$ , to estimate such a parameter by:

$$z_{RA} = \left[\frac{P_c \cdot v_{L,\exp}^{sat}\left(T_r^{ref}\right)}{RT_c}\right]^{\left[\frac{1}{1+\left(1-T_r^{ref}\right)^{2/7}}\right]} \tag{5.24}$$

Following Péneloux [39], many process simulation software programs however express $c \cdot P_c/(RT_c)$ as a linear function of $z_{RA}$ . We believe that 35 years after Péneloux, it is time to update such correlations which are routinely used in many industrial sectors. In his paper, Péneloux developed in fact a unique correlation applicable to the RK EoS. Such a correlation was finalized by considering light n-alkanes only and we know by experience that it cannot be accurately extended to heavy n-alkanes or to other chemical families. In this study, in order to develop non-biased correlations, it was decided to work with the 475 compounds, available in the DIPPR database, for which the four parameters: $T_c$ , $P_c$ , $\omega$ and $v_L^{sat,DIPPR}$ are all known with an error lower than 5%. The α-function used in this section is the gen. Twu88 [see Eq. (5.20) and Eq. (5.21)]. For each of the 475 chemicals, $z_{RA}$ was determined by Eq. (5.13) and *c* calculated for each EoS by Eq. (5.23). Figure 5.8 highlights that $c \cdot P_c/(RT_c)$ can be reasonably correlated to $z_{RA}$ using a linear dependence. The obtained correlations are:

$$\begin{cases} c_{PR} = \dfrac{RT_c}{P_c}\left(0.1398 - 0.5294 z_{RA}\right) & \text{for the PR CEoS} \\ c_{RK} = \dfrac{RT_c}{P_c}\left(0.1487 - 0.5052 z_{RA}\right) & \text{for the RK CEoS} \end{cases} \quad (5.25)$$

Four compounds had a $z_{RA}$ value outside the typical range 0.22–0.35 and were excluded from the linear regression.

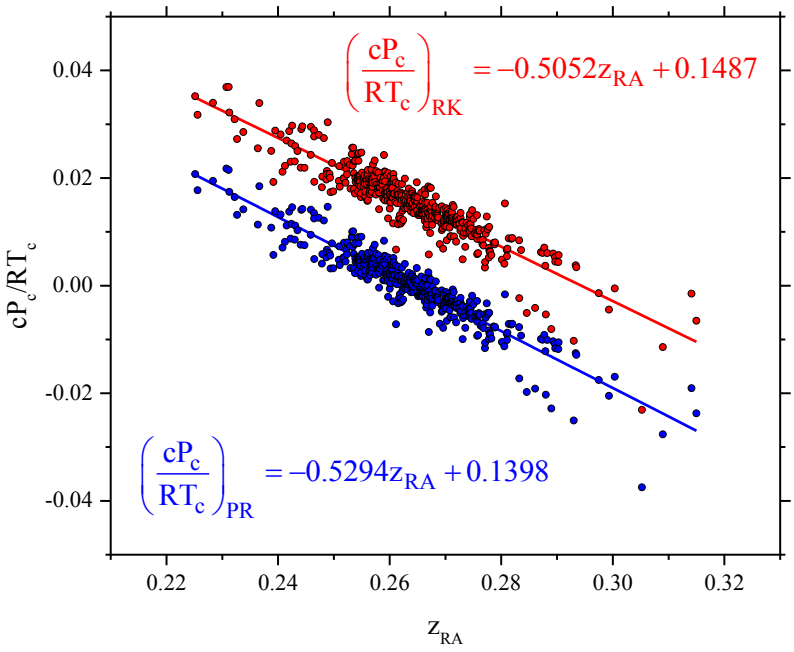



Figure 5.8. Changes of $c \cdot P_c/(RT_c)$ with respect to $z_{RA}$ for the RK and PR CEoS

To conclude this section it was decided to relate directly the volume-translation parameter $c$ to $\omega$. Such a relation could indeed be useful to estimate the volume correction in the case where no experimental density is available. We however know by experience that relating $c$ to $\omega$ without an important loss of accuracy on the liquid density calculation is not possible. It is indeed well-established that liquid molar volumes cannot be represented by CEoS that obey the 3-parameter corresponding states theorem. In addition to $T_c$, $P_c$ and $\omega$, a fourth parameter like $z_{RA}$ or an experimental density value must be added. Aware of the inherent limitations of a correlation between $c$ and $\omega$, a linear regression over the 475 compounds for which the four parameters: $T_c$, $P_c$, $\omega$ and $v_L^{sat,DIPPR}$ are all known with an error lower than 5%, leads to the following relations:

$$\begin{cases} c_{PR} = \dfrac{RT_c}{P_c}(-0.0065 + 0.0198\omega) & \text{for the PR CEoS} \\ c_{RK} = \dfrac{RT_c}{P_c}(0.0096 + 0.0172\omega) & \text{for the RK CEoS} \end{cases} \quad (5.26)$$

With such correlations, MAPEs on $v_L^{sat}$, over 997 components modeled with the gen. Twu88 $\alpha$-function, in a temperature range so that $T_r \leq 0.9$, as predicted by the PR and RK EoS are 7.2% and 7.6% respectively. The MAPEs on the molar critical volume are 19.5% and 23.9% respectively.

A comparison with the deviations given in Table 5.3 makes it possible to conclude that the MAPEs on $v_L^{sat}$ have at least doubled. If the use of such a correlation with the PR EoS loses interest (the average deviation on $v_L^{sat}$ is only slightly better than the one obtained with a null volume translation), it remains extremely useful with the RK EoS.

### 5.5. Conclusion

In this paper, *translated* and *consistent* versions of the Peng-Robinson and Redlich-Kwong cubic equations of state, the acronyms of which are *tc*-PR and *tc*-RK were developed. The adjective *consistent* means that the $\alpha$-function used in such models passes the consistency test recently proposed by Le Guennec et al. [20] that guarantees safe extrapolation to the supercritical region and safe VLE calculation in multi-component systems. In this study a consistent version of the Twu91 $\alpha$-function was used. The 3 (*L*, *M*, *N*) parameters were determined for 1116 compounds by minimizing an objective function which takes into account the deviations between calculated and experimental vapor pressures $\left(P^{sat}\right)$, enthalpies of vaporization $\left(\Delta_{vap}H\right)$ and saturated liquid heat capacities $\left(c_{P,L}^{sat}\right)$. The adjective *translated* means that a volume translation aimed at exactly reproducing the experimental saturated liquid volume at a reduced temperature of 0.8 was used. For both EoS, the numerical value of such a volume correction was determined for 997 chemicals. The key conclusion of this paper is that the *tc*-PR EoS is certainly the safest and the most accurate 3-parameter cubic EoS ever published. Indeed the average deviations over roughly 1000 compounds belonging to different chemical families are: $\Delta P^{sat} < 1\%$, $\Delta_{vap}H = \Delta c_{P,L}^{sat} = 2\%$ and $\Delta v_L^{sat}(T_r < 0.9) = 2.3\%$. Such a model can be safely applied in any ranges of pressure

and temperature. Its unique limitation is the liquid density prediction in the critical region.

In order the *tc*-PR and *tc*-RK CEoS could be applied to components not included in the DIPPR database, a generalized version of such models was developed. The 3-parameter Twu91 α-function was substituted by the 2-parameter Twu88 function and the parameters *L* and *M* were correlated to the acentric factor. This generalized α-function, applicable to molecules having a positive acentric factor lower than 1.5, performs slightly better than the Soave α-function in the subcritical temperature range but can safely extrapolate in the supercritical temperature range since it passes the consistency test for α-function developed in a previous study [20]. In order to estimate the volume translation for molecules not included in the DIPPR, it is advised to use one experimental density available at a reference temperature, to estimate the Rackett compressibility factor with Eq. (5.24) and then to estimate *c* with Eq. (5.23). It is also possible to use the updated correlations, developed in this work, that directly link the volume translation to $z_{RA}$. In the case $z_{RA}$ cannot be estimated, and as a last resort, it is possible to use the less-accurate correlations developed in this paper which make it possible to estimate the volume translation from the mere knowledge of the acentric factor.

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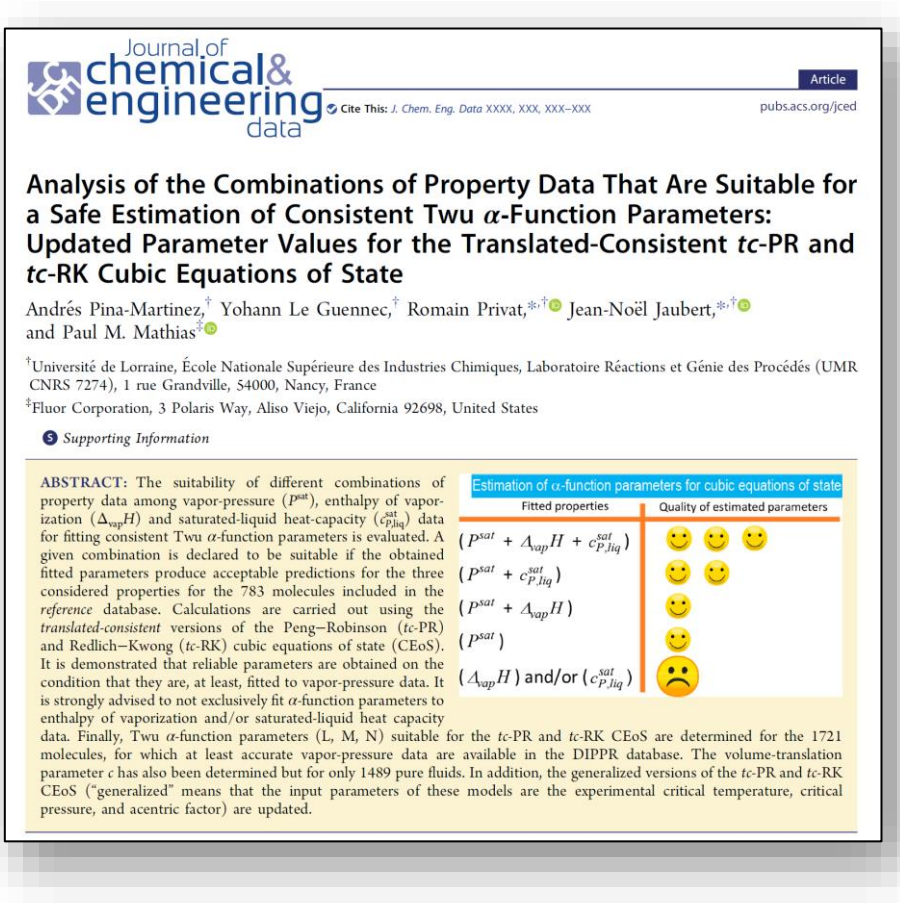
Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.fluid.2016.09.003.

# Chapitre 6. Article “Analysis of the combinations of property data that are suitable for a safe estimation of consistent Twu α-function parameters. Updated parameter values for the translated-consistent tc-PR and tc-RK cubic equations of state.”

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**Analysis of the Combinations of Property Data That Are Suitable for a Safe Estimation of Consistent Twu α-Function Parameters: Updated Parameter Values for the Translated-Consistent *tc*-PR and *tc*-RK Cubic Equations of State**

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Supporting Information

**ABSTRACT:** The suitability of different combinations of property data among vapor-pressure ($P^{sat}$), enthalpy of vaporization ($\Delta_{vap}H$) and saturated-liquid heat-capacity ($c^{sat}_{P,liq}$) data for fitting consistent Twu α-function parameters is evaluated. A given combination is declared to be suitable if the obtained fitted parameters produce acceptable predictions for the three considered properties for the 783 molecules included in the *reference* database. Calculations are carried out using the *translated-consistent* versions of the Peng−Robinson (*tc*-PR) and Redlich−Kwong (*tc*-RK) cubic equations of state (CEoS). It is demonstrated that reliable parameters are obtained on the condition that they are, at least, fitted to vapor-pressure data. It is strongly advised to not exclusively fit α-function parameters to enthalpy of vaporization and/or saturated-liquid heat capacity data. Finally, Twu α-function parameters (L, M, N) suitable for the *tc*-PR and *tc*-RK CEoS are determined for the 1721 molecules, for which at least accurate vapor-pressure data are available in the DIPPR database. The volume-translation parameter *c* has also been determined but for only 1489 pure fluids. In addition, the generalized versions of the *tc*-PR and *tc*-RK CEoS (“generalized” means that the input parameters of these models are the experimental critical temperature, critical pressure, and acentric factor) are updated.




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**Abstract**

The suitability of different combinations of property data among vapor-pressure ($P^{sat}$), enthalpy of vaporization ($\Delta_{vap}H$) and saturated-liquid heat-capacity ($c_{P,liq}^{sat}$) data for fitting consistent Twu α-function parameters is evaluated. A given combination is declared to be suitable if the obtained fitted parameters produce acceptable predictions for the 3 considered properties for the 783 molecules included in the *reference* database. Calculations are carried out using the *translated-consistent* versions of the Peng-Robinson (*tc*-PR) and Redlich-Kwong (*tc*-RK) cubic equations of state (CEoS). It is demonstrated that reliable parameters are obtained on the condition that they are – at least – fitted to vapor-pressure data. It is strongly advised to not exclusively fit α-function parameters to enthalpy of vaporization and/or saturated-liquid heat capacity data.

Finally, Twu α-function parameters (*L*, *M*, *N*) suitable for the *tc*-PR and *tc*-RK CEoS are determined for the 1721 molecules, for which at least accurate vapor-pressure data are available in the DIPPR database. The volume-translation parameter *c* has also been determined but for only 1489 pure fluids. In addition, the generalized versions of the *tc*-PR and *tc*-RK CEoS ('generalized' means that the input parameters of these models are the experimental critical temperature, critical pressure and acentric factor) are updated.

### 6.1. Introduction

Most of the 2-parameter cubic equations of state (CEoS) obey the general formulation:

$$P(T,v) = \frac{RT}{v-b} - \frac{a(T)}{(v-r_1 b)(v-r_2 b)} \tag{6.1}$$

where parameter $a$ is a measure of the attractive forces between molecules; parameter $b$ is the so-called covolume, which attempts to correct the perfect-gas law for the fact that molecules have a finite volume; and $r_1$ and $r_2$ are two universal constants that depend on the selected EoS. The temperature-dependent $a$ parameter of any CEoS is classically written as:

$$a(T) = a_c \times \alpha(T) \tag{6.2}$$

that is, as the product of the value of the attractive parameter at the critical temperature ($a_c$) multiplied by a so-called α-function, which is dimensionless. It is possible to distinguish two types of α-functions: *generalized* and *component-dependent*. The coefficients of the generalized α-functions are usually determined using correlations that only depend on the acentric factor ($\omega$), while the parameters of the component-dependent α-functions must be regressed, component by component, from experimental data. It is worth noting that the generalized α-functions, although less accurate than the component-dependent α-functions, are extremely useful when experimental data to fit the specific parameters of a given α-function are not available. Moreover, generalized α-functions are easy to implement because the acentric factor is known for thousands of pure components or can be estimated by well-established correlations or group-contribution methods [81].

As recently highlighted by Le Guennec et al. [20,59], α-functions cannot be freely chosen. The temperature dependence of α-functions must indeed obey the following list of constraints to guarantee safe property predictions in both subcritical and supercritical domains:

$$\alpha(T_c)=1 \text{ and for all T: } \begin{cases} \alpha \geq 0 & \text{and } \alpha(T_r) \text{ continuous} \\ \dfrac{d\alpha}{dT_r} \leq 0 & \text{and } \dfrac{d\alpha}{dT_r} \text{ continuous} \\ \dfrac{d^2\alpha}{dT_r^2} \geq 0 & \text{and } \dfrac{d^2\alpha}{dT_r^2} \text{ continuous} \\ \dfrac{d^3\alpha}{dT_r^3} \leq 0 & \end{cases} \tag{6.3}$$

An α-function that fulfills all of the conditions reported in Eq. (6.4)was described as *consistent* by Le Guennec et al. These authors also demonstrated that the highly flexible 3-parameter α-function developed by Twu et al. in 1991 [19] (denoted hereafter as Twu91):

$$\alpha(T_r)=T_r^{N(M-1)}\exp\left[L\left(1-T_r^{MN}\right)\right] \tag{6.4}$$

became consistent if the following constraints were added to the 3 parameters:

$$\begin{cases} \delta<0 \\ L\gamma>0 \\ \gamma<1-\delta \end{cases} \quad \text{or} \quad \begin{cases} \delta<0 \\ L\gamma>0 \\ \gamma<1-2\delta+2\sqrt{\delta(\delta-1)} \\ 4Y^3+4ZX^3+27Z^2-18XYZ-X^2Y^2>0 \end{cases}$$

$$\text{with: } \begin{cases} \delta=N(M-1) \\ \gamma=MN \\ X=-3(\gamma+\delta-1) \\ Y=\gamma^2+3\delta\gamma-3\gamma+3\delta^2-6\delta+2 \\ Z=-\delta\left(\delta^2-3\delta+2\right) \end{cases} \tag{6.5}$$

Le Guennec et al. coupled this noteworthy α-function to the volume translation concept [40,112] discovered by Péneloux et al. [39] in 1982 to define the *translated-consistent* versions of the Peng-Robinson [8] (PR) and Redlich-Kwong[6] (RK) EoS. The volume correction, denoted hereafter as *c*, was selected to exactly reproduce the experimental saturated liquid volume at a reduced temperature of 0.8 [$v_{liq,\exp}^{sat}(T_r=0.8)$], that is:

$$c=v_L^{sat,\boldsymbol{u}-CEoS}(T_r=0.8)-v_{L,\exp}^{sat}(T_r=0.8) \text{ with } T_r=\frac{T}{T_c} \tag{6.6}$$

where $v_L^{sat,\boldsymbol{u}-CEoS}(T_r = 0.8)$ is the molar volume calculated with the original (*untranslated*) CEoS at $T_r = 0.8$.

These EoS, for which safe property predictions are guaranteed in both subcritical and supercritical domains because the α-function passes the consistency test proposed by Le Guennec et al. are also almost certainly the most accurate 3-parameter CEoS ever published. They can be expressed as:

$$\underline{\underline{tc-PR:}}$$

$$P(T,v) = \frac{RT}{v-b} - \frac{a_c \cdot \alpha(T_r)}{(v+c)(v+b+2c)+(b+c)(v-b)}$$

$$with: \begin{cases} \alpha(T_r) = T_r^{N(M-1)} \exp\left[L\left(1-T_r^{MN}\right)\right] \\ c = v_{liq}^{sat,\boldsymbol{u}-PR}(T_r = 0.8) - v_{liq,\exp}^{sat}(T_r = 0.8) \\ \eta_c = \left[1 + \sqrt[3]{4-2\sqrt{2}} + \sqrt[3]{4+2\sqrt{2}}\right]^{-1} \approx 0.25308 \\ a_c = \dfrac{40\eta_c + 8}{49 - 37\eta_c} \dfrac{R^2 T_{c,\exp}^2}{P_{c,\exp}} \approx 0.45724 \dfrac{R^2 T_{c,\exp}^2}{P_{c,\exp}} \\ b = \dfrac{\eta_c}{\eta_c + 3} \dfrac{RT_{c,\exp}}{P_{c,\exp}} - c \approx 0.07780 \dfrac{RT_{c,\exp}}{P_{c,\exp}} - c \end{cases} \quad (6.7)$$

$$\underline{\underline{tc-RK:}}$$

$$P(T,v) = \frac{RT}{v-b} - \frac{a_c \cdot \alpha(T)}{(v+c)(v+b+2c)}$$

$$with: \begin{cases} \alpha(T_r) = T_r^{N(M-1)} \exp\left[L\left(1-T_r^{MN}\right)\right] \\ c = v_{liq}^{sat,\boldsymbol{u}-RK}(T_r = 0.8) - v_{liq,\exp}^{sat}(T_r = 0.8) \\ a_c = \dfrac{1}{9\left(\sqrt[3]{2}-1\right)} \dfrac{R^2 T_{c,\exp}^2}{P_{c,\exp}} \\ b = \dfrac{\sqrt[3]{2}-1}{3} \dfrac{RT_{c,\exp}}{P_{c,\exp}} - c \end{cases} \quad (6.8)$$

By working with 1116 pure fluids, Le Guennec et al. [60] not only published a library of consistent parameters that are suitable for the *tc*-PR and *tc*-RK EoS but also developed a generalized version of the Twu α-function for both CEoS (RK and PR). Recently, Bell et al.[113] also published consistent Twu parameters for more than 2500 pure fluids. While the overall aims of these studies were similar, a noticeable difference should be highlighted: Bell et al.[113] directly employed experimental data from the

ThermoDataEngine (TDE) database of NIST, while Le Guennec et al. [60] fitted the 3 parameters of the α-function on pseudo-experimental data generated from correlations available in the DIPPR database. Indeed, the DIPPR database provides a set of temperature-dependent correlations, the coefficients of which are fit to actual experimental data, making it possible to estimate, among other properties, vapor pressures, enthalpies of vaporization and saturated-liquid heat capacities of pure components. Note that for each component and each property, an experimental error is provided. The benefit of using DIPPR correlations instead of raw experimental data is the ability to carry out fitting procedures on pseudo-experimental data that are regularly distributed between the triple point and critical point. By doing so, the optimization results (i.e., α-function parameters) are not biased by experimental data points that are concentrated in a specific temperature range. The approach also eliminates the opportunity for independent evaluation of the raw data.

It is worth noting that Le Guennec et al. [60] determined α-function parameters for 1116 pure compounds by minimizing an objective function accounting for deviations between calculated and pseudo-experimental vapor pressure ($P^{sat}$) and/or enthalpy of vaporization ($\Delta_{vap}H$) and/or saturated-liquid heat capacity ($c_{P,liq}^{sat}$) data. For many components, thanks to the DIPPR correlations, it was possible to generate accurate pseudo-experimental data for all 3 properties, whereas for other components, only 2 or even 1 accurate property could be generated. Therefore, each set of α-function parameters was fitted on one out of the seven different possible combinations of the pseudo-experimental data properties shown in Table 6.1.

| Type of pure fluid | Properties for which accurate data are available (that were considered in the fitting procedure of α-function parameters by Le Guennec et al. [60]) |
|---|---|
| 1 | $(P^{sat})$ |
| 2 | $(\Delta_{vap}H)$ |
| 3 | $(c_{P,liq}^{sat})$ |
| 4 | $(P^{sat} + \Delta_{vap}H)$ |
| 5 | $(P^{sat} + c_{P,liq}^{sat})$ |
| 6 | $(\Delta_{vap}H + c_{P,liq}^{sat})$ |
| 7 | $(P^{sat} + \Delta_{vap}H + c_{P,liq}^{sat})$ |

Table 6.1. Possible combinations of accurate pseudo-experimental data available in the DIPPR database for a given pure component. The pure fluid type is an arbitrary index that indicates which properties among $P^{sat}$, $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ are associated with accurate data and can thus be used to fit α-function parameters.

In view of this situation, the key questions we address in this paper are:

- Are all of the possible arrangements of the properties listed in Table 6.1 suitable for parameter fitting? If not, some of the parameters we published in 2016[60] should not be used.
- Which property combinations are the most appropriate for parameter fitting?

As previously explained, Bell et al.[113] published Twu parameters for more than 2500 pure fluids, while the library published by Le Guennec[60] contains parameters for less than half the number of pure components. This is because Le Guennec et al. only considered a DIPPR correlation to be acceptable if its experimental error (reported in the DIPPR database) was lower or equal to 5%. However, it is believed that, in many cases, this error is overestimated. Thus, another objective of this paper is to review the uncertainty of the correlations reported in the DIPPR database and to develop a new procedure to evaluate error of DIPPR correlations. This new procedure makes it possible to notably increase the number of compounds for which the Twu parameters can be determined.

In the first section of this study, an error evaluation of DIPPR correlations is performed in order to draw up a list of compounds for which accurate data of interest ( $P^{sat}$ and/or $\Delta_{vap}H$ and/or $c_{P,liq}^{sat}$) are available in the DIPPR database. The next section presents the combinations of the property data that are suitable for parameter regression. Finally, an update of the Twu91 α-function and volume-translation parameters with respect to Le Guennec et al.'s initial study is proposed. Component-dependent parameters are determined for 1721 pure fluids. The updated versions of the generalized Twu88 α-functions and volume-translation correlations for both the PR and RK EoS are also provided.

## 6.2. Overview of the DIPPR database

### 6.2.1. Error evaluation of the DIPPR correlations

As previously stated, this paper addresses the fitting of consistent Twu91 α-function parameters on vapor pressure ( $P^{sat}$ ), enthalpy of vaporization ( $\Delta_{vap}H$ ) and saturated-liquid heat capacity ($c_{P,liq}^{sat}$ ) data. It is thus decided to draw up the list of pure components for which the DIPPR database has reasonable experimental error for at least one out of the three aforementioned properties.

At this step, it should be noted that only the residual part of the isobaric heat capacity can be estimated from a CEoS. The $c_P$ of the fluid is obtained by adding the heat capacity of the corresponding perfect gas to the residual contribution expressed from the EoS:

$$c_P(T,v) = c_{P,perfect\ gas}(T) + c_{P,residual}(T,v) \tag{6.9}$$

The heat capacities of perfect gases can be estimated from DIPPR correlations. Consequently, the error of four correlations per compound must be taken into account when evaluating a pure component: $P^{sat}$ , $\Delta_{vap}H$ , $c_{P,liq}^{sat}$ and $c_{P,perfect\ gas}$ . Henceforth, in this work, when it is stated that $c_{P,liq}^{sat}$ data can be accurately generated, it is implied that both the $c_{P,liq}^{sat}$ and $c_{P,perfect\ gas}$ pseudo-experimental data can be accurately generated.

In this study, the 11.1.0 version (May 2016) of the DIPPR database is used. It should be noted that in the DIPPR database:

- for a series of experimental data, the single attribute ERROR that is reported is the experimental uncertainty of the measured values. This uncertainty can either be provided by the source or calculated by the DIPPR staff.
- for a temperature-dependent correlation, the way that the attribute ERROR is calculated is not known with certainty. Generally, ERROR is equal to the maximum error among those of the data series used to fit correlation parameters.

For certain compounds it is found that the ERROR reported in the DIPPR was overestimated. Indeed, for such cases, the DIPPR reported uncertainty (henceforth called type I error), set to the maximum uncertainty among the data series, was much higher than the average uncertainty value and did not reflect the confidence we could have on the experimental data. Therefore, the actual average uncertainty is calculated (henceforth called type II error) for each of the four temperature-dependent properties ( $P^{sat}$ , $\Delta_{vap}H$ , $c_{P,liq}^{sat}$ and $c_{P,perfect\ gas}$ ) and for all pure compounds in the DIPPR database. For a given property and a given pure fluid, a type II error is calculated as:

$$Type\ II\ error = \frac{\sum_{j=1}^{n_{series}} N_{data,j} \times Error_j}{\sum_{j=1}^{n_{series}} N_{data,j}} \tag{6.10}$$

where $N_{data,j}$ is the number of experimental data points available in the series *j* and $Error_j$ the corresponding experimental error.

A third strategy to evaluate the correlation errors is to compare pseudo-experimental data with calculated values obtained using the *generalized* version of the *tc*-PR model, which was developed by Le Guennec et al. [60]. Based on the predictive performance of the model, it is possible to state that if a correlation is well represented by the generalized model, it is implied that there is no reason to reject the pseudo-experimental data, and the correlation is considered to be accurate.

For type III errors, the threshold of acceptance (noted *TH*) for each property is defined as:

- For $P^{sat}$ : the mean absolute percentage error (MAPE) on $P^{sat}$ calculated by the generalized *tc*-PR EoS (see Table 5.6) from a database including 980 compounds + one standard deviation:

$$TH_{P^{sat}}^{type\ III} = 2.0\% + 1.2\% = 3.2\% \tag{6.11}$$

- For $\Delta_{vap}H$ : the mean absolute percentage error (MAPE) on $\Delta_{vap}H$ calculated by the generalized *tc*-PR EoS (see Table 5.6) from a database including 805 compounds + one standard deviation:

$$TH_{\Delta_{vap}H}^{type\ III} = 2.8\% + 1.5\% = 4.3\% \tag{6.12}$$

- For $c_{P,liq}^{sat}$ : the mean absolute percentage error (MAPE) on $c_{P,liq}^{sat}$ calculated by the generalized *tc*-PR EoS (see Table 5.6) from a database including 529 compounds + one standard deviation – 5% (maximum allowed error for $c_{P,perfect\ gas}$ ). The maximum error of the perfect gas heat capacity was subtracted to focus on the deviation on the residual heat capacity, which is the sole property calculable from the EoS:

$$TH_{c_{P,liq}^{sat}}^{type\ III} = 6.7\% + 4.3\% - 5\% = 6\% \tag{6.13}$$

The thresholds of the three types of error are reported in Table 6.2.

| Error type | Acceptance thresholds for each property | | | |
|---|---|---|---|---|
| | $P^{sat}$ | $\Delta_{vap}H$ | $c_{P,liq}^{sat}$ | $c_{P,perfect\ gas}$ |
| Type I (error reported in the DIPPR database) | 5% | 5% | 5% | 5% |
| Type II (average exp. error calculated by Eq.(6.10)) | 5% | 5% | 5% | 5% |
| Type III (deviation calculated by the gen. *tc*-PR EoS) | 3.2% | 4.3% | 6% | - |

Table 6.2. Acceptance thresholds for the different property correlations and types of error.

Finally, it is considered that a property can be accurately estimated by a DIPPR correlation if at least one out of the three types of error is less than or equal to its respective threshold.

### 6.2.2. Drawing up of a list of compounds potentially suitable for parameter fitting

First, the use of cubic equations of state requires critical temperature ($T_c$) and critical pressure ($P_c$) data. Whether a generalized α-function is used, the acentric factor ($\omega$) is also needed. Therefore, the first criterion that suitable molecules must meet is that the three experimental constants, $T_c$, $P_c$ and $\omega$, are simultaneously reported in the DIPPR database. Additionally, molecules for which none of the three saturation properties of interest ($P^{sat}$, $\Delta_{vap}H$, $c_{P,liq}^{sat}$) can be accurately generated are removed. Application of these criteria results in 1887 suitable molecules among 2162 available in the DIPPR database. The properties of some compounds, especially metals with a critical temperature higher than 2000 K (Li, K, Ca, LiI) or quantum fluids (He-3 and p-$H_2$) that are not of industrial interest, were removed from the database, leaving 1881 compounds. In comparison to the work by Le Guennec et al., who only considered type I errors, the definition of two new types of error (type II and type III) makes it possible to significantly increase the number of potentially suitable components for parameter

fitting. Let us recall that 1116 pure fluids were considered by Le Guennec et al., whereas 1881 pure fluids are considered in this study.

In Table 6.3, these 1881 molecules are distributed along the 7 fluid types defined in Table 6.1 (i.e., according to the number and type of accurate properties that can be generated for each of them), and a comparison is made with the previous work of Le Guennec et al. Among the 1116 molecules considered by Le Guennec et al., 684 kept the same fluid *type,* whereas 432 moved to a new fluid type. For instance, if type I error is solely considered to evaluate the uncertainty of the correlations (as in Le Guennec et al.), only $c_{P,liq}^{sat}$ can be estimated for 1-hexene, and consequently, it belongs to type 3 (as defined by Table 6.1 and Table 6.3). If type II and III errors are also considered, all three of the temperature-dependent properties, $P^{sat}$ , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ , can be estimated and 1-hexene moves to type 7.

| Type of pure fluid | Accurate property data available | Le Guennec et al. | This work |
|---|---|---|---|
| 1 | ($P^{sat}$) | 166 | 217 |
| 2 | ($\Delta_{vap}H$) | 20 | 25 |
| 3 | ($c_{P,liq}^{sat}$) | 98 | 53 |
| 4 | ($P^{sat}$ + $\Delta_{vap}H$) | 401 | 705 |
| 5 | ($P^{sat}$ + $c_{P,liq}^{sat}$) | 47 | 80 |
| 6 | ($\Delta_{vap}H$ + $c_{P,liq}^{sat}$) | 18 | 18 |
| 7 | ($P^{sat}$ + $\Delta_{vap}H$ + $c_{P,liq}^{sat}$) | 366 | 783 |
| TOTAL | | 1116 | 1881 |

Table 6.3. Comparison of the number of molecules included in the database by Le Guennec et al. and this work.

### 6.3. Suitable combinations of property data for the safe estimation of consistent Twu91 α-function parameters

Table 6.1 indicates that it was possible to define 7 types of pure fluids depending on the availability of accurate pseudo-experimental data. As explained in the introduction,

our key concern is to determine which of these 7 types are suitable for safely fitting consistent Twu91 α-function parameters and to order these types. To answer this question, the approach proposed in this section is aimed at fitting Twu91 α-function parameters for type 7 pure-compounds, such that all three temperature-dependent properties, $P^{sat}$ , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ , can be accurately estimated from DIPPR correlations. The interest in choosing these pure-compounds is that if it is decided to fit the (*L*, *M*, *N*) parameters using not three but one or two of the selected properties, it becomes possible to predict the remaining ones and to compare them with pseudo-experimental values. It is thus possible to determine whether taking specific combinations of 1 or 2 properties into account for parameter fitting may lead to non-reliable sets of (*L*, *M*, *N*) parameters. Consequently, for the 783 type 7 fluids (see Table 6.3), seven different fittings were carried out, as shown in Table 6.5. In the second column, the properties that were taken into account for each fitting are presented. In the third column, the properties predicted by the CEoS with the fitted (*L*, *M*, *N*) parameters are provided.

| Fitting procedure index | Property data included in the Twu parameter fitting procedure | Properties predicted with the optimized Twu parameter set |
|---|---|---|
| 1 | $(P^{sat})$ | $(\Delta_{vap}H + c_{P,liq}^{sat})$ |
| 2 | $(\Delta_{vap}H)$ | $(P^{sat} + c_{P,liq}^{sat})$ |
| 3 | $(c_{P,liq}^{sat})$ | $(P^{sat} + \Delta_{vap}H)$ |
| 4 | $(P^{sat} + \Delta_{vap}H)$ | $(c_{P,liq}^{sat})$ |
| 5 | $(P^{sat} + c_{P,liq}^{sat})$ | $(\Delta_{vap}H)$ |
| 6 | $(\Delta_{vap}H + c_{P,liq}^{sat})$ | $(P^{sat})$ |
| 7 | $(P^{sat} + \Delta_{vap}H + c_{P,liq}^{sat})$ | - |

Table 6.4. Arrangements of the properties for Twu91 α-function parameter fitting.

### 6.3.1. Fitting procedure

- In this study, generation of the pseudo-experimental data obeys the following rules:

1) Regardless of the considered property among $P^{sat}$, $\Delta_{vap}H$ and $c_{P,liq}^{sat}$, 50 equidistant pseudo-experimental data points are generated in their valid temperature range, $[T_{\min};T_{\max}]$.

2) For the $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ correlations, in the case that $T_{\max}$ exceeds $0.98T_c$, $T_{\max}=0.98T_c$ is set. The reason for this choice is simple: $\Delta_{vap}H$ goes to zero at the critical temperature and the calculation of the relative deviation with the experimental data induces a division by zero. Similarly, $c_{P,liq}^{sat}$ goes to infinity at the critical temperature so that, once again, the relative deviation with the experimental value cannot be calculated.

3) For the $P^{sat}$ correlations, $T_{\max}=T_c$ is set. However, in the case where $P^{sat}(T_{\min})<0.1\ bar$, the value of $T_{\min}$ is increased to enforce that $P^{sat}(T_{\min})=0.1\ bar$ (considering that most industrial processes operate at higher values of pressure and that $P^{sat}$ is highly uncertain at low pressures, say less than 1 torr).

- The optimal set of (*L*, *M*, *N*) parameters is the one which minimizes the generic objective function depicted in Eq.(6.14), which is a ponderation of the Mean Absolute Percentage Error (MAPE) on $P^{sat}$, $\Delta_{vap}H$ and $c_{P,liq}^{sat}$. The objective function is obviously adapted according to the fitting procedure index defined in Table 6.4. As an example, for fitting procedure number 1, the objective function only considers the MAPE on $P^{sat}$. The fitting procedure is conducted by imposing the mathematical constraints necessary to obtain consistent parameters, as explained by Le Guennec et al. and recalled from the introduction.

$$OF_{\alpha} = \frac{100}{50}\sum_{i=1}^{50}\left[\left|\frac{P^{sat,DIPPR}\left(T_i^{P^{sat}}\right)-P^{sat,EoS}\left(T_i^{P^{sat}}\right)}{P^{sat,DIPPR}\left(T_i^{P^{sat}}\right)}\right| + \left|\frac{\Delta_{vap}H^{DIPPR}\left(T_i^{\Delta_{vap}H}\right)-\Delta_{vap}H^{EoS}\left(T_i^{\Delta_{vap}H}\right)}{\Delta_{vap}H^{DIPPR}\left(T_i^{\Delta_{vap}H}\right)}\right| + WF\left|\frac{c_{P,liq}^{sat,DIPPR}\left(T_i^{c_{P,liq}^{sat}}\right)-c_{P,liq}^{sat,EoS}\left(T_i^{c_{P,liq}^{sat}}\right)}{c_{P,liq}^{sat,DIPPR}\left(T_i^{c_{P,liq}^{sat}}\right)}\right|\right] \quad (6.14)$$

For fitting procedure 6, the weighting factor on $c_{P,liq}^{sat}$ (denoted as $WF$ in Eq.(6.14)) is set to 1. In turn, for fitting procedures 5 and 7, special attention is devoted to the estimation of $WF$ ; as an initial choice, it is set to 1. Nevertheless, for certain compounds, deviations on $c_{P,liq}^{sat}$ are found to be much smaller than those on $P^{sat}$. In these cases, the deviation on $c_{P,liq}^{sat}$ is reduced to better correlate $P^{sat}$ (i.e., to obtain smaller deviations on $P^{sat}$). This goal is made possible by carrying out successive minimizations by changing the value of $WF$ from 1 to 0.1, with a step of 0.1. In practice, this procedure is run for a considered compound if:

- The MAPE on $P^{sat}$ is larger than 2% (which corresponds to the average MAPE plus one standard deviation calculated for the 782 considered compounds when $WF = 1$) and the MAPE on $c_{P,liq}^{sat}$ is smaller than that on $P^{sat}$.
- The MAPE on $c_{P,liq}^{sat}$ is considerably smaller (two times) than that on $P^{sat}$ and the MAPE on $c_{P,liq}^{sat}$ is larger than 1%.

These conditions are summarized in Eq.(6.15) :

$$\begin{aligned} &MAPE \text{ on } P^{sat} > 2\% \; and \; MAPE \text{ on } c_{P,liq}^{sat} < MAPE \text{ on } P^{sat} \\ &2 \times MAPE \text{ on } c_{P,liq}^{sat} < MAPE \text{ on } P^{sat} \; and \; MAPE \text{ on } c_{P,liq}^{sat} > 1\% \end{aligned} \quad (6.15)$$

In a second step, the weighing factor is selected on a case by case basis to obtain what we consider to be the best compromise between the MAPE on the vapor pressures and MAPE on the saturated-liquid heat capacities.

### 6.3.2. Results

The Mean Absolute Percentage Error (MAPE) on $P^{sat}$, $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ is reported in Table 6.5 for the seven fitting procedures described in Table 6.4. Procedure 7, for which the 3 properties are simultaneously considered, serves as a reference. It is observed that fitting procedures that are carried out when only considering $c_{P,liq}^{sat}$ (procedure 3) yield extremely high deviations: 24.8% and 16.0% for the predicted properties $P^{sat}$ and $\Delta_{vap}H$, respectively. Conversely, it is crucial to include experimental $c_{P,liq}^{sat}$ data in the fitting procedure to obtain a MAPE on $c_{P,liq}^{sat}$ lower than 5% (see procedures 1, 2 and 4 in Table 6.5). Procedures 2 and 6, for which no vapor pressure data are considered, seem to yield acceptable average deviations for the predicted properties. However, the deviations on $P^{sat}$ are higher than the average deviation plus one standard deviation of the reference case (procedure 7). Moreover, for certain molecules, the average deviation on $P^{sat}$ unfortunately reaches 20%. We thus strongly recommend against fitting α-function parameters when experimental $P^{sat}$ data are not available.

| Fitting N° procedure | Property taken into account for fitting | MAPE on $P^{sat}$ (783 compounds) | MAPE on $\Delta_{vap}H$ (783 compounds) | MAPE on $c_{P,liq}^{sat}$ (783 compounds) |
|---|---|---|---|---|
| 1 | ($P^{sat}$) | 0.7% | 2.7% | 6.8% |
| 2 | ($\Delta_{vap}H$) | 2.1% | 1.4% | 5.1% |
| 3 | ($c_{P,liq}^{sat}$) | 24.8% | 16.0% | 0.6% |
| 4 | ($P^{sat}$ + $\Delta_{vap}H$) | 0.9% | 1.6% | 5.1% |
| 5 | ($P^{sat}$ + $c_{P,liq}^{sat}$) | 1.3% | 2.8% | 1.7% |
| 6 | ($\Delta_{vap}H$ + $c_{P,liq}^{sat}$) | 3.1% | 2.3% | 1.7% |
| 7 | ($P^{sat}$ + $\Delta_{vap}H$ + $c_{P,liq}^{sat}$) | 1.1% | 2.2% | 2.3% |

Table 6.5. MAPE on $P^{sat}$, $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ according to the property considered for parameter fitting.

For procedure 5, very accurate predictions are achieved. To sum up, if we accept deviations on $c_{P,liq}^{sat}$ higher than 5%, it is recommended to only estimate consistent Twu91 α-functions parameters for molecules for which at least the pseudo-experimental data of $P^{sat}$ can be accurately generated (procedures 1, 4, 5 and 7 in Table 6.6).

After the reference case for which the 3 experimental properties are available, the most favorable case is that for which $P^{sat}$ and $c_{P,liq}^{sat}$ are available (procedure 5), followed by procedure 4, for which $P^{sat}$ and $\Delta_{vap}H$ are experimentally known, and procedure 1, for which only $P^{sat}$ is known. The grading of the 4 procedures is as follows: procedure 7 > procedure 5 > procedure 4 > procedure 1. The number of molecules belonging to each of these 4 categories of fluids for which vapor pressure data are available are summarized in Table 6.6.

| Type of pure fluid | Accurate property data available | This work |
|---|---|---|
| 1 | ($P^{sat}$) | 217 |
| 4 | ($P^{sat}$ + $\Delta_{vap}H$) | 705 |
| 5 | ($P^{sat}$ + $c_{P,liq}^{sat}$) | 80 |
| 7 | ($P^{sat}$ + $\Delta_{vap}H$ + $c_{P,liq}^{sat}$) | 783 |
| TOTAL: | | 1785 |

Table 6.6. Number of molecules for which at least the pseudo-experimental data of $P^{sat}$ can be accurately generated.

Among the 1116 molecules studied by Le Guennec et al. [60] for which L,M,N parameters are published, it is recommended not to use these values for 34 molecules (see the Supporting Information) since they were estimated by only taking experimental $\Delta_{vap}H$ data or experimental $c_{P,liq}^{sat}$ data, or both of them, into account (fluids of types 2, 3 or 6 in Table 6.3).

### 6.4. Updated consistent Twu91 α-function parameters

Following the conclusion of the previous section, a safe estimation of consistent Twu91 α-functions parameters is carried out only for molecules for which at least $P^{sat}$

pseudo-experimental data can be accurately generated from DIPPR correlations. The objective function, imposed constraints and data generation rules used in this section are identical to those used previously.

### 6.4.1. Constitution of a pure-compound database

As highlighted in Table 6.6, among the 2162 molecules available in the DIPPR database, it is possible to accurately generate at least experimental $P^{sat}$ data for 1785 of them.

It should be noted that among these 1785 molecules, there are 4 quantum fluids (He, $H_2$, Ne and deuterium), which require special treatment [60]. The (*L*, *M*, *N*) parameters for these fluids are presented in the Supporting Information section, but are identical to those published by Le Guennec et al. [60].

In this paper, deviations are thus calculated for 1781 non-quantum fluids for which accurate $P^{sat}$ and/or $\Delta_{vap}H$ and/or $c_{P,liq}^{sat}$ data are available (see Table 6.7).

| Property | Number of compounds |
|---|---|
| ($P^{sat}$) | 1781 |
| ($\Delta_{vap}H$) | 1487 |
| ($c_{P,liq}^{sat}$) | 863 |

Table 6.7. Number of *non-quantum* compounds for which the experimental properties can be accurately estimated.

### 6.4.2. Results

Among the 1781 studied molecules, it is found that by working with the *tc*-PR EoS, 61 reach a mean deviation on at least one property among $P^{sat}$, $\Delta_{vap}H$ or $c_{P,liq}^{sat}$ greater than the average MAPE ($\bar{X}$) calculated for the 1781 compounds plus 3 times the standard deviation (σ). These thresholds are provided in Table 6.8.

These molecules are considered to be outliers, and it is decided not to publish the corresponding values of the L, M, N parameters (i.e., to remove them from the consolidated database) except for mercury, which is considered to be a molecule of interest as shown by a number of recent research articles. Among these 60 molecules, 14 were unfortunately considered as reliable by Le Guennec et al. and α-function parameters should not have been published [60]. These large deviations are justified as follows:

1) Some of these 60 molecules do not obey the 3-parameter corresponding-state theorem, so that their properties cannot be modeled with an EoS from the mere knowledge of $T_c$, $P_c$ and $\alpha(T)$. This behavior is detected when the acentric factor does not reflect at all the size of the molecule. As an example, the acentric factor of trimethylolpropane ($C_6H_{14}O_3$) is 1.6; by comparison, a similar value is reached in the alkane family for n-hexatriacontane (n-$C_{36}$) (its acentric factor is equal to 1.5).

2) There is a problem with the experimental data that was not detected by the correlation selection procedure.

| Property | Average MAPE over 1781 fluids ($\bar{x}$) | Standard deviation over 1781 fluids ($\sigma$) | Threshold ($\bar{x}+3\sigma$) |
|---|---|---|---|
| ($P^{sat}$) | 1.2% | 1.6% | 6% |
| ($\Delta_{vap}H$) | 2.0% | 2.0% | 8% |
| ($c_{P,liq}^{sat}$) | 2.3% | 3.4% | 13% |

Table 6.8. Rejection thresholds for molecule selection.

| Type of pure fluid | Accurate property data available | This work |
|---|---|---|
| 1 | ($P^{sat}$) | 198 |
| 4 | ($P^{sat}$ + $\Delta_{vap}H$) | 694 |
| 5 | ($P^{sat}$ + $c_{P,liq}^{sat}$) | 70 |
| 7 | ($P^{sat}$ + $\Delta_{vap}H$ + $c_{P,liq}^{sat}$) | 759 |
| TOTAL | | 1721 |

Table 6.9. Distribution of the 1721 retained molecules according to the available accurate property data.

The regressed parameters of the 1721 remaining molecules (Table 6.9) are reported in Appendix 1-A and 1-B for both the PR and the RK EoS. The MAPE on $P^{sat}$, $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ are reported in Table 6.10 for both *consistent*-PR and *consistent*-RK EoS.

It can be stated that the PR or RK EoS, coupled with a consistent Twu91 α-function, are capable of accurately reproducing the properties of interest. The MAPE on vapor

pressures for more than 1700 compounds is only 1 %, while the deviations on $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ are approximately 2%. It is possible to observe that the addition of up to 600 compounds with respect to that used in Le Guennec et al. did not affect the mean deviations on the studied properties.

Furthermore, it is possible to compare the MAPE on $P^{sat}$, $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ obtained in this work with those calculated by Bell et al.[113]. It is observed that the average deviation on $P^{sat}$ in this work is five-fold lower than that obtained by Bell et al. (see Table 6.10). Conversely, the MAPE on $c_{P,liq}^{sat}$ is two-fold greater than that obtained by Bell et al.[113]. This difference is probably due to the mathematical expressions of the objective functions, which are different in the two studies and to the fact that vapor pressures considered in this work were cut off at 0.1 bar whereas Bell et al. accepted – as part of the fitting exercise – much lower vapor pressures for which it is not scarce to get large relative deviations.

| Source | EoS | MAPE on $P^{sat}$ | MAPE on $\Delta_{vap}H$ | MAPE on $c_{P,L}^{sat}$ |
|---|---|---|---|---|
| This work (1721 fluids) | | (1721 compounds) | (1453 compounds) | (829 compounds) |
| | *consistent*-PR | 1.0% | 1.9% | 2.0% |
| | *consistent*-RK | 1.2% | 1.9% | 2.2% |
| Le Guennec et al. [60] (1116 fluids) | | (980 compounds) | (805 compounds) | (529 compounds) |
| | *consistent*-PR | 0.9% | 2.0% | 2.0% |
| | *consistent*-RK | 1.1% | 2.1% | 2.2% |
| Bell et al.[113] (2571 fluids) | | (2571 compounds) | (764 compounds) | (414 compounds) |
| | *consistent*-PR | 4.9% | 1.5% | 0.9% |

Table 6.10. MAPE on $P^{sat}$, $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ as predicted from the updated *consistent* PR and RK EoS.

### 6.5. Updated volume-translation parameters *c*

To calculate the volume-translation parameter, it is imposed to exactly reproduce the pseudo-experimental saturated-liquid molar volume returned by the DIPPR

correlation at a reduced temperature of 0.8, as described by Le Guennec et al. [60]. The volume translation parameter is thus calculated as:

$$c = v_{liq}^{sat,u-CEoS}(T_r = 0.8) - v_{liq,\exp}^{sat}(T_r = 0.8) \quad (6.16)$$

where $v_{liq}^{sat,u-CEoS}(T_r = 0.8)$ is the molar volume calculated with the original (*untranslated*) CEoS at $T_r = 0.8$.

### 6.5.1. Results

To estimate the MAPE on the liquid molar volumes, it is necessary to identify the molecules for which the pseudo-experimental liquid densities can be accurately generated following the procedure described in section 2.1 (i.e., error reported in the DIPPR database or average experimental error calculated by Eq. (6.10)is lower than 5%). As highlighted in Table 6.11, among the 1721 compounds included in the database, 1489 have accurate correlations for the liquid molar volume data.

| Type of pure fluid | Accurate property data available | This work | Accurate property data available | This work |
|---|---|---|---|---|
| 1 | ($P^{sat}$) | 198 | ($P^{sat}$ + $v_{liq}^{sat}$) | 164 |
| 4 | ($P^{sat}$ + $\Delta_{vap}H$) | 694 | ($P^{sat}$ + $\Delta_{vap}H$ + $v_{liq}^{sat}$) | 543 |
| 5 | ($P^{sat}$ + $c_{P,liq}^{sat}$) | 70 | ($P^{sat}$ + $c_{P,liq}^{sat}$ + $v_{liq}^{sat}$) | 65 |
| 7 | ($P^{sat}$ + $\Delta_{vap}H$ + $c_{P,liq}^{sat}$) | 759 | ($P^{sat}$ + $\Delta_{vap}H$ + $c_{P,liq}^{sat}$ + $v_{liq}^{sat}$) | 717 |
| TOTAL | | 1721 | | 1489 |

Table 6.11. Distribution of the 1489 molecules for which at least $P^{sat}$ and $v_{liq}^{sat}$ can be accurately generated from the DIPPR database.

As previously done for the $P^{sat}$, $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ properties, for each of these 1489 compounds, the DIPPR correlation was used to generate 50 equidistant liquid molar volume data points between $T_{\min}$ and $T_{\max} = 0.9T_c$. Here, $T_{\min}$ is the minimum temperature at which $v_{liq}^{sat}$ can be estimated from the DIPPR correlation, whereas

$T_{max} = 0.9T_c$ is the highest temperature at which the volume-translation concept has beneficial effect. By denoting $v_{liq}^{sat,t-CEoS}$, the molar volume calculated with the translated EoS, the MAPE on $v_{liq}^{sat}$ is calculated as:

$$MAPE = \frac{100}{50}\sum_{i=1}^{50}\left|\frac{v_{liq}^{sat,DIPPR}\left(T_i^{v_{liq}^{sat}}\right) - v_{liq}^{sat,t-CEoS}\left(T_i^{v_{liq}^{sat}}\right)}{v_{liq}^{sat,DIPPR}\left(T_i^{v_{liq}^{sat}}\right)}\right| \quad (6.17)$$

These MAPE are reported in Table 6.12 for both the PR and RK EoS in their translated and original versions. The calculated volume-translation parameters are reported in the Supporting Information for both the PR and RK EoS. It is observed that the reproduction of the $v_{liq}^{sat}$ data is dramatically improved for both models.

In addition, the average deviations on the molar critical volume are reported in Table 6.13. At the critical point, the volume-translation parameter *c* has too weak an influence on the calculated critical volume ($v_c$) to obtain a good match with the experimental value. Although the influence of the volume translation concept is more visible on the RK EoS, the PR CEoS yields better predictions of $v_c$.

| EoS | MAPE on $v_{liq}^{sat}\left(T_r < 0.9\right)$ (1489 compounds) | |
|---|---|---|
| | Untranslated EoS | Translated EoS |
| *consistent*-PR | 8.7% | 2.2% |
| *consistent*-RK | 19.2% | 3.7% |

Table 6.12. MAPE on $v_{liq}^{sat}$ as predicted by the *consistent* PR and RK EoS on an updated database. Effect of the volume translation.

| EoS | MAPE on $v_c$ (1489 compounds) | |
|---|---|---|
| | Untranslated EoS | Translated EoS |
| *consistent*-PR | 21% | 20% |
| *consistent*-RK | 31% | 24% |

Table 6.13. MAPE on $v_c$ as predicted by the *consistent* PR and RK EoS. Effect of the selected volume translation.

In Table 6.14, the accurate results obtained with the *tc*-PR and *tc*-RK CEoS using the updated parameters determined in this study are summarized. This table highlights that the accuracies of both EoS are very similar, with the exception of the molar volumes, which are better correlated with the PR EoS.

| EoS | MAPE on | | | | | | |
|---|---|---|---|---|---|---|---|
| | $P^{sat}$ (1721 fluids) | $\Delta_{vap}H$ (1453 fluids) | $c_{P,liq}^{sat}$ (829 fluids) | $v_{liq}^{sat}$ (1489 fluids) ($T_r < 0.9$) | $v_c$ (1489 fluids) | $T_c$ (1721 fluids) | $P_c$ (1721 fluids) |
| *tc*-PR | 1.0% | 1.9% | 2.0% | 2.2% | 20% | 0% | 0% |
| *tc*-RK | 1.2% | 2.0% | 2.2% | 3.7% | 24% | 0% | 0% |

Table 6.14. MAPE on $P^{sat}$, $\Delta_{vap}H$, $c_{P,liq}^{sat}$, $v_{liq}^{sat}$, $v_c$, $T_c$, and $P_c$ as predicted by the *translated-consistent* PR and RK EoS with the updated parameters determined in this study.

In Table 6.14, the MAPEs on the critical temperature and critical pressure, which are necessarily zero, are reported to remind the reader that these errors are not null with EoS that do not satisfy the critical constraints, e.g., SAFT-type EoS. A proper prediction of the pure-component critical coordinates is, however, a prerequisite to accurately predict the global phase equilibrium diagrams (GPED) of binary systems [24,96].

### 6.6. Updated generalized Twu88 α-functions suitable for the *tc*-PR and *tc*-RK EoS

This section aims to update the generalized formulations for the *tc*-PR and *tc*-RK EoS. It is recalled that the interest of these formulations is that they can be applied to

components for which consistent Twu91 α-function parameters cannot be determined from experimental data since no vapor pressure data are available in the literature.

As explained in our previous paper [60], parameter *N* is set to 2 in order to work with the so-called Twu88 [35] α-function whereas *L* and *M* are correlated as second order polynomials with respect to the acentric factor $\omega$ (see Eq.(6.18)):

$$\begin{cases} \alpha(T_r) = T_r^{2(M-1)} \exp\left[L\left(1-T_r^{2M}\right)\right] \\ L(\omega) = L_1\omega^2 + L_2\omega + L_3 \\ M(\omega) = M_1\omega^2 + M_2\omega + M_3 \end{cases} \quad (6.18)$$

To update the polynomial expressions for parameters L and M, the 759 molecules that have simultaneously accurate correlations for the $P^{sat}$, $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ properties are used (see Table 6.11). The resulting expressions, for both the PR and RK CEoS, are:

$$PRCEoS: \begin{cases} L(\omega) = 0.0925\omega^2 + 0.6693\omega + 0.0728 \\ M(\omega) = 0.1695\omega^2 - 0.2258\omega + 0.8788 \end{cases} \quad (6.19)$$

$$RK\ CEoS: \begin{cases} L(\omega) = 0.0611\omega^2 + 0.7535\omega + 0.1359 \\ M(\omega) = 0.1709\omega^2 - 0.2063\omega + 0.8787 \end{cases} \quad (6.20)$$

As proposed by Le Guennec et al., a comparison of the MAPEs obtained with the following three α-functions is performed:

i. the component-dependent Twu91 α-function with the updated parameters determined in this paper,
ii. the updated generalized Twu88 α-function, and
iii. the Soave α-function.

Table 6.15 highlights that the 2 generalized α-functions, namely "generalized Twu88" and Soave have similar accuracy with, however, an advantage to the first one, especially when predicting $P^{sat}$ and $c_{P,liq}^{sat}$ with the PR EoS. Conversely, it is observed that the results are strongly improved if the deviations calculated for the gen. Twu88 α-function are compared with those calculated for the component-dependent Twu91 α-function. The conclusions are identical to those drawn previously and with the exception of molar volumes which are better correlated with the PR EoS, Table 6.15 does not make it possible to conclude which of the PR or RK EoS is the most accurate. Working with

the Soave α-function, the RK EoS is the best-suited but the reverse situation occurs when considering the Twu88 or Twu91 α-functions.

| **α**-function | Peng-Robinson | | | Redlich-Kwong | | |
|---|---|---|---|---|---|---|
| | Twu91 | gen. Twu88 | Soave | Twu91 | gen. Twu88 | Soave |
| MAPE on $P^{sat}$ (1721 compounds) | 1.0% | 1.8% | 2.8% | 1.2% | 2.1% | 2.3% |
| MAPE on $\Delta_{vap}H$ (1453 compounds) | 1.9% | 2.7% | 3.1% | 1.9% | 2.9% | 2.9% |
| MAPE on $c_{P,liq}^{sat}$ (829 compounds) | 2.0% | 4.1% | 7.1% | 2.2% | 4.3% | 5.3% |
| MAPE on $v_{liq}^{sat}$ (1489 compounds) ($T_r < 0.9$) | 2.2% | 2.2% | 2.2% | 3.7% | 3.8% | 3.8% |

Table 6.15. Comparison of the MAPEs calculated with the 3-parameter Twu91, generalized Twu88 and Soave α-functions for the translated PR and RK EoS.

Many process simulation software programs however express $cP_c / (RT_c)$ as a linear function of the Rackett compressibility factor ($z_{RA}$), appearing in the improvement of the original Rackett equation [42] proposed by Spencer and Danner [41]. In this study, it was decided to work with the 1489 compounds, for which $v_{liq}^{sat}$ can be accurately estimated. The obtained correlations are:

$$\begin{cases} c_{PR} = \dfrac{RT_c}{P_c}\left(0.1975 - 0.7325 z_{RA}\right) \\ c_{RK} = \dfrac{RT_c}{P_c}\left(0.2150 - 0.7314 z_{RA}\right) \end{cases} \tag{6.21}$$

With such correlations, MAPEs on $v_{liq}^{sat}$ data, over 1489 compounds modeled with the gen. Twu88 α-function, in a temperature range so that $T_r \leq 0.9$, coupled with the PR and RK EoS, are 3.0% and 4.0%, respectively.

To conclude this section, the updated correlations of volume-translation parameters to $\omega$ are presented below:

$$\begin{cases} c_{PR} = \dfrac{RT_c}{P_c}\left(0.0096 + 0.0048\omega\right) \\ c_{RK} = \dfrac{RT_c}{P_c}\left(0.0227 + 0.0093\omega\right) \end{cases} \quad (6.22)$$

We know by experience that these correlations are not very accurate but can be useful in the case where $T_c$, $P_c$ and $\omega$ are the unique data available for a given compound, which is often the case for the pseudo-components encountered in the oil and gas industry.

### 6.7. Conclusion

In this study, the suitable combinations of properties among vapor pressures, enthalpies of vaporization and saturated liquid heat capacities for fitting Twu91 α-function parameters were investigated. The study reveals that reliable (L, M, N) parameters are obtained if the fitting includes at least vapor pressure data. Fitting with only the enthalpies of vaporization and/or saturated liquid heat capacities are wholly inadvisable.

One thousand seven hundred twenty-one compounds, for which at least accurate vapor-pressure data could be generated, were found in the DIPPR database, and the 3 (L, M, N) parameters were determined for these fluids. Using these parameters, the *tc*-PR EoS leads to the following very small average deviations: $\Delta P^{sat} = 1\,\%$, $\Delta_{vap}H = \Delta c_{P,L}^{sat} = 2\,\%$ and $\Delta v_L^{sat}(T_r < 0.9) = 2.2\,\%$. Moreover, for the *tc*-PR and *tc*-RK CEoS to be applied to components not included in the DIPPR database, a generalized version of these models was developed. The 3-parameter Twu91 α-function was substituted by the 2-parameter Twu88 function, and the parameters L and M were correlated to the acentric factor.

In comparison with the previous work of Le Guennec et al. and as explained notably in sections 3.2 and 4.2, 52 molecules that were considered to be suitable by these authors for fitting α-function parameters were declared non-reliable in this study. The reject of these 52 molecules is justified as follows:

- for 34 molecules, no vapor pressure data were available (see section 3.2).
- For 14 molecules, the deviations between experimental and calculated properties were abnormally high so that such molecules were considered to be outliers (see section 4.2)

- 4 molecules (Ca, K, Li and LiI) are metals with critical temperature higher than 2000 K which we believe can not be seriously modeled by a CEoS.

In return, 661 new molecules were added to the library developed in this work.

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- At DOI: 10.1021/acs.jced.8b00640
- In Appendices A-1 and A-2

# Partie 2

# Étude des mélanges

# Chapitre 7. Mise au point de règles de mélange pour la modélisation des mélanges par une équation d'état cubique

## 7.1. Des règles de mélange classiques aux règles de mélange complexes

En vertu de la théorie à un fluide, l'équation d'état cubique appliquée à un mélange admet la même forme mathématique que lorsqu'elle est appliquée aux corps purs. Les deux paramètres des corps purs de l'équation d'état (covolume et paramètre attractif) doivent alors être remplacés par des paramètres caractéristique du mélange étudié. Dans une équation d'état cubique des mélanges, le covolume $b$ du mélange dépend de sa composition et le paramètre attractif $a$ du mélange dépend de sa composition (représentée par le vecteur $x$ des fractions molaires) ainsi que de sa température $T$. L'équation d'état, dans laquelle $v$ désigne le volume molaire du mélange, s'écrit alors :

$$P(T,v,x)=\frac{RT}{v-b(x)}-\frac{a(T,x)}{\left[v-r_1 b(x)\right]\left[v-r_2 b(x)\right]} \tag{7.1}$$

Les paramètres $r_1$ et $r_2$ sont les mêmes que pour les corps purs : l'équation de Van der Waals des mélanges est obtenue en choisissant $r_1=0$ et $r_2=0$, l'équation de Redlich-Kwong des mélanges est obtenue en choisissant $r_1=-1$ et $r_2=0$ tandis que l'équation de Peng-Robinson est obtenue en choisissant $r_1=-1-\sqrt{2}$ et $r_2=-1+\sqrt{2}$.

Pour paramétrer une équation d'état cubique des mélanges, on utilise des règles de mélange permettant d'exprimer les paramètres $a$ et $b$ du mélange en fonction des paramètres $a_i$ et $b_i$ des corps purs. Dans sa thèse, Van der Waals a proposé les règles de mélange suivantes (dites règles de mélange classiques ou règles de mélange de Van der Waals) [1] :

$$\begin{cases} a(T,x)=\sum_{i=1}^{N}\sum_{j=1}^{N}x_i x_j\sqrt{a_i(T)\times a_j(T)} \\ b(x)=\sum_{i=1}^{N}\sum_{j=1}^{N}x_i x_j\left(\frac{b_i+b_j}{2}\right)=\sum_{i=1}^{N}x_i b_i \end{cases} \tag{7.2}$$

Afin de gagner en flexibilité, il est habituel d'ajouter respectivement aux expressions de $a$ et $b$, des paramètres d'interaction binaires $k_{ij}$ et $l_{ij}$. Les expressions de $a$ et de $b$ s'écrivent alors :

$$\begin{cases} a(T,x) = \sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j \sqrt{a_i(T)\times a_j(T)}\left(1-k_{ij}\right) \\ b(x) = \sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j \left(\frac{b_i+b_j}{2}\right)\left(1-l_{ij}\right) \end{cases} \quad (7.3)$$

Les paramètres $k_{ij}$ et $l_{ij}$ peuvent être soit ajustés sur des données expérimentales, calculés par des corrélations ou autres méthodes plus avancées parfois prédictives. À titre d'exemple, le modèle PPR78 [23], pour lequel $l_{ij} = 0$, permet de prédire, à toute température, la valeur du paramètre $k_{ij}$ du mélange à partir de la seule connaissance de la structure chimique des molécules. Cependant, l'introduction d'une dépendance en température dans le paramètre $k_{ij}$ n'est pas suffisante pour représenter certains mélanges, en particulier ceux contenant des molécules très polaires et associées. Certaines expressions de $k_{ij}$ fonctions de la température et de la composition du mélange ont été proposées [121–123] mais ces expressions, non prédictives, sont principalement empiriques et donc peu fiables en extrapolation.

En parallèle de ces modèles de $k_{ij}$ dépendant de la température et éventuellement de la composition ont été développées des règles de mélange pour le paramètre $a/b$ déduites de la combinaison d'une équation d'état et de modèles empiriques ou théoriques dits de coefficient d'activité. Cette approche prétend combiner les avantages des deux types de modèles thermodynamiques : les équations d'état cubiques sont applicables à toute température, toute pression et toute composition mais peinent à représenter les mélanges contenant des molécules polaires et associées tandis que les modèles de coefficients d'activité les plus performants peuvent représenter les comportements de phases de mélanges polaires et associés mais ne sont applicables que sur le domaine des basses pressions.

Dans un premier temps, quelques modèles de coefficient d'activité seront détaillés afin de définir leurs avantages et leurs inconvénients par rapport aux équations d'état cubiques. Dans un second temps, les règles de mélange pour le paramètre $a$ d'Huron-

Vidal [98] et de MHV [124], utilisant des modèles de coefficient d'activité, seront établies. Les limitations de ces règles de mélange seront alors discutées, conduisant à définir de nouvelles règles de mélange.

### 7.2. Les modèles de coefficient d'activité

Les modèles de coefficient d'activité sont des expressions de l'énergie de Gibbs molaire d'excès, notée $g^E$ qui caractérisent la non-idéalité d'une solution liquide. Les différents modèles de $g^E$ qui ont été développés au cours du XXe siècle résultent d'approches semi-théoriques (et en particulier, de la thermodynamique statistique) ou empiriques.

Les modèles permettant de représenter les effets combinatoires, c'est-à-dire la non-idéalité causée par le mélange de molécules de tailles et formes différentes en solution sont d'abord présentés. Par souci de clarté, les modèles sont exprimés dans le cas des systèmes binaires. Si elles existent, leurs extensions à des mélanges contenant plus de composés sont disponibles dans les publications originales.

Les auteurs de ces modèles de coefficient d'activité se concentrant principalement sur la modélisation des liquides, l'hypothèse d'incompressibilité du fluide, judicieuse sous pression basse à modérée, a alors toujours été effectuée, conduisant ainsi à une indépendance des modèles de coefficient d'activité par rapport à la pression. Une conséquence est que le volume molaire d'excès calculé $\left(v^{E,\gamma} = \left(\partial g^{E,\gamma} / \partial P\right)_{T,x}\right)$ par les modèles de coefficient d'activité est toujours nul :

$$v^{E,\gamma} = 0 \tag{7.4}$$

Une conséquence est que les modèles de coefficient d'activité ne s'extrapolent pas de manière satisfaisante à haute pression où l'hypothèse d'incompressibilité du liquide est mise en défaut. Ainsi, les modèles de coefficient d'activité sont contraints à être utilisés dans le domaine des pressions basses à modérées.

*Remarque :* l'énergie de Helmholtz d'excès se déduit de celle de Gibbs d'excès par la relation :

$$a^{E,\gamma}(T,x) = g^{E,\gamma}(T,x) - P\underset{0}{v^{E,\gamma}} = g^{E,\gamma}(T,x) \tag{7.5}$$

Ainsi, tous les modèles d'énergie de Gibbs d'excès peuvent être identifiés à des modèles d'énergie d'Helmholtz d'excès. De plus, il a été observé expérimentalement que l'énergie d'Helmholtz d'excès, contrairement à l'énergie de Gibbs d'excès est quasiment invariante par rapport à la pression [125].

De plus, par définition de l'énergie de Gibbs d'excès, cette propriété peut être décomposée en un terme « combinatoire », associé à l'entropie d'excès du mélange, et un terme « résiduel », associé à l'enthalpie d'excès du mélange :

$$\underset{\text{terme résiduel/ enthalpique}}{g^E} \equiv \underset{\text{terme résiduel/ enthalpique}}{h^E} - T \times \underset{\text{terme combinatoire/ entropique}}{s^E} \tag{7.6}$$

La valeur du terme résiduel est proportionnelle aux différences d'interactions énergétiques entre les molécules en solution tandis que celle du terme combinatoire est proportionnelle aux différences de tailles et de formes des molécules du mélange. Il est alors commun de définir les quantité $g^E_{res} = h^E$ et $g^E_{comb} = -Ts^E$, permettant ainsi de réécrire l'équation (7.6) de la façon suivante :

$$g^E = g^E_{res} + g^E_{comb} \tag{7.7}$$

Puisque les termes $g^E_{res}$ et $g^E_{comb}$ représentent des effets physiques très différentes, il n'est étonnant de constater que des modèles de coefficient d'activité visant à reproduire les effets entropiques ont été développés indépendamment de ceux visant à la reproduction des effets enthalpiques.

### 7.2.1. Modèles de coefficient d'activité permettant la reproduction des effets entropiques

Le modèle de Flory-Huggins [126,127] est obtenu à partir de théories issues du domaine de la physique statistique. Ce modèle décrit les effets entropiques en solution. En tant que tel, ce modèle est donc principalement appliqué aux mélanges pour lesquels les effets enthalpiques sont négligeables tels que les mélanges de polymères. Ce modèle s'écrit :

$$\frac{g^{E,FH}_{comb}(T,x)}{RT} = x_1 \ln\left(\frac{\Phi_1}{x_1}\right) + x_2 \ln\left(\frac{\Phi_2}{x_2}\right) \tag{7.8}$$

Où $\Phi_i$ désigne la fraction volumique du composé $i$ calculée par la relation :

$$\Phi_i = \frac{x_i v_i^*}{\sum_{j=1}^{N} x_j v_j^*} \tag{7.9}$$

Dans cette expression, *N* désigne le nombre de composés du mélange et $x_i$ désigne la fraction molaire du composé $i$ .

Le caractère purement combinatoire de ce modèle se retrouve par l'absence de contribution enthalpique du modèle. En effet, par définition de l'entropie d'excès :

$$s_{comb}^{E,FH} = -\left(\frac{\partial g_{comb}^{E,FH}}{\partial T}\right) = -R\left[x_1 \ln\left(\frac{\Phi_1}{x_1}\right) + x_2 \ln\left(\frac{\Phi_2}{x_2}\right)\right] = -\frac{g_{comb}^{E,FH}}{T}$$

En combinant cette expression à la relation $g_{comb}^{E,FH} = h_{comb}^{E,FH} - Ts_{comb}^{E,FH}$ , il vient : $h_{comb}^{E,FH} = 0$ .

Les volumes molaires $v_i^*$ de l'équation (7.9) doivent donc être choisis constants pour ne pas introduire de contribution enthalpique (ou résiduelle) dans le modèle de Flory-Huggins.

D'autres expressions de la fraction volumique $\Phi_i$ ont été utilisées au fil des ans [128]. Il est commun d'introduire un volume adimensionnel dans l'équation (7.9) en divisant les volumes molaires des corps purs par celui d'une molécule de référence, par exemple celui du méthane. On a alors $r_i = v_i^* / v_{CH_4}$ et l'équation (7.9) devient :

$$\Phi_i = \frac{x_i r_i}{\sum_{j=1}^{N} x_j r_j} \tag{7.10}$$

Si les volumes molaires des corps purs sont inconnus, les paramètres $r_i$ peuvent être estimés par la méthode de contribution de groupes de Bondi [129]. Il a cependant été rapidement remarqué que l'équation (7.10) conduit à surestimer les effets combinatoires en solution.

Donohue et Prausnitz [130] ont alors proposé l'expression suivante :

$$\Phi_i = \frac{x_i \left(r_i\right)^{p_i}}{\sum_{j=1}^{N} x_j \left(r_j\right)^{p_j}} \tag{7.11}$$

Le paramètre $p_i$ doit être ajusté pour chaque composé du mélange. Une valeur universelle égale à 2/3, permettant une bonne représentation de mélanges d'alcanes aliphatiques, a été proposée par Kikic et al. [128]. Si les paramètres $p_i$ sont choisis égaux à 1, l'équation (7.10) est retrouvée.

On notera que la modification proposée par Donohue et Prausnitz est purement empirique. Une approche plus théorique issue du domaine de la thermodynamique statistique permet de fournir une expression corrigée du modèle de Flory-Huggins original. Ce modèle est celui de Staverman-Guggenheim. Le modèle de coefficient d'activité proposé est alors composé du modèle de Flory-Huggins original auquel un terme supplémentaire correctif, dit de Staverman-Guggenheim, est accolé :

$$\frac{g^E_{comb}(T,x)}{RT} = \overbrace{x_1 \ln\left(\frac{\Phi_1}{x_1}\right) + x_2 \ln\left(\frac{\Phi_2}{x_2}\right)}^{g^{E,FH}_{comb}/RT} + \overbrace{\frac{z}{2}\left[q_1 x_1 \ln\left(\frac{\theta_1}{\Phi_1}\right) + q_2 x_2 \ln\left(\frac{\theta_2}{\Phi_2}\right)\right]}^{g^{E,SG}_{comb}/RT} \tag{7.12}$$

La quantité $\theta_i$ est la fraction surfacique du composé $i$ et est calculée comme suit :

$$\theta_i = \frac{x_i q_i}{\sum_{j=1}^{N} x_j q_j} \tag{7.13}$$

À ce jour, les modèles de Flory-Huggins et de Staverman-Guggenheim sont les seuls termes combinatoires utilisés dans les modèles de coefficient d'activité. Cependant ces termes combinatoires permettent uniquement de représenter des systèmes pour lesquels les interactions énergétiques entre les molécules sont négligeables. Pour qu'un modèle de coefficient d'activité soit complet, et puisse représenter tous les types de mélanges, il est nécessaire d'ajouter une contribution résiduelle à la contribution combinatoire choisie. Cette contribution résiduelle est caractérisée par une dépendance en température que le terme combinatoire n'a pas.

### 7.2.2. Modèles de coefficient d'activité permettant la reproduction des effets enthalpiques et, parfois, entropiques

Proposé en 1895, le modèle de Margules constitue le premier modèle de coefficient d'activité permettant de modéliser des effets énergétiques (aussi qualifiés d'enthalpiques ou de résiduels) [131] :

$$\frac{g^{E,\text{Margules}}(T,x)}{RT} = A(T)x_1x_2 \tag{7.14}$$

Ce modèle est purement empirique mais a ouvert la voie à d'autres travaux. Quelques modèles importants sont analysés.

Le modèle de Van Laar [132] publié en 1910 dérive de l'équation d'état de Van der Waals. Pour un système binaire, ce modèle s'écrit :

$$\frac{g^{E,\text{Van Laar}}(T,x)}{RT} = x_1x_2 \times \frac{A_{21}(T)\times A_{12}(T)}{A_{12}(T)x_1 + A_{21}(T)x_2} \tag{7.15}$$

Les fonctions $A_{12}(T)$ et $A_{21}(T)$ sont choisies comme des fonctions de la température ayant un certain nombre de paramètres ajustables, permettant ainsi une représentation acceptable de la phase liquide d'un système [133]. Parmi les modèles dérivant de l'équation de Van der Waals, on peut aussi citer le modèle de Scatchard-Hildebrand [134].

A ces modèles dérivant de l'équation de Van der Waals, d'autres modèles obtenus à partir d'une approche statistique leur ont succédé. Ces modèles plus récents supposent que les molécules en phase liquide ne sont pas distribuées aléatoirement dans le fluide mais que ces dernières se regroupent par affinité. On parle alors de concept de *composition locale*. Ainsi, ces modèles permettent une représentation plus réaliste des phénomènes physiques pouvant se produire dans un liquide.

Les modèles de coefficient d'activité les plus connus dérivant de cette approche sont les modèles de Wilson [99], le modèle NRTL [135] ainsi que le modèle UNIQUAC [136], dont le modèle UNIFAC [137] est une version prédictive.

Le modèle de *Wilson* s'écrit [99] :

$$\begin{cases} \dfrac{g^{E,Wilson}(T,x)}{RT} = -x_1 \ln\left(x_1 + x_2\Lambda_{12}\right) - x_2 \ln\left(x_2 + x_1\Lambda_{21}\right) \\ \Lambda_{ij} = \dfrac{v_j^*}{v_i^*} \exp\left(-\dfrac{\lambda_{ij} - \lambda_{ii}}{RT}\right) \end{cases} \tag{7.16}$$

Le paramètres $\lambda_{ij}$ quantifie les interactions énergétiques entre l'espèce $i$ et l'espèce $j$. Ce modèle contient à la fois une contribution résiduelle et une contribution combinatoire, bien que cette dernière ne soit pas explicite dans l'équation (7.16). Afin d'isoler la contribution combinatoire, on annule les effets de non idéalité liés aux différences d'interactions énergétiques entre les molécules en posant $\lambda_{ij} = \lambda_{ji} = \lambda_{ii} = \lambda_{jj}$. On obtient alors un terme combinatoire identique à celui de Flory-Huggins :

$$\frac{g^E_{comb}(T,x)}{RT} = \frac{g^{E,FH}_{comb}(T,x)}{RT} = x_1 \ln\left(\frac{\Phi_1}{x_1}\right) + x_2 \ln\left(\frac{\Phi_2}{x_2}\right) \tag{7.17}$$

La fraction de volume est calculée par l'équation (7.9). Une fois ce terme injecté dans l'équation (7.16), on obtient alors la décomposition suivante du modèle de Wilson :

$$\begin{aligned} \frac{g^{E,\text{Wilson}}(T,x)}{RT} = & \overbrace{\left[x_1 \ln\left(\frac{\Phi_1}{x_1}\right) + x_2 \ln\left(\frac{\Phi_2}{x_2}\right)\right]}^{g^{E,\text{Wilson}}_{comb}/RT = g^{E,\text{FH}}_{comb}/RT} \\ & \underbrace{+\left[-x_1\left[\Phi_1 + \Phi_2 \exp\left(-\frac{\lambda_{12} - \lambda_{21}}{RT}\right)\right] - x_2\left[\Phi_2 + \Phi_2 \exp\left(-\frac{\lambda_{21} - \lambda_{12}}{RT}\right)\right]\right]}_{g^{E,\text{Wilson}}_{res}/RT} \end{aligned} \tag{7.18}$$

Un autre modèle fréquemment rencontré dans la littérature est le modèle NRTL. Il s'écrit [135] :

$$\begin{cases} \dfrac{g^{E,NRTL}(T,x)}{RT} = \overbrace{x_1 x_2\left(\dfrac{\tau_{21}G_{21}}{x_1 + x_2 G_{21}} + \dfrac{\tau_{12}G_{12}}{x_2 + x_1 G_{12}}\right)}^{g^{E,\text{NRTL}}_{res}/RT} \\ \tau_{ij} = \dfrac{g_{ij} - g_{jj}}{RT} \\ G_{ij} = \exp\left(-\alpha_{ij}\tau_{ij}\right) \end{cases} \tag{7.19}$$

Ce modèle possède uniquement un terme résiduel car $g^{E,NRTL} = 0$ si l'on pose $g_{ij} = g_{jj} = g_{ji} = g_{ii}$ , les paramètres $g_{ij}$ étant les paramètres d'interactions

énergétiques entre les molécules *i* et *j*. Les paramètres $\alpha_{ij}$ sont des paramètres ajustables révélateurs de la déviation de la phase liquide à un état hypothétique où les molécules seraient réparties de manière aléatoire dans la phase liquide. Si l'on pose $\alpha_{ij}=0$, le modèle de Margules est retrouvé. Par défaut, il est recommandé de poser $\alpha_{ij}=0.3$, tout en sachant que ce paramètre varie généralement dans l'intervalle $[0.2;0.47]$ [138].

Enfin, le modèle *UNIQUAC* s'écrit [136] :

$$\frac{g^{E,\mathrm{UNIQUAC}}}{RT}=\overbrace{\overbrace{x_1\ln\left(\frac{\Phi_1}{x_1}\right)+x_2\ln\left(\frac{\Phi_2}{x_2}\right)}^{g_{comb}^{E,\mathrm{FH}}/RT}+\overbrace{\frac{z}{2}\left[q_1x_1\ln\left(\frac{\theta_1}{\Phi_1}\right)+q_2x_2\ln\left(\frac{\theta_2}{\Phi_2}\right)\right]}^{g_{comb}^{E,\mathrm{SG}}/RT}}^{g_{comb}^{E,\mathrm{UNIQUAC}}/RT}+\underbrace{\left[-q_1x_1\ln\left(\theta_1+\theta_2\tau_{21}\right)-q_2x_2\ln\left(\theta_2+\theta_1\tau_{12}\right)\right]}_{g_{res}^{E,\mathrm{UNIQUAC}}/RT} \quad (7.20)$$

Le terme combinatoire utilisé dans le modèle UNIQUAC est le terme de Flory-Huggins corrigé par le terme de Staverman-Guggenheim (cf. équation (7.12)). L'équation (7.10) est quant à elle utilisée pour calculer les fractions volumiques. Les paramètres $r_i$ et $q_i$ étant estimés par la méthode de Bondi [129] aucun terme ajustable n'est présent dans la partie combinatoire du modèle UNIQUAC.

### 7.2.3. Des modèles de coefficient d'activité aux règles de mélange avancées pour l'équation d'état cubique

Les équations d'état cubiques peuvent prédire les régions subcritiques, critiques et supercritiques des diagrammes de phases mais ne permettent pas de représenter de manière satisfaisante les propriétés thermodynamiques de certains mélanges complexes (contenant des molécules fortement polaires et associées).

Les modèles de coefficient d'activité, limités au domaine des pressions basses à modérées, permettent une représentation satisfaisante des liquides complexes. Lorsqu'ils sont combinés à une équation d'état pour la phase gaz, il n'est possible de décrire les équilibres liquide-vapeur des mélanges que sous basse pression car cette approche ne permet ni de prédire les phénomènes critiques liquide-vapeur, ni les états supercritiques.

Une idée alors développée par Huron et Vidal [98] puis reprise, entre autres, par Michelsen [124] consiste à utiliser un modèle de coefficient d'activité pour définir la règle de mélange pour le paramètre $a/b$ de l'équation d'état cubique. De cette manière, les auteurs espèrent combiner les points forts respectifs des modèles de coefficient d'activité et des équations d'état cubiques afin de représenter de manière satisfaisante des mélanges complexes sur tout le domaine de température, pression et composition.

La méthode choisie par ces deux auteurs a consisté à égaler l'expression mathématique de l'énergie de Gibbs d'excès issue d'un modèle de coefficient d'activité ( $g^{E,\gamma} = a^{E,\gamma}$ ) à celle de l'énergie de Gibbs d'excès calculée à partir d'une équation d'état cubique dont l'expression est la suivante (cf. Annexe) :

$$\begin{aligned} g^{E,\varphi}(T,P,x) = RT\sum_{i=1}^{N} x_i \ln\left(\frac{v_i^* - b_i}{v-b}\right) \\ -\frac{a}{b(r_1-r_2)}\times\ln\left(\frac{v-r_2 b}{v-r_1 b}\right) + \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i(r_1-r_2)}\times\ln\left(\frac{v_i^* - r_2 b_i}{v_i^* - r_1 b_i}\right) \\ \underbrace{+P\left(v - \sum_{i=1}^{N} x_i \times v_i^*\right)}_{Pv^{E,\varphi}} \end{aligned} \quad (7.21)$$

Les contributions combinatoires et résiduelles de l'équation d'état sont identifiées de la manière suivante :

$$g^{E,\varphi}(T,P,x) = a_{comb}^{E,\varphi}(T,P,x) + a_{res}^{E,\varphi}(T,P,x) + Pv^{E,\varphi} \quad (7.22)$$

Avec :

$$\begin{cases} a_{comb}^{E,\varphi} = RT\sum_{i=1}^{N} x_i \ln\left(\frac{v_i^* - b_i}{v-b}\right) \\ a_{res}^{E,\varphi} = -\frac{a}{b(r_1-r_2)}\times\ln\left(\frac{v-r_2 b}{v-r_1 b}\right) + \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i(r_1-r_2)}\times\ln\left(\frac{v_i^* - r_2 b_i}{v_i^* - r_1 b_i}\right) \end{cases} \quad (7.23)$$

### 7.3. Les règles de mélange pour le paramètre $a/b$

Le point de départ des règles de mélange de Huron-Vidal et de Michelsen est l'égalité entre l'expression de l'énergie de Gibbs d'excès venant de l'équation d'état cubique (équation (7.21)) dépendant de la température, de la pression et de la composition du système et celle issue des modèles de coefficient d'activité dépendant uniquement de

la température et de la composition. Pour réaliser l'égalité de ces deux expressions, il est alors nécessaire de fixer la pression dans l'équation (7.21) à une pression de référence $P^{ref}$ . On écrira alors :

$$\lim_{P \to P^{ref}} g^{E,\varphi}(T,P,x) = g^{E,\gamma}(T,x) \tag{7.24}$$

Cette égalité constitue le point de départ des règles de mélange de Huron-Vidal et MHV-1.

### 7.3.1. La règle de mélange de Huron-Vidal

La règle de mélange de Huron-Vidal [98] est obtenue en imposant une pression de référence infinie. L'équation (7.24) se réécrit alors :

$$\lim_{P \to +\infty} g^{E,\varphi}(T,P,x) = g^{E,\gamma}(T,x) \tag{7.25}$$

L'équation (7.21) doit alors être évaluée lorsque la pression est infinie. Une première conséquence est que le volume molaire et les volumes molaires des corps purs tendent respectivement vers le covolume du mélange et les covolumes des corps purs :

$$\begin{cases} \lim_{P \to \infty} v = b \\ \lim_{P \to \infty} v_i^* = b_i \end{cases} \tag{7.26}$$

L'équation (7.21) devient alors :

$$\begin{aligned} \lim_{P \to +\infty} g^{E,\varphi}(T,P,x) = RT \times \lim_{P \to +\infty} \sum_{i=1}^{N} x_i \overbrace{\ln\left(\frac{v_i^* - b_i}{v-b}\right)}^{F_1} \\ - \frac{1}{r_1 - r_2} \times \ln\left(\frac{1-r_2}{1-r_1}\right) \times \left(\frac{a}{b} - \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i}\right) \\ + \lim_{P \to +\infty} \underbrace{P\left(v - \sum_{i=1}^{N} x_i \times v_i^*\right)}_{F_2} \end{aligned} \tag{7.27}$$

Afin de simplifier l'équation (7.27), il faut remarquer que l'équation d'état cubique des mélanges permet d'écrire la relation suivante pour $v-b$ :

$$P=\frac{RT}{v-b}-\frac{a}{(v-r_1b)(v-r_2b)}\Rightarrow v-b=\frac{1}{\frac{P}{RT}+\frac{a}{RT}\times\frac{1}{(v-r_1b)(v-r_2b)}} \tag{7.28}$$

Pour les corps purs, une expression analogue est obtenue pour la quantité $v_i-b_i$ :

$$P=\frac{RT}{v_i^*-b_i}-\frac{a_i}{(v_i^*-r_1b_i)(v_i^*-r_2b_i)}\Rightarrow v_i^*-b_i=\frac{1}{\frac{P}{RT}+\frac{a_i}{RT}\times\frac{1}{(v_i^*-r_1b_i)(v_i^*-r_2b_i)}} \tag{7.29}$$

En combinant les équations (7.28) et (7.29), le terme $F_1$ peut être réécrit de la manière suivante :

$$\ln\left(\frac{v_i^*-b_i}{v-b}\right)=\ln\left(\frac{1}{\frac{P}{RT}+\frac{a_i}{RT}\times\frac{1}{(v_i^*-r_1b_i)(v_i^*-r_2b_i)}}\times\frac{\frac{P}{RT}+\frac{a}{RT}\times\frac{1}{(v-r_1b)(v-r_2b)}}{1}\right) \tag{7.30}$$

Par sommation et passage à la limite :

$$\lim_{P\to+\infty}\sum_{i=1}^{N}x_i\ln\left(\frac{v_i^*-b_i}{v-b}\right)=\sum_{i=1}^{N}x_i\times\ln 1=0 \tag{7.31}$$

La comparaison entre les équations (7.31) et (7.23), montre que sous pression infinie l'énergie de Gibbs d'excès combinatoire de l'équation d'état cubique $g_{comb}^{E,\varphi}$ est nulle :

$$\lim_{P\to+\infty}g_{comb}^{E,\varphi}=0 \tag{7.32}$$

La forme indéterminée $F_2$ se réécrit :

$$\begin{aligned}F_2&=P\left(v-\sum_{i=1}^{N}x_i\times v_i^*\right)\\&=P\left(b-\sum_{i=1}^{N}x_ib_i\right)+P\left((v-b)-\sum_{i=1}^{N}x_i\times\left(v_i^*-b_i\right)\right)\end{aligned} \tag{7.33}$$

Afin que le valeur de $F_2$ reste finie à pression infinie, les auteurs choisissent une règle de mélange linéaire pour le covolume du mélange :

$$b = \sum_{i=1}^{N} x_i b_i \tag{7.34}$$

Par utilisation des équations (7.28) et (7.29), l'équation (7.33) devient alors :

$$F_2 = \frac{1}{\frac{1}{RT} + \frac{a}{PRT} \times \frac{1}{(v - r_1 b)(v - r_2 b)}} - \sum_{i=1}^{N} x_i \times \frac{1}{\frac{1}{RT} + \frac{a_i}{PRT} \times \frac{1}{\left(v_i^* - r_1 b_i\right)\left(v_i^* - r_2 b_i\right)}} \tag{7.35}$$

Ainsi en faisant tendre la pression vers l'infini :

$$\lim_{P \to +\infty} F_2 = \lim_{P \to +\infty} P v^{E,\varphi} = RT - \sum_{i=1}^{N} x_i \times RT = 0 \tag{7.36}$$

Si la règle de mélange sur $b$ n'avait pas été choisie linéaire on aurait eu $\lim_{P \to +\infty} F_2 = +\infty$ ,rendant impossible la suite de l'identification des termes de $g^E$ .

Tous calculs faits, l'équation (7.27) devient :

$$\lim_{P \to +\infty} g^{E,\varphi}(T,P,x) = -\frac{1}{r_1 - r_2} \times \ln\left(\frac{1 - r_2}{1 - r_1}\right) \times \left(\frac{a}{b} - \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i}\right) \tag{7.37}$$

Sachant que l'on impose $\lim_{P \to +\infty} g^{E,\varphi}(T,P,x) = g^{E,\gamma}(T,x)$ , on peut alors réécrire l'équation (7.37) sous la forme :

$$\left(\frac{a}{b}\right)_{P \to +\infty} = \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i} + \frac{g^{E,\gamma}(T,x)}{C} \text{ avec } \begin{cases} C = -\frac{1}{r_1 - r_2} \times \ln\left(\frac{1 - r_2}{1 - r_1}\right) \\ b = \sum_{i=1}^{N} x_i b_i \end{cases} \tag{7.38}$$

Le système d'équations (7.38) permet de déterminer une expression explicite du paramètre *a* du mélange et est connu sous le nom de règles de mélange de Huron-Vidal. Dans leur publication originale, le modèle de coefficient d'activité utilisé est le modèle NRTL (cf. équation (7.19)).

Comme représenté sur la Figure 7.1, cette règle de mélange permet une nette amélioration de la représentation de systèmes binaires qui étaient auparavant modélisés par une équation d'état cubique utilisant les règles de mélange de Van der

Waals [98]. Comme expliqué par les auteurs, les paramètres du modèle NRTL doivent être redéterminés spécifiquement pour les règles de mélange de Huron-Vidal.

On peut démontrer que les règles de mélange du modèle PPR78 sont équivalentes à celles de Huron-Vidal lorsqu'un modèle de coefficient d'activité de Van Laar est utilisé. En effet, pour un système multi constituants, le modèle de Van Laar s'écrit :

$$\frac{g^{E,\text{Van Laar}}(T,x)}{RT} = C \times \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j b_i b_j E_{ij}(T,x)}{2\sum_{j=1}^{N} x_j b_j} \tag{7.39}$$

Avec $E_{ij}$ une fonction mathématique complexe dépendant de la composition et de la température du mélange mais aussi de la décomposition des molécules du mélange en sous-groupes élémentaires.

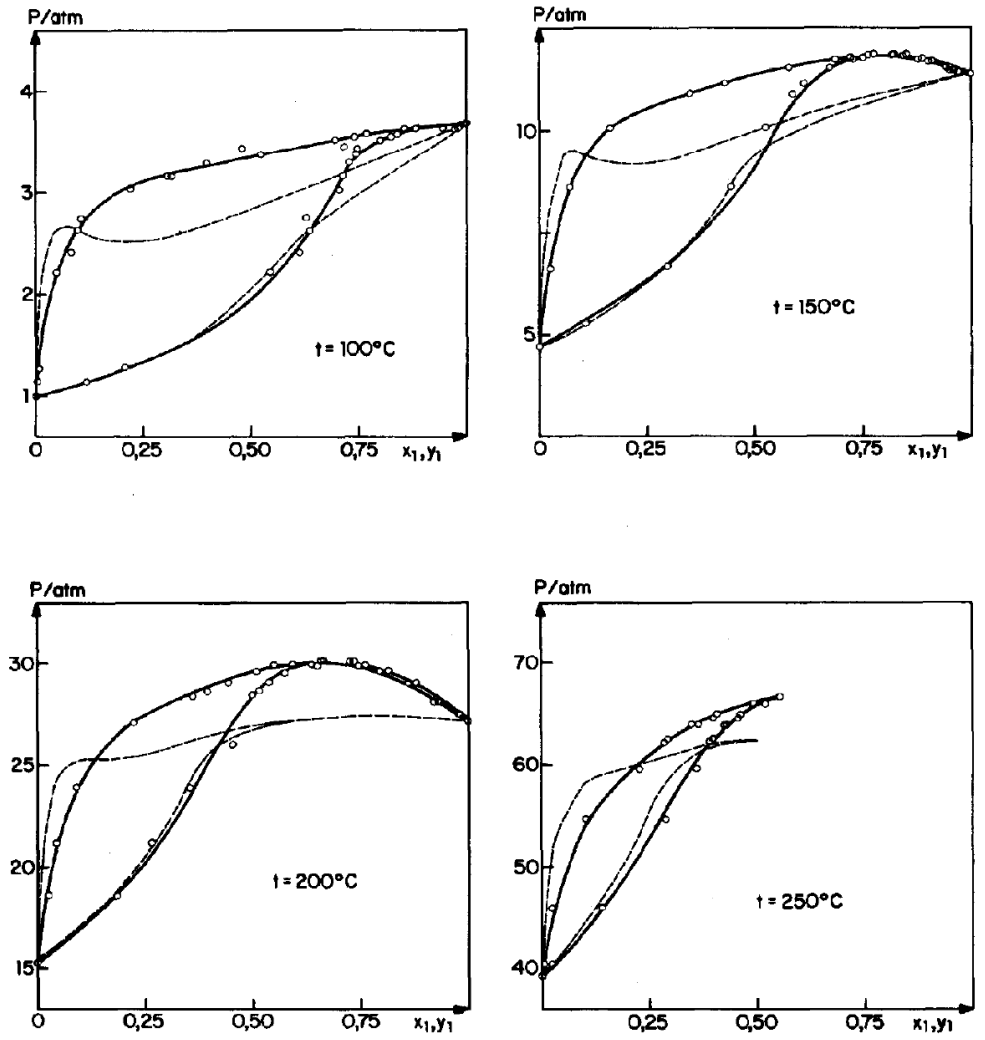



Figure 7.1. Modélisation du système binaire eau-acétone. Les cercles représentent les points expérimentaux, les courbes en pointillés correspondent à la modélisation obtenue lorsque les règles de mélange de Van der Waals sont utilisées dans l'équation d'état tandis que les traits pleins correspondent à la modélisation obtenue lorsque la règle de mélange de Huron-Vidal utilisant le modèle de coefficient d'activité NRTL est employée [98].

On peut alors montrer que le paramètre d'interaction binaire utilisé dans le modèle PPR78 s'écrit :

$$k_{ij}^{PPR78}(T,x) = \frac{E_{ij}(T,x) - \left(\frac{\sqrt{a_i(T)}}{b_i} - \frac{\sqrt{a_j(T)}}{b_j}\right)^2}{2 \times \frac{\sqrt{a_i(T)}}{b_i} \times \frac{\sqrt{a_j(T)}}{b_j}} \tag{7.40}$$

La règle de mélange sur le paramètre $b$ du modèle PPR78 étant linéaire, la contrainte imposée par la règle de mélange de Huron-Vidal est respectée. Finalement, on peut écrire :

$$\left(\frac{a}{b}\right)_{PPR78} = \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j \sqrt{a_i a_j}\left(1-k_{ij}^{PPR78}\right)}{\sum_{i=1}^{N} x_i b_i} = \sum_{i=1}^{N} x_i \frac{a_i}{b_i} + \frac{g^{E,\text{Van Laar}}(T,x)}{C} = \left(\frac{a}{b}\right)_{HV} \tag{7.41}$$

### 7.3.2. La règle de mélange MHV

La règle de mélange de Huron-Vidal présente l'inconvénient de ne pas permettre de réutiliser les paramètres des modèles de coefficient d'activité ajustés à basse pression puisque le raccordement entre les modèles a été effectué à pression infinie. Ceci est particulièrement problématique, car à l'époque du développement de la règle de mélange de Huron-Vidal, des campagnes de compilation des paramètres optimaux à basse pression des modèles de coefficient d'activité avaient été initiées par la DECHEMA, rendant ce travail inutilisable. À propos des équations d'état cubiques utilisant les règles de mélange de Huron-Vidal, Michelsen écrit [139] : « The resulting model was capable of correlating high temperature phase equilibrium but could not directly utilize parameter tables from existing $g^E$ models, correlated from low temperature data. » Michelsen [124] a donc proposé en 1990 une nouvelle règle de mélange établie à partir du raccordement des modèles à pression nulle dans l'espoir de pouvoir utiliser les paramètres tabulés des modèles de coefficient d'activité.

#### 7.3.2.1. Règle de mélange MHV implicite

Sous pression nulle on impose que $\lim_{P\to 0} g^{E,\varphi}(T,P,x) = g^{E,\gamma}(T,x)$. L'équation (7.21) devient alors :

$$g^{E,\gamma}(T,x) = \lim_{P\to 0} RT\sum_{i=1}^{N} x_i \ln\left(\frac{v_i^* - b_i}{v-b}\right) + \lim_{P\to 0}\left[-\frac{a}{b(r_1-r_2)}\times\ln\left(\frac{v-r_2 b}{v-r_1 b}\right) + \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i(r_1-r_2)}\times\ln\left(\frac{v_i^* - r_2 b_i}{v_i^* - r_1 b_i}\right)\right] \tag{7.42}$$

Le terme $P\left(v-\sum x_i \times v_i^*\right)$ ayant conduit Huron et Vidal à supposer une règle de mélange linéaire pour $b$ disparaît naturellement en faisant tendre la pression vers 0, libérant ainsi le paramètre $b$ de cette contrainte.

Sous pression nulle et pour une valeur de température donnée, l'équation d'état cubique des mélanges s'écrit :

$$0=\frac{RT}{v-b}-\frac{a}{(v-r_1 b)(v-r_2 b)} \tag{7.43}$$

L'équation (7.43) peut alors se réécrire sous forme polynomiale :

$$v^2-\left(\frac{a}{bRT}+r_1+r_2\right)bv+b^2\left(r_1 r_2+\frac{a}{bRT}\right)=0 \tag{7.44}$$

Le discriminant de l'équation (7.44) est :

$$\Delta=b^2\times\left[\left(\frac{a}{bRT}+r_1+r_2\right)^2-4\left(r_1 r_2+\frac{a}{bRT}\right)\right] \tag{7.45}$$

Ce polynôme étant de degré 2, il est alors possible de calculer :

- Une racine liquide métastable sous pression nulle ($v_{liq,0}$) et une racine instable sous pression nulle ($v_{ins,0}$), éventuellement confondues, si $\Delta \geq 0$
- Aucune racine si $\Delta < 0$

La même méthode de résolution que pour l'équation d'état cubique pour les corps purs est possible et permet de calculer des valeurs de $v_{i,liq,0}^*$ et $v_{i,ins,0}^*$ pour chaque composé. Définissons les grandeurs adimensionnelles suivantes : $\Gamma = a/(bRT)$, $\Gamma_i = a_i/(b_i RT)$, $\eta_0 = b/v_{liq,0}$ et $\eta_{i,0}^* = b_i/v_{i,liq,0}^*$. Les volumes molaires des corps purs et des mélanges peuvent être exprimés de la manière suivante :

$$\begin{cases} \eta_0 = \dfrac{b}{v_{liq,0}} = \eta(a/(bRT)) = \eta(\Gamma) \\ \eta_{i,0}^* = \dfrac{b_i}{v_{i,liq,0}^*} = \eta(a_i/(b_i RT)) = \eta(\Gamma_i) \end{cases} \tag{7.46}$$

Avec $\eta(x)$ la fonction suivante :

$$\eta(x)=\left[\frac{x+r_1+r_2-\sqrt{(x+r_1+r_2)^2-4(r_1r_2+x)}}{2}\right]^{-1} \tag{7.47}$$

L'équation (7.42) ne peut donc être écrite que s'il est possible de calculer au moins un volume molaire pour le mélange ainsi que pour tous les corps purs sous pression nulle et à la température choisie. Les modèles de coefficient d'activité s'appliquant aux phases liquides, Michelsen choisit que les volumes molaires utilisés dans l'équation (7.42) soient les volumes molaires liquides métastables.

L'équation (7.42) se réécrit donc :

$$\begin{aligned} &g^{E,\gamma}(T,x)= \\ &RT\sum_{i=1}^{N}x_i\ln\left[\frac{b_i}{b}\cdot\frac{\eta(\Gamma)}{\eta(\Gamma_i)}\cdot\frac{1-\eta(\Gamma_i)}{1-\eta(\Gamma)}\right] \\ &+\left[-\frac{a}{b(r_1-r_2)}\times\ln\left[\frac{1-\eta(\Gamma)r_2}{1-\eta(\Gamma)r_1}\right]+\sum_{i=1}^{N}x_i\times\frac{a_i}{b_i(r_1-r_2)}\times\ln\left[\frac{1-\eta(\Gamma_i)r_2}{1-\eta(\Gamma_i)r_1}\right]\right] \end{aligned} \tag{7.48}$$

À température et composition fixées, l'équation (7.48) constitue une règle de mélange implicite pour le paramètre $\Gamma = a/(bRT)$. Si l'on suppose connue la règle de mélange sur le paramètre $b$, l'équation (7.48) constitue une règle de mélange implicite pour le paramètre $a$ dont c'est l'unique inconnue. Une procédure de résolution itérative permet de déterminer la valeur de $a$ solution de cette équation à température, pression et composition fixées.

Cependant, cette procédure présente les inconvénients suivants :

- La procédure de calcul de $a$ est itérative et peut donc être couteuse en temps de calcul.
- L'équation (7.48) ne peut être résolue que s'il existe une racine liquide à pression nulle, c'est-à-dire que l'inégalité $\Delta \geq 0$ est vérifiée. Cette inégalité étant vérifiée à basse température, la règle de mélange implicite de Michelsen ne peut donc pas être utilisée à haute température.

#### 7.3.2.2. Approximation de la règle de mélange MHV permettant de la rendre explicite : règle de mélange MHV-1

Face à ces limitations, Michelsen a proposé une variante de cette règle de mélange contournant ces défauts.

L'équation (7.48) peut alors se réécrire :

$$\begin{cases} \dfrac{g^{E,\gamma}(T,x)}{RT} = \displaystyle\sum_{i=1}^{N} x_i \ln\left(\frac{b_i}{b}\right) + Q(\Gamma) - \sum_{i=1}^{N} x_i Q(\Gamma_i) \\ Q(x) = -\ln\left[\dfrac{1-\eta(x)}{\eta(x)}\right] - \dfrac{x}{r_1 - r_2} \times \ln\left[\dfrac{1-r_2\eta(x)}{1-r_1\eta(x)}\right] \end{cases} \tag{7.49}$$

Michelsen a remarqué que la fonction $Q$ est approximativement affine. Cette représentation est faite sur la Figure 7.2.

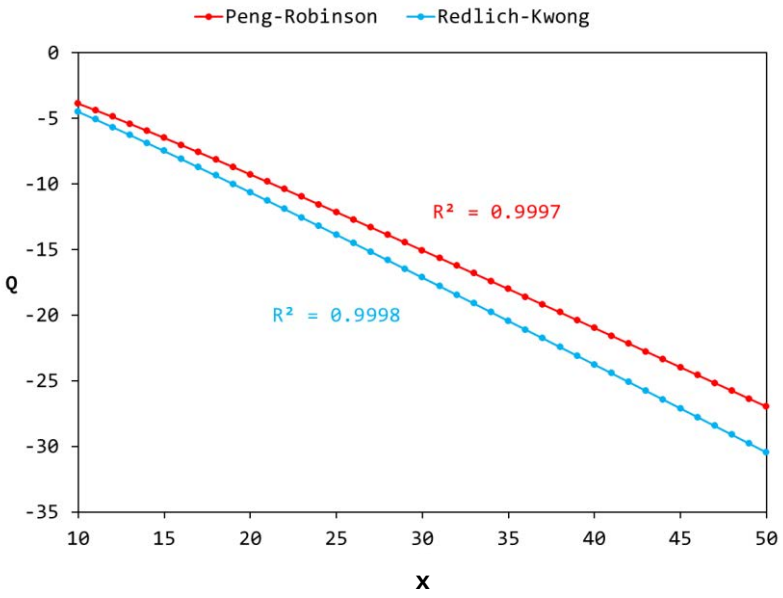



Figure 7.2. Représentation de la fonction $Q$ pour les modèles de Peng-Robinson et de Redlich-Kwong.

La fonction $Q$ est alors approximée par une fonction affine selon l'expression :

$$Q(x) = q_0 + x q_1 \tag{7.50}$$

Si l'on combine les équations (7.49) et (7.50), on obtient alors :

$$\begin{aligned} \frac{g^{E,\gamma}(T,x)}{RT} &= \sum_{i=1}^{N} x_i \ln\left(\frac{b_i}{b}\right) + q_0 + \Gamma q_1 - \sum_{i=1}^{N} x_i \left(q_0 + \Gamma_i q_1\right) \\ &= \sum_{i=1}^{N} x_i \ln\left(\frac{b_i}{b}\right) + \Gamma q_1 - q_1 \sum_{i=1}^{N} x_i \Gamma_i \end{aligned} \tag{7.51}$$

En substituant $\Gamma$ par $a/(bRT)$ et $\Gamma_i$ par $a_i/(b_i RT)$ la règle de mélange finalement obtenue s'écrit :

$$\left(\frac{a}{b}\right)_{\text{MHV-1}} = \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i} + \frac{1}{q_1}\left[ g^{E,\gamma} - RT \sum_{i=1}^{N} x_i \ln\left(\frac{b_i}{b}\right)\right] \qquad (7.52)$$

L'équation (7.52) constitue la règle de mélange MHV-1 (pour Modified Huron-Vidal combinée à une approximation de la fonction $Q$ par un polynôme de degré 1). Ce nom a été choisi par Michelsen à cause des similitudes pouvant exister entre sa règle de mélange et celle de Huron et Vidal. Cette règle de mélange, bien que relativement similaire à celle de Huron-Vidal, présente les différences suivantes :

- Apparition d'un terme $\sum x_i \ln(b_i / b)$ assimilé à un terme combinatoire, car très similaire à celui de Flory-Huggins (cf. équation (7.8)). En effet, pour une phase liquide $v \approx b$ et $v_i \approx b_i$ donc :

$$\sum x_i \ln(b_i / b) \approx \sum x_i \ln(v_i^* / v) = \sum x_i \ln(\Phi_i / x_i) = g_{comb}^{E,\text{FH}} / RT \qquad (7.53)$$

- La règle de mélange sur le paramètre $b$ peut être choisie librement.
- La valeur du coefficient pondérant le terme $g^{E,\gamma}$ (l'inverse du paramètre $q_1$ pour MHV-1) est obtenue par régression linéaire de la fonction $Q$ et ne résulte pas d'une expression analytique comme c'est le cas pour la règle de mélange de Huron-Vidal. Les valeurs de $q_1$ varient en fonction de l'équation d'état utilisée ainsi que du domaine de $x$ utilisé pour la régression. Michelsen ayant réalisé la régression linéaire de $Q(x)$ pour des valeurs de $x$ comprises entre 10 et 13 il obtient les valeurs suivantes des paramètres $q_1$ (les valeurs de $q_0$ ne sont pas indiquées, car elles n'interviennent pas dans l'expression finale de la règle de mélange) :

$$\begin{cases} q_{1,SRK} = -0.593 \\ q_{1,PR} = -0.53 \end{cases} \qquad (7.54)$$

Comme illustré sur la Figure 7.3, la règle de mélange MHV-1 permet donc d'utiliser les paramètres des modèles de coefficient d'activité tabulés dans les tables de la DECHEMA dans l'équation d'état cubique sans dégradation des résultats.

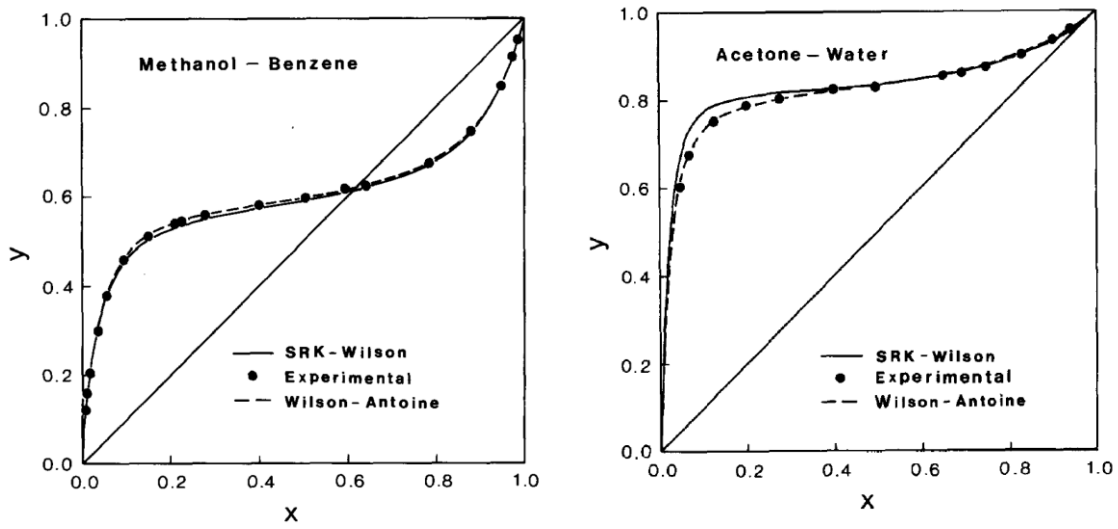



Figure 7.3. Plans xy à 0.99 bar des systèmes binaires méthanol-benzène (à gauche) et eau-acétone (à droite). Le modèle SRK-Wilson correspond au modèle SRK utilisant la règle de mélange MHV-1 dans laquelle le modèle de coefficient d'activité de Wilson est intégré ( $g^{E,\gamma} = g^{E,WILSON}$ ) et une règle de mélange linéaire sur le paramètre $b$ est utilisée. En comparaison, le modèle Wilson-Antoine combine un modèle de coefficient d'activité de type Wilson pour la phase liquide, une équation d'Antoine pour les pressions de vapeur saturante des corps purs et la loi des gaz parfaits pour la phase gaz. Le modèle Wilson-Antoine n'utilise donc pas d'équation d'état cubique. Les mêmes coefficients d'interactions binaires du modèle de Wilson sont utilisés dans les modèles SRK-Wilson et Wilson-Antoine, démontrant ainsi la capacité de l'équation d'état cubique ainsi paramétrée à reproduire les résultats du modèle de coefficient d'activité à basse pression. [124]

Les points communs et différences entre les règles de mélange de Huron-Vidal et MHV-1 sont compilés dans le Tableau 7.1 .

### 7.3.3. Problèmes soulevés par l'identification des énergies de Gibbs d'excès de l'équation d'état et des modèles de coefficient d'activité

Pour des mélanges dans lesquels les effets entropiques sont prédominants (molécules de tailles très différentes et peu d'interactions énergétiques entre les molécules), il a été observé que les règles de mélange de Huron-Vidal et de MHV-1 donnent de meilleurs résultats lorsque les différentes contributions combinatoires sont supprimées [140]. Les règles de mélange de Huron-Vidal et MHV-1 ont été modifiées par différents auteurs pour aboutir aux expressions suivantes :

$$\begin{cases} \left(\frac{a}{b}\right)_{\substack{\text{modification de } HV \\ \text{proposée par certains auteurs}}} = \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i} + \frac{g_{res}^{E,\gamma}}{C} \\ \left(\frac{a}{b}\right)_{\substack{\text{modification de MHV-1} \\ \text{proposée par certains auteurs}}} = \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i} + \frac{g_{res}^{E,\gamma}}{q_1} \end{cases} \quad (7.55)$$

La règle de mélange modifiée de Huron-Vidal est utilisée dans le modèle PPR78 [23] tandis que la règle de mélange MHV-1 modifiée est utilisée dans les modèles VTPR [141] et NRTL-PR [25].

Dans ce cas, les deux règles de mélange ne diffèrent que par le choix de la règle de mélange sur $b$ (linéaire pour Huron-Vidal et libre pour MHV-1) et la valeur du paramètre universel $C / q_1$.

L'égalité $\lim_{P \to +\infty} g^{E,\varphi}(T,P,x) = g^{E,\gamma}(T,x)$ semble donc remise en question par certains développeurs de modèles.

| | Huron-Vidal | MHV-1 |
|---|---|---|
| Pression de raccordement des modèles | Pression infinie | Pression nulle |
| Expression de $a / b$ | $\frac{a}{b} = \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i} + \frac{g_{res}^{E,\gamma} + g_{comb}^{E,\gamma}}{C}$ | $\frac{a}{b} = \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i} + \frac{g_{res}^{E,\gamma} + g_{comb}^{E,\gamma} - RT \overbrace{\sum_{i=1}^{N} x_i \ln(b_i / b)}^{\lim_{P\to 0} g_{comb}^{E,\varphi}}}{q_1}$ |
| Expression de $b$ | $b = \sum_{i=1}^{N} x_i b_i$ | L'expression peut être choisie librement |
| Méthode de calcul de $C / q_1$ | $C = -\frac{1}{r_1 - r_2} \times \ln\left(\frac{1-r_2}{1-r_1}\right)$ | $q_1$ doit être déterminé par régression linéaire de $Q(x)$ défini par l'équation (7.49) |
| Valeurs de $C / q_1$ | $\begin{cases} C_{SRK} \approx -0.6931 \\ C_{PR} \approx -0.6232 \end{cases}$ | $\begin{cases} q_{1,SRK} = -0.593 \\ q_{1,PR} = -0.53 \end{cases}$ |

Tableau 7.1. Comparaison des règles de mélange de Huron-Vidal et MHV-1

Le paragraphe qui suit propose une justification de la suppression des termes combinatoires dans certaines règles de mélange de la littérature ; il s'inspire d'explications fournies par quelques études récentes [140,142]. Le problème majeur de l'identification des modèles de $g^E$ complets – comprenant donc un terme résiduel et un terme combinatoire – est qu'elle n'impose pas l'égalité des énergies de Gibbs d'excès combinatoires et résiduelles provenant de l'équation d'état cubique et du modèle de coefficient d'activité choisis :

$$\lim_{P\to P^*} g^{E,\varphi} = g^{E,\gamma} \Rightarrow \begin{cases} \lim_{P\to P^*} g_{res}^{E,\varphi} = g_{res}^{E,\gamma} \\ \lim_{P\to P^*} g_{comb}^{E,\varphi} = g_{comb}^{E,\gamma} \end{cases} \tag{7.56}$$

Un premier exemple est donné par la règle de mélange de Huron-Vidal.

Durant la démonstration de la règle de mélange, on aboutit à la conclusion que le terme combinatoire de l'équation d'état cubique à pression infinie ainsi que le terme $Pv^{E,\varphi}$

sont nuls (cf. équations (7.32) et (7.36)). Or ce n'est pas le cas du terme combinatoire issu du modèle de coefficient d'activité qui est généralement au moins composé du terme de Flory-Huggins (cas des modèles UNIQUAC, UNIFAC, Wilson). Ainsi, écrire $\lim_{P\to+\infty} g^{E,\varphi} = g^{E,\gamma}$ est équivalent à écrire :

$$\begin{aligned} &\cancel{\lim_{P\to+\infty} a_{comb}^{E,\varphi}} + \lim_{P\to+\infty} a_{res}^{E,\varphi} + \overbrace{\cancel{\lim_{P\to+\infty} Pv^{E,\varphi}}}^{\text{si } b \text{ linéaire}} = a_{comb}^{E,\gamma} + a_{res}^{E,\gamma} + \cancel{Pv^{E,\gamma}} \\ &\Leftrightarrow \lim_{P\to+\infty} a_{res}^{E,\varphi} = a_{res}^{E,\gamma} + a_{comb}^{E,\gamma} \end{aligned} \tag{7.57}$$

Un tel résultat va à l'encontre du principe de séparation des effets combinatoires et résiduels dans les modèles thermodynamiques. La seule solution est alors de choisir un modèle de coefficient d'activité sans terme combinatoire ($a_{comb}^{E,\gamma} = 0$) tel que les modèles NRTL ou Van Laar. On notera :

- Qu'il s'agit là du choix fait par Huron et Vidal dans l'article original relatif à leurs règles de mélange et qu'il s'agit également du choix des développeurs du modèle PPR78. En effet, le modèle de coefficient d'activité de Van Laar étant contenant uniquement une contribution énergétique, on a $g^{E,\text{Van Laar}} = a_{res}^{E,\text{Van Laar}}$ et l'équation (7.41) se réécrit :

$$\left(\frac{a}{b}\right)_{PPR78} = \sum_{i=1}^{N} x_i \frac{a_i}{b_i} + \frac{a_{res}^{E,\text{Van Laar}}(T,x)}{C} \tag{7.58}$$

- Qu'afin de représenter les mélanges dissymétriques, Soave [143] supprime le terme combinatoire du modèle UNIFAC lorsque ce modèle de coefficient d'activité est utilisé dans la règle de mélange de Huron-Vidal.
- Que la règle de mélange de Huron-Vidal telle qu'utilisée en pratique est obtenue en posant $g_{comb}^{E,\gamma} = 0$, ce qui est équivalent à poser $a_{comb}^{E,\gamma} = 0$ (puisque ces modèles ne prévoient pas de volume molaire d'excès).

Ces trois exemples montrent qu'en pratique, il serait souhaitable que l'équation (7.57) s'écrive :

$$\lim_{P\to+\infty} a_{res}^{E,\varphi} = a_{res}^{E,\gamma} \tag{7.59}$$

Sous pression nulle, à la différence du cas à pression infinie, le terme combinatoire issu de l'équation d'état n'est pas nul. Ainsi, écrire $\lim_{P\to+\infty} g^{E,\varphi} = g^{E,\gamma}$ est équivalent à écrire

$$\begin{aligned}
&\lim_{P\to 0} g^{E,\varphi} = g^{E,\gamma} \\
\Leftrightarrow\ &\lim_{P\to 0} a_{comb}^{E,\varphi} + \lim_{P\to+0} a_{res}^{E,\varphi} + \cancel{\lim_{P\to+0} Pv^{E,\varphi}} = a_{comb}^{E,\gamma} + a_{res}^{E,\gamma} + \cancel{Pv^{E,\gamma}} \\
\Leftrightarrow\ &\lim_{P\to 0} a_{comb}^{E,\varphi} + \lim_{P\to 0} a_{res}^{E,\varphi} = a_{res}^{E,\gamma} + a_{comb}^{E,\gamma} \\
\Leftrightarrow\ &\lim_{P\to 0} a_{res}^{E,\varphi} = a_{res}^{E,\gamma} + \underbrace{\left(a_{comb}^{E,\gamma} - \lim_{P\to 0} a_{comb}^{E,\varphi}\right)}_{\substack{\text{différence de}\\ \text{deux termes}\\ \text{combinatoire}}}
\end{aligned} \tag{7.60}$$

Le paramètre $a$ étant contenu dans l'expression de $a_{res}^{E,\varphi}$, la règle de mélange résultant est alors de la forme :

$$\frac{a}{b}\left(\frac{a_i}{b_i},\ a_{res}^{E,\gamma},\ a_{comb}^{E,\gamma} - \lim_{P\to 0} a_{comb}^{E,\gamma}\right) \tag{7.61}$$

La séparation des effets combinatoires et résiduels serait exacte si et seulement si l'égalité suivante était respectée :

$$a_{comb}^{E,\gamma} = \lim_{P\to 0} a_{comb}^{E,\varphi} \tag{7.62}$$

Par défaut, l'équation (7.62) n'est pas vérifiée. Ainsi, toute règle de mélange sur le paramètre énergétique $a/b$ dérivant de l'équation (7.62) inclura une différence de termes combinatoires provenant du modèle de coefficient d'activité et de l'équation d'état cubique. Comme observé par Mollerup en 1986 [144], ces deux contributions ayant la même fonctionnalité, ils devraient s'annuler («The last two terms […] are both Flory-Huggins terms and should in principle cancel »).

Comme expliqué par Kontogeorgis et al. [140], de nombreuses modifications apportées à la règle de mélange MHV-1 visent à satisfaire l'équation (7.62). On citera notamment la réévaluation des paramètres $r_i$ et $q_i$ utilisés dans le calcul du terme de Flory-Huggins du modèle UNIFAC [145], le développement du modèle LCVM [146] ainsi que l'ajustement du paramètre universel $s$ de la règle de mélange sur le covolume du modèle UMR-PR [57]. Toutes ces méthodes conduisent à une nette amélioration de la représentation des systèmes dissymétriques. On en déduit donc que la condition

$a_{comb}^{E,\gamma} = \lim_{P\to 0} a_{comb}^{E,\varphi}$ est nécessaire à la bonne reproduction de l'ensemble des systèmes binaires. Dans ce cas, l'équation (7.60) devient :

$$\lim_{P\to 0} a_{res}^{E,\varphi} = a_{res}^{E,\gamma} \tag{7.63}$$

En conclusion, que la pression de référence soit la pression infinie ou la pression nulle, toutes les modifications apportées aux règles de mélange conduisent à :

$$\lim_{P\to P^{ref}} a_{res}^{E,\varphi} = a_{res}^{E,\gamma} \quad avec : P^{ref} \in \{0;+\infty\} \tag{7.64}$$

Dans le cas où $P^{réf} \to +\infty$, une règle de mélange pour le paramètre $b$ devait être adoptée. L'équation (7.64), sans contrainte sur la règle de mélange à choisir pour le paramètre $b$, constitue le point de départ des règles de mélange proposées par Jaubert et Privat [147] et paramétrées dans le cadre de cette thèse.

### 7.4. Dérivation d'une nouvelle règle de mélange pour le paramètre *a/b*

Ce paragraphe reprend les bases sur lesquelles repose la règle de mélange proposée par Jaubert et Privat à l'occasion du congrès ESAT 2012 [147] . Deux démonstrations sont présentées, l'une en choisissant une pression de raccordement infinie entre le modèle de coefficient d'activité et l'équation d'état, l'autre en choisissant une pression de raccordement nulle.

#### 7.4.1. Règle de mélange à pression infinie

Par une procédure analogue à celle suivie par Huron et Vidal, on réalise ici l'égalisation des termes $a_{res}^{E}$ provenant d'un modèle de coefficient d'activité et d'une équation d'état cubique à pression infinie :

$$\lim_{P\to+\infty} a_{res}^{E,\varphi}(T,P,x) = a_{res}^{E,\varphi}(T,x) \tag{7.65}$$

Pour rappel, l'expression de $a_{res}^{E,\varphi}(T,P,x)$ est la suivante :

$$a_{res}^{E,\varphi} = -\frac{a}{b(r_1-r_2)} \times \ln\left(\frac{v-r_2 b}{v-r_1 b}\right) + \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i(r_1-r_2)} \times \ln\left(\frac{v_i^* - r_2 b_i}{v_i^* - r_1 b_i}\right) \tag{7.66}$$

Contrairement au cas où l'on identifie les expressions de $g^E$, le passage à la limite de l'équation (7.66) est immédiat :

$$\lim_{P\to+\infty} a_{res}^{E,\varphi}(T,P,x) = \underbrace{-\frac{1}{r_1-r_2}\times\ln\left(\frac{1-r_2}{1-r_1}\right)}_{C}\times\left(\frac{a}{b}-\sum_{i=1}^{N}x_i\times\frac{a_i}{b_i}\right) \tag{7.67}$$

À pression infinie, la règle de mélange obtenue est alors :

$$\left(\frac{a}{b}\right)_{P\to+\infty} = \sum_{i=1}^{N}x_i\times\frac{a_i}{b_i}+\frac{a_{res}^{E,\gamma}(T,x)}{C} \tag{7.68}$$

Cette règle de mélange est très proche de celle de Huron-Vidal, aux différences suivantes :

- Seul le terme résiduel du modèle de coefficient d'activité apparaît
- La règle de mélange sur le paramètre $b$ peut être choisie librement, car le terme $Pv^{E,\varphi}$ n'est pas présent dans l'équation (7.66)

### 7.4.2. Règle de mélange à pression nulle

Par une procédure analogue à celle suivie par Michelsen, on réalise ici l'égalisation des termes $a_{res}^{E}$ provenant d'un modèle de coefficient d'activité et d'une équation d'état cubique à pression nulle :

$$\lim_{P\to 0} a_{res}^{E,\varphi}(T,P,x) = a_{res}^{E,\varphi}(T,x) \tag{7.69}$$

En suivant la même procédure que celle proposée par Michelsen, on aboutit à la règle de mélange implicite suivante :

$$\begin{cases} \dfrac{a_{res}^{E,\gamma}(\Gamma,\Gamma_i)}{RT} = Q'(\Gamma)-\displaystyle\sum_{i=1}^{N}x_iQ_i'(\Gamma_i) \\ Q'(x) = -\dfrac{x}{r_1-r_2}\times\ln\left(\dfrac{1-r_2\eta(x)}{1-r_1\eta(x)}\right) \\ \eta(x) = \left[\dfrac{x+r_1+r_2-\sqrt{(x+r_1+r_2)^2-4(r_1r_2+x)}}{2}\right]^{-1} \end{cases} \tag{7.70}$$

On remarque que l'expression $Q'(x)$ est différente de l'expression $Q(x)$ de l'équation (7.49).

On peut montrer que la grandeur $Q'(x)$ peut être approximée par une expression affine et s'écrire sous la forme : $Q'(x)\approx q_0'+xq_1'$. Les coefficients $q_0'$ et $q_1'$ peuvent

être déterminés par régression linéaire sur $Q'(x)$. L'équation (7.70) peut alors être réécrite de la façon suivante :

$$\frac{a_{res}^{E,\gamma}(\Gamma,\Gamma_i)}{RT} = q'_0 + \Gamma q'_1 - \sum_{i=1}^{N} x_i \left(q'_0 + \Gamma_i q'_1\right) \tag{7.71}$$

Une fois l'équation (7.71) réarrangée, on obtient la règle de mélange à pression nulle :

$$\left(\frac{a}{b}\right)_{P=0} = \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i} + \frac{a_{res}^{E,\gamma}(T,x)}{q'_1} \tag{7.72}$$

Cette règle de mélange est très proche de celle de Michelsen aux différences suivantes :

- Le terme combinatoire $\sum x_i \ln(b_i / b)$ a disparu
- Le paramètre $q_1$ a été remplacé par $q'_1$.

### 7.4.3. Valeurs numériques des paramètres $q_1$ et C

Cette étude, ainsi que celles présentées dans les paragraphes suivants ont été réalisées dans le cadre de cette thèse.

La valeur du paramètre $C$ des règles de mélange à pression infinie est déterminée par application de l'équation :

$$C = -\frac{1}{r_1 - r_2} \times \ln\left(\frac{1 - r_2}{1 - r_1}\right) \tag{7.73}$$

Les valeurs de $C$ calculées pour les équations d'état de Redlich-Kwong et Peng-Robinson sont alors :

$$\begin{cases} C_{RK} = -\ln 2 \approx -0.6931 \\ C_{PR} = -\dfrac{1}{2\sqrt{2}} \times \ln\left(\dfrac{2+\sqrt{2}}{2-\sqrt{2}}\right) \approx -0.6232 \end{cases} \tag{7.74}$$

À l'inverse du paramètre $C$, la valeur du paramètre $q'_1$ n'est pas définie de manière absolue, car sa valeur dépend du domaine de $x$ considéré pour réaliser la régression linéaire sur les points de la fonction $Q'$. Dans sa publication relative à MHV-1 [124], Michelsen réalise cette linéarisation pour $x$ compris entre 10 et 13. Ces bornes ont été choisies car elles correspondent aux valeurs de $\Gamma_i$ généralement obtenues pour les corps purs à leur température normale d'ébullition.

On s'intéresse désormais à $Q'(x=\Gamma_i)$. L'objectif de cette section est de définir quel domaine de $\Gamma_i$ est équivalent à un domaine de température allant, pour un corps pur, de son point triple, la plus petite température pour laquelle un état liquide existe, jusqu'à son point critique, la plus haute température pour laquelle un état liquide existe. Par définition, $\Gamma_i = a_i / (b_i RT) = a_{c,i}\alpha_i / (b_i RT)$. Sachant que la fonction $\alpha_i$ est décroissante avec la température et que le dénominateur croit avec la température, on en déduit que $\Gamma_i$ est maximum à la température triple du corps pur. Ainsi :

$$\Gamma_{i,max} = \frac{a_i(T_{tr,i})}{b_i R T_{tr,i}} = \frac{\Omega_a}{\Omega_b} \times \frac{\alpha_i(T_{tr,i})}{T_{tr,i}} \tag{7.75}$$

Il a été choisi de calculer $\Gamma_{i,max}$ pour un certain nombre d'alcanes linéaires allant du méthane à l'hexatriacontane (n-$C_{36}$). La fonction $\alpha$ utilisée est celle de Soave et les valeurs de température triple sont issues de la DIPPR. Les valeurs de $\Gamma_{i,max}$ ont été tracées en fonction du facteur acentrique des molécules, pour les équations de Peng-Robinson et Redlich-Kwong, sur la Figure 7.4.

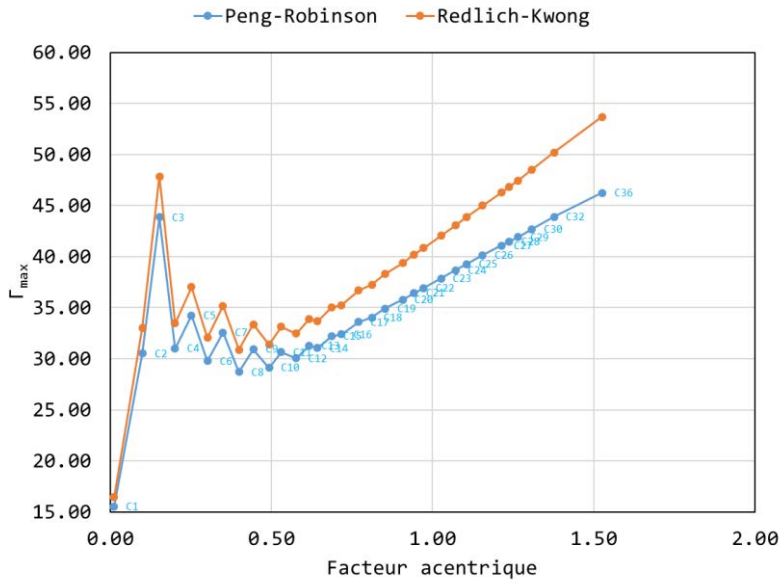



Figure 7.4. Calcul des valeurs de $\Gamma_{max}$ pour des alcanes linéaires

On remarque que les valeurs de $\Gamma_{i,max}$ ainsi calculées peuvent atteindre des valeurs de 50, aussi bien pour un composé léger tel que le propane que pour des composés lourds. Il est donc choisi de fixer la valeur de $\Gamma_{i,max}$ à 50, soit bien plus que la valeur de 13 choisie par Michelsen.

Les régressions linéaires de la fonction $Q'$ de l'équation (7.70) pour les équations de Peng-Robinson et de Redlich-Kwong et avec $x$ compris entre 10 et 50, conduisent aux expressions affines suivantes :

$$\begin{cases} Q'_{SRK} = \overbrace{-0.6965}^{q'_1} \times x + \overbrace{1.1742}^{q'_0} \\ Q'_{PR} = -0.6281 \times x + 1.2463 \end{cases} \tag{7.76}$$

Les valeurs de $q'_1$ et $C$ calculées pour les nouvelles règles de mélange proposées sont résumées dans le Tableau 7.2:

| Paramètre de la règle de mélange | Redlich-Kwong | Peng-Robinson |
|---|---|---|
| $q_1$ par identification des $g^E$ $\Gamma \in ]10;13[$ (valeurs Michelsen pour MHV-1) | -0.593 | -0.53 |
| $q'_1$ par identification des $a^E_{res}$ $\Gamma \in [10;50]$ | -0.6965 | -0.6281 |
| $C$ | -0.6931 | -0.6232 |

Tableau 7.2. Valeurs de C et de $q_1$ et $q'_1$ calculées selon le domaine de $\Gamma$ choisi ainsi que selon les grandeurs d'excès identifiées.

On remarque que les valeurs de $q'_1$ calculées pour un domaine de $\Gamma$ compris entre 10 et 50 pour les nouvelles règles de mélange sont très proches des valeurs de $C$ (moins de 1% d'écart). Il ne semble donc pas nécessaire de maintenir la distinction entre les paramètres $C$ et $q_1$. Désormais, un seul paramètre noté $\Lambda$ peut être utilisé pour la nouvelle règle de mélange car il a été établi qu'il est quasi-indépendant du choix de la pression de raccordement.

La nouvelle règle de mélange, indépendante de la pression de raccordement, s'écrit de la façon suivante :

$$\begin{cases} \dfrac{a}{b} = \sum_{i=1}^{N} x_i \times \dfrac{a_i}{b_i} + \dfrac{a_{res}^{E,\gamma}(T,x)}{\Lambda} \\ \Lambda = -\dfrac{1}{r_1 - r_2} \times \ln\left(\dfrac{1-r_2}{1-r_1}\right) \end{cases} \tag{7.77}$$

On en conclut que :

- Le choix de la pression de raccordement est négligeable lorsque l'identification des $a_{res}^{E}$ est effectuée. Ce résultat n'est pas surprenant, car il est couramment fait l'hypothèse que, contrairement à l'énergie de Gibbs d'excès, l'énergie de Helmholtz d'excès est relativement invariante par effet de la pression [125]. Cette observation est d'ailleurs à la base du développement de la règle de mélange de Wong et Sandler [148].
- Le paramètre $\Lambda$ est un paramètre universel défini uniquement par l'équation d'état du mélange.

Pour que la nouvelle règle de mélange développée puisse être appliquée, il est désormais nécessaire de définir la règle de mélange pour le paramètre $b$.

## 7.5. Choix d'une règle de mélange pour le covolume

### 7.5.1. Règles de mélange possibles pour le covolume

La règle de mélange sur $b$ la plus simple est la règle de mélange dite linéaire :

$$b = \sum_{i=1}^{N} x_i b_i \tag{7.78}$$

Bien que l'équation (7.78) présente l'avantage de la simplicité, elle présente l'inconvénient d'être peu flexible, car aucun paramètre ajustable, même universel, n'est présent. On préfère alors utiliser une expression plus générale :

$$b = \sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j \left(\frac{b_i^{1/s} + b_j^{1/s}}{2}\right)^{s} \tag{7.79}$$

Le paramètre $s$ est un paramètre universel ajusté afin d'améliorer la représentation des mélanges. On remarque que la règle de mélange linéaire est obtenue si $s=1$.

Parmi les modèles fréquemment rencontrés, les valeurs suivantes du paramètre $s$ sont utilisées :

- NRTL-PR [25] : $s=1$, une règle de mélange linéaire est choisie. Aucune justification n'est donnée.
- VTPR [141] : $s=4/3\approx1.333$. D'après les auteurs du modèle VTPR, cette valeur a été choisie, car elle correspond à la valeur inverse de l'exposant utilisé dans l'expression de Flory-Huggins modifiée issue du modèle UNIFAC-Dortmund [149].
- UMR-PRU [57] : $s=2$. Cette valeur est choisie, car elle permet de minimiser l'effet du double terme combinatoire $g_{comb}^{E,\gamma}-RT\sum x_i \ln(b_i/b)$ de la règle de mélange MHV-1.

Dans les cas où une valeur différente de 1 pour le paramètre $s$ est retenue (modèles VTPR et UMR-PRU), la bonne représentation des systèmes binaires n'est jamais au centre de la justification. Il est donc choisi de déterminer la valeur du paramètre $s$ permettant de minimiser les erreurs sur les compositions en phase liquide et vapeur par l'équation d'état cubique pour un certain nombre de systèmes binaires détaillés par la suite.

$$f=\sum_{\substack{\text{données}\\ \text{exp. de tous les}\\ \text{système binaire}}}\left[\left|\frac{x_i^{eos}(T,P)-x_i^{\exp}}{x_i^{\exp}}\right|+\left|\frac{y_i^{eos}(T,P)-y_i^{\exp}}{y_i^{\exp}}\right|\right] \tag{7.80}$$

### 7.5.2. Procédure de régression du paramètre *s*

Les mélanges d'alcanes sont des mélanges athermiques, c'est-à-dire des mélanges pour lesquels les effets enthalpiques en solution peuvent être considérés négligeables. Par conséquent, ils peuvent être théoriquement représentés par les règles de mélange suivantes où seuls les effets entropiques sont pris en compte :

$$\begin{cases}\dfrac{a}{b}=\displaystyle\sum_{i=1}^{N}x_i\times\frac{a_i}{b_i}\\ b=\displaystyle\sum_{i=1}^{N}\sum_{j=1}^{N}x_i x_j\left(\frac{b_i^{1/s}+b_j^{1/s}}{2}\right)^s\end{cases} \tag{7.81}$$

L'équation (7.81) correspond à l'équation (7.77) pour laquelle on impose $a_{res}^{E,\gamma}(T,x)=0$. Pour ces systèmes, le seul paramètre ajustable est donc le paramètre $s$. Ainsi, optimiser la représentation des mélanges d'alcanes est équivalent à trouver la valeur optimale du paramètre $s$. Cette procédure permet donc de séparer

l'optimisation de la représentation des effets énergétiques nécessitant le terme $a_{res}^{E}$ dans la règle de mélange de celle des effets combinatoires.

Pour les alcanes plus lourds que l'eicosane (n-$C_{20}$), les valeurs des températures critiques et des pressions critiques expérimentales sont incertaines, car les molécules tendent à se décomposer thermiquement avant d'atteindre leur point critique [45,150]. Seuls des mélanges binaires pour lesquels des alcanes ayant 20 atomes de carbones ou moins ont été considérés. En raison du nombre de données expérimentales disponibles, les 18 systèmes binaires suivants ont été retenus :

- $C_2$ + {n$C_6$ [151,152]; n$C_7$ [153]; n$C_8$ [154,155]; n$C_{10}$ [156,157]; n$C_{16}$ [158]; n$C_{20}$ [159]}
- $C_3$ + {n$C_7$ [160]; n$C_8$ [161]; n$C_9$ [162]; n$C_{10}$ [162,163]; n$C_{12}$ [156]}
- n$C_4$ + {n$C_8$ [161]; n$C_{10}$ [164]}
- n$C_5$ + n$C_{18}$ [165]
- n$C_6$ + n$C_{16}$ [166]
- n$C_7$ + {n$C_{12}$ [167]+ n$C_{19}$ [165]}
- n$C_8$ + n$C_{12}$ [168]

Le méthane pouvant avoir un comportement différent des autres alcanes linéaires, les systèmes binaires contenant cette molécule n'ont pas été inclus dans l'ajustement.

Pour cette étude, l'équation d'état de Peng-Robinson est utilisée.

La variation de la fonction objectif $f$ en fonction de la valeur du paramètre $s$ est représentée sur la Figure 7.5 :

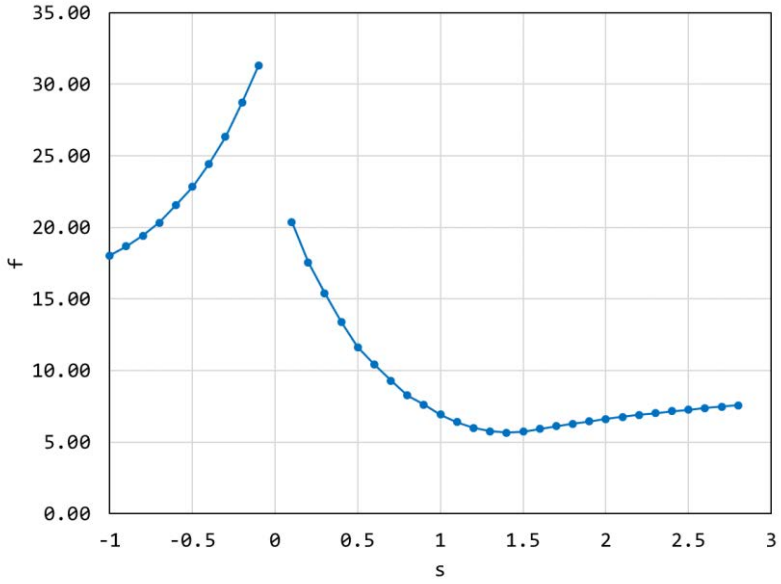



Figure 7.5. Variation de la fonction objectif définie par l'équation (7.80) en fonction du paramètre $s$

Les conclusions suivantes peuvent être faites :

- une valeur du paramètre $s$ égale à 1 n'est pas optimale. La valeur de la fonction objectif est de 6.92 et ne correspond pas au minimum global.
- à cause des incertitudes expérimentales, il peut être considéré que la valeur optimale de $s$ se situe entre 1.3 et 1.5.

Une analyse visuelle des diagrammes de phase calculés pour des valeurs de $s$ comprises entre 1.3 et 1.5 montre que la valeur $s=1.5$ permet une très bonne représentation de la courbe de bulle. La valeur de $s$ retenue pour la règle de mélange sur le covolume est donc de 1.5. La règle de mélange pour le paramètre $b$ s'écrit :

$$b=\sum_{i=1}^{N}\sum_{j=1}^{N}x_i x_j\left(\frac{b_i^{2/3}+b_j^{2/3}}{2}\right)^{3/2} \qquad (7.82)$$

Le passage d'une valeur de $s=1$ à $s=1.5$ est illustré sur la Figure 7.6 pour le système éthane – n-décane. En comparaison avec la règle de mélange linéaire, une bien meilleure représentation du fuseau est obtenue avec la nouvelle règle de mélange. On remarque cependant qu'il n'est pas possible de représenter de manière satisfaisante l'ensemble du fuseau : ici la bonne représentation de la courbe de bulle et de la courbe de rosée loin du point critique est favorisée par rapport à la représentation du point critique.

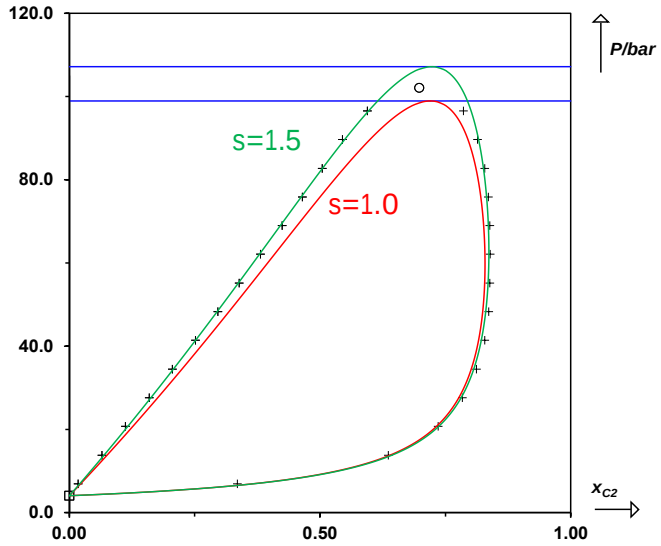



Figure 7.6. Effet de la valeur du paramètre *s* sur la représentation d'un fuseau d'équilibre liquide-vapeur du système éthane-décane lorsque l'éthane est supercritique

### 7.6. Choix d'une règle de mélange pour le paramètre de translation volumique

Un paramètre de translation volumique $c(x)$ du mélange peut être utilisé afin d'améliorer la reproduction des volumes molaires liquides. D'une façon analogue à celle des corps purs, l'équation d'état des mélanges translatée s'écrit :

$$P(T,v,x)=\frac{RT}{v+c(x)-b(x)}-\frac{a(T,x)}{\left[v+c(x)-r_1 b(x)\right]\left[v+c(x)-r_2 b(x)\right]} \tag{7.83}$$

Avec :

$$\begin{cases} \dfrac{a}{b}=\displaystyle\sum_{i=1}^{N} x_i \times \frac{a_i}{b_i}+\frac{g_{res}^{E,\gamma}(T,x)}{\Lambda} \\ b=\displaystyle\sum_{i=1}^{N}\sum_{j=1}^{N} x_i x_j \left(\frac{b_i^{2/3}+b_j^{2/3}}{2}\right)^{3/2} \\ c=f\left(x_i,c_i\right) \end{cases} \tag{7.84}$$

Comme pour les corps purs, il est souhaité que la règle de mélange pour le paramètre $c$ du mélange ne conduise pas à modifier les conditions d'équilibre entre phases ainsi que les grandeurs de mélange calculées avec l'équation d'état non translatée. De cette manière, il serait possible de décorréler la représentation des équilibres entre phases de la reproduction des volumes molaires du liquide bouillant et la valeur optimale du

paramètre $s$ de la règle de mélange sur $b$ n'aura pas à être modifiée. Cette étude est menée dans l'article « *Incorporation of a volume translation in an equation of state for fluid mixtures: which combining rule? Which effect on properties of mixing?* » [112] faisant suite à ce chapitre.

### 7.7. Développement d'une base de données de systèmes binaires pour le choix du modèle de coefficient d'activité optimal à intégrer dans l'expression du paramètre *a*

Au regard des développements théoriques récents dans les modèles d'équations d'état [78,79,169], on remarque qu'une importance significative est donnée aux mélanges dits associés c'est-à-dire aux mélanges dans lesquels des interactions intermoléculaires fortes (liaisons hydrogène par exemple) donnent naissance à des édifices polymoléculaires s'approchant de dimères ou de polymères (à la différence près que les molécules au sein de ces édifices ne sont pas liées entre elles par des liaisons chimiques). Ainsi, les molécules associées en mélange n'existent pas ou peu sous la forme de monomères. Dès lors, les équations d'état les plus simples ne parviennent pas à reproduire ce phénomène d'association et des déviations importantes entre les valeurs expérimentales et les valeurs calculées par le modèle sont obtenues. C'est par exemple le cas des mélanges contenant de l'eau ou des alcools dont l'intérêt industriel est patent. Il existe donc un réel intérêt industriel à la bonne représentation de tels systèmes.

Maintenant que les expressions générales des règles de mélange pour les paramètres $a$, $b$ et $c$ sont connues, il reste à déterminer l'expression de $a_{res}^{\gamma}$ permettant d'obtenir la meilleure représentation des données expérimentales pour un grand nombre de systèmes binaires. Afin d'établir l'expression de $a_{res}^{E,\gamma}$ optimale, il est nécessaire d'avoir à disposition une base de données représentative de la diversité des mélanges pouvant être rencontrés en pratique. Il est donc important que l'expression de $a_{res}^{\gamma}$ soit testée sur des systèmes simples, c'est-à-dire non associés, mais aussi sur des systèmes associés. Or il n'existe pas à l'heure actuelle une telle base de données.

Le développement de cette base de données est rapporté dans le second article faisant suite à ce chapitre.

### 7.8. Conclusions

Ce chapitre a été l'occasion de réaliser un tour d'horizon des modèles de coefficient d'activité ainsi que leur incorporation dans la règle de mélange sur le paramètre $a$ / $b$.

Dans un premier temps, les démonstrations des règles de mélange originales de Huron-Vidal et de MHV, respectivement obtenues en égalant les expressions de $g^{E,\gamma}$ et $g^{E,\varphi}$ à pression infinie et à pression nulle, ont été rappelées. Les limites inhérentes à cette approche ont été listées et en particulier, la présence de doubles termes combinatoires dans l'expression du paramètre $a/b$ ou l'annulation à pression infinie de $g^{E,\varphi}_{comb}$.

Jaubert et Privat [147] ont montré qu'en identifiant des expressions de $a^{E}_{res}$ provenant de l'équation d'état cubique et du modèle de coefficient d'activité choisi, il devient possible d'obtenir des règles de mélange sur le paramètre $a/b$ ne différent que par les valeur des paramètres $C$ et $q_1^{'}$. Il a été prouvé que les valeurs prises par les paramètres $C$ et $q_1$ sont suffisamment proches pour considérer qu'il existe une unique expression de $a/b$, indépendante de la pression de raccordement choisie.

Dans le cadre de cette thèse, les valeurs des paramètres universels de cette règle de mélange ont été déterminés. Le paramètre $s$ de la règle de mélange sur le paramètre $b$ a été choisi afin d'améliorer la représentation des systèmes alcane-alcane pour lesquels les effets en solution sont purement entropiques. Une valeur optimale $s=1.5$ a ainsi été obtenue.

L'équation d'état cubique des mélanges obtenue s'écrit alors :

$$P(T,v,x)=\frac{RT}{v-b(x)}-\frac{a(T,x)}{\left[v-r_1 b(x)\right]\left[v-r_2 b(x)\right]}$$

$$\text{avec}\begin{cases}\dfrac{a}{b}=\displaystyle\sum_{i=1}^{N}x_i\times\frac{a_i}{b_i}+\frac{a^{E,\gamma}_{res}(T,x)}{\Lambda}\\ \Lambda=-\dfrac{1}{r_1-r_2}\times\ln\left(\dfrac{1-r_2}{1-r_1}\right)\\ b=\displaystyle\sum_{i=1}^{N}\sum_{j=1}^{N}x_i x_j\left(\frac{b_i^{2/3}+b_j^{2/3}}{2}\right)^{3/2}\end{cases} \qquad (7.85)$$

Afin d'améliorer la représentation des propriétés volumiques, un paramètre de translation volumique peut être intégré à l'équation (7.85). La règle de mélange sur le paramètre de translation volumique $c$ est l'objet du premier article faisant suite à ce

chapitre. De façon analogue au cas des corps purs, l'accent a été mis sur le choix d'une règle de mélange ne modifiant pas les conditions d'équilibre entre phases.

La création d'une base de données représentative de la plupart des interactions existant en solution non-électrolytique a été réalisée. Celle-ci pourra alors être utilisée pour comparer les performances des différents modèles de coefficient d'activité pouvant être intégrés dans la règle de mélange sur le paramètre $a / b$ et sélectionner le modèle de coefficient d'activité optimal à combiner avec la règle de mélange proposée. Le développement de cette banque de données est l'objet du second article faisant suite à ce chapitre.

## 7.9. Annexe : calcul de l'énergie de Gibbs d'excès par une équation d'état cubique

### 7.9.1. Prérequis au calcul

En vertu de l'identité d'Euler, l'énergie de Gibbs molaire d'un mélange de gaz parfaits s'écrit :

$$g^{\bullet}(T,P,x)=\sum_{i=1}^{N}x_i\bar{g}_i^{\bullet}(T,P,x) \tag{7.86}$$

La quantité $\bar{g}_i^{\bullet}$ est appelée potentiel chimique du composé $i$ dans l'état gaz parfait.

*Potentiel chimique d'un constituant en solution idéale*

Par définition, le potentiel chimique du composé $i$ dans une solution idéale s'écrit :

$$\bar{g}_i^{id}(T,P,x)\equiv g_i^{*}(T,P,x)+RT\ln x_i \tag{7.87}$$

L'exposant $*$ désigne les propriétés calculées pour les corps purs par l'équation d'état cubique.

Le mélange de gaz parfaits étant un cas particulier de solution idéale, l'équation (7.87) peut être appliquée au mélange de gaz parfait :

$$\bar{g}_i^{\bullet}(T,P,x)=g_i^{\bullet}(T,P,x)+RT\ln x_i \tag{7.88}$$

L'exposant $\bullet$ désigne les propriétés calculées pour les corps purs par application de la loi des gaz parfaits.

### 7.9.2. Calcul de l'énergie de Gibbs d'excès pour l'ensemble des équations d'état explicites en pression

L'énergie de Gibbs d'excès du mélange est définie par la relation :

$$g^{E}(T,P,x)=g(T,P,x)-g^{id}(T,P,x) \tag{7.89}$$

Par définition, le potentiel chimique du composé $i$ en solution idéale s'écrit (équation(7.87)) :

$$\bar{g}_i^{id}(T,P,x)=g_i^{*}(T,P,x)+RT\ln x_i \tag{7.90}$$

Par application de l'identité d'Euler, on obtient alors comme expression de $g^{id}$ :

$$g^{id}(T,P,x)=\sum_{i=1}^{N}x_i\left[g_i^*(T,P,x)+RT\ln x_i\right] \tag{7.91}$$

Ainsi :

$$g^{E}(T,P,x)=g(T,P,x)-\sum_{i=1}^{N}x_i\left[g_i^*(T,P,x)+RT\ln x_i\right] \tag{7.92}$$

Dans les calculs suivants, $a$ désigne l'énergie de Helmholtz et $v$ le volume molaire :

$$\begin{aligned}
g^{E}(T,P,x) &= a(T,P,x)+Pv-\sum_{i=1}^{N}x_i a_i^*(T,P)-\sum_{i=1}^{N}x_i Pv_i^*-\sum_{i=1}^{N}x_i\ln x_i \\
&= a(T,v,x)+Pv-\sum_{i=1}^{N}x_i a_i^*\left(T,v_i^*\right)-\sum_{i=1}^{N}x_i Pv_i^*-\sum_{i=1}^{N}x_i\ln x_i \\
&= a^{\bullet}(T,v,x)+a^{éc}(T,v,x)+Pv-\sum_{i=1}^{N}x_i a_i^{\bullet}\left(T,v_i^*\right) \\
&\quad -\sum_{i=1}^{N}x_i a_i^{éc}\left(T,v_i^*\right)-\sum_{i=1}^{N}x_i Pv_i^*-\sum_{i=1}^{N}x_i\ln x_i \\
&= a^{\bullet}(T,v,x)-\sum_{i=1}^{N}x_i a_i^{\bullet}\left(T,v_i^*\right)+a^{éc}(T,v,x)-\sum_{i=1}^{N}x_i a_i^{éc,*}\left(T,v_i^*\right) \\
&\quad +P\left(v-\sum_{i=1}^{N}x_i v_i^*\right)-\sum_{i=1}^{N}x_i\ln x_i
\end{aligned} \tag{7.93}$$

Finalement :

$$\begin{aligned}
g^{E}(T,P,x) &= a^{éc}(T,v,x)-\sum_{i=1}^{N}x_i a_i^{éc}\left(T,v_i^*\right) \\
&\quad +a^{\bullet}(T,v,x)-\sum_{i=1}^{N}x_i a_i^{\bullet}\left(T,v_i^*\right)-\sum_{i=1}^{N}x_i\ln x_i \\
&\quad +P\left(v-\sum_{i=1}^{N}x_i v_i^*\right)
\end{aligned} \tag{7.94}$$

Par définition :

$$\begin{cases}
a^{\bullet}(T,v,x)=g^{\bullet}(T,v,x)-(Pv)^{\bullet}=g^{\bullet}\left(T,P=\dfrac{RT}{v},x\right)-RT \\
a_i^{\bullet}\left(T,v_i^*\right)=g_i^{\bullet}\left(T,v_i^*\right)-\left(Pv_i^*\right)^{\bullet}=g_i^{\bullet}\left(T,P=\dfrac{RT}{v_i^*}\right)-RT
\end{cases} \tag{7.95}$$

En incorporant les équations (7.86) et (7.88) dans l'équation précédente :

$$a^{\bullet}(T,v,x)-\sum_{i=1}^{N}x_i a_i^{\bullet}\left(T,v_i^*\right)= \\ \sum_{i=1}^{N}x_i\left[g_i^{\bullet}\left(T,P=\frac{RT}{v}\right)+RT\ln x_i-g_i^{\bullet}\left(T,P=\frac{RT}{v_i^*}\right)\right] \tag{7.96}$$

Or à température constante $dg_i^{\bullet,*}(T,P)=v_i^{\bullet,*}(T,P)dP$ :

$$g_i^{\bullet}\left(T,P=\frac{RT}{v}\right)-g_i^{\bullet}\left(T,P=\frac{RT}{v_i^*}\right)=\int_{RT/v_i^*}^{RT/v}v^{\bullet}dP=\int_{RT/v_i^*}^{RT/v}\frac{RT}{P}dP=RT\ln\left(\frac{v_i^*}{v}\right) \tag{7.97}$$

Donc :

$$a^{\bullet}(T,v,x)-\sum_{i=1}^{N}x_i a_i^{\bullet}\left(T,v_i^*\right)-RT\sum_{i=1}^{N}x_i\ln x_i=RT\sum_{i=1}^{N}x_i\ln\left(\frac{v_i^*}{v}\right) \tag{7.98}$$

En combinant les équations (7.94) et (7.98), on obtient :

$$g^E(T,P,x)=a^{éc}(T,v,x)-\sum_{i=1}^{N}x_i a_i^{éc}\left(T,v_i^*\right)+RT\sum_{i=1}^{N}x_i\ln\left(\frac{v_i^*}{v}\right) \\ +P\left(v-\sum_{i=1}^{N}x_i v_i^*\right) \tag{7.99}$$

L'équation (7.99) peut être utilisée pour estimer l'énergie de Gibbs d'excès d'un mélange à partir de l'expression d'une équation d'état explicite en pression.

### 7.9.3. Calcul de l'énergie de Gibbs d'excès pour l'ensemble des équations d'état cubiques

Par définition d'une grandeur d'écart :

$$a^{éc}(T,v,x)=a(T,v,x)-a^{\bullet}(T,v,x) \tag{7.100}$$

Par ailleurs, on sait que le comportement du fluide réel tend vers celui du gaz parfait lorsque le volume molaire tend vers l'infini :

$$a(T,v\to+\infty,x)=a^{\bullet}(T,v\to+\infty,x) \tag{7.101}$$

L'équation (7.100) peut donc se réécrire :

$$\begin{aligned} a^{éc}(T,v,x) = &\left[a(T,v=v,x) - a(T,v\to+\infty,x)\right] \\ &-\left[a^{\bullet}(T,v=v,x) - a^{\bullet}(T,v\to+\infty,x)\right] \end{aligned} \tag{7.102}$$

L'expression de la différentielle de l'énergie de Helmholtz d'un corps pur dans le jeu de variable température et volume molaire s'écrit :

$$da = -Pdv - sdT \tag{7.103}$$

Ainsi, l'équation (7.102) s'écrit :

$$a^{éc}(T,v,x) = -\int_{+\infty}^{v}\left[P(T,v,x) - P^{\bullet}(T,v,x)\right]dv \tag{7.104}$$

En injectant l'expression de $P^{\bullet}(T,v,x)$, on obtient finalement :

$$a^{éc}(T,v,x) = -\int_{+\infty}^{v}\left[P(T,v,x) - \frac{RT}{v}\right]dv \tag{7.105}$$

Pour un corps pur, un résultat analogue est obtenu :

$$a_i^{éc}\left(T,v_i^*\right) = -\int_{+\infty}^{v_i^*}\left[P^*\left(T,v_i^*\right) - \frac{RT}{v}\right]dv \tag{7.106}$$

L'intégrale de l'équation (7.105) peut être calculée explicitement si l'on injecte l'expression de l'équation d'état cubique (cf. équation (7.1)) :

$$\begin{aligned} a^{éc}(T,v) &= -\int_{+\infty}^{v}\left[\frac{RT}{v-b} - \frac{a}{(v-r_1b)(v-r_2b)} - \frac{RT}{v}\right]dv \\ &= \underbrace{-RT\int_{+\infty}^{v}\left(\frac{1}{v-b} - \frac{1}{v}\right)dv}_{I_1} + \underbrace{\int_{+\infty}^{v}\frac{a}{(v-r_1b)(v-r_2b)}dv}_{I_2} \end{aligned} \tag{7.107}$$

L'intégrale $I_1$ peut être intégrée :

$$I_1 = RT\ln\left(\frac{v}{v-b}\right) \tag{7.108}$$

Le calcul de l'intégrale $I_2$ nécessite de réaliser la décomposition en éléments simples de la quantité à intégrer :

$$I_2 = \int_{+\infty}^{v} \frac{a}{(v-r_1 b)(v-r_2 b)} dv = -\frac{a}{(r_1-r_2)b} \times \int_{+\infty}^{v} \left( \frac{1}{v-r_2 b} - \frac{1}{v-r_1 b} \right) dv \qquad (7.109)$$

L'intégrale $I_2$ peut alors être intégrée :

$$I_2 = -\frac{a}{(r_1-r_2)b} \times \ln\left( \frac{v-r_2 b}{v-r_1 b} \right) \qquad (7.110)$$

On obtient finalement :

$$a^{éc}(T,v) = RT \ln\left( \frac{v}{v-b} \right) - \frac{a}{(r_1-r_2)b} \times \ln\left( \frac{v-r_2 b}{v-r_1 b} \right) \qquad (7.111)$$

Par une procédure analogue, on démontre que la quantité $a_i^*$ peut être calculée par la formule :

$$a_i^*\left(T, v_i^*\right) = RT \ln\left( \frac{v_i^*}{v_i^* - b_i} \right) - \frac{a_i}{(r_1-r_2)b_i} \times \ln\left( \frac{v_i^* - r_2 b_i}{v_i^* - r_1 b_i} \right) \qquad (7.112)$$

Une fois les équations (7.111) et (7.112) injectée dans l'équation (7.99), on obtient :

$$\begin{aligned} g^E(T,P,x) = {} & RT \ln\left( \frac{v}{v-b} \right) - RT \sum_{i=1}^{N} x_i \ln\left( \frac{v_i^*}{v_i^* - b_i} \right) + RT \sum_{i=1}^{N} x_i \ln\left( \frac{v_i^*}{v} \right) \\ & - \frac{a}{(r_1-r_2)b} \times \ln\left( \frac{v-r_2 b}{v-r_1 b} \right) + \sum_{i=1}^{N} x_i \times \frac{a_i}{(r_1-r_2)b_i} \times \ln\left( \frac{v_i^* - r_2 b_i}{v_i^* - r_1 b_i} \right) \\ & + P\left( v - \sum_{i=1}^{N} x_i v_i^* \right) \end{aligned} \qquad (7.113)$$

L'équation (7.113) peut alors s'écrire de manière « simplifiée » :

$$\begin{aligned} g^E(T,P,x) = {} & RT \sum_{i=1}^{N} x_i \ln\left( \frac{v_i^* - b_i}{v-b} \right) \\ & - \frac{a}{b(r_1-r_2)} \times \ln\left( \frac{v-r_2 b}{v-r_1 b} \right) + \sum_{i=1}^{N} x_i \times \frac{a_i}{b_i(r_1-r_2)} \times \ln\left( \frac{v_i^* - r_2 b_i}{v_i^* - r_1 b_i} \right) \\ & + P\left( v - \sum_{i=1}^{N} x_i \times v_i^* \right) \end{aligned} \qquad (7.114)$$

Le premier terme à droite du signe égal de l'équation (7.114) provient du terme $RT/(v-b)$ de l'équation d'état cubique qui est un terme combinatoire tandis que le second terme à droite du signe égal de l'équation (7.114) a pour origine le terme $a/\left[(v-r_1 b)(v-r_2 b)\right]$ de l'équation d'état qui est un terme résiduel.

Sachant que $a^E = g^E - Pv^E$, l'équation (7.114) s'écrit aussi :

$$a^E(T,P,x) = a^E_{comb}(T,P,x) + a^E_{res}(T,P,x)$$

avec (7.115)

$$\begin{cases} a^E_{comb} = RT\sum_{i=1}^{N} x_i \ln\left(\dfrac{v_i^* - b_i}{v-b}\right) \\ a^E_{res} = -\dfrac{a}{b(r_1-r_2)} \times \ln\left(\dfrac{v-r_2 b}{v-r_1 b}\right) + \sum_{i=1}^{N} x_i \times \dfrac{a_i}{b_i(r_1-r_2)} \times \ln\left(\dfrac{v_i^* - r_2 b_i}{v_i^* - r_1 b_i}\right) \end{cases}$$

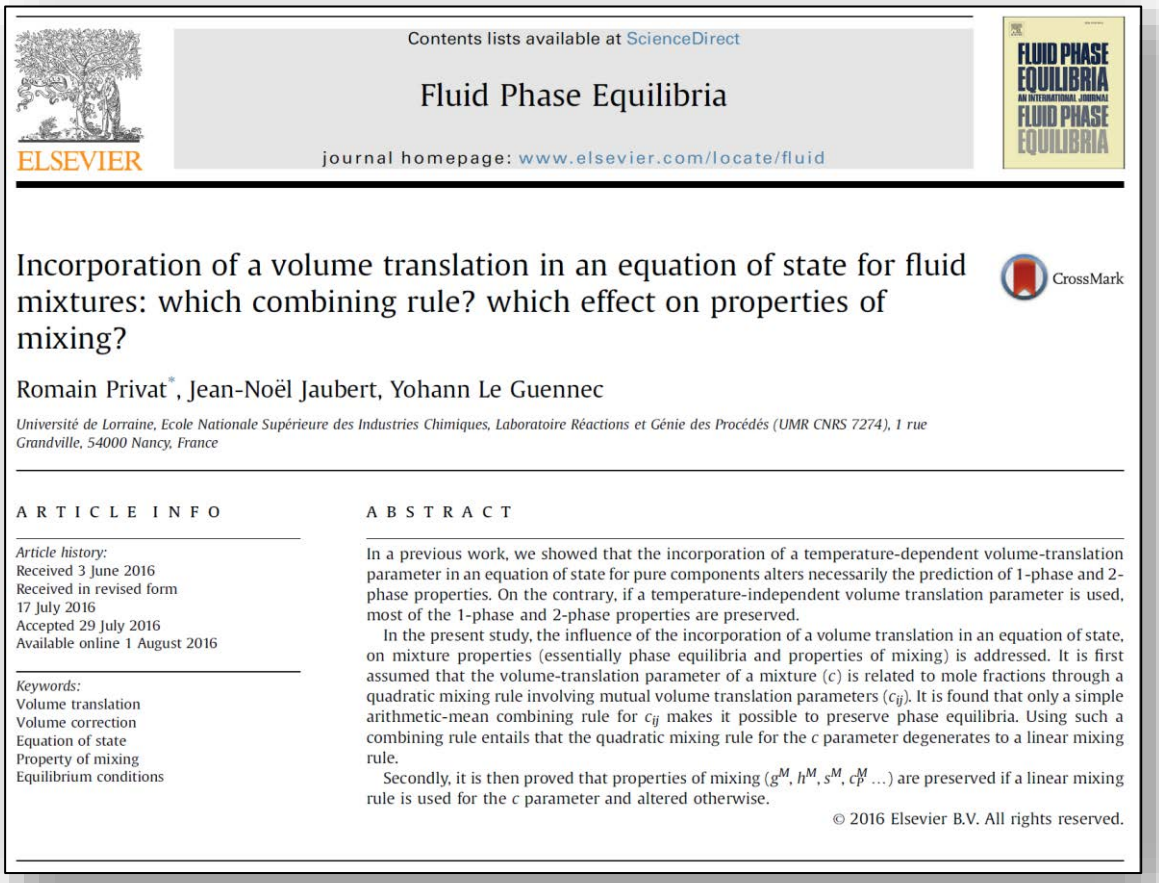
# Chapitre 8. Article “Incorporation of a volume translation in an equation of state for fluid mixtures: which combining rule? which effect on properties of mixing?”

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ABSTRACT

In a previous work, we showed that the incorporation of a temperature-dependent volume-translation parameter in an equation of state for pure components alters necessarily the prediction of 1-phase and 2-phase properties. On the contrary, if a temperature-independent volume translation parameter is used, most of the 1-phase and 2-phase properties are preserved.

In the present study, the influence of the incorporation of a volume translation in an equation of state, on mixture properties (essentially phase equilibria and properties of mixing) is addressed. It is first assumed that the volume-translation parameter of a mixture ($c$) is related to mole fractions through a quadratic mixing rule involving mutual volume translation parameters ($c_{ij}$). It is found that only a simple arithmetic-mean combining rule for $c_{ij}$ makes it possible to preserve phase equilibria. Using such a combining rule entails that the quadratic mixing rule for the $c$ parameter degenerates to a linear mixing rule.

Secondly, it is then proved that properties of mixing ($g^M$, $h^M$, $s^M$, $c_P^M$ ...) are preserved if a linear mixing rule is used for the $c$ parameter and altered otherwise.

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**Abstract**

In a previous work, we showed that the incorporation of a temperature-dependent volume-translation parameter in an equation of state for pure components alters necessarily the prediction of 1-phase and 2-phase properties. On the contrary, if a temperature-independent volume translation parameter is used, most of the 1-phase and 2-phase properties are preserved.

In the present study, the influence of the incorporation of a volume translation in an equation of state, on mixture properties (essentially phase equilibria and properties of mixing) is addressed. It is first assumed that the volume-translation parameter of a mixture ($c$) is related to mole fractions through a quadratic mixing rule involving mutual volume translation parameters ($c_{ij}$). It is found that only a simple arithmetic-mean combining rule for $c_{ij}$ makes it possible to preserve phase equilibria. Using such a combining rule entails that the quadratic mixing rule for the c parameter degenerates to a linear mixing rule.

Secondly, it is then proved that properties of mixing ($g^M$, $h^M$, $s^M$, $c_P{}^M$ ...) are preserved if a linear mixing rule is used for the c parameter and altered otherwise.

**Keywords**

volume translation; volume correction; equation of state; property of mixing; equilibrium conditions

## 8.1. Introduction

In a recent work [40], a list of pure-component properties altered by the application of a volume translation to any equation of state (EoS) was established. Although applied to cubic equations of state in practice, the concept of volume translation, introduced by Péneloux et al. [39,70], could be introduced actually in any type of EoS (e.g., SAFT-type or virial-type EoS). Note that working specifically on cubic EoS, Leibovici [69] was able to identify a series of properties not influenced by a temperature-independent volume translation, but however did not realize that his conclusions did not depend on the mathematical expression of the EoS and never discussed the case of a temperature-dependent volume translation.

Considering the very general framework of pressure-explicit EoS (i.e., EoS expressing explicitly the pressure of a pure fluid as a function of its temperature and molar volume) combined to a temperature-dependent volume translation, our previous study [40] highlighted that while the strict majority of 1-phase properties estimable from an EoS are altered (volume, enthalpy, entropy, fugacity, heat capacity, second virial coefficient and so on), vapor pressures remain unchanged as well as most of properties of vaporization.

As largely described in the literature, the use of temperature-dependent volume-translation parameters has to be avoided since it mainly leads to two undesirable effects [68,170]:

- negative heat capacities at high temperatures,
- isotherm crossings in the pressure-volume plane.

When a temperature-independent volume translation is considered, it was showed that results are slightly different [40]: all 2-phase properties are unaffected by the introduction of such a parameter; a larger number of 1-phase properties are not altered at the noticeable exception of the volume, the enthalpy, the fugacity, the second virial coefficient and the speed of sound.

The present article aims at extending the scope of our first study to volume-translation parameters incorporated in equations of state for mixtures. To do so, a mixing rule relating the volume-translation parameter to the composition of the mixture has to be defined. According to classical practices, mainly two types of mixing rules are generally considered:

- *linear mixing rule:* the volume-translation parameter of the mixture $c(T,z)$ is obtained by summing pure-component volume-translation parameters $c_i(T)$ weighted by their corresponding mole fractions $z_i$ ,

$$c(T,z)=\sum_i z_i c_i(T) \tag{8.1}$$

- *quadratic mixing rule:* in this case, the volume-translation parameter of a mixture is a quadratic function of the component mole fractions:

$$c(T,\mathrm{z})=\sum_i\sum_j z_i z_j c_{ij}(T) \tag{8.2}$$

The $c_{ij}(T)$ parameter (with $i\neq j$ ) is called *mutual volume-translation parameter*; $c_{ii}(T)$ is the volume-translation parameter of pure *i* which is alternatively denoted $c_i(T)$ in the present article. The mathematical relation linking parameter $c_{ij}$ to pure-component parameters is a so-called *combining rule*. A limited number of combining rules are used in practice:

- Simple arithmetic-mean combining rule:

$$c_{ij}=\frac{1}{2}\left(c_i+c_j\right) \tag{8.3}$$

Note that the association of this combining rule with a quadratic mixing rule is strictly equivalent to the use of a linear mixing rule:

$$c(T,\mathrm{z})=\sum_i\sum_j z_i z_j\left[\tfrac{1}{2}\left(c_i(T)+c_j(T)\right)\right]=\sum_i z_i c_i(T) \tag{8.4}$$

- Arithmetic-mean combining rule involving a binary interaction parameter ( $\chi_{ij}$ ):

$$c_{ij}=\frac{1}{2}\left(c_i+c_j\right)\left(1-\chi_{ij}\right) \tag{8.5}$$

- Simple geometric-mean combining rule:

$$c_{ij}=\sqrt{c_i c_j} \tag{8.6}$$

- Geometric-mean combining rule involving a binary interaction parameter ( $\chi_{ij}$ ):

$$c_{ij} = \sqrt{c_i c_j}\left(1 - \chi_{ij}\right) \tag{8.7}$$

Since a linear mixing rule can be seen as a particular case of a quadratic mixing rule (i.e., association of a quadratic mixing rule and a simple arithmetic-mean combining rule), a quadratic mixing rule will be assumed to express the volume-translation parameter along this study.

In the present article, it is mainly intended to answer the two following questions:

- Can the combining rule for the mutual volume-translation parameters $c_{ij}$ be freely chosen?
- What are the mixture properties altered by the use of (1) a temperature-dependent volume translation? (2) a temperature-independent volume translation? A special attention will be paid to property changes on mixing.

## 8.2. Modification of the two-phase equilibrium conditions when an EoS for mixtures is translated

The translation of molar volumes at fixed temperature $T$, pressure $P$ and mole fraction vector $\mathrm{z}$ is expressed by the basic transform:

$$v_t\left(T,P,\mathrm{z}\right) = v_o\left(T,P,\mathrm{z}\right) - c(T,\mathrm{z}) \tag{8.8}$$

where subscripts t and o refer to the original (i.e., untranslated) and translated EoS, respectively. In terms of total volumes, this transform writes:

$$V_t\left(T,P,\mathrm{n}\right) = V_o\left(T,P,\mathrm{n}\right) - n \cdot c(T,\mathrm{n}) \tag{8.9}$$

where $\mathrm{n}$ is a mole number vector, $n = \sum_i n_i$ and $n_i$ is the mole number of species i.

As mentioned in the introduction, a volume-translation parameter $c$ depends a priori on the temperature $T$ and the composition $\mathrm{z}$ of the mixture even though, the use of temperature-dependent volume-translation terms is not advised [40,68,170]. Despite this, the instance of temperature-dependent volume-translation parameter will be anyway considered throughout this study to keep the most general framework.

This section is devoted to detail how the two-phase equilibrium conditions are affected by the volume-translation transform, for a given EoS. To do so, the changes of some

specific properties (partial molar volumes, fugacity coefficients and fugacities) resulting from a volume-translation transform are first addressed.

The volume-translation parameter of a given mixture being assumed to be a quadratic function of the composition (see Equation (8.2)), one has:

$$c(T,\mathrm{n}) = \frac{1}{n^2}\sum_i\sum_j n_i n_j c_{ij}(T) \tag{8.10}$$

The partial molar property of component i related to the total property $n \cdot c(T,\mathrm{n})$ is:

$$\bar{c}_i = \left[\frac{\partial\left(nc(T,\mathrm{n})\right)}{\partial n_i}\right]_{T,n_{j\neq i}} = -c(T,\mathrm{n}) + \frac{2}{n}\sum_j n_j c_{ij}(T) = -c(T,\mathrm{z}) + 2\sum_j z_j c_{ij}(T) \tag{8.11}$$

We can now take benefit of this preliminary calculation to estimate the partial molar volume change accompanying a volume-translation transform.

$$\begin{aligned}
\bar{v}_{i,t} &= \left(\frac{\partial V_t(T,P,\mathrm{n})}{\partial n_i}\right)_{T,P,n_{j\neq i}} \\
&= \left[\frac{\partial\left(V_o(T,P,\mathrm{n}) - nc(T,\mathrm{n})\right)}{\partial n_i}\right]_{T,P,n_{j\neq i}} \\
&= \bar{v}_{i,o} - \bar{c}_i \\
&= \bar{v}_{i,o} + c(T,\mathrm{z}) - 2\sum_j z_j c_{ij}(T)
\end{aligned} \tag{8.12}$$

According to classical thermodynamics, the fugacity coefficient of component i is given by:

$$\ln\varphi_{i,t}(T,P,\mathrm{z}) = \int_0^P\left(\frac{\bar{v}_{i,t}}{RT} - \frac{1}{P}\right)dP \tag{8.13}$$

By combining Equations (8.12) and (8.13), one obtains:

$$\ln \varphi_{i,t}(T,P,\mathrm{z}) = \int_0^P \left( \frac{\bar{v}_{i,o} + c(T,\mathrm{z}) - 2\sum_j z_j c_{ij}(T)}{RT} - \frac{1}{P} \right) dP$$

$$= \int_0^P \left( \frac{\bar{v}_{i,o}}{RT} - \frac{1}{P} \right) dP + \frac{P}{RT}\left[ c(T,\mathrm{z}) - 2\sum_j z_j c_{ij}(T) \right] \qquad (8.14)$$

$$= \ln \varphi_{i,o}(T,P,\mathrm{z}) + \frac{P}{RT}\left[ c(T,\mathrm{z}) - 2\sum_j z_j c_{ij}(T) \right]$$

The fugacity change of component i along a volume-translation transform is simply deduced from:

$$\ln f_{i,t}(T,P,\mathrm{z}) = \ln P + \ln z_i + \ln \varphi_{i,t}(T,P,\mathrm{z}) \qquad (8.15)$$

From Equations (8.14) and (8.15), one has thus:

$$\ln f_{i,t}(T,P,\mathrm{z}) = \ln P + \ln z_i + \ln \varphi_{i,o}(T,P,\mathrm{z}) + \frac{P}{RT}\left[ c(T,\mathrm{z}) - 2\sum_j z_j c_{ij}(T) \right]$$

$$= \ln f_{i,o}(T,P,\mathrm{z}) + \frac{P}{RT}\left[ c(T,\mathrm{z}) - 2\sum_j z_j c_{ij}(T) \right] \qquad (8.16)$$

Fugacities being explicitly involved in two-phase equilibrium conditions, Equation (8.16) makes it possible to understand how these conditions are affected by a volume-translation transform.

The application of the isofugacity criterion to species i represented by an untranslated EoS, simply writes:

$$\ln f'_{i,o}(T,P,\mathrm{x}'_o) = \ln f''_{i,o}(T,P,\mathrm{x}''_o) \qquad (8.17)$$

where superscripts ′ and ″ refer to the two phases in equilibrium.

The application of the same criterion when considering the corresponding translated EoS gives:

$$\ln f'_{i,t}(T,P,\mathrm{x}'_t) = \ln f''_{i,t}(T,P,\mathrm{x}''_t) \qquad (8.18)$$

Combination of Equations (8.16) and (8.18) leads to the final expression of the two-phase equilibrium conditions:

$$\ln f'_{i,o}(T,P,\mathrm{x}'_t)+\frac{P}{RT}\left[c(T,\mathrm{x}'_t)-2\sum_j x'_{t,j}\cdot c_{ij}(T)\right] = \ln f''_{i,o}(T,P,\mathrm{x}''_t)+\frac{P}{RT}\left[c(T,\mathrm{x}''_t)-2\sum_j x''_{t,j}\cdot c_{ij}(T)\right] \tag{8.19}$$

### 8.3. Derivation of combining rules for mutual volume-translation parameters making it possible to preserve phase-equilibrium conditions

Comparison of Equations (8.17) and (8.19) clearly shows that the isofugacity criterion at fixed temperature and pressure is a priori affected by a volume-translation transform (i.e., at given temperature and pressure, $\mathrm{x}'_t \neq \mathrm{x}'_o$ and $\mathrm{x}''_t \neq \mathrm{x}''_o$). Such an effect is not in agreement with the philosophy of the volume-translation transform that was introduced by Péneloux to improve volumetric-property predictions from EoS by preserving at the same time, the phase-equilibrium conditions.

In this section, still assuming a quadratic mixing rule for parameter $c$, it is intended to derive a combining rule for parameter $c_{ij}$ which preserves the phase-equilibrium conditions, i.e., such that: $\begin{cases}\mathrm{x}'_t=\mathrm{x}'_o\\ \mathrm{x}''_t=\mathrm{x}''_o\end{cases}$. For the sake of simplicity, the phase-equilibrium compositions are simply denoted $\mathrm{x}'$ and $\mathrm{x}''$ below (subscripts t and o are deliberately omitted). The two isofugacity equations for a given component i, that are:

$$\ln f'_{i,t}(T,P,\mathrm{x}')=\ln f''_{i,t}(T,P,\mathrm{x}'') \text{ and } \ln f'_{i,o}(T,P,\mathrm{x}')=\ln f''_{i,o}(T,P,\mathrm{x}'') \tag{8.20}$$

return the same compositions provided:

$$\forall \mathrm{x}',\mathrm{x}'':\quad c(T,\mathrm{x}')-2\sum_j x'_j c_{ij}(T)=c(T,\mathrm{x}'')-2\sum_j x''_j c_{ij}(T) \tag{8.21}$$

Or equivalently, if:

$$\forall \mathrm{x}',\mathrm{x}'':\quad c(T,\mathrm{x}'')-c(T,\mathrm{x}')=2\sum_j\left(x''_j-x'_j\right)c_{ij}(T) \tag{8.22}$$

Parameter $c$ being assumed to be a quadratic function of mole fractions, one has:

$$\forall \mathrm{x}',\mathrm{x}'':\quad \sum_k\sum_j\left(x''_k x''_j-x'_k x'_j\right)c_{kj}(T)=2\sum_j\left(x''_j-x'_j\right)c_{ij}(T) \tag{8.23}$$

The right-hand side (rhs) term is converted into two terms involving the summation indices $j$ and $k$, respectively:

$$\forall \mathrm{x}', \mathrm{x}'': \quad \sum_k \sum_j \left( x''_k x''_j - x'_k x'_j \right) c_{kj}(T) = \sum_j \left( x''_j - x'_j \right) c_{ij}(T) + \sum_k \left( x''_k - x'_k \right) c_{ik}(T) \tag{8.24}$$

Remembering that the summation of mole fractions over all the components of a given phase is equal to one (i.e., $\sum_m x''_m = \sum_m x'_m = 1$ with $m = i, j, k$), simple sums of the rhs term of Equation (8.24) can be converted into double sums:

$$\forall \mathrm{x}', \mathrm{x}'': \quad \sum_k \sum_j \left( x''_k x''_j - x'_k x'_j \right) c_{kj}(T) = \sum_k \sum_j \left( x''_k x''_j - x'_k x'_j \right) \left( c_{ij}(T) + c_{ik}(T) \right) \tag{8.25}$$

Equation (8.25) can now be written in a more compact way:

$$\forall \mathrm{x}', \mathrm{x}'': \quad \sum_k \sum_j \left( x''_k x''_j - x'_k x'_j \right) \lambda_{i,jk} = 0, \text{ with } \lambda_{i,jk} = c_{kj}(T) - c_{ij}(T) - c_{ik}(T) \tag{8.26}$$

To sum up, combining rules for parameter $c_{ij}$ such that the equilibrium conditions are preserved through a volume-translation transform verify both Equation (8.26) and the summation constraint on mole fractions:

$$\begin{cases} \forall \mathrm{x}', \mathrm{x}'': \quad \sum_k \sum_j x''_k x''_j \lambda_{i,jk} = \sum_k \sum_j x'_k x'_j \lambda_{i,jk} \\ \textit{subject to} \sum_m x''_m = \sum_m x'_m = 1 \end{cases} \tag{8.27}$$

This last equation can be equivalently written using matrix notations:

$$\begin{cases} \forall \mathrm{x}', \mathrm{x}'': \quad \left( \mathrm{x}' \right)^{\mathrm{T}} \boldsymbol{\lambda}_{\mathrm{i}} \, \mathrm{x}' = \left( \mathbf{x}'' \right)^{\mathrm{T}} \boldsymbol{\lambda}_{\mathrm{i}} \, \mathbf{x}'' \\ \textit{subject to} \sum_m x''_m = \sum_m x'_m = 1 \end{cases} \tag{8.28}$$

It can be mathematically proved that the unique matrix $\boldsymbol{\lambda}_{\mathrm{i}}$ which is solution to Equation (8.27) (or similarly, of Equation (8.28)) verifies:

$$\forall (j,k), \quad \lambda_{i,jk} = \text{constant (denoted } \lambda_i \text{)} \text{ (where index i refers to species i)} \tag{8.29}$$

In other words, the coefficients of the matrix $\boldsymbol{\lambda}_i$ have all the same value $\lambda_i$ (they do not depend on indices $j$ and $k$).

*Remark:* in order to convince the reader that $\lambda_{i,jk} = \lambda_i$ is a solution of Equation (8.27), it is shown below that by replacing $\lambda_{i,jk}$ by $\lambda_i$, an obvious equality is obtained.

$$\begin{cases} \forall \mathrm{x}', \mathrm{x}'': \quad \lambda_i \sum_k {}' \sum_j {}' x''_k x''_j = \lambda_i \sum_k {}' \sum_j {}' x'_k x'_j \\ \textit{subject to} \sum_m x''_m = \sum_m x'_m = 1 \end{cases} \Rightarrow \begin{cases} \forall \mathrm{x}', \mathrm{x}'': \quad \sum_k x''_k \sum_j x''_j = \sum_k x'_k \sum_j x'_j = 1 \\ \textit{subject to} \sum_m x''_m = \sum_m x'_m = 1 \end{cases} \tag{8.30}$$

Finally, it can be claimed that 2-phase equilibrium compositions at fixed *T* and *P* remain unchanged provided mutual volume translation coefficients verify the constraint:

$$c_{kj}(T) - c_{ij}(T) - c_{ik}(T) = \lambda_i(T) \tag{8.31}$$

It is again recalled that $\lambda_i$ denotes a quantity which may solely depend on species index *i* but is independent of indices *j* and *k*.

The adequacy of constraint (8.31) with four classically-used combining rules is now investigated.

(a) Simple arithmetic-mean combining rule: $c_{mn} = \frac{1}{2}(c_m + c_n)$

$$c_{kj} - c_{ij} - c_{ik} = \frac{1}{2}\left(c_k + c_j - c_i - c_j - c_i - c_k\right) = -c_i \tag{8.32}$$

Conclusion: constraint (8.31) is satisfied and the arithmetic-mean combining rule for the mutual volume translation preserves the phase-equilibrium compositions

(b) Arithmetic-mean combining rule involving a binary interaction parameter: $c_{mn} = \frac{1}{2}(c_m + c_n)(1 - \chi_{mn})$

$$c_{kj} - c_{ij} - c_{ik} = -c_i - \frac{1}{2}\left[\left(c_k + c_j\right)\chi_{kj} - \left(c_i + c_j\right)\chi_{ij} - \left(c_i + c_k\right)\chi_{ik}\right] \tag{8.33}$$

Conclusion: constraint (8.31) is not satisfied.

(c) Simple geometric-mean combining rule: $c_{mn} = \sqrt{c_n c_m}$

$$c_{kj} - c_{ij} - c_{ik} = \sqrt{c_k c_j} - \sqrt{c_i c_j} - \sqrt{c_k c_i} \tag{8.34}$$

Conclusion: constraint (8.31) is not satisfied.

(d) Geometric-mean combining rule involving a binary interaction coefficient: $c_{mn} = \sqrt{c_n c_m}\left(1 - \chi_{mn}\right)$

Since a simple geometric-mean combining rule does not satisfy constraint (8.31), more complex combining rule such as the geometric-mean combining rule involving a binary interaction coefficient can even less satisfy constraint (8.31).

It follows that constraint (8.31) is only satisfied if a simple arithmetic-mean combining rule is used. In this particular case, the volume-translation parameter is actually a linear combination of mole fractions:

$$\begin{cases} c_{ij}(T) = \dfrac{1}{2}\left[c_i(T) + c_j(T)\right] \\ c(T,\mathrm{z}) = \displaystyle\sum_i \sum_j z_i z_j c_{ij}(T) = \frac{1}{2}\sum_i \sum_j z_i z_j \left[c_i(T) + c_j(T)\right] \\ \qquad\quad = \displaystyle\sum_i z_i c_i(T) \end{cases} \tag{8.35}$$

This conclusion offers for the first time (to the best of our knowledge), an a posteriori justification of the choice intuited by Péneloux in his seminal article [39] to apply a linear mixing rule to the volume-translation parameter $c(T,\mathrm{z})$. In the rest of the present article, it is assumed that $c(T,\mathrm{z})$ is a linear function of the mole fractions.

*Remark:* more generally, it can be proved that any combining rule such that $c_{mn} = f\left(c_m\right) + f\left(c_n\right)$, where $f$ is an arbitrary function, makes it possible to preserve the phase-equilibrium conditions through a volume-translation transform.

Eventually, by combining Equations (8.16) and (8.35), the fugacity of a component *i* writes:

$$\begin{aligned}\ln f_{i,t}(T,P,\mathrm{z}) &= \ln f_{i,o}(T,P,\mathrm{z}) + \frac{P}{RT}\left[\sum_i z_i c_i(T) - 2\sum_j z_j\left[\tfrac{1}{2}\left(c_i(T)+c_j(T)\right)\right]\right] \\ &= \ln f_{i,o}(T,P,\mathrm{z}) - \frac{P}{RT}c_i \end{aligned} \qquad (8.36)$$

Note that this last expression can be found in Peneloux's article [39].

### 8.4. Effect of a volume translation on properties of mixing when a linear mixing rule is used to express the mixture volume-translation parameter

The molar Gibbs energy is a so-called *characteristic function* in the $(T,P)$ variable set; it is here meant that the simple knowledge of the molar Gibbs energy in the $(T,P)$ variable set makes it possible to express all the other thermodynamic functions ($h$, $s$, $c_P$ …) in the same variable set. In order to understand how properties of mixing are affected by a volume-translation transform, it is thus necessary to calculate first the molar Gibbs energy change and the molar Gibbs energy of mixing change through a volume-translation transform.

#### 8.4.1. Total molar Gibbs energy and total molar Gibbs energy of mixing

$$\begin{aligned} g_t(T,P,\mathrm{z}) &= g^{\bullet}(T,P,\mathrm{z}) + \int_0^P \left[ v_t(T,P,\mathrm{z}) - \frac{RT}{P} \right] dP \\ &= g^{\bullet}(T,P,\mathrm{z}) + \int_0^P \left[ v_o\left(T,P,\mathrm{z}\right) - c(T,\mathrm{z}) - \frac{RT}{P} \right] dP \\ &= g^{\bullet}(T,P,\mathrm{z}) + \int_0^P \left[ v_o\left(T,P,\mathrm{z}\right) - \frac{RT}{P} \right] dP - \int_0^P c(T,\mathrm{z}) dP \\ &= g_o(T,P,\mathrm{z}) - c(T,\mathrm{z})\cdot P \end{aligned} \qquad (8.37)$$

The Gibbs energy of mixing is given by:

$$\begin{aligned} g_t^M(T,P,\mathrm{z}) &= g_t(T,P,\mathrm{z}) - \sum_i z_i g_{t,pure\,i}(T,P) \\ &= g_o(T,P,\mathrm{z}) - c(T,\mathrm{z})\cdot P - \sum_i z_i \left[ g_{o,pure\,i}(T,P) - c_i(T)\cdot P \right] \\ &= g_o(T,P,\mathrm{z}) - \sum_i z_i g_{o,pure\,i}(T,P) - P\left[ c(T,\mathrm{z}) - \sum_i z_i c_i(T) \right] \\ &= g_o^M(T,P,\mathrm{z}) - c^M(T,\mathrm{z})\cdot P \end{aligned} \tag{8.38}$$

where:

$$c^M(T,\mathrm{z}) = c(T,\mathrm{z}) - \sum_i z_i c_i(T) \tag{8.39}$$

can be seen as a *volume-translation parameter change on mixing*. The introduction of parameter $c^M$ highlights the similarity between the relation $g_t^M(T,P,\mathrm{z})$ *versus* $g_o^M(T,P,\mathrm{z})$ and the relation $g_t(T,P,\mathrm{z})$ *versus* $g_o(T,P,\mathrm{z})$.

If a linear mixing rule is used to relate $c(T,\mathrm{z})$ to the composition, then:

$$\begin{cases} c^M(T,\mathrm{z}) = 0 \\ g_t^M(T,P,\mathrm{z}) = g_o^M(T,P,\mathrm{z}) \end{cases} \tag{8.40}$$

### 8.4.2. Total molar entropy and total molar entropy of mixing

The total molar entropy is a partial derivative of $g$ with respect to the temperature:

$$s = -(\partial g/\partial T)_{P,\mathrm{z}} \tag{8.41}$$

By deriving the relation between $g_t$ and $g_o$ (see Equation (8.37)), one obtains:

$$s_t(T,P,\mathrm{z}) = s_o(T,P,\mathrm{z}) + P\cdot c'(T,\mathrm{z}) \text{ with: } c'(T,\mathrm{z}) = \left(\frac{\partial c}{\partial T}\right)_{\mathrm{z}} \tag{8.42}$$

For a pure component:

$$s_{t,pure\,i}(T,P) = s_{o,pure\,i}(T,P) + c_i'(T)\cdot P \tag{8.43}$$

As a consequence, the total molar entropy change on mixing is:

$$\begin{aligned} s_t^M(T,P,\mathrm{z}) &= s_t(T,P,\mathrm{z}) - \sum_i z_i s_{t,pure\,i}(T,P) \\ &= s_o(T,P,\mathrm{z}) + c'(T,\mathrm{z})\cdot P - \sum_i z_i \left[ s_{o,pure\,i}(T,P) + c_i'(T)\cdot P \right] \\ &= s_o^M(T,P,\mathrm{z}) + P\cdot\left[ c'(T,\mathrm{z}) - \sum_i z_i c_i'(T) \right] \\ &= s_o^M(T,P,\mathrm{z}) + P\cdot\left[ c^M \right]'(T,\mathrm{z}) \end{aligned} \tag{8.44}$$

With :

$$\left[ c^M \right]' = \left( \frac{\partial c^M}{\partial T} \right)_{\mathrm{z}} \tag{8.45}$$

If an arithmetic-mean combining rule is used to express the volume-translation parameter, one has:

$$\begin{cases} \left[ c^M \right]' = 0 \\ s_t^M(T,P,\mathrm{z}) = s_o^M(T,P,\mathrm{z}) \end{cases} \tag{8.46}$$

### 8.4.3. Total molar enthalpy and total molar enthalpy of mixing

The total molar enthalpy is deduced from functions $g$ and $s$ :

$$h = g + Ts \tag{8.47}$$

Thus:

$$\begin{cases} g_t(T,P,\mathrm{z}) = g_o(T,P,\mathrm{z}) - c(T,\mathrm{z})\cdot P \\ Ts_t(T,P,\mathrm{z}) = Ts_o(T,P,\mathrm{z}) + Tc'(T,\mathrm{z})\cdot P \end{cases} \Rightarrow h_t(T,P,\mathrm{z}) = h_o(T,P,\mathrm{z}) + \left[ Tc'(T,\mathrm{z}) - c(T,\mathrm{z}) \right]\cdot P \tag{8.48}$$

For a pure component:

$$h_{t,pure\,i}(T,P,\mathrm{z}) = h_{o,pure\,i}(T,P,\mathrm{z}) + \left[ Tc_i'(T,\mathrm{z}) - c_i(T,\mathrm{z}) \right]\cdot P \tag{8.49}$$

Consequently, the total molar enthalpy change on mixing is:

$$
\begin{aligned}
h_t^M(T,P,\mathrm{z}) &= h_t(T,P,\mathrm{z}) - \sum_i z_i h_{t,pure\,i}(T,P) \\
&= h_o(T,P,\mathrm{z}) + \left[Tc'(T,\mathrm{z}) - c(T,\mathrm{z})\right]\cdot P \\
&\quad - \sum_i z_i \left[h_{o,pure\,i}(T,P) + \left[Tc_i'(T) - c_i(T)\right]\cdot P\right] \\
&= h_o^M(T,P,\mathrm{z}) + T\cdot P\left[c'(T,\mathrm{z}) - \sum_i z_i c_i'(T)\right] \\
&\quad - P\left[c(T,\mathrm{z}) - \sum_i z_i c_i(T)\right] \\
&= h_o^M(T,P,\mathrm{z}) + T\cdot P\cdot\left[c^M\right]'(T,\mathrm{z}) - P\cdot c^M(T,\mathrm{z})
\end{aligned}
\tag{8.50}
$$

If an arithmetic-mean combining rule is used to express the volume-translation parameter, one has:

$$
\begin{cases}
c^M = \left[c^M\right]' = 0 \\
h_t^M(T,P,\mathrm{z}) = h_o^M(T,P,\mathrm{z})
\end{cases}
\tag{8.51}
$$

### 8.4.4. Total molar constant-pressure heat capacity and total molar constant-pressure heat capacity of mixing

By definition:

$$c_P = (\partial h/\partial T)_{P,\mathrm{z}} \tag{8.52}$$

By deriving the relation between $h_t$ and $h_o$ (see Equation (8.48)), one obtains:

$$c_{P,t}(T,P,\mathrm{z}) = c_{P,o}(T,P,\mathrm{z}) + TPc''(T,\mathrm{z}) \tag{8.53}$$

For a pure component:

$$c_{P,t,pure\,i}(T,P) = c_{P,o,pure\,i}(T,P) + TPc_i''(T) \tag{8.54}$$

The heat capacity change on mixing is:

$$
\begin{aligned}
c^{M}_{P,t}(T,P,\mathrm{z}) &= c_{P,t}(T,P,\mathrm{z}) - \sum_i z_i c_{P,t,pure\,i}(T,P) \\
&= c_{P,o}(T,P,\mathrm{z}) + T\cdot P\cdot c''(T,\mathrm{z}) - \sum_i z_i \left[ c_{P,o,pure\,i}(T,P) + T\cdot P\cdot c''_i(T,\mathrm{z}) \right] \\
&= c^{M}_{P,o}(T,P,\mathrm{z}) + T\cdot P\cdot \left[ c''(T,\mathrm{z}) - \sum_i z_i c''_i(T,\mathrm{z}) \right] \\
&= c^{M}_{P,o}(T,P,\mathrm{z}) + T\cdot P\cdot \left[ c^{M} \right]''(T,\mathrm{z})
\end{aligned}
\tag{8.55}
$$

With:

$$
\left[ c^{M} \right]'' = \left( \frac{\partial^2 c^{M}}{\partial T^2} \right)_{\mathrm{z}} \tag{8.56}
$$

As previous, if an arithmetic-mean combining rule is used to express the volume-translation, parameter, one has:

$$
\begin{cases} \left[ c^{M} \right]'' = 0 \\ c^{M}_{P,t}(T,P,\mathrm{z}) = c^{M}_{P,o}(T,P,\mathrm{z}) \end{cases} \tag{8.57}
$$

### 8.5. Main results and discussion

In this section, answers to the two questions posed in the introduction part are proposed.

*Question 1: can the combining rule for the mutual volume-translation parameters $c_{ij}$ be freely chosen?*

This study demonstrates that the sole combining rule for the mutual volume-translation parameter $c_{mn}$ which preserves the phase-equilibrium conditions through a volume-translation transform is the simple arithmetic-mean combining rule.

$$
c_{mn} = \frac{1}{2}\left( c_m + c_n \right) \tag{8.58}
$$

By incorporating this combining rule in the expression of the volume-translation parameter $c(T,\mathrm{z})$ expressed with a quadratic mixing rule, a linear mixing rule is eventually obtained:

$$c(T,z) = \sum_i z_i c_i(T) \tag{8.59}$$

It can be concluded that using such a mixing rule, the same isothermal Pxy and isobaric Txy phase diagrams are obtained from the translated and untranslated versions of an EoS.

It has been also shown that the simple use of a linear mixing rule for the $c(T,z)$ parameter always leads to the same properties of mixing ( $g^M$ , $s^M$ , $h^M$ , $c_P^M$ ), regardless of whether the EoS is translated or untranslated, regardless of whether the volume-translation parameter are made temperature-dependent or not. It can be highlighted that the selection of linear mixing rules for the volume-translation parameter of the mixture annihilates the effect of making pure-component volume-translation parameters temperature-dependent or not, while our previous study [40] showed that such a choice influences dramatically the prediction of pure-component properties.

*Question 2: what are the mixture properties altered by the use of (1) a temperature-dependent volume translation? (2) a temperature-independent volume translation?*

Table 1 summarizes the changes undergone by the properties of mixing through a volume-translation transform when a non-linear mixing rule is used for the $c(T,z)$ parameter:

| Molar property of mixing $x^M$ | Change through a volume-translation transform $x_t^M(T,P,z)-x_o^M(T,P,z)$ when a non linear mixing rule is chosen for parameter c |
|---|---|
| $g^M$ | $-c^M(T,z)\cdot P$ |
| $s^M$ | $P\cdot\left[c^M\right]'(T,z)$ |
| $h^M$ | $T\cdot P\cdot\left[c^M\right]'(T,z)-P\cdot c^M(T,z)$ |
| $c_P^M$ | $T\cdot P\cdot\left[c^M\right]''(T,z)$ |

Table 8.1. Change of properties of mixing when a volume-translation parameter is introduced in a given EoS. The quantity $c^M$ and its derivatives are defined by Equations (8.39), (8.45) and (8.56)

Table 1 clearly shows that the use of temperature-dependent volume-translation parameters with quadratic mixing rules for $c(T,z)$ affects all properties of mixing ($g^M$, $s^M$, $h^M$, $c_P^M$).

Otherwise, the use of temperature-independent volume-translation parameters and the selection of a quadratic mixing rule for $c(z)$ induce that the entropy of mixing and the constant-pressure heat capacity of mixing as well, are not affected by a volume-translation transform, contrary to the enthalpy of mixing and the Gibbs energy of mixing.

### 8.6. Conclusion

The outcomes of this study could be of practical importance for thermodynamicists developing EoS for mixtures since it is now possible to assert that the use of a linear mixing rule to express the volume-translation parameter $c(T,z)$ makes it possible to uncouple the problem of reproducing liquid densities from the problems of predicting phase-equilibrium properties and properties of mixing.

For instance, working with cubic EoS, the development of correlations for the binary interaction coefficient or the search for parameters involved in advanced mixing rules are not influenced by the incorporation of a volume-translation parameter in the EoS. In other words, it becomes easy to apply a volume-translation transform to a cubic EoS

which was initially developed to well reproduce pure-component properties, phase equilibria of mixture and properties of mixing as well: using temperature-independent volume-translation parameters for pure components and a linear mixing rule for the volume-translation parameter of the mixture ensures both to preserve the aforementioned properties and to improve density predictions.

On the contrary, if using a quadratic mixing rule for the volume-translation parameter, it becomes necessary to consider simultaneously the problem of reproducing liquid densities and the problems of predicting phase-equilibrium properties and properties of mixing.

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# Chapitre 9. Article "A benchmark database containing binary-system-high-quality-certified data for assessing accuracy and cross-comparing thermodynamic models."

## 9.1. Introduction

In order to assess the accuracy of a thermodynamic model or to cross-compare two models, one must confront model predictions to experimental data. In order to make comparisons between models meaningful, the experimental data must be the same from one comparison to another, leading the path to thermodynamic reference databases. Reference databases are not meant to be updated regularly but to be used as landmarks through a long period. Therefore, the DETHERM database [171] which records an 8% growth per year in terms of available experimental data and the NIST-TRC database TDE [172] which is "dynamically curated" cannot be considered as a reference database. Relating to the existence of numerous databases, Hendriks et al. wrote that *"the existing databases will become less useful as the tendency to target quantity rather than quality will intensify,"* making the emphasis on the need for databases composed of a high-quality restrained number of experimental data.

To our knowledge, the sole reference database for non-electrolytic and non-polymeric systems commonly cited in the literature is the one proposed by Danner and Gess in 1990 [173]. This reference database shows the following aspects:

- Only subcritical vapor-liquid equilibrium (VLE) data are available
- Data quality is ensured by performing consistency tests
- Pure compounds are classified based on their polarity, from nonpolar to very strongly polar, and their capacity to form hydrogen bonds
- Binary systems are classified with respect to their deviations to ideality
- Data are evenly distributed among all kinds of systems (ideal, non-ideal, with or without hydrogen bonds)

Unfortunately, this reference database was only cited 49 times during its 28 years of existence while more than 20,000 articles relating to the Peng-Robinson equation of state were released during the same period. Therefore, one can conclude that (i) this reference database is not widely used and that (ii) all newly published models

performances cannot be fairly compared. In our opinion, the database of Danner and Gess is not used for the following reasons:

- Not only VLE data should be used. Indeed, as stated by Hendriks et al., "although VLE remains the most common [property], other types of phase equilibria (LLE, SLE) are nowadays also in demand. Furthermore, there is an increasing need for enthalpic properties (heat of mixing, heat capacities) and transport properties."
- The reference database should be easily accessible. Indeed, the one of Danner and Gess can only be *"provided on a $5^{1/4}$ or $3^{1/2}$ inch MS-DOS formatted disk"* [173].

Therefore, it is time to suggest a new reference database based on an updated work of Danner and Gess that could be used for the comparison of thermodynamic models and reach a general acceptance among the community of thermodynamicists. To do so, the following questions must be answered (these key questions are also addressed in Figure 2 of [174]):

- What systems must be included?
- What properties must be included?
- How much data must be included?

The next sections of this article are dedicated to answering these questions in order to build a new reference database.

### 9.2. What properties must be included?

For fluid systems, most commonly available experimental data are phase-equilibrium data, energetic mixing property data and critical point data. Such data are routinely measured because they are of practical interest for process engineers:

- A good reproduction of phase equilibrium data is mandatory to ensure that processes meet their compositional specifications. Depending on the temperature and pressure conditions, phase equilibrium data can involve either two subcritical compounds, a subcritical and a supercritical compound or possibly two supercritical compounds. For some systems, azeotropic behavior and 3-phase liquid-liquid-vapor equilibrium can also be observed. Because of such diversity, it is important to embed all kinds of phase equilibrium data in a reference database. It should be emphasized that any new model should be tested on wide temperature

and pressure conditions, including ones for which the model was not intentionally developed, as it is a common thing that a model becomes *"modified and extended to model more processes than their original creators dreamed about"* [175].

- A good reproduction of energetic mixing properties allows a good quantification of the energy needs and losses of a process. Such knowledge is required if one wants to perform, for example, the energetic integration of a process. Mixing properties such as mixing enthalpy and mixing heat capacity are valuable energetic data which calculation, contrarily to the phase equilibrium calculation, involves the derivative of the thermodynamic model with respect to temperature. Therefore, one can have excellently correlated phase diagrams but poorly calculated mixing properties. This observation is also made by Agarval et al. [175]: *"...if you are modeling a system with significant excess enthalpies using a Gibbs free-energy-based EOS and you have a good VLE fit, this does not automatically ensure you have a good overall model from an energy balance point of view."* A consequence would be an inaccurate calculation of the energy balance of any installation using this thermodynamic model. On the other hand, Qian et al. [24] demonstrated that it is possible for an equation of state to accurately correlate both fluid-phase equilibria and mixing properties if both types of data are included in the regression procedure. This short discussion highlights the importance of mixing enthalpies and mixing heat capacities data, explaining why they will be included in the proposed reference database. Thus, someone developing a new thermodynamic model should care about the reproduction of mixing properties by the model and this is why we consider that such experimental data should be included in our reference database.
- For a binary mixture, a good representation of the critical loci [96] are of the highest importance because such lines fix the topology [176] of the isothermal and isobaric phase diagrams, whatever the temperature and the pressure. From our experience, a thermodynamic model which is able to represent the critical loci will not have much difficulty to accurately predict phase diagrams on the whole temperature and pressure range. We are thus convinced that critical points are of the utmost importance and have to be included in our database. Consequently, a special emphasis was made to include systems for which such data were available.

To sum up, we answer the question, "What properties must be included?" considering that the following data should be included in our database:

- Phase equilibrium data of all kinds (VLE, LLE, VLLE, gas-gas, azeotropes)
- Critical points
- Mixing enthalpy and mixing heat capacity

### 9.3. What systems must be included?

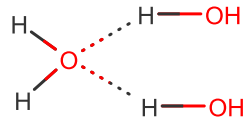
Danner and Gess's database retained our attention as it does not only compile experimental data but also provides a classification for binary systems based on mixtures ideality. Moreover, pure compounds are discriminated over their polarity which is, in the article of Danner and Gess, related to their ability to form hydrogen bonds in solution. In the same article, ideality of a mixture is considered as the most relevant classification criteria while polarity, or equivalently association, comes only as second. Contrary to Danner and Gess, we believe that the difficulty to model a thermodynamic system is more related to its capacity to show association phenomena than exhibiting deviations to ideality. Indeed, several thermodynamic models are able to represent non-ideal systems that do not exhibit associations between their components [23,56,57]. On the other hand, a good representation of associated systems requires the use of a supplementary term in the thermodynamic models dedicated to explicitly account of the association phenomenon [169,177]. Thus, any new thermodynamic model should focus on its ability to represent associated systems more than representing non-ideal systems.

Next sections are dedicated to the establishment of general rules to determine if, in a first time, a pure compound and, in a second time, binary mixtures can show hydrogen bonds. Once these criteria are defined, an insight is given to the determination of a mixture's ideality.

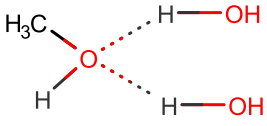
#### 9.3.1. A rule of thumb to predicting the association phenomena in solution

As previously stated, the main criteria to classify the binary systems inside our database is their capability to exhibit an association behavior. In our methodology, hydrogen bonds between molecules in solution are considered as the single cause for association phenomena. Following the IUPAC [178], hydrogen bonds are defined as "an attractive interaction between a hydrogen atom from a molecule or a molecular fragment X–H in which X is more electronegative than H, and an atom or a group of atoms in the same or a different molecule, in which there is evidence of bond formation."

We considered a more restrictive case in which hydrogen bonds can only result from the energetic interactions between a labile hydrogen and a lone pair of electrons, which can be located on the same molecule or on two different molecules. Thus, such phenomena can occur either with a pure compound or in a binary mixture as illustrated on Figure 9.1.




Hydrogen bonds between water molecules



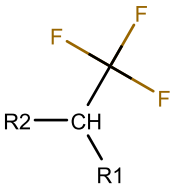
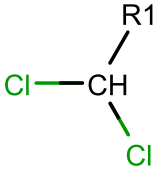
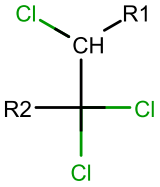
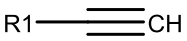
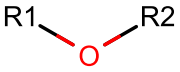
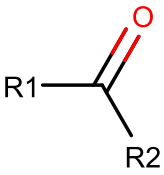
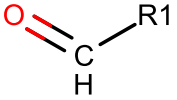
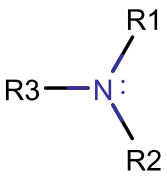

Hydrogen bonds between methanol and water

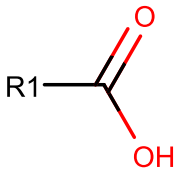
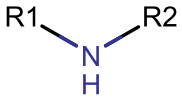
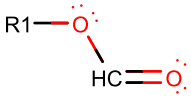
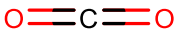
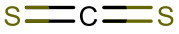
Figure 9.1. Hydrogen bonds between the same molecules (left, water and water) or different molecules (right, water and methanol)

For a pure compound the following four cases exist:

- Case 1 (noted NA for “Not Associated”): the molecule has no labile hydrogen atom and no lone pair of electrons. Molecules like alkanes and mono-halogenated compounds are included in this family.
- Case 2 (noted H for “Hydrogen donor”): the molecule has a labile hydrogen atom but no lone pair of electrons. Molecules like di-, tri-halogenated compounds or the ones with a terminal alkyne group are included in this family. The labile hydrogen earns his acidity from the electronegativity of his closest neighbors.
- Case 3 (noted E for “Electronic receiver”): the molecule has no labile hydrogen atom but a lone pair of electrons. Molecules like ketones, aldehydes, ether and ternary amines are included in this family.
- Case 4 (noted SA for “Self Associated”): the molecule has a labile hydrogen atom and a lone pair of electrons. Such molecules fulfill the two necessary and sufficient conditions to be self-associated. Molecules like water, alcohols and carboxylic acids are included in this family.

Table 9.1. details the chemical groups involved in the molecules contained in our database and that have a labile hydrogen, a lone pair of electrons or both.

| Group name or its description | Schematic group | Has a labile hydrogen atom? | Has a lone pair of electrons? |
|---|---|---|---|
| -$CX_3$, X = Br, Cl or F |  | | |
| two halogens on the carbon atom possessing an H |  | Y | N |
| on halogen on the carbon atom possessing an H plus two halogens on the carbon atom in α position |  | | |
| terminal alkyne group |  | | |
| ether |  | | |
| ketones |  | | |
| aldehydes |  | N | Y |
| ternary amines |  | | |

| Group name or its description | Schematic group | Has a labile hydrogen atom? | Has a lone pair of electrons? |
|---|---|---|---|
| alcohols |  | | |
| carboxylic acids |  | Y | Y |
| primary and secondary amines |  | | |
| formate |  | | |
| special molecules | | | |
| oxygen |  | | |
| carbon dioxide |  | | |
| sulfur dioxide |  | | |
| carbon disulfide |  | N | Y |
| hydrogen sulfide |  | | |
| carbon monoxyde |  | | |

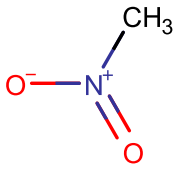
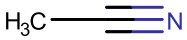
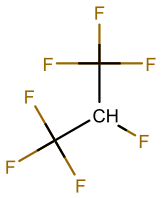
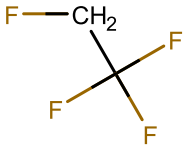
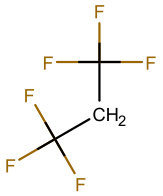
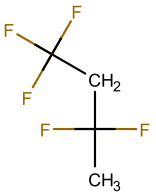
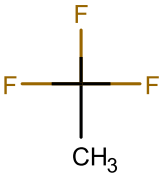
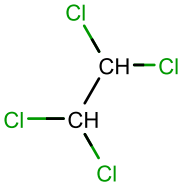
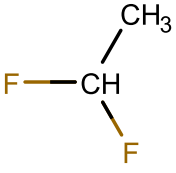
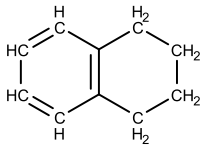
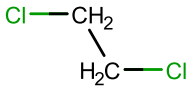
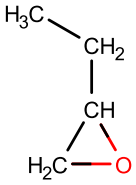
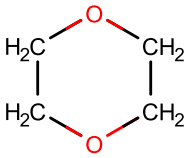
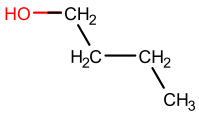
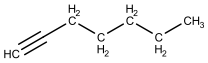
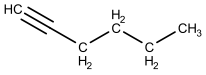
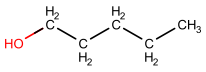
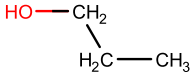
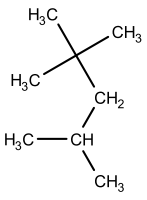
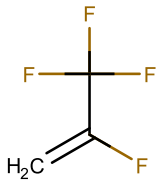
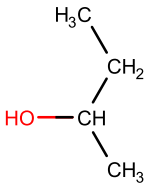
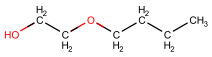
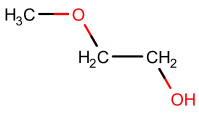
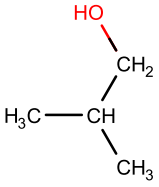
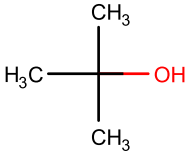
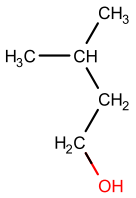
| Group name or its description | Schematic group | Has a labile hydrogen atom? | Has a lone pair of electrons? |
|---|---|---|---|
| nitromethane |  | | |
| acetonitrile |  | Y | Y |
| water | $H_2O$ | | |

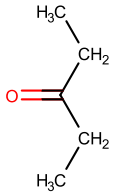
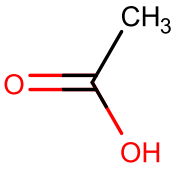
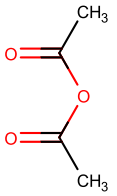
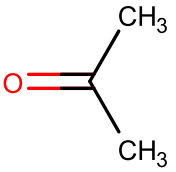
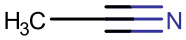
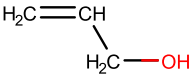
Table 9.1. Chemical groups having a labile hydrogen group, a lone pair of electrons or both (only groups involved in our database)

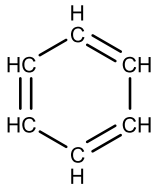
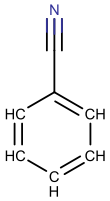
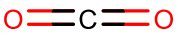
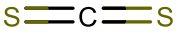
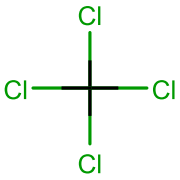
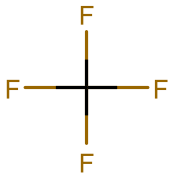
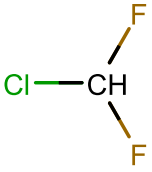
Table 9.2. lists all the pure compounds included in the proposed database and indicates its corresponding association code among “Not associated” (NA), “Hydrogen donor” (H), “Electronic receiver” (E) or “Self Associated” (SA).

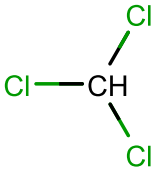
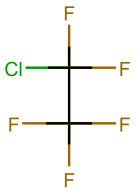
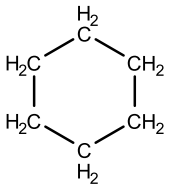
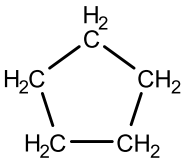
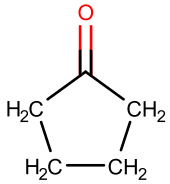
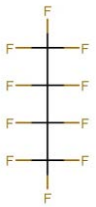
| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| 1,1,1,2,3,3,3-heptafluoropropane |  | Y | N | H |
| 1,1,1,2-tetrafluoroethane |  | Y | N | H |
| 1,1,1,3,3,3-hexafluoropropane |  | Y | N | H |
| 1,1,1,3,3-pentafluorobutane |  | Y | N | H |
| 1,1,1-trifluoroethane |  | Y | N | H |
| 1,1,2,2-tetrachloroethane |  | Y | N | H |
| 1.1-difluoroethane |  | Y | N | H |

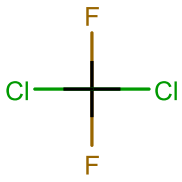
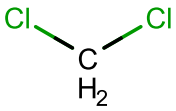
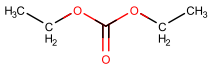
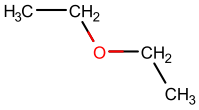
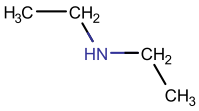
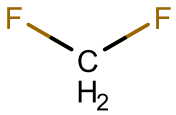
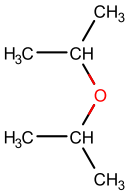
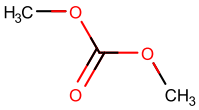
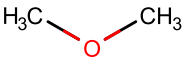
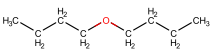
| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| 1,2,3,4-tetrahydronaphthalene |  | N | N | NA |
| 1.2-dichloroethane |  | N | N | NA |
| 1,2-epoxybutane |  | N | Y | E |
| 1.4-dioxane |  | N | Y | E |
| 1-butanol |  | Y | Y | SA |
| 1-heptyne |  | Y | N | H |
| 1-hexyne |  | Y | N | H |
| 1-pentanol |  | Y | Y | SA |
| 1-propanol |  | Y | Y | SA |
| 2,2,4-trimethylpentane |  | N | N | NA |

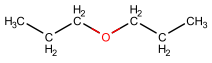
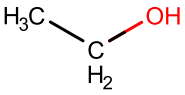
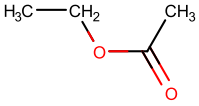
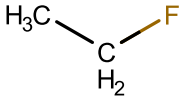
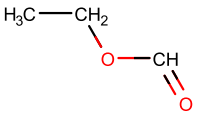
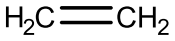
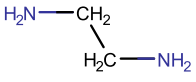
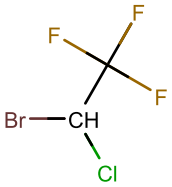
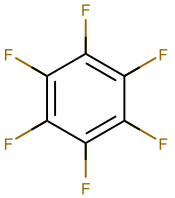
| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| 2,3,3,3-tetrafluoropropene |  | N | N | NA |
| 2-butanol |  | Y | Y | SA |
| 2-butoxyethanol |  | Y | Y | SA |
| 2-methoxyethanol |  | Y | Y | SA |
| 2-methyl-1-propanol |  | Y | Y | SA |
| 2-methyl-2-propanol |  | Y | Y | SA |
| 3-methyl-1-butanol |  | Y | Y | SA |

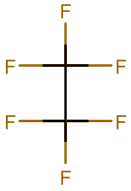
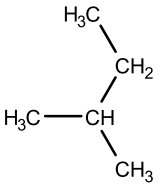
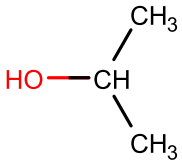
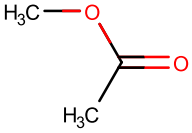
| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| 3-pentanone |  | N | Y | E |
| acetic acid |  | Y | Y | SA |
| acetic anhydride |  | N | Y | E |
| acetone |  | N | Y | E |
| acetonitrile |  | Y | Y | SA |
| allyl alcohol |  | Y | Y | SA |
| ammonia | $NH_3$ | Y | Y | SA |
| argon | Ar | N | N | NA |

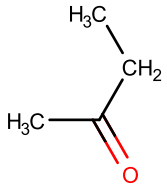
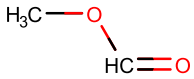
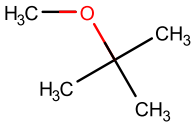
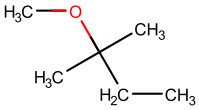
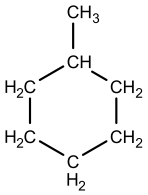
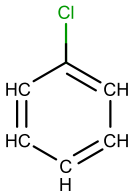
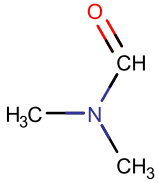
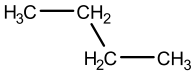
| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| benzene |  | N | N | NA |
| benzonitrile |  | N | Y | E |
| carbon dioxide |  | N | Y | E |
| carbon disulfide |  | N | Y | E |
| carbon monoxide |  | N | Y | E |
| carbon tetrachloride |  | N | N | NA |
| carbon tetrafluoride |  | N | N | NA |
| chlorodifluoro methane |  | Y | N | H |

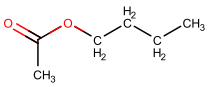
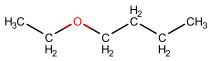
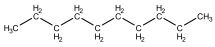
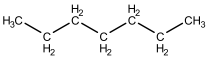
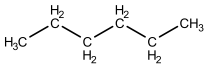
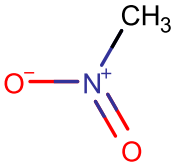
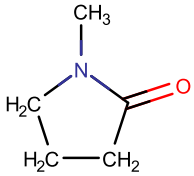
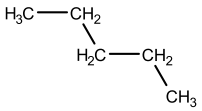
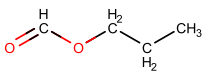
| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| chloroform |  | Y | N | H |
| chloropentafluoroethane |  | N | N | NA |
| cyclohexane |  | N | N | NA |
| cyclopentane |  | N | N | NA |
| cyclopentanone |  | N | Y | E |
| decafluorobutane |  | N | N | NA |

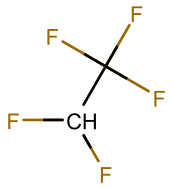
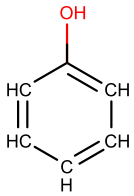
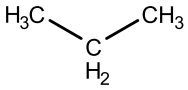
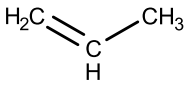
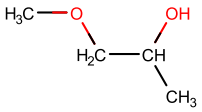
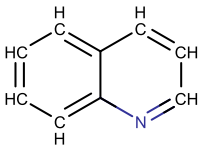
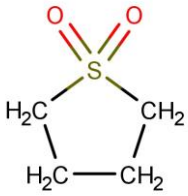
| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| dichlorodifluoromethane |  | N | N | NA |
| dichloromethane |  | Y | N | H |
| diethyl carbonate |  | N | Y | E |
| diethyl ether |  | N | Y | E |
| diethylamine |  | Y | Y | SA |
| difluoromethane |  | Y | N | H |
| diisopropyl ether |  | N | Y | E |
| dimethyl carbonate |  | N | Y | E |
| dimethyl ether |  | N | Y | E |
| di-n-butyl ether |  | N | Y | E |

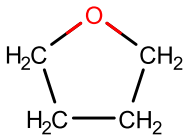
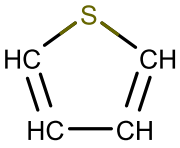
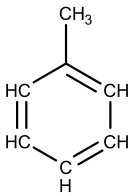
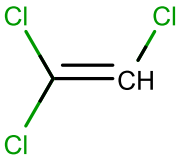
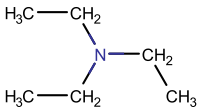
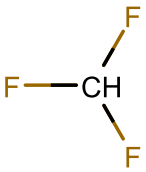
| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| di-n-propyl ether |  | N | Y | E |
| ethane |  | N | N | NA |
| ethanol |  | Y | Y | SA |
| ethyl acetate |  | N | Y | E |
| ethyl fluoride |  | N | N | NA |
| ethyl formate |  | Y | Y | SA |
| ethylene |  | N | N | NA |
| ethylenediamine |  | Y | Y | SA |
| halothane |  | Y | N | H |
| hexafluorobenzene |  | N | N | NA |

| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| hexafluoroethane |  | N | N | NA |
| hydrogen sulfide | $H_2S$ | N | Y | E |
| isopentane |  | N | N | NA |
| isopropanol |  | Y | Y | SA |
| methane | $CH_4$ | N | N | NA |
| methanol |  | Y | Y | SA |
| methyl acetate |  | N | Y | E |

| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| methyl ethyl ketone |  | N | Y | E |
| methyl formate |  | Y | Y | SA |
| methyl tert-butyl ether |  | N | Y | E |
| methyl tert-pentyl ether |  | N | Y | E |
| methylcyclohexane |  | N | N | NA |
| monochlorobenzene |  | N | N | NA |
| n, n-dimethylformamide |  | N | Y | E |
| n-butane |  | N | N | NA |

| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| n-butyl acetate |  | N | Y | E |
| n-butyl ethyl ether |  | N | Y | E |
| n-decane |  | N | N | NA |
| n-heptane |  | N | N | NA |
| n-hexane |  | N | N | NA |
| nitrogen |  | N | N | NA |
| nitromethane |  | Y | Y | SA |
| n-methyl-2-pyrrolidone |  | N | Y | E |
| n-pentane |  | N | N | NA |
| n-propyl formate |  | Y | Y | SA |
| oxygen |  | N | Y | E |

| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| pentafluoroethane |  | Y | N | H |
| phenol |  | Y | Y | SA |
| propane |  | N | N | NA |
| propylene |  | N | N | NA |
| propylene glycol monomethyl ether |  | Y | Y | SA |
| quinoline |  | N | N | NA |
| sulfolane |  | N | Y | N |
| sulfur dioxide |  | N | Y | E |

| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| tetrahydrofuran |  | N | Y | E |
| thiophene |  | N | Y | E |
| toluene |  | N | N | NA |
| trichloroethylene |  | Y | N | H |
| triethylamine |  | N | Y | E |
| trifluoromethane |  | Y | N | H |
| water | $H_2O$ | Y | Y | SA |

| Name | Formula | Has a labile hydrogen atom? | Has a lone pair of electrons? | Association code for pure compound |
|---|---|---|---|---|
| xenon | Xe | N | N | NA |

Table 9.2. Pure compounds in the database

Once each pure compound is assigned to one of the four previous categories it is immediately possible to determine the hydrogen bonds that might occur when two of them are mixed. Indeed, the minimal requirement for hydrogen bonds remains the existence of both a labile hydrogen atom and a lone pair of electrons than can now originate from the two different species. It is notable that two pure compounds H and E that do not exhibit hydrogen bonds will meet the requirement for the existence of hydrogen bonds when mixed together. In this case, the hydrogen bond is said to be formed by the "cross-association" between molecules.

Exactly ten cases, identified by the so-called Association Code (AC), can be derived for binary systems:

*Mixtures without association*

- AC 1: combining NA and NA pure compounds (NA-NA mixture).
- AC 2: combining NA and E pure compounds (NA-E mixture).
- AC 3: combining NA and H pure compounds (NA-H mixture).
- AC 4: combining E and E pure compounds (E-E mixture).
- AC 5: combining H and H pure compounds (H-H mixture).

For AC from 1 to 5, the mixture compounds do not satisfy the necessary and sufficient conditions for a binary system to show hydrogen-bonds. Therefore, mixtures in these families are expected to be easily represented by all modern thermodynamic models.

*Mixtures in which cross association takes place*

- AC 6: combining E and H pure compounds (E-H mixture).

AC 6 results from the mixing of one compound with a labile hydrogen with another molecule possessing a lone pair of electrons, causing the cross association phenomenon. Therefore, such molecules were not associated at their pure compound state but exhibit hydrogen bonds in mixture. Therefore, the molecules are more attracted to each other's in mixture than when they were pure.

*Mixtures in which self-association takes place*

- AC 7: combining NA and SA pure compounds (NA-SA mixture).

Association family 7 is made of self-associated molecules that face not associated ones. Because the non-associated molecules will hardly break through the hydrogen bond mesh, partial immiscibility is observed for this family. All binary systems of type water + alkanes or alcohol + alkanes belong to this family.

*Mixtures in which both cross-association and self-association take place*

- AC 8: combining E and SA pure compounds (E-SA mixture).
- AC 9: combining H and SA pure compounds (H-SA mixture).
- AC 10: combining SA and SA pure compounds (SA-SA mixture).

For association codes 8 to 10, very complex phenomena occur as a self-associated compound is mixed with another molecule to which it can bind through hydrogen-bonds. Therefore, it is not possible to determine how the mixture will behave and if the mixing leads to an increase or a decrease of the hydrogen bonds number.

From our experience, much less experimental data are reported for AC 4 (E-E) and 5 (H-H) than for any other family. Indeed, binary systems involving at least a SA or NA compound are much more measured than other binary systems, due to the over-representation of water (SA) and alkanes (NA) based mixtures. Moreover, H molecules

are mostly refrigerants generally used as pure compounds, explaining the lack of binary systems experimental data. Therefore, we decided to merge AC 4 and 5, both unassociated mixtures, into a single family, reducing the number of association families to 9:

- AC 1: combining NA and NA pure compounds (NA-NA mixture).
- AC 2: combining NA and E pure compounds (NA-E mixture).
- AC 3: combining NA and H pure compounds (NA-H mixture).
- AC 4: combining E and E pure compounds (E-E mixture) and H and H pure compounds (H-H mixture).
- AC 5: combining NA and SA pure compounds (NA-SA mixture).
- AC 6: combining E and H pure compounds (E-H mixture).
- AC 7: combining H and SA pure compounds (H-SA mixture).
- AC 8: combining E and SA pure compounds (E-SA mixture).
- AC 9: combining SA and SA pure compounds (SA-SA mixture).

### 9.3.2. Ideality of binary mixtures

Once a binary system has been assigned one of the 9 association codes, the way it deviates from ideality can be determined. Qualitatively, a system will be classified as ideal if it is made of molecules having (i) similar sizes (ii) similar shapes and (iii) similar energetic interactions whatever the temperature, pressure and composition [179]. On the contrary, a system exhibits deviations to ideality if it does not simultaneously satisfy the three aforementioned criteria. If deviations to ideality are the consequence of a difference in molecule sizes and shapes, the solution is athermal ($h^E=0$) and consequently $g^E=-Ts^E$. It is said that deviations to ideality are the consequence of entropic effects. Symmetrically if deviations to ideality are solely caused by a difference in energetic interactions, the solution is regular ($s^E = 0$) and $g^E = h^E$. In such a case, enthalpic effects are at the origin of the deviations to ideality. Naturally, both effects can co-exist in a non-ideal solution and in this case it is said that deviations to ideality are the consequence of both enthalpic and entropic effects. Such an overview of the three possible causes of deviation to ideality is important as many thermodynamic models are built by adding the contributions of an enthalpic (relating to the energetic interactions in the system) and an entropic terms (relating to the size of the molecules).

For each of the nine association codes (AC), our ambition is to find binary systems for which deviations to ideality are the consequence of enthalpic, entropic or mixed effects.

We indeed want to provide a reference database that will be challenging for all kinds of models and can be potentially used to identify lacks in their enthalpic and entropic contributions. Quantitative details about how to define whether a binary system is ideal or exhibits deviations to ideality originating from entropic, enthalpic or mixed effects are now detailed. To start, it is worth noting that the classification of a binary system as *ideal* or *non-ideal* can only be conducted when low-pressure vapor-liquid equilibria data are available. If it is not the case, the ideal character of the binary system was labeled *undetermined*.

For each binary system, low-pressure vapor-liquid phase equilibrium data and enthalpies of mixing (when available) were used to adjust the following 4 parameters ($p_1$, $p_2$, $p_3$, $p_4$) of the Margules excess Gibbs energy model:

$$\begin{cases} \dfrac{g^E(T,x)}{RT} = x_1 x_2 \times A(T) \\ A(T) = p_1 - p_2 T - p_3 \ln T + p_4 \exp\left(\dfrac{1}{T}\right) \end{cases} \tag{9.1}$$

The so-called $\gamma$-$\varphi$ approach was used assuming the gas phase perfect and neglecting the Poynting factor. In other words, the following classical VLE relation was used:

$$Py_i = P_i^{sat} x_i \gamma_i \tag{9.2}$$

The vapor pressures were calculated with the help of correlations extracted from the DIPPR database. In order to be able to consider perfect the gas phase, only experimental data for which the pressure was lower than 15 bar were selected. Moreover, since the $\gamma$-$\varphi$ approach can not be used with supercritical compounds, only experimental data for which the pressure was lower than 0.9 time the minimal critical pressure of the two compounds in the mixture and for which the temperature was lower than 0.98 time the minimal critical temperature of the two compounds of the mixture were selected. In addition, experimental liquid mole fraction lower than 0.01 or higher than 0.99 were rejected to get parameters well representative of the whole composition range [0;1].

Once the adjustment is performed, one can use equation (9.1) to quantify the excess enthalpy and excess entropy of the binary system in the temperature range used for the regression. In this study, $g^E$, $h^E$ and $s^E$ were calculated after fixing the composition at 0.5 as most of the systems show an extremum Gibbs excess energy at this composition making it easier to detect non-ideal binary systems. Based on our personal analysis, a

binary system can be considered as ideal if $\left|g^E / RT\right|_{x=0.5} < 0.1$ on the whole experimental temperature range. If not, the system is declared non-ideal. Once done:

1) if $h^M$ data are available and:

- If for all temperatures $\left|\left(h^E / RT\right) / \left(s^E / R\right)\right|_{x=0.5} > 2$, the non-ideality originates from enthalpic effects
- If for all temperatures $\left|\left(h^E / RT\right) / \left(s^E / R\right)\right|_{x=0.5} < 1/2$, the non-ideality originated from entropic effects
- Else, deviations to ideality are the consequence of both enthalpic and entropic effects in solution and none is dominant over the second. The system non-ideality cause is said to be mixed.

2) if $h^M$ data are unavailable, the non-ideality cause cannot be properly stated and the binary system is considered as non-ideal but with an undetermined cause. Indeed, the prediction of the binary system excess enthalpy can be very uncertain when not included in the regression procedure and should be avoided.

The structure of the database with respect to the association code and ideality criterion is resumed in Figure 9.2.

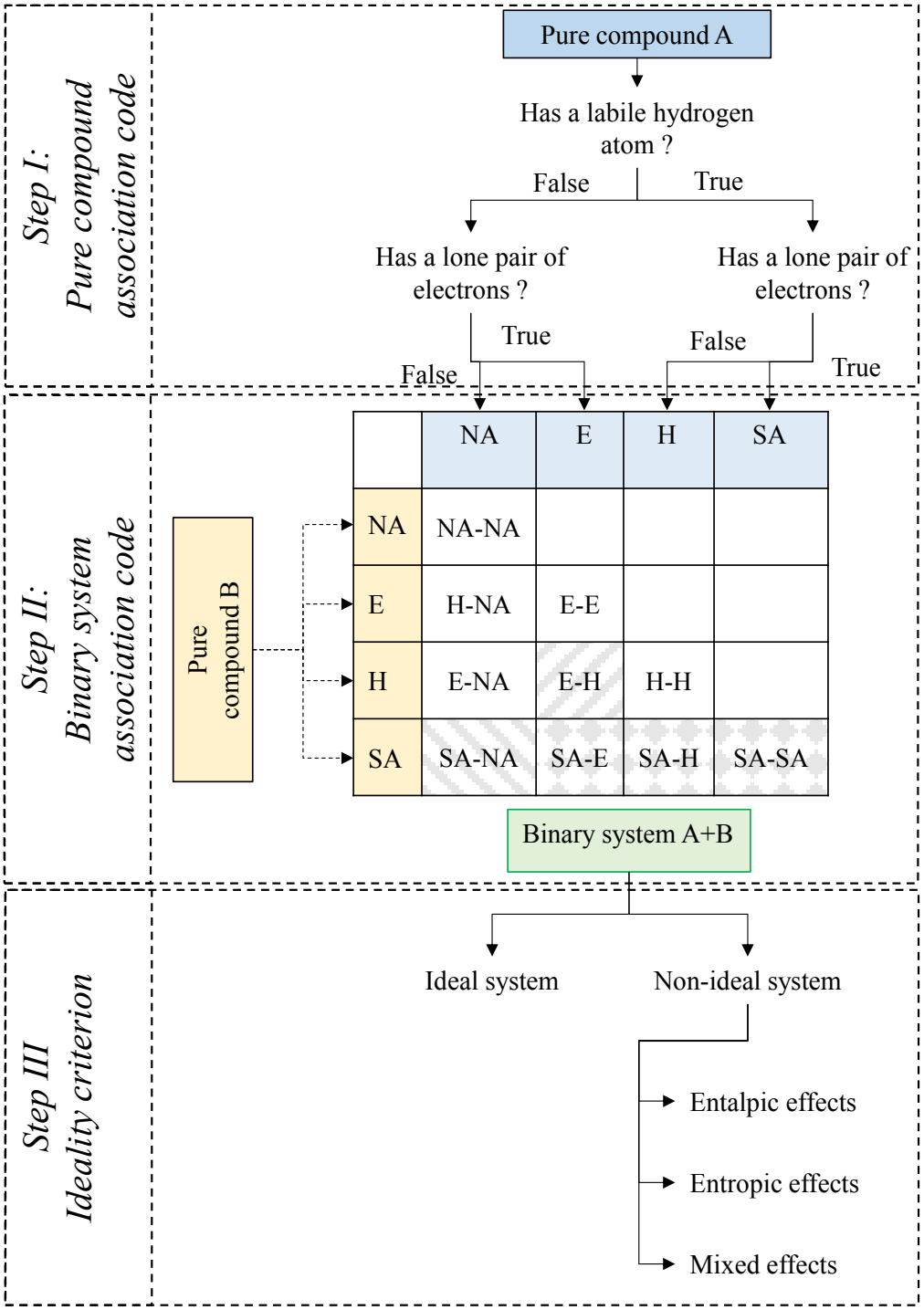



Figure 9.2. Classification procedure of a binary system with respect to its association phenomena in solution and its ideality

### 9.4. How many data must be included?

We collected experimental data for more than 20,000 binary systems from the literature. Their binary association codes were then determined on the basis of their chemical structure as discussed in Section 9.3.1. After this step, the ideal character of the systems: ideal, non-ideal (enthalpic dominant, entropic dominant, mixed, undetermined) was established using the procedure described in Section 9.3.2. At this

step, our objective was to embed about 20 binary systems in each of the 9 families, each defined by an association code, with the following proportions of ideal and non-ideal systems:

- 1/3 of ideal systems
- 2/3 of non-ideal systems
    - 1/3 of non-ideal systems with enthalpic causes
    - 1/3 of non-ideal systems with entropic causes
    - 1/3 of non-ideal systems with mixed causes

When it is not possible to fill one or more of these non-ideal subcategories, due to a lack of experimental data, non-ideal systems with an undetermined cause are used as replacement.

Another key point is to only retain high-quality-certified data explaining why the consistency of the data were checked with the help of four consistency tests: the point test [180], the integral test [181], the differential test and the infinite dilution test [182], all performed with the DPP software. It is however worth noting that the aforementioned tests can only be applied for phase equilibrium data for which both compounds are subcritical meaning that only the quality of these data in our database can be guaranteed. For an ideal binary system, passing the point test was considered as a sufficient consistency condition while for non-ideal systems, the point test and two of the three remaining tests had to be passed in order to keep the experimental data in our database.

At the end, the proposed database is composed of 200 binary systems and contains about 37000 data points. As previously discussed, we made our best in order the selected systems are those for which phase equilibrium data (VLE, LLE, VLLE, azeotrope) and mixing properties ($h^M$, $c_P{}^M$) are abundant in large temperature, pressure and composition ranges. An overview of the database can be found in Table 9.3 and 9.4 whereas Table 9.5 to 9.13 give for each of the 9 association codes, the list of the selected systems, information about the origin of the deviations to ideality and the list of references in which the experimental data can be found. All the experimental values are given in Appendices B-1 and B-2.

| Association Code | Subcritical phase equilibrium data | Supercritical phase equilibrium data | Azeotropic point | Critical point | Enthalpy of mixing | Heat capacity of mixing | Sum | % |
|---|---|---|---|---|---|---|---|---|
| 1 | 1480 | 2219 | 18 | 270 | 2480 | 231 | 6698 | 18% |
| 2 | 1071 | 319 | 44 | 51 | 352 | 30 | 1867 | 5% |
| 3 | 1429 | 1272 | 22 | 339 | 3949 | 46 | 7057 | 19% |
| 4 | 912 | 462 | 7 | 61 | 598 | 15 | 2055 | 6% |
| 5 | 1250 | 466 | 37 | 133 | 2680 | 175 | 4741 | 13% |
| 6 | 1048 | 416 | 19 | 74 | 500 | 99 | 2156 | 6% |
| 7 | 711 | 0 | 10 | 0 | 514 | 26 | 1261 | 3% |
| 8 | 2044 | 967 | 31 | 242 | 2566 | 144 | 5994 | 16% |
| 9 | 2149 | 119 | 20 | 49 | 2427 | 507 | 5271 | 14% |
| Sum | 12094 | 6240 | 208 | 1219 | 16066 | 1273 | 37100 | |
| % | 32.60% | 16.82% | 0.56% | 3.29% | 43.30% | 3.43% | | |
| % merged | | 53.26% | | | 46.74% | | | |

Table 9.3. Number of experimental data in the database

| Association Code | Undetermined | Ideal | Non ideal (enthalpic reasons) | Non ideal (entropic reasons) | Non ideal (enthalpic and entropic reasons) | Non ideal with undetermined causes |
|---|---|---|---|---|---|---|
| 1 | 32.00% | 20.00% | 16.00% | 4.00% | 20.00% | 8.00% |
| 2 | 9.52% | 28.57% | 9.52% | 0.00% | 19.05% | 33.33% |
| 3 | 29.17% | 25.00% | 12.50% | 8.33% | 16.67% | 8.33% |
| 4 | 27.27% | 36.36% | 13.64% | 4.55% | 9.09% | 9.09% |
| 5 | 31.58% | 15.79% | 21.05% | 0.00% | 21.05% | 10.53% |
| 6 | 28.00% | 16.00% | 4.00% | 0.00% | 28.00% | 24.00% |
| 7 | 43.75% | 0.00% | 6.25% | 25.00% | 25.00% | 0.00% |
| 8 | 23.08% | 19.23% | 26.92% | 3.85% | 19.23% | 7.69% |
| 9 | 9.09% | 31.82% | 22.73% | 9.09% | 13.64% | 13.64% |

Table 9.4. Ideality of the binary systems in the database

| Ideality | Molecule 1 | Molecule 2 | References |
|---|---|---|---|
| Undetermined | methane | propane | [183–196] |
| | methane | n-hexane | [185,197–204] |
| | methane | n-heptane | [185,205–209] |
| | nitrogen | ethane | [210–217] |
| | methane | n-decane | [218–223] |
| | ethane | n-heptane | [153,224–228] |
| | nitrogen | n-pentane | [229–232] |
| | nitrogen | n-decane | [233,234] |
| Ideal | n-hexane | cyclohexane | [235–248] |
| | benzene | toluene | [249–258] |
| | propane | isopentane | [259] |
| | cyclohexane | methylcyclohexane | [235,254,260–263] |
| | hexafluorobenzene | benzene | [264–269] |
| Non-ideal with undetermined causes | ethane | propane | [270–282] |
| | methane | n-butane | [185,197,283–287] |
| Non-ideal (enthalpic reasons) | argon | methane | [288–298] |
| | n-heptane | monochlorobenzene | [299–306] |
| | cyclohexane | monochlorobenzene | [260,300,307–311] |
| | 1,2-dichloroethane | carbon tetrachloride | [312–317] |
| Non-ideal (enthalpic and entropic reasons) | nitrogen | methane | [318–320,211,321–323,292,324,325,297,326,298] |
| | methane | ethane | [185,186,194,211,214,327–330] |
| | benzene | n-heptane | [235,254,299,331–347] |
| | benzene | cyclohexane | [242,245,343,348–366] |
| | ethylene | xenon | [367–369] |
| Non-ideal (entropic reasons) | 1,2-dichloroethane | toluene | [249,370–374] |

Table 9.5. Binary systems for which BAC = NA-NA (25 systems)

| Ideality | Molecule 1 | Molecule 2 | References |
|---|---|---|---|
| Undetermined | ethylene | dichloromethane | [375] |
| | nitrogen | chlorodifluoromethane | [376–379] |
| Ideal | chloroform | benzene | [249,380–387] |
| | chloroform | 1,2-dichloroethane | [388,389] |
| | chloroform | carbon tetrachloride | [383,390–395] |
| | 1,1,1-trifluoroethane | 2,3,3,3-tetrafluoropropene | [396] |
| | ethyl fluoride | 1,1,1,2-tetrafluoroethane | [397] |
| | propylene | chlorodifluoromethane | [398] |
| Non-ideal with undetermined causes | difluoromethane | propane | [399–403] |
| | trifluoromethane | ethane | [404–406] |
| | carbon tetrafluoride | chlorodifluoromethane | [407,408] |
| | pentafluoroethane | propane | [402,403,409–411] |
| | carbon tetrafluoride | trifluoromethane | [407,412] |
| | hexafluoroethane | 1,1,1,2-tetrafluoroethane | [398,413] |
| | decafluorobutane | 1,1,1,3,3-pentafluorobutane | [414] |
| Non-ideal (enthalpic reasons) | chlorodifluoromethane | dichlorodifluoromethane | [415–420] |
| | dichloromethane | carbon tetrachloride | [312,315,394,421] |
| Non-ideal with $h^E$ and $s^E$ causes | chlorodifluoromethane | chloropentafluoroethane | [416,422] |
| | chloroform | n-hexane | [423–429] |
| | chloroform | n-heptane | [423–425,427,430,431] |
| | dichloromethane | n-pentane | [432–434] |

Table 9.6. Binary systems for which BAC = H-NA (21 systems)

| Ideality | Molecule 1 | Molecule 2 | References |
|---|---|---|---|
| Undetermined | carbon dioxide | toluene | [435–450] |
| | carbon dioxide | n-decane | [451,451–462] |
| | methane | carbon dioxide | [193,330,463–473] |
| | carbon dioxide | cyclopentane | [474,475] |
| | nitrogen | carbon dioxide | [210,463,464,471,473,476–489] |
| | methane | hydrogen sulfide | [490–492] |
| | oxygen | carbon dioxide | [482,485,488,493–495] |
| Ideal | methyl tert-butyl ether | n-heptane | [496–500] |
| | ethyl acetate | toluene | [501–505] |
| | carbon tetrachloride | 1,4-dioxane | [506–513] |
| | methyl ethyl ketone | benzene | [514–517] |
| | methyl tert-pentyl ether | n-heptane | [518–521] |
| | methyl tert-butyl ether | toluene | [522–525] |
| Non-ideal with undetermined causes | ethylene | carbon dioxide | [526–532] |
| | carbon dioxide | propane | [190,193,282,487,533–541] |
| Non-ideal (enthalpic reasons) | acetone | n-hexane | [542–550] |
| | n-pentane | acetone | [544,547,548,551,552] |
| | acetone | cyclohexane | [238,363,553–560] |
| Non-ideal (enthalpic and entropic reasons) | carbon dioxide | ethane | [537,561–571] |
| | carbon dioxide | n-butane | [282,479,530,533,534,537,539,572–579] |
| | n-hexane | methyl ethyl ketone | [334,515,546,580–582] |
| | acetone | benzene | [363,384,508,583–590] |
| Non-ideal (entropic reasons) | benzene | n-methyl-2-pyrrolidone | [591–597] |
| | benzene | benzonitrile | [598–601] |

Table 9.7. Binary systems for which BAC = E-NA (24 systems)

| Ideality | Molecule 1 | Molecule 2 | References |
|---|---|---|---|
| Undetermined | carbon dioxide | dimethyl ether | [602–604] |
| | carbon dioxide | hydrogen sulfide | [605–608] |
| | carbon dioxide | ethyl acetate | [609–614] |
| | carbon dioxide | carbon disulfide | [615,616] |
| | carbon dioxide | dimethyl carbonate | [617–622] |
| | carbon monoxide | carbon dioxide | [623–625] |
| Ideal | pentafluoroethane | 1,1,1,2-tetrafluoroethane | [626–630] |
| | difluoromethane | pentafluoroethane | [631,632] |
| | chlorodifluoromethane | 1,1,1,2-tetrafluoroethane | [633,634] |
| | difluoromethane | 1,1,1,2-tetrafluoroethane | [626–629,635–639] |
| | 1,1,1,2-tetrafluoroethane | 1,1-difluoroethane | [398,640,641] |
| | ethyl acetate | 1,4-dioxane | [513,642–644] |
| | dimethyl carbonate | diethyl carbonate | [645–647] |
| | 1,2-epoxybutane | dimethyl carbonate | [648,649] |
| Non-ideal with undetermined causes | dimethyl ether | sulfur dioxide | [650–652] |
| | trifluoromethane | chlorodifluoromethane | [653,654] |
| Non-ideal (enthalpic reasons) | diethyl ether | acetone | [383,655,656] |
| | carbon disulfide | acetone | [657–659] |
| | triethylamine | 1,4-dioxane | [660–662] |
| Non-ideal ((enthalpic and entropic reasons) | tetrahydrofuran | n,n-dimethylformamide | [663,664] |
| | n-butyl acetate | n,n-dimethylformamide | [665,666] |
| Non-ideal (entropic reasons) | thiophene | sulfolane | [667] |

Table 9.8. Binary systems for which BAC = H-H or E-E (22 systems)

| Ideality | Molecule 1 | Molecule 2 | References |
|---|---|---|---|
| Undetermined | n-butane | water | [668–672] |
| | water | benzene | [673–675] |
| | ethane | 1-propanol | [676–681] |
| | nitrogen | ammonia | [682–684] |
| | ethane | water | [668] |
| | nitrogen | water | [295,685–694] |
| Ideal | 1,2,3,4-tetrahydronaphthalene | quinoline | [695,696] |
| | diethylamine | benzene | [299,697,698] |
| | diethylamine | monochlorobenzene | [299,699] |
| Non-ideal with undetermined causes | ethane | methanol | [151,679,700–704] |
| | propane | methanol | [705–710] |
| Non-ideal (enthalpic reasons) | 1-propanol | benzene | [355,711–721] |
| | ethanol | benzene | [336,341,366,381,712,718,721–730] |
| | isopropanol | 2,2,4-trimethylpentane | [731–737] |
| | 2-butanol | cyclohexane | [738–743] |
| Non-ideal (enthalpic and entropic reasons) | 1-propanol | n-hexane | [744–750] |
| | ethanol | n-heptane | [336,751–766] |
| | methanol | n-hexane | [746,764,767–775] |
| | methanol | benzene | [235,712,718,721,776–785] |

Table 9.9. Binary systems for which BAC = SA-NA (19 systems)

| Ideality | Molecule 1 | Molecule 2 | References |
|---|---|---|---|
| Undetermined | carbon dioxide | chlorodifluoromethane | [377,379,654,786] |
| | carbon dioxide | 1,1,1,2-tetrafluoroethane | [787–790] |
| | carbon dioxide | 1,1,1,2,3,3,3-heptafluoropropane | [791,792] |
| | trifluoromethane | carbon disulfide | [654] |
| | chloroform | diisopropyl ether | [427,661,793,794] |
| | 1,1,1-trifluoroethane | dimethyl ether | [795] |
| | chloroform | n-butyl ethyl ether | [794,796] |
| Ideal | carbon dioxide | difluoromethane | [637,797–800] |
| | difluoromethane | dimethyl ether | [801–803] |
| | difluoromethane | sulfur dioxide | [804] |
| | ethyl acetate | trichloroethylene | [805] |
| Non-ideal with undetermined causes | sulfur dioxide | 1,1,1,2,3,3,3-heptafluoropropane | [806] |
| | chlorodifluoromethane | dimethyl ether | [807,808] |
| | chlorodifluoromethane | carbon disulfide | [654] |
| | pentafluoroethane | dimethyl ether | [409,809] |
| | 3-pentanone | 1,1,2,2-tetrachloroethane | [810] |
| | dimethyl ether | 1,1,1,3,3,3-hexafluoropropane | [811,812] |
| Non-ideal (enthalpic reasons) | dichloromethane | carbon disulfide | [813,814] |
| Non-ideal (enthalpic and entropic reasons) | acetone | chloroform | [386,427,428,583,590,661,815–822] |
| | chloroform | ethyl acetate | [823–826] |
| | chloroform | tetrahydrofuran | [427,827–831] |
| | chloroform | di-n-propyl ether | [427,793,794,796,832,833] |
| | methyl acetate | chloroform | [427,825,834,835] |
| | cyclopentanone | 1,1,2,2-tetrachloroethane | [836–838] |
| | ethyl acetate | 1,1,2,2-tetrachloroethane | [267,269,839] |

Table 9.10. Binary systems for which BAC = E-H (25 systems)

| Ideality | Molecule 1 | Molecule 2 | References |
|---|---|---|---|
| Undetermined | chloroform | 1-butanol | [380,840,841] |
| | 1-propanol | trichloroethylene | [842,843] |
| | trichloroethylene | 1-butanol | [843,844] |
| | isopropanol | trichloroethylene | [842,845] |
| | 2-butanol | trichloroethylene | [844,845] |
| | 1-hexyne | acetonitrile | [846] |
| | isopropanol | chloroform | [840,847,848] |
| Non-ideal (enthalpic reasons) | ethanol | 1-heptyne | [849,850] |
| Non-ideal (enthalpic and entropic reasons) | chloroform | acetonitrile | [851–856] |
| | ethyl formate | chloroform | [825,826] |
| | chloroform | 1-propanol | [383,840,857–859] |
| | n-propyl formate | 1,1,2,2-tetrachloroethane | [267,269,839] |
| Non-ideal (entropic reasons) | ethanol | chloroform | [380,431,840,860–865] |
| | chloroform | acetic acid | [390,391,866–869] |
| | methanol | halothane | [870–872] |
| | trichloroethylene | 2-methoxyethanol | [873,874] |

Table 9.11. Binary systems for which BAC = H-SA (16 systems)

| Ideality | Molecule 1 | Molecule 2 | References |
|---|---|---|---|
| Undetermined | carbon dioxide | water | [875–894] |
| | carbon dioxide | ethanol | [448,450,453,681,746,886,895–911] |
| | ethanol | methyl tert-butyl ether | [496,912–916] |
| | carbon dioxide | 2-methyl-1-propanol | [917–922] |
| | carbon monoxide | methanol | [923–925] |
| | carbon dioxide | 1-pentanol | [453,919,926] |
| Ideal | diethylamine | ethyl acetate | [642,643] |
| | diethylamine | triethylamine | [927–930] |
| | acetic acid | acetic anhydride | [931,932] |
| | 2-methyl-2-propanol | methyl tert-butyl ether | [933–936] |
| | acetonitrile | 1,4-dioxane | [856,937,938] |
| Non-ideal with undetermined causes | dimethyl ether | water | [603,939–941] |
| | carbon dioxide | methanol | [442,450,453,603,746,773,900,901,909,923,942–952] |
| Non-ideal (enthalpic reasons) | methanol | ethyl acetate | [953–960] |
| | isopropanol | diisopropyl ether | [736,914,961,962] |
| | methanol | n-butyl acetate | [957,963–966] |
| | diethyl ether | ethanol | [967–969] |
| | methanol | 1,4-dioxane | [970–976] |
| | methanol | thiophene | [782] |
| | ethanol | di-n-butyl ether | [969,977–979] |
| Non-ideal (enthalpic and entropic reasons) | methanol | methyl tert-butyl ether | [496,498,499,912,980–985] |
| | ethanol | ethyl acetate | [956,957,960,979,986–993] |
| | acetone | water | [235,554,558,994–1006] |
| | ethanol | methyl ethyl ketone | [517,1007–1014] |
| | ethanol | acetone | [757,1015–1020] |
| Non-ideal (entropic reasons) | methanol | diisopropyl ether | [914,981,1021,1022] |

Table 9.12. Binary systems for which BAC = E-SA (26 systems)

| Ideality | Molecule 1 | Molecule 2 | References |
|---|---|---|---|
| Undetermined | water | ethylenediamine | [1023–1025] |
| | water | 1-pentanol | [1026–1030] |
| Ideal | methanol | 1-butanol | [235,1031–1035] |
| | ethanol | acetic acid | [990,1036–1039] |
| | methanol | ethanol | [823,1033,1040–1046] |
| | 2-methyl-2-propanol | 1-butanol | [1047–1049] |
| | ethanol | 3-methyl-1-butanol | [1050–1052] |
| | methanol | 3-methyl-1-butanol | [1052–1054] |
| | methanol | 1-propanol | [766,998,1033,1045,1046,1055–1058] |
| Non-ideal with undetermined causes | ammonia | water | [1059–1069] |
| | ammonia | acetonitrile | [909] |
| | water | allyl alcohol | [1070,1071] |
| Non-ideal (enthalpic reasons) | water | phenol | [1072–1078] |
| | methyl formate | methanol | [1079–1083] |
| | ethyl formate | water | [1084,1085] |
| | ethanol | ethyl formate | [1080,1086–1088] |
| | 1-butanol | nitromethane | [1045,1089–1094] |
| Non-ideal (enthalpic and entropic reasons) | ethanol | water | [558,902,960,988,998,1042,1095–1117] |
| | water | acetonitrile | [1118–1130] |
| | methanol | water | [241,1000,1095,1096,1131–1151] |
| Non-ideal (entropic reasons) | water | 2-butoxyethanol | [1152–1157] |
| | water | propylene glycol monomethyl ether | [1152] |

Table 9.13. Binary systems for which BAC = SA-SA (22 systems)

The last part of this article is dedicated to explain how the proposed database has to be used to benchmark a thermodynamic model. For illustration purpose, the Peng-Robinson equation of state with a temperature dependent binary interaction parameter was benchmarked.

### 9.5. Calculating models deviations and grading of a thermodynamic model

The experimental data being selected, it is worth detailing the deviation calculation procedure between experimental and values returned by a thermodynamic model as there is not a single way to do it since the phase rule only indicates the number of intensive variables to specify in order to define an equilibrium state. The following arbitrary choices were made (a summary is given in Table 9.14):

- For systems of variance 2 (2-phase equilibrium binary systems), temperature and pressure are specified and phase compositions are calculated.
- For systems of variance 1 (critical binary system, azeotropic binary system, 3-phase equilibrium binary systems), temperature is specified and other variables (critical pressure and composition, azeotropic pressure and composition, 3-phase pressure and compositions) are calculated.
- For mixing properties, they are reported at fixed temperature and pressure as a function of the global composition $z_1$ but depending on $z_1$, the binary system can either be in a 1-phase or a 2-phase region. Consequently, a flash calculation is first performed at specified temperature, pressure and global composition in order to determine the number of phases in equilibrium, their composition and their proportions. Once done, $h^M$ and $c_P^M$ can be calculated. More details about the calculation of the mixing properties are given in [24]. It is worth noting that the authors do not always specify the pressure at which the mixing properties are measured although such a value is required to perform the calculation. In such a case the pressure is determined by trial and errors in order the calculated physical state of the system agrees with the experimental data. The first guessed pressure is always 1 bar.

| Property | Variance | Variables | Fixed variables | Calculated variables |
|---|---|---|---|---|
| Critical point | 1 | $T,P,x$ | $T$ | $P,x$ |
| Azeotropic point | | $T,P,x,y$ | | $P,x$ |
| Phase equilibrium data | 2 | $\begin{cases} T,P,x,y \text{ for VLE} \\ T,P,x^{\alpha},x^{\beta} \text{ for LLE} \end{cases}$ | $T,P$ | $\begin{cases} x,y \text{ for VLE} \\ x^{\alpha},x^{\beta} \text{ for LLE} \end{cases}$ |
| Enthalpy of mixing | 3 | $T,P,z,h^{M}$ | $T,P,z$ | $h^{M}$ |
| Heat capacity of mixing | | $T,P,z,c_P^{M}$ | | $c_P^{M}$ |

Table 9.14. Specified and calculated variables for the different properties involved in the database

For any calculated property $X$, the Mean Absolute Percentage Error [MAPE - see Equ.(9.3)] was selected to determine the deviations with the experimental data:

$$MAPE_X = 100 \sum_{i=1}^{N_{data}} \left| \frac{X_i^{MODEL} - X_i^{EXP}}{X_i^{EXP}} \right| \tag{9.3}$$

At this step it becomes possible to grade a given thermodynamic model in order to cross-compare it with another one. Our idea is to start giving a mark over 20 to each of the nine association codes (AC). Such a mark is in fact the average value of 8 marks (one for each of the 8 calculated properties defined in the last column of Table 9.14 and that are: critical pressure, critical composition, azeotropic pressure, azeotropic composition, liquid phase composition, gas phase composition, mixing enthalpy, mixing heat capacity). Once done, we thus have 9 marks (one for each AC). In a second step, the number of marks is reduced from 9 to 4 by averaging the marks got by some AC in order to only retain 4 families of systems based on the type of association they exhibit:

- the marks obtained by AC1 + AC2 + AC3 + AC4 are averaged because all these systems do not exhibit association. The grouping of AC1 + AC2 + AC3 + AC4 defines the “No association” family

- the mark obtained by AC5 is kept because all these systems exhibit self-association. AC5 is also called “Self-association” family.

- the mark obtained by AC6 is kept because all these systems exhibit cross-association. AC6 is also called “Cross-association” family.

- the marks obtained by AC7 + AC8 + AC9 are averaged because all these systems both exhibit self-association and cross-association. The grouping of AC7 + AC8 + AC9 defines the “Self-association + Cross-association” family.

The unique final mark given to a thermodynamic model is obtained by averaging these 4 marks.

The procedure aiming at giving a mark over 20 to a given AC is now detailed. As previously stated, such a mark is in fact the average value of 8 marks (in critical pressure $P_c$, critical composition $x_c$, azeotropic pressure $P_{az}$, azeotropic composition $x_{az}$, liquid phase composition $x_{liq}$, gas phase composition $x_{gas}$, mixing enthalpy $h^M$, mixing heat capacity $c_P{}^M$) defined as follows:

$$\text{Mark in critical pressure } (P_c) = 20 - 0.75 \times \text{MAPE on } P_c\,(\%) \tag{9.4}$$

$$\text{Mark in azeotropic pressure } (P_{az}) = 20 - 0.5 \times \text{MAPE on } P_{az}\,(\%) \tag{9.5}$$

$$\text{Mark in phase composition } (x_c, x_{az}, x_{liq}, x_{gas}) = 20 - 0.5 \times \text{MAPE on } x\,(\%) \tag{9.6}$$

$$\text{Mark in mixing enthalpy } (h^M) = 20 - 0.25 \times \text{MAPE on } h^M\,(\%) \tag{9.7}$$

$$\text{Mark in mixing heat capacity } (c_P^M) = 20 - 0.125 \times \text{MAPE on } c_P^M\,(\%) \tag{9.8}$$

Moreover any mark below zero is raised to zero. In conclusion 8 marks (at the most) are attributed to all the binary systems belonging to an AC. It is obvious that the absence of experimental data may render impossible the calculation of a mark. It is worth noting that the previous equations give the greatest importance to the critical pressures whereas less attention is given to mixing enthalpies and even less to mixing heat capacities.

### 9.6. Benchmark of the Peng-Robinson equation of state

The following Peng-Robinson equation was used:

$$P(T,v,x)=\frac{RT}{v-b(x)}-\frac{a(T,x)}{v\times[v+b(x)]+b(x)\times[v-b(x)]}$$

Pure compounds

$$X=\frac{-1+\sqrt[3]{6\sqrt{2}+8}-\sqrt[3]{6\sqrt{2}-8}}{3}$$

$$\Omega_a=\frac{8(5X+1)}{49-37X}$$

$$a_{c,i}=\Omega_a\times\frac{\left(RT_{c,i}\right)^2}{P_{c,i}}$$

$$a_i(T)=a_{c,i}\times\alpha\left(T/T_{c,i}\right)$$

$$\alpha\left(T/T_{c,i}\right)=\left[1+m\left(\omega_i\right)\left(1-\sqrt{T/T_{c,i}}\right)\right]^2$$

$$m\left(\omega_i\le 0.491\right)=0.37464+1.54226\omega_i-0.26992\omega_i^2$$

$$m\left(\omega_i>0.491\right)=0.379642+1.48503\omega_i-0.164423\omega_i^2+0.016666\omega_i^3$$

$$\Omega_b=\frac{X}{X+3}$$

$$b_i=\Omega_b\times\frac{RT_{c,i}}{P_{c,i}}$$

Mixtures

$$a(T,x)=\sum_{i=1}^{N}\sum_{j=1}^{N}x_ix_j\sqrt{a_i(T)a_j(T)}\times\left[1-k_{ij}(T)\right]$$

$$k_{ij}(T)=\frac{A\left(\frac{298.15}{T}\right)^{\frac{B}{A}-1}-\left(\frac{\sqrt{a_i}}{b_i}-\frac{\sqrt{a_j}}{b_j}\right)^2}{2\times\frac{\sqrt{a_i}}{b_i}\times\frac{\sqrt{a_j}}{b_j}}$$

$$b(x)=\sum_{i=1}^{N}x_ib_i \qquad (9.9)$$

The equation giving the changes of $k_{ij}$ with respect to temperature comes from the PPR78 model [23,24] in which each compound is considered as an elementary group. The 2 parameters $A$ and $B$ are determined for each binary system by minimizing an objective function accounting for the deviations between experimental data (vapor-liquid equilibrium data, critical data, azeotropic data, heat capacity of mixing data, enthalpy of mixing data ...) and model predictions. The objective function expression is:

$$F_{\text{obj}} = \frac{F_{\text{obj, bubble}} + F_{\text{obj, dew}} + F_{\text{obj, crit.comp}} + F_{\text{obj, crit.pressure}}}{n_{\text{bubble}} + n_{\text{dew}} + 2n_{\text{crit}} + 2n_{\text{az}} + n_{\text{mix,enthalpy}} + n_{\text{mix,heat capacity}}} + \frac{F_{\text{obj, az.comp}} + F_{\text{obj, az.pressure}} + F_{\text{obj, mix,enthalpy}} + F_{\text{obj, mix,heat capacity}}}{n_{\text{bubble}} + n_{\text{dew}} + 2n_{\text{crit}} + 2n_{\text{az}} + n_{\text{mix,enthalpy}} + n_{\text{mix,heat capacity}}}$$

$$\begin{cases} F_{\text{obj, bubble}} = 100 \sum_{i=1}^{n_{\text{bubble}}} 0.5 \left( \frac{|\Delta x|}{x_{1,\text{exp}}} + \frac{|\Delta x|}{x_{2,\text{exp}}} \right)_i \\ F_{\text{obj, dew}} = 100 \sum_{i=1}^{n_{\text{dew}}} 0.5 \left( \frac{|\Delta y|}{y_{1,\text{exp}}} + \frac{|\Delta y|}{y_{2,\text{exp}}} \right)_i \text{ with } |\Delta y| = |y_{1,\text{exp}} - y_{1,\text{cal}}| = |y_{2,\text{exp}} - y_{2,\text{cal}}| \\ F_{\text{obj, crit, comp}} = 100 \sum_{i=1}^{n_{\text{crit}}} 0.5 \left( \frac{|\Delta x_{\text{c}}|}{x_{\text{c1,exp}}} + \frac{|\Delta x_{\text{c}}|}{x_{\text{c2,exp}}} \right)_i \\ F_{\text{obj, crit, pressure}} = 100 \sum_{i=1}^{n_{\text{crit}}} \left( \frac{|P_{\text{c,exp}} - P_{\text{c,cal}}|}{P_{\text{c,exp}}} \right)_i \\ F_{\text{obj, az, comp}} = 100 \sum_{i=1}^{n_{\text{az}}} 0.5 \left( \frac{|\Delta x_{\text{az}}|}{x_{\text{az1,exp}}} + \frac{|\Delta x_{\text{az}}|}{x_{\text{az2,exp}}} \right)_i \text{ with } |\Delta x_{\text{az}}| = |x_{\text{az1,exp}} - x_{\text{az1,cal}}| = |x_{\text{az2,exp}} - x_{\text{az2,cal}}| \\ F_{\text{obj, az, pressure}} = 100 \sum_{i=1}^{n_{\text{az}}} \left( \frac{|P_{\text{az,exp}} - P_{\text{az,cal}}|}{P_{\text{az,exp}}} \right)_i \\ F_{\text{obj, mix, enthalpy}} = 100 \sum_{i=1}^{n_{\text{mix,enthalpy}}} \left( \frac{\Delta h^{\text{M}}}{|h^{\text{M}}_{\text{exp}}|} \right)_i \text{ with } \Delta h^{\text{M}} = |h^{\text{M}}_{\text{exp}} - h^{\text{M}}_{\text{cal}}| \\ F_{\text{obj, mix, heat capacity}} = 100 \sum_{i=1}^{n_{\text{mix,heat capacity}}} \left( \frac{\Delta c_P^M}{|c_{P,\text{exp}}^M|} \right)_i \text{ with } \Delta c_P^M = |c_{P,\text{exp}}^M - c_{P,cal}^M| \end{cases}$$

(9.10)

### 9.6.1. Grading of the PR EoS

For each association code, the MAPEs on critical pressure $P_c$, critical composition $x_c$, azeotropic pressure $P_{az}$, azeotropic composition $x_{az}$, liquid phase composition $x_{liq}$, gas phase composition $x_{gas}$, mixing enthalpy $h^M$ and mixing heat capacity $c_P{}^M$ are resumed in Table 9.15:

| | | MAPE | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Association Code | Association family | $x_{liq}$ | $x_{gas}$ | $x_c$ | $P_c$ | $x_{az}$ | $P_{az}$ | $h^M$ | $c_P^M$ |
| 1 (NA - NA) | No association | 16.7 | 10.2 | 11.3 | 9.6 | 33.4 | 1.3 | 28.6 | 43.2 |
| 2 (NA-E) | | 13.9 | 7.5 | 18.5 | 7.7 | 9.0 | 0.6 | 25.6 | 94.3 |
| 3 (NA-H) | | 7.0 | 6.3 | 17.7 | 5.3 | 5.5 | 1.2 | 12.0 | 58.3 |
| 4 (E-E + H-H) | | 8.9 | 9.2 | 13.7 | 3.1 | 11.8 | 0.3 | 16.0 | |
| 5 (NA-SA) | Self-association | 33.6 | 15.8 | 58.3 | 27.7 | 19.4 | 9.4 | 32.7 | 87.3 |
| 6 (E-H) | Cross-association | 8.0 | 8.4 | 24.3 | 4.1 | 9.2 | 1.7 | 15.9 | 58.2 |
| 7 (H-SA) | Self-association + Cross-association | 17.0 | 13.6 | | | 3.9 | 1.5 | 65.3 | 78.8 |
| 8 (E-SA) | | 21.4 | 14.5 | 19.9 | 13.0 | 10.9 | 2.2 | 46.1 | 60.4 |
| 9 (SA-SA) | | 27.5 | 16.5 | 10.2 | 5.9 | 24.3 | 7.4 | 42.6 | 66.3 |

Table 9.15. MAPE between experimental data and values calculated with the Peng-Robinson equation of state (only deviations below 100% are taken into account not to give too much importance to binary systems that are very poorly represented).

Such MAPEs make it possible to give a mark over 20 to each of the 9 AC by averaging the 8 marks in $x_{liq}$, $x_{gas}$, $x_c$, $P_c$, $x_{az}$, $P_{az}$, $h^M$ and $c_P{}^M$. Such marks can be found in Table 9.16. At the end, as previously explained some AC are grouped together to define 4 association families (AC1-AC4; AC5; AC6; AC7-AC9). The marks for these association families are simply the average marks got by the AC that compose them. By averaging these 4 values, the PR EoS receives the mark of 12.4/20.

| | | Mark (/20) | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Association Code | Association family | $x_{liq}$ | $x_{gas}$ | $x_c$ | $P_c$ | $x_{az}$ | $P_{az}$ | $h^M$ | $c_P^M$ | Association **code's** mark | Association **families'** mark | **PR EoS' mark** |
| 1 (NA - NA) | No association | 11.7 | 14.9 | 14.4 | 12.8 | 3.3 | 19.4 | 12.9 | 14.6 | 13.0 | 14.7 | 12.4 |
| 2 (NA-E) | | 13.1 | 16.3 | 10.8 | 14.2 | 15.5 | 19.7 | 13.6 | 8.2 | 13.9 | | |
| 3 (NA-H) | | 16.5 | 16.9 | 11.2 | 16.0 | 17.3 | 19.4 | 17.0 | 12.7 | 15.9 | | |
| 4 (E-E + H-H) | | 15.6 | 15.4 | 13.2 | 17.7 | 14.1 | 19.9 | 16.0 | | 16.0 | | |
| 5 (NA-SA) | Self-association | 3.2 | 12.1 | 0.0 | 0.0 | 10.3 | 15.3 | 11.8 | 9.1 | 7.7 | 7.7 | |
| 6 (E-H) | Cross-association | 16.0 | 15.8 | 7.9 | 16.9 | 15.4 | 19.2 | 16.0 | 12.7 | 15.0 | 15.0 | |
| 7 (H-SA) | Self-association + cross-association | 11.5 | 13.2 | | | 18.1 | 19.3 | 3.7 | 10.2 | 12.6 | 12.1 | |
| 8 (E-SA) | | 9.3 | 12.8 | 10.1 | 10.3 | 14.6 | 18.9 | 8.5 | 12.5 | 12.1 | | |
| 9 (SA-SA) | | 6.3 | 11.8 | 14.9 | 15.6 | 7.9 | 16.3 | 9.4 | 11.7 | 11.7 | | |

Table 9.16. Scores calculated for each property for each association code

### 9.6.2. Discussion about the accuracy of the PR EoS

At this step, it is possible to analyze in detail the results obtained with the PR EoS. The 8 MAPEs reported in Table 9.15 are plotted in Figure 9.3 for each association code.

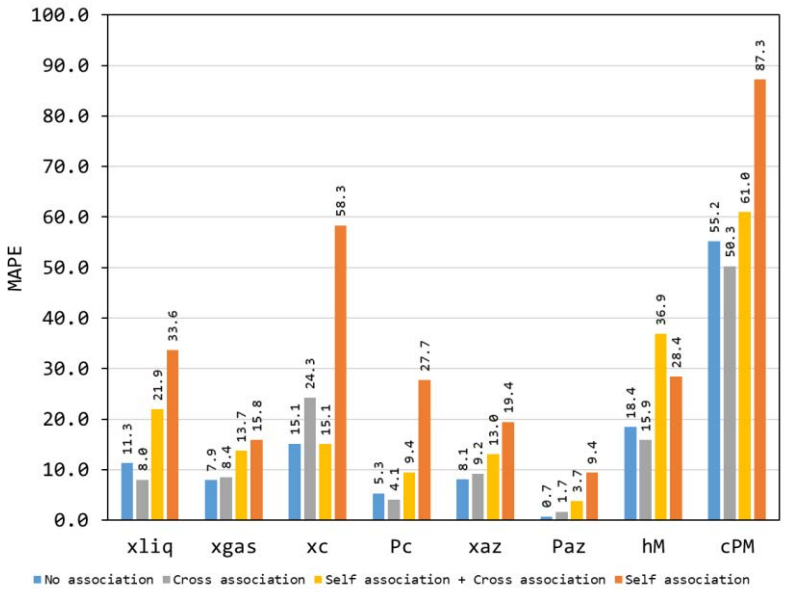



Figure 9.3. MAPE calculated for the four association-based families

From Figure 9.3, one can see that:

- In some cases, the smallest deviations are obtained for the "Cross association" family. In this family, molecules in mixture form hydrogen bonds that stabilize the liquid phase and avoid phase splits.
- The highest deviations are obtained for the "Self-association" family. In this family, self-association occurs for one of the pure compounds while the second one shows no associative behavior. When both are mixed, the non-associated compound tends to break the hydrogen bonds formed by the self-associated compound, leading to phases split. The most common case being the water – oil phase split.
- Similar deviations are obtained for the "No association" and "Self-association + Cross association" family. For the "No association" family, no hydrogen bond is formed or broken when pure compounds are mixed. On the other hand, the "Self-association + Cross association" family leads to both the break of hydrogen bonds from self-associated molecules and the creation of cross-associated hydrogen bonds when pure compounds are mixed. In the ideal case where the number of cross-associated hydrogen bonds formed equals the number of self-associated hydrogen bonds broken, the total amount of hydrogen bonds in solution remains the same. Thus, the "Self-association + Cross association" family members can, in

a way, behave like binary mixtures from the “No association” family, leading to similar deviations.

This analysis, highlights that the Peng-Robinson equation of state is able to properly correlate the creation of hydrogen bonds in mixture but is totally unable to describe their breaking.

A similar analysis can be performed from the viewpoint of the systems ideality:

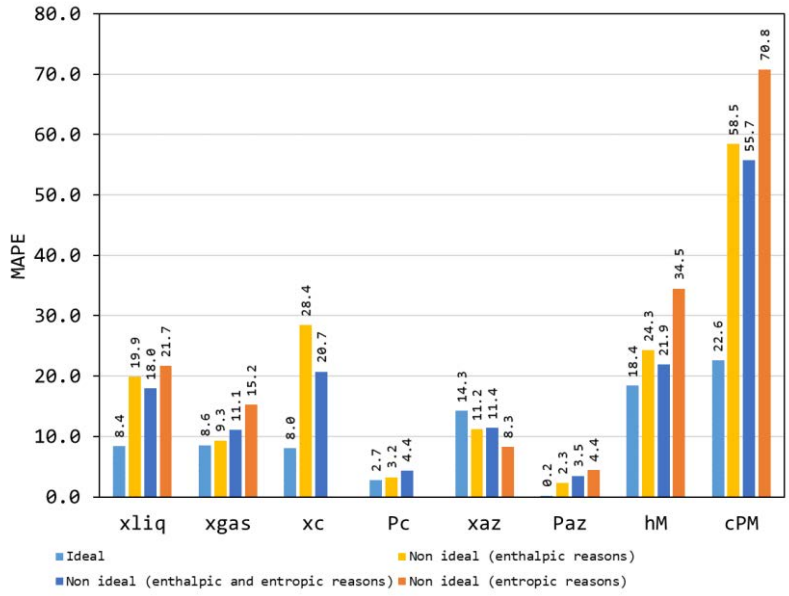



Figure 9.4. MAPE calculated for the five ideality-based families

Figure 9.4 shows that the vapor molar composition, the critical pressure and the azeotropic pressure and composition are represented with a similar accuracy for both ideal and non-ideal systems. Deviations on enthalpies and heat capacities of mixing are smaller for ideal than for non-ideal systems. Such smaller deviations are however not significant because for ideal systems, $h^M$ and $c_P{}^M$ are extremely small.

Figure 9.4 thus only highlights that the liquid phase composition (including the critical composition) is better correlated for ideal solutions than for non-ideal solutions. Deviations to ideality is thus not the key property that makes it possible to highlight the strengths and the weaknesses of a model.

A classification based on the degree of association, like the one proposed in this paper (see Figure 9.2) is much more pertinent.

The following conclusions can be drawn for the PR EoS:

- Systems exhibiting cross-association are accurately correlated.

- The model satisfactorily represents non-associated mixtures
- Associated mixtures can be accurately correlated when cross association simultaneously takes place (i.e. when the hydrogen bond number is more or less constant).
- The model poorly represents mixtures of self-associated compounds.
- The amplitude of the deviations to ideality is not a good indicator of whether a system will be accurately correlated.

This section highlights that the proposed reference database coupled with the way of benchmarking a model make it possible to highlight the strengths and the weaknesses of a thermodynamic model and eventually make recommendations for future developments.

### 9.7. Conclusion

We developed a thermodynamic reference database that could be used to compare thermodynamic models. Following the idea of Danner and Gess, emphasis was made on including both non-associated and associated mixtures, leading us to define 9 association codes. For each of them, ideal and non-ideal mixtures were included in our database. In the end, the proposed database embeds 200 binary mixtures uniformly distributed among the 9 association codes and with a wide type of data including both phase equilibrium data and energetic data. For each property, a detailed procedure explaining how deviations should be estimated with a thermodynamic model is provided.

Finally, the performances of the Peng-Robinson equation of state with a temperature dependent binary interaction parameter were evaluated on the full database and a discussion on its strengths and weaknesses is made. A last observation from Hendriks et al. [174] should convince the reader of the interest of such reference database: *"The new models are published very frequently, but unfortunately most, if not all, of these models are tested against only a few data sets. A large, standardized set of data against which all models may be tested will be of great benefit, as it will allow models to be compared on equal footing."*

# Conclusion

Cette thèse fut l'occasion de poser les fondations pour le développement d'une nouvelle équation d'état des mélanges. Ce travail a été réalisé en deux temps :

Concernant les corps purs :

- Il a été démontré que l'ajustement des paramètres des fonctions α doit être réalisé au moins sur des données de pression de saturation. Si des données d'enthalpie de vaporisation et de capacité calorifique à saturation sont disponibles il est alors recommandé de les considérer dans la procédure d'ajustement.
- La liste des contraintes mathématiques auxquelles les fonctions α doivent absolument se conformer ont été établies. D'un point de vue pratique, l'application de ces contraintes permet d'ajuster les paramètres de la fonction α sur des données subcritiques et de garantir une extrapolation fiable et thermodynamiquement cohérente dans le domaine supercritique.
- Une liste des propriétés invariantes par translation volumique a été établie. Cela permet de conclure qu'il est possible d'ajuster séparément les paramètres de la fonction α et le paramètre de translation volumique.

Afin de pouvoir découpler l'ajustement des paramètres de la fonction α de celui du paramètre de correction volumique, la liste des propriétés invariantes par translation volumique a été établie. Cette étude conclut qu'il est recommandé d'ajuster les paramètres de la fonction α sur des données d'équilibre liquide-vapeur (pressions de vapeur, enthalpies de vaporisation …) et dans un deuxième temps le paramètre de translation volumique sur des données de densité liquide.

- Deux équations d'état (tc-PR et tc-RK) ont été développées pour les corps purs. Elles permettent une représentation très précise des équilibres de phases mais aussi des propriétés énergétiques (y compris dans le domaine supercritique).

Pour chacune de ces équations d'état, des expressions généralisées permettant d'estimer la fonction α de Twu et le paramètre de translation volumique à partir de la seule connaissance du facteur acentrique ont été développées.

Concernant les mélanges :

- Les bases d'une nouvelle règle de mélange proposée lors du congrès ESAT 2012 ont été rappelées. Il a notamment été montré qu'une nouvelle dérivation des règles de mélange de Huron-Vidal et MHV-1 conduisait à la même règle de mélange pour le

paramètre *a*/*b*. Cette unique règle de mélange, considérée donc comme universelle, est obtenue lorsque les énergies d'Helmholtz résiduelles de l'équation d'état cubique et du modèle de coefficient d'activité sont identifiées.

- La valeur optimale du paramètre universel *s* intervenant dans la règle de mélange du paramètre *b* a été déterminée afin de représenter au mieux les conditions d'équilibre entre phases de systèmes présentant des effets entropiques marqués (mélanges d'alcanes linéaires de tailles différentes).
- Il a été démontré que seule une règle de mélange linéaire pour le paramètre de translation volumique laisse invariantes les conditions d'équilibre entre phases ainsi que les grandeurs de mélange. Ce résultat, analogue à celui obtenu pour les corps purs, permet de découpler la représentation des propriétés volumiques de celle des autres grandeurs (équilibre entre phases, grandeurs de mélange…), simplifiant ainsi les futures procédures d'optimisation des paramètres du modèle.
- Une base de données pour le développement, la validation et surtout la comparaison des modèles thermodynamiques a été proposée. Cette base de données est proposée comme un outil à l'intention des développeurs de modèles afin de présenter les performances de ces derniers sur une base de comparaison commune.

Elle devrait prochainement être utilisée afin de définir le modèle de coefficients d'activité le mieux adapté à notre règle de mélange universelle. Il est notamment envisagé de comparer les modèles de Wilson, NRTL et UNIQUAC.

Une fois l'équation d'état des mélanges établie, les améliorations suivantes pourront être envisagées :

- Rendre prédictif le modèle par une approche type contributions de groupes. Par ce processus, l'équation d'état pourra être utilisée sans qu'il soit nécessaire d'utiliser des données expérimentales afin d'ajuster les paramètres du modèle, ces derniers étant estimés à partir de la simple décomposition des molécules du mélange en sous-groupes élémentaires. La faisabilité de ce travail est avérée comme le montre la méthode de contribution de groupe utilisée dans l'équation d'état prédictive VTPR qui utilise le modèle de coefficient d'activité UNIFAC.
- L'ajout d'un terme d'association afin d'améliorer la représentation des systèmes associés. On sait d'après les résultats de la littérature que l'ajout d'un terme d'association permet une nette amélioration de la reproduction des données expérimentales de systèmes dont les interactions énergétiques sont dominées par

les liaisons hydrogène. Si l'on opte pour l'approche dérivée de la théorie de Wertheim, la forme mathématique de l'équation d'état devient beaucoup plus complexe (elle n'est plus cubique). De plus, la détermination (voire la prédiction) des schémas d'association de chaque espèce est un problème significatif car il n'existe pas à l'heure actuelle une méthode permettant de les déterminer de manière fiable à partir de la seule connaissance de la structure chimique de la molécule (une méthode type essai-erreur est fréquemment employée). Le modèle CPA ainsi que les équations de type SAFT semblent montrer qu'il existe un avantage réel à tenir compte des phénomènes d'association pour la bonne représentation des mélanges complexes (fortement associés).

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# Annexe A-1

# Modélisations des corps purs Paramètres et déviations du modèle tc-PR

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| (3-METHYLACRYLOXYPROPYL)TRICHLOROSILANE | 708,1 | 21,13 | 0,6267 | 0,2457 | 1,1215 | 0,8855 | 1,0933 | 18,1828 | 0,58% | 1,20% | | 1,75% | 26,25% |
| (Z)-1,3-DICHLORO-2-BUTENE | 617 | 37,8 | 0,2370 | 0,2508 | 1,1767 | 0,9689 | 0,5983 | 14,7605 | 2,10% | | 0,27% | 2,37% | 21,95% |
| [3-(2,3-EPOXYPROXY)PROPYL]TRIMETHOXYSILANE | 701,4 | 18,12 | 0,7605 | 0,2336 | 0,7928 | 0,8225 | 1,6955 | 40,9453 | 0,71% | 1,77% | 0,37% | 2,58% | 29,56% |
| [3-(MERCAPTO)PROPYL]TRIETHOXYSILANE | 647,5 | 18,63 | 0,8370 | 0,2587 | 0,6337 | 0,8623 | 2,3632 | -15,3185 | 1,06% | | | 3,76% | 22,78% |
| 1-(4-ETHYLPHENYL)-2-(4-ETHYLPHENYL)ETHANE | 780,9 | 19,17 | 0,5860 | | 0,4913 | 0,8110 | 2,0505 | | 0,59% | 2,22% | | | |
| 1-(4-ETHYLPHENYL)-2-PHENYLETHANE | 771 | 21,7 | 0,5782 | | 1,1185 | 0,9028 | 1,0406 | | 0,75% | 1,04% | 3,33% | | |
| 1,1,1,2,2,3,4,5,5,5-DECAFLUOROPENTANE | 454,2 | 22,88 | 0,5000 | 0,2605 | 1,3682 | 1,0000 | 0,7623 | -1,2289 | 2,48% | 2,99% | | 1,23% | 18,28% |
| 1,1,1,2,2-PENTAFLUOROPROPANE | 380,11 | 31,372 | 0,3046 | 0,2658 | 1,1242 | 1,0000 | 0,7096 | -0,8342 | 0,50% | 1,19% | | 1,22% | 13,66% |
| 1,1,1,2,3,3,3-HEPTAFLUOROPROPANE | 374,83 | 29,116 | 0,3552 | 0,2650 | 1,1900 | 1,0000 | 0,7259 | -1,7055 | 0,37% | 0,97% | | 1,22% | 20,71% |
| 1,1,1,2,3,3-HEXAFLUOROPROPANE | 412,38 | 34,116 | 0,3688 | 0,2649 | 0,2305 | 0,8216 | 2,4768 | -1,9507 | 0,39% | 0,91% | | 1,07% | 15,15% |
| 1,1,1,2-TETRACHLORODIFLUOROETHANE | 552 | 33,4 | 0,2570 | 0,2615 | 0,1535 | 0,7882 | 2,1533 | 3,8810 | 0,84% | 3,16% | | 2,18% | 19,24% |
| 1,1,1,2-TETRACHLOROETHANE | 624 | 40,2 | 0,2422 | 0,2615 | 0,1999 | 0,8182 | 2,0925 | 4,8893 | 1,49% | 2,49% | | 1,33% | 20,57% |
| 1,1,1,2-TETRAFLUOROETHANE | 374,18 | 40,56 | 0,3269 | 0,2590 | 0,2842 | 0,8321 | 2,1218 | 2,2694 | 0,26% | 0,72% | 3,82% | 1,45% | 17,46% |
| 1,1,1,3,3,3-HEXAFLUOROPROPANE | 398,07 | 32,192 | 0,3905 | 0,2645 | 0,9448 | 0,8718 | 0,9521 | -2,3048 | 0,61% | 1,70% | | 1,13% | 19,68% |
| 1,1,1,3,3-PENTACHLOROPROPANE | 670,9 | 32,96 | 0,3241 | 0,2568 | 1,5632 | 1,0000 | 0,5102 | 8,7508 | 0,69% | 1,84% | | 1,59% | 17,58% |
| 1,1,1,3,3-PENTAFLUOROBUTANE | 473,7 | 33,92 | 0,2571 | 0,2742 | 0,0000 | 0,4391 | 1,1562 | -4,9886 | 1,31% | | | 0,93% | 16,75% |
| 1,1,1,3,3-PENTAFLUOROPROPANE | 427,2 | 36,4 | 0,3755 | 0,2630 | 1,5935 | 1,0000 | 0,5416 | -0,5819 | 0,63% | 1,61% | | 1,34% | 16,04% |
| 1,1,1-TRICHLOROETHANE | 545 | 43 | 0,2183 | 0,2707 | 0,1493 | 0,8507 | 2,5381 | -2,4584 | 0,48% | 1,87% | 1,32% | 1,13% | 16,16% |
| 1,1,1-TRICHLOROFLUOROETHANE | 565 | 39,9 | 0,2501 | | 1,0710 | 1,0000 | 0,6770 | | 0,64% | 1,31% | | | |
| 1,1,1-TRICHLOROTRIFLUOROETHANE | 483 | 33,2 | 0,2667 | 0,2655 | 0,1813 | 0,8499 | 2,5503 | -1,0762 | 3,54% | 1,60% | 0,19% | 1,96% | 16,17% |
| 1,1,1-TRIFLUOROETHANE | 345,88 | 37,64 | 0,2614 | 0,2565 | 0,2844 | 0,8435 | 1,9314 | 4,8500 | 0,35% | 1,65% | 0,71% | 1,95% | 17,95% |
| 1,1,2,2,3-PENTAFLUOROPROPANE | 447,57 | 39,25 | 0,3531 | 0,2665 | 1,1029 | 1,0000 | 0,7901 | -2,4814 | 0,52% | 1,51% | | 1,07% | 14,82% |
| 1,1,2,2-TETRACHLOROETHANE | 645 | 40,9 | 0,2467 | 0,2545 | 0,0000 | 0,4300 | 1,1100 | 11,8121 | 1,67% | | | 2,79% | 20,39% |
| 1,1,2,2-TETRAFLUOROETHANE | 391,8 | 46,4 | 0,2660 | 0,2691 | 0,2310 | 0,8629 | 2,3548 | -1,7814 | 3,23% | 2,57% | | 1,01% | 13,93% |
| 1,1,2,2-TETRAPHENYLETHANE | 827 | 16,7 | 0,7322 | | 0,6019 | 0,7981 | 2,0170 | | 0,64% | 1,29% | 1,10% | | |
| 1,1,2-TRICHLOROETHANE | 602 | 44,8 | 0,2591 | 0,2591 | 0,1669 | 0,8226 | 2,3608 | 6,2930 | 0,51% | 2,02% | 0,06% | 1,16% | 19,98% |
| 1,1,2-TRICHLOROTRIFLUOROETHANE | 487,25 | 34,1 | 0,2515 | 0,2719 | 0,4985 | 0,8401 | 1,2736 | -4,9288 | 0,85% | 1,59% | 0,50% | 1,16% | 13,89% |
| 1,1,2-TRIFLUOROETHANE | 429,8 | 52,41 | 0,3265 | 0,2622 | 0,9201 | 0,8598 | 0,8740 | 0,7414 | 0,40% | 1,14% | | 1,37% | 16,68% |
| 1,1,2-TRIMETHYLCYCLOPENTANE | 579,54 | 29,385 | 0,2523 | 0,2613 | 0,2074 | 0,8205 | 2,1149 | 4,5476 | 0,61% | 2,25% | | 2,06% | 19,79% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1,1,2-TRIPHENYLETHANE | 840 | 20,4 | 0,6116 | | 1,0779 | 0,8904 | 1,1202 | | 0,79% | 1,07% | 1,27% | | |
| 1,1,3-TRIMETHYLCYCLOHEXANE | 611,3 | 29,78 | 0,2753 | 0,2783 | 0,2027 | 0,8505 | 2,4950 | -15,2345 | 0,90% | 2,23% | | 1,66% | 15,11% |
| 1,1,3-TRIMETHYLCYCLOPENTANE | 569,54 | 28,268 | 0,2119 | 0,2608 | 1,3254 | 1,0000 | 0,5011 | 6,3045 | 1,66% | 1,61% | | 2,48% | 21,98% |
| 1,1-DIBROMOETHANE | 628 | 60,3 | 0,1250 | 0,3016 | 0,2784 | 0,0000 | 0,5139 | -18,2097 | 4,23% | 6,18% | | 2,15% | 3,04% |
| 1,1-DICHLORO-1-FLUOROETHANE | 478,85 | 43,4 | 0,2211 | 0,2756 | 0,1886 | 0,8489 | 2,2880 | -5,3725 | 0,56% | 1,25% | 2,00% | 1,13% | 13,59% |
| 1,1-DICHLOROETHANE | 523 | 50,7 | 0,2339 | 0,2751 | 0,5696 | 0,8152 | 1,0619 | -4,5259 | 0,49% | 1,63% | 0,82% | 1,24% | 11,74% |
| 1,1-DICHLOROPROPANE | 560 | 42,4 | 0,2529 | 0,2572 | 0,3488 | 0,8027 | 1,5171 | 4,7204 | 0,35% | 1,21% | 1,60% | 4,05% | 14,38% |
| 1,1-DICHLOROTETRAFLUOROETHANE | 418,55 | 33 | 0,2533 | 0,2748 | 0,1906 | 0,8435 | 2,3735 | -6,4585 | 0,19% | 1,67% | 5,02% | 0,98% | 12,46% |
| 1,1-DIETHYLCYCLOHEXANE | 643 | 25,7 | 0,4036 | 0,2567 | 1,0433 | 0,9540 | 0,9048 | 7,1248 | 0,87% | 1,41% | 3,23% | 1,77% | 18,42% |
| 1,1-DIFLUOROETHANE | 386,44 | 45,198 | 0,2751 | 0,2534 | 0,2964 | 0,8463 | 1,9520 | 5,6960 | 0,36% | 0,98% | 4,88% | 1,99% | 18,90% |
| 1,1-DIFLUOROETHYLENE | 302,8 | 44,6 | 0,1362 | 0,2725 | 0,1422 | 0,8645 | 2,3323 | -0,6234 | 2,47% | | 2,28% | 0,97% | 13,08% |
| 1,1-DIMETHOXYETHANE | 507,8 | 37,73 | 0,3277 | 0,2660 | 0,1532 | 0,8322 | 2,8613 | -1,5783 | 1,25% | 5,83% | 2,54% | 1,32% | 16,35% |
| 1,1-DIMETHYLCYCLOHEXANE | 591,15 | 29,3843 | 0,2326 | 0,2605 | 1,3829 | 1,0000 | 0,4902 | 8,0765 | 0,31% | 0,96% | 0,41% | 1,86% | 12,47% |
| 1,1-DIMETHYLCYCLOPENTANE | 547 | 34,45 | 0,2724 | 0,2786 | 0,3589 | 0,8341 | 1,6350 | -11,5218 | 1,60% | 0,78% | 3,02% | 1,39% | 15,93% |
| 1,1-DIPHENYLETHANE | 775 | 26,8 | 0,4566 | 0,2559 | 0,6969 | 0,8274 | 1,3393 | 9,3260 | 0,62% | 1,38% | | 2,01% | 20,82% |
| 1,2,3,4-TETRAHYDRONAPHTHALENE | 720 | 36,5 | 0,3353 | 0,2597 | 0,4128 | 0,8260 | 1,6580 | 3,2432 | 0,66% | 3,10% | 0,45% | 1,43% | 22,78% |
| 1,2,3,4-TETRAMETHYLBENZENE | 693 | 31,1 | 0,4172 | 0,2564 | 0,2555 | 0,8409 | 2,7014 | 6,0453 | 2,07% | 2,73% | | 1,21% | 18,63% |
| 1,2,3,4-TETRAMETHYLCYCLOHEXANE | 642 | 25,7 | 0,4016 | 0,2564 | 0,7400 | 0,8286 | 1,1754 | 7,5453 | 0,57% | 1,51% | 2,51% | 1,48% | 19,49% |
| 1,2,3,5-TETRAETHYLBENZENE | 708 | 20,7 | 0,5940 | 0,2494 | 1,2438 | 1,0000 | 0,9627 | 14,8773 | 1,33% | 4,14% | 2,67% | 1,80% | 22,23% |
| 1,2,3,5-TETRAMETHYLBENZENE | 679 | 29,7 | 0,4242 | 0,2543 | 0,4709 | 0,8430 | 1,8073 | 8,7976 | 0,95% | 1,87% | 0,67% | 1,31% | 19,40% |
| 1,2,3,6-TETRAHYDROBENZALDEHYDE | 655 | 40,3 | 0,3638 | 0,2607 | 0,3296 | 0,8045 | 1,9259 | 1,3544 | 0,47% | 3,62% | 2,84% | 1,50% | 20,02% |
| 1,2,3-BENZENETRIOL | 830 | 88,1 | 0,9452 | | 0,6834 | 0,8591 | 2,4093 | | 5,42% | | | | |
| 1,2,3-TRICHLOROBENZENE | 734 | 45,1 | 0,4263 | 0,2848 | 0,4553 | 0,8411 | 1,8351 | -20,0494 | 0,66% | 2,03% | 0,32% | 2,66% | 10,38% |
| 1,2,3-TRICHLOROPROPANE | 652 | 38,7 | 0,3056 | 0,2393 | 0,2844 | 0,8001 | 1,8723 | 21,8715 | 0,44% | 2,42% | 2,31% | 4,63% | 22,37% |
| 1,2,3-TRIETHYLBENZENE | 683 | 23,8 | 0,5054 | | 0,6790 | 0,8594 | 1,5206 | | 1,01% | 1,48% | 1,63% | | |
| 1,2,3-TRIMETHYL-4-ETHYLBENZENE | 702,7 | 27,95 | 0,4574 | 0,2543 | 0,8539 | 0,8721 | 1,1573 | 8,7016 | 0,62% | 1,67% | | 1,35% | 19,37% |
| 1,2,3-TRIMETHYLBENZENE | 664,5 | 34,54 | 0,3666 | 0,2560 | 0,4191 | 0,8441 | 1,8018 | 5,2133 | 0,49% | 0,98% | 1,25% | 1,87% | 17,51% |
| 1,2,3-TRIMETHYLINDENE | 726 | 27,7 | 0,4419 | 0,2427 | 0,9973 | 0,9992 | 1,0229 | 26,3827 | 1,67% | 0,92% | 6,44% | 1,44% | 21,64% |
| 1,2,4,5-TETRAISOPROPYLBENZENE | 703 | 15,56 | 0,6360 | | 0,3564 | 0,7669 | 2,4302 | | 0,27% | 1,56% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1,2,4,5-TETRAMETHYLBENZENE | 676 | 29 | 0,4217 | 0,2481 | 0,7740 | 0,8998 | 1,2351 | 15,2278 | 0,74% | 1,02% | 2,52% | 2,13% | 20,45% |
| 1,2,4-TRICHLOROBENZENE | 725 | 37,2 | 0,3581 | 0,2524 | 0,6126 | 0,8313 | 1,2780 | 12,1382 | 1,11% | 1,71% | 0,13% | 1,42% | 23,03% |
| 1,2,4-TRIETHYLBENZENE | 684 | 23,8 | 0,5011 | 0,2513 | 0,4150 | 0,8462 | 2,2435 | 12,4036 | 0,58% | 3,43% | 0,50% | 2,04% | 20,36% |
| 1,2,4-TRIMETHYL-3-ETHYLBENZENE | 697,3 | 27,95 | 0,4569 | 0,2562 | 0,5508 | 0,8982 | 1,8266 | 5,2782 | 0,42% | | | 1,53% | 19,09% |
| 1,2,4-TRIMETHYL-5-ETHYLBENZENE | 687,3 | 26,78 | 0,4638 | 0,2531 | 0,5562 | 0,8481 | 1,6844 | 10,0543 | 0,44% | 1,88% | | 1,34% | 19,61% |
| 1,2,4-TRIMETHYLBENZENE | 649,1 | 32,32 | 0,3787 | 0,2557 | 0,4151 | 0,8395 | 1,8302 | 6,8924 | 0,23% | 0,79% | 0,77% | 1,30% | 17,77% |
| 1,2-BENZENE DICARBOXYLIC ACID, HEPTYL, UNDECYL ESTER | 878 | 10,7 | 1,0205 | 0,2217 | 0,5135 | 0,8219 | 3,0699 | 101,2589 | 0,68% | | | 2,07% | 45,69% |
| 1,2-BENZENEDICARBOXYLIC ACID, HEPTYL, NONYL ESTER | 841 | 11,6 | 1,0944 | 0,2275 | 0,5321 | 0,8188 | 3,1380 | 66,0347 | 0,56% | | | 2,74% | 40,71% |
| 1,2-BENZENEDIOL | 764 | 74,9 | 0,6937 | 0,3102 | 0,6565 | 0,8897 | 2,0143 | -31,3646 | 5,91% | 4,73% | | 3,59% | 2,64% |
| 1,2-BUTADIENE | 452 | 43,6 | 0,1659 | 0,2627 | 1,1125 | 0,9395 | 0,5387 | 4,4502 | 1,75% | 2,44% | 0,31% | 1,48% | 18,42% |
| 1,2-BUTANEDIOL | 680 | 52,1 | 0,6305 | 0,2557 | 1,6181 | 1,0000 | 0,7356 | -0,3086 | 0,65% | 0,68% | | 1,51% | 10,20% |
| 1,2-DIBROMOETHANE | 650,15 | 54,769 | 0,2067 | 0,2663 | 1,2790 | 1,0000 | 0,5009 | 1,2274 | 0,76% | 1,28% | 0,62% | 1,80% | 15,51% |
| 1,2-DIBROMOTETRAFLUOROETHANE | 487,8 | 33,93 | 0,2431 | 0,2710 | 0,1382 | 0,8425 | 2,6732 | -4,0293 | 0,47% | 0,95% | | 1,21% | 8,94% |
| 1,2-DICHLORO-1,1,2-TRIFLUOROETHANE | 461,6 | 36,1 | 0,2410 | 0,2642 | 0,2843 | 0,8238 | 1,7539 | 1,7895 | 0,29% | 1,44% | 5,17% | 1,38% | 16,91% |
| 1,2-DICHLORO-4-NITROBENZENE | 758 | 36 | 0,5385 | 0,2438 | 0,6554 | 0,8276 | 1,5755 | 16,8259 | 0,61% | 1,13% | | 1,27% | 19,57% |
| 1,2-DICHLOROBUTANE | 600 | 36,8 | 0,2988 | 0,2503 | 0,4213 | 0,8312 | 1,5511 | 11,2506 | 0,35% | 1,10% | | 3,52% | 18,21% |
| 1,2-DICHLOROETHANE | 561,6 | 53,7 | 0,2866 | 0,2659 | 0,2198 | 0,8567 | 2,4452 | -0,5534 | 2,02% | 2,78% | 2,77% | 1,05% | 21,75% |
| 1,2-DICHLOROHEXAFLUOROCYCLOBUTANE | 497 | 27,3 | 0,2330 | | 0,2347 | 0,8283 | 1,9499 | | 0,44% | 1,86% | | | |
| 1,2-DICHLOROPROPANE | 572 | 42,4 | 0,2564 | 0,2604 | 0,1969 | 0,8261 | 2,1983 | 4,5362 | 0,42% | 3,66% | 1,03% | 1,44% | 16,93% |
| 1,2-DICHLOROTETRAFLUOROETHANE | 418,85 | 32,6 | 0,2520 | 0,2725 | 0,1523 | 0,8446 | 2,6386 | -5,0568 | 0,54% | 2,03% | 4,28% | 1,11% | 13,41% |
| 1,2-DIETHOXYETHANE | 561 | 29,3 | 0,4818 | 0,2535 | 0,1860 | 0,8175 | 3,1662 | 3,4919 | 1,42% | 5,34% | 6,71% | 1,99% | 20,86% |
| 1,2-DIFLUOROBENZENE | 566 | 42,99 | 0,2792 | 0,2646 | 0,2047 | 0,8522 | 2,5148 | 0,3606 | 0,79% | 2,19% | | 1,08% | 15,91% |
| 1,2-DIFLUOROETHANE | 445 | 43,4 | 0,2224 | 0,2286 | 0,1829 | 0,8585 | 2,4184 | 22,1486 | 0,54% | 2,89% | | 4,66% | 23,03% |
| 1,2-DIMETHOXYETHANE | 536,15 | 38,7061 | 0,3475 | 0,2587 | 1,2596 | 1,0000 | 0,6717 | 2,1768 | 0,52% | 0,98% | | 1,89% | 30,01% |
| 1,2-DIMETHOXYPROPANE | 543 | 34,46 | 0,3522 | 0,2674 | 1,1561 | 0,9947 | 0,7470 | -3,9126 | 0,61% | 1,32% | | 1,09% | 16,19% |
| 1,2-DIMETHYL-3-PROPYLBENZENE | 687,7 | 27,24 | 0,4531 | 0,2615 | 0,6541 | 0,8665 | 1,4715 | 1,8917 | 0,61% | 1,48% | | 2,41% | 9,79% |
| 1,2-DIPHENYLETHANE | 780 | 26,5 | 0,4885 | 0,2518 | 0,2802 | 0,8358 | 2,7926 | 12,6100 | 0,31% | 0,94% | | 1,18% | 20,08% |
| 1,2-EPOXY-2-METHYLPROPANE | 521 | 46,6 | 0,1709 | 0,2674 | 0,5395 | 0,8422 | 0,9964 | 0,5916 | 0,46% | 3,27% | 0,75% | 2,24% | 17,83% |
| 1,2-EPOXY-3-PHENOXYPROPANE | 720 | 29,5 | 0,5943 | 0,2317 | 0,2544 | 0,8171 | 3,1750 | 33,6108 | 1,17% | 2,03% | | 1,47% | 27,20% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1,2-EPOXYBUTANE | 526 | 43,9 | 0,2345 | 0,2570 | 0,6675 | 0,8160 | 0,9451 | 6,9415 | 0,41% | 2,65% | 0,24% | 1,80% | 16,01% |
| 1,2-ETHANEDITHIOL | 663 | 53,6 | 0,2570 | 0,2566 | 1,1168 | 0,9999 | 0,6547 | 5,8013 | 0,65% | 1,38% | | 1,67% | 48,49% |
| 1,2-HEXADIENE | 526 | 33,5 | 0,2762 | 0,2564 | 1,2482 | 1,0000 | 0,5973 | 8,0288 | 0,53% | 1,93% | 0,61% | 1,72% | 18,82% |
| 1,2-PENTADIENE | 500 | 38 | 0,1542 | 0,2570 | 1,1211 | 1,0000 | 0,5433 | 8,9486 | 4,35% | 4,87% | 0,70% | 2,61% | 18,60% |
| 1,2-PROPANEDIAMINE | 587 | 52,7 | 0,4738 | 0,2798 | 0,6805 | 0,8498 | 1,4295 | -10,2907 | 0,23% | 0,69% | | 3,03% | 6,65% |
| 1,2-PROPYLENE OXIDE | 482,25 | 49,2 | 0,2683 | 0,2456 | 0,3360 | 0,8300 | 1,6871 | 10,4198 | 1,61% | 2,62% | 0,69% | 3,44% | 29,09% |
| 1,3,5,7-CYCLOOCTATETRAENE | 641,4 | 44,2 | 0,2870 | | 0,1981 | 0,8497 | 2,5539 | | 0,44% | 2,35% | 0,79% | | |
| 1,3,5-TRICHLOROBENZENE | 718 | 37,2 | 0,3596 | 0,2566 | 1,0137 | 1,0000 | 0,8744 | 7,8292 | 1,03% | 1,74% | | 1,06% | 14,23% |
| 1,3,5-TRIETHYLBENZENE | 678 | 23 | 0,5077 | 0,2476 | 0,6078 | 0,8500 | 1,6627 | 17,4137 | 0,57% | 2,66% | 0,72% | 1,60% | 24,12% |
| 1,3,5-TRIISOPROPYLBENZENE | 696,6 | 19,5 | 0,5324 | | 1,0138 | 0,8406 | 1,0692 | | 0,66% | 1,35% | | | |
| 1,3,5-TRI-tert-BUTYLBENZENE | 717,8 | 16,56 | 0,4865 | | 1,4794 | 0,8049 | 0,7096 | | 0,57% | 1,84% | | | |
| 1,3-BENZENEDIOL | 810 | 74,9 | 0,6767 | 0,2911 | 1,3743 | 1,0000 | 0,9313 | -22,5197 | 1,92% | 1,83% | 1,02% | 1,97% | 0,36% |
| 1,3-BUTADIENE | 425 | 43,2 | 0,1950 | 0,2708 | 0,1609 | 0,8589 | 2,4120 | -1,6099 | 0,66% | 1,68% | 1,36% | 1,22% | 14,50% |
| 1,3-BUTANEDIOL | 676 | 40,2 | 0,7043 | 0,2106 | 1,6949 | 1,0000 | 0,7507 | 35,4139 | 1,61% | 2,52% | 9,25% | 6,78% | 29,30% |
| 1,3-CYCLOHEXADIENE | 558 | 47,3 | 0,2308 | 0,2823 | 0,3483 | 0,8292 | 1,5190 | -8,8397 | 1,36% | 1,75% | 1,69% | 2,96% | 12,04% |
| 1,3-DICHLOROHEXAFLUOROPROPANE | 449 | 25,7 | 0,3286 | 0,2570 | 1,1546 | 1,0000 | 0,7186 | 4,9252 | 0,59% | 1,10% | | 2,33% | 19,68% |
| 1,3-DICHLOROPROPANE | 603 | 41,5 | 0,2916 | 0,2456 | 0,4465 | 0,8100 | 1,4001 | 15,3373 | 1,97% | 2,95% | 2,22% | 3,14% | 22,35% |
| 1,3-DIFLUOROBENZENE | 548,4 | 42,99 | 0,2862 | 0,2710 | 0,2283 | 0,8569 | 2,4419 | -4,2674 | 0,94% | 2,34% | | 1,14% | 13,12% |
| 1,3-DIMETHYL UREA | 787,1 | 48,7 | 0,5900 | | 0,4594 | 0,8019 | 2,1177 | | 0,33% | 1,67% | | | |
| 1,3-DIMETHYL-2-IMIDAZOLIDINONE | 749,9 | 42,75 | 0,3701 | 0,2485 | 0,7955 | 0,9024 | 1,1091 | 14,1868 | 0,61% | 1,84% | | 1,44% | 19,93% |
| 1,3-DIMETHYL-5-NITROBENZENE | 787,7 | 33,13 | 0,4745 | | 0,6179 | 0,8265 | 1,5217 | | 0,63% | 2,17% | | | |
| 1,3-DIMETHYLADAMANTANE | 708 | 30 | 0,2935 | 0,2785 | 0,2295 | 0,8410 | 2,3211 | -18,9470 | 0,41% | 2,39% | 0,88% | 1,29% | 9,15% |
| 1,3-DIOXANE | 590 | 51,5 | 0,2891 | 0,2703 | 1,2454 | 1,0000 | 0,6123 | -2,5768 | 0,64% | 1,93% | 1,40% | 1,52% | 23,59% |
| 1,3-DIPHENYLTRIAZENE | 845 | 28,3 | 0,6173 | | 0,5654 | 0,8114 | 1,9110 | | 0,57% | 0,97% | | | |
| 1,3-DI-TERT-BUTYL GLYCERIN | 667,1 | 21,86 | 0,6502 | 0,2721 | 0,6137 | 0,8259 | 1,8961 | -29,0774 | 0,50% | 1,21% | | 2,40% | 17,25% |
| 1,3-PROPANEDIAMINE | 608 | 51,2 | 0,5063 | 0,2737 | 0,3505 | 0,8481 | 2,5799 | -5,7318 | 0,89% | | | 4,16% | 2,14% |
| 1,3-PROPYLENE GLYCOL | 724 | 95 | 0,7385 | 0,3022 | 0,4868 | 0,8467 | 2,6036 | -23,7610 | 4,71% | 2,07% | | 2,59% | 0,71% |
| 1,3-PROPYLENE OXIDE | 520 | 57,5 | 0,2005 | 0,2535 | 0,1445 | 0,8422 | 2,3839 | 7,6174 | 0,47% | 2,04% | 0,39% | 2,50% | 18,89% |
| 1,4-BENZENEDICARBOXYLIC ACID, 2-HYDROXYETHYL METHYL ESTER | 832 | 26,75 | 0,8033 | | 0,5083 | 0,8125 | 2,5246 | | 0,68% | 1,34% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1,4-BIS(3-AMINOPROPYL)PIPERAZINE | 750,3 | 22,66 | 0,8314 | 0,2553 | 0,3989 | 0,8190 | 3,1324 | -0,6228 | 0,65% | | 2,72% | 3,95% | 13,83% |
| 1,4-BUTANEDIISOCYANATE | 724,3 | 29,47 | 0,4258 | 0,2245 | 0,4290 | 0,8440 | 1,9574 | 49,4806 | 0,66% | 2,19% | 0,62% | 2,81% | 26,08% |
| 1,4-CYCLOHEXANEDICARBOXYLIC ACID | 819,8 | 37,36 | 1,0050 | | 0,5154 | 0,8216 | 3,0236 | | 0,44% | 2,29% | | | |
| 1,4-DIBROMOBENZENE | 738,15 | 44,72 | 0,4257 | 0,2748 | 0,5521 | 0,9137 | 1,7630 | -12,7570 | 3,35% | | | 1,45% | 17,15% |
| 1,4-DICHLOROBUTANE | 641 | 36,1 | 0,3260 | 0,2414 | 0,4825 | 0,7807 | 1,3654 | 21,4179 | 0,45% | 2,13% | 0,75% | 3,61% | 26,07% |
| 1,4-DICHLORO-cis-2-BUTENE | 640 | 37,8 | 0,3299 | 0,2434 | 0,6910 | 0,8209 | 1,1013 | 19,9122 | 0,57% | 2,15% | 0,28% | 2,29% | 20,36% |
| 1,4-DICHLORO-trans-2-BUTENE | 646 | 37,8 | 0,3282 | 0,2432 | 0,6941 | 0,8216 | 1,0951 | 20,2679 | 0,53% | 2,01% | 0,32% | 2,49% | 20,38% |
| 1,4-DICYANO-2-BUTENE | 755 | 29,5 | 0,6668 | 0,2004 | 0,4582 | 0,8090 | 2,3543 | 74,9953 | 0,60% | 1,58% | | 4,06% | 35,95% |
| 1,4-DIFLUOROBENZENE | 556,9 | 44 | 0,2985 | 0,2722 | 0,2308 | 0,8554 | 2,4644 | -4,5462 | 1,03% | 2,56% | | 1,04% | 9,38% |
| 1,4-DIOXANE | 587 | 52,081 | 0,2793 | 0,2679 | 0,1971 | 0,8198 | 2,2484 | -1,7643 | 0,69% | 1,64% | 7,34% | 1,17% | 21,78% |
| 1,4-DI-tert-BUTYLBENZENE | 708 | 23 | 0,5023 | 0,2705 | 0,2651 | 0,8300 | 2,8881 | -18,0871 | 1,87% | 1,49% | 1,00% | 1,33% | 9,95% |
| 1,4-HEXADIENE | 510 | 33,5 | 0,2800 | 0,2636 | 1,2181 | 1,0000 | 0,6108 | 1,8606 | 1,86% | 2,28% | 4,25% | 1,50% | 16,99% |
| 1,4-PENTADIENE | 479 | 37,4 | 0,0837 | 0,2770 | 1,9155 | 1,0000 | 0,2615 | -1,0849 | 5,22% | 5,38% | 2,48% | 3,73% | 8,39% |
| 1,5,9-CYCLODODECATRIENE | 745 | 29,9 | 0,4031 | 0,2717 | 0,8277 | 0,9834 | 1,1833 | -15,0183 | 0,68% | | | 1,88% | 15,78% |
| 1,5-CYCLOOCTADIENE | 645 | 39 | 0,2858 | 0,2803 | 0,6714 | 0,8370 | 1,0621 | -11,4034 | 0,98% | 1,29% | | 3,96% | 18,61% |
| 1,5-DICHLOROPENTANE | 668 | 31,9 | 0,3766 | 0,2406 | 0,8914 | 0,8167 | 0,9544 | 24,8571 | 0,37% | 3,42% | 2,58% | 2,78% | 28,88% |
| 1,5-HEXADIENE | 508 | 33,5 | 0,2259 | 0,2633 | 1,0360 | 1,0000 | 0,6687 | 2,6762 | 0,66% | 0,99% | | 1,83% | 13,54% |
| 1,5-NAPHTHALENE DIISOCYANATE | 818 | 27,2 | 0,7301 | | 0,3302 | 0,8168 | 3,1833 | | 0,54% | 1,29% | | | |
| 1,5-PENTANEDIAMINE | 642 | 37,35 | 0,5874 | 0,2647 | 0,5973 | 0,8916 | 1,9931 | -3,4768 | 0,96% | | | 3,47% | 4,93% |
| 1,5-PENTANEDIOL | 673 | 41,5 | 1,2216 | 0,2260 | 0,9297 | 0,8731 | 2,2156 | 8,2031 | 4,08% | | 9,09% | 2,34% | 17,76% |
| 1,9-DECADIENE | 606,8 | 22,67 | 0,5110 | 0,2538 | 0,8716 | 0,8817 | 1,2250 | 7,9099 | 0,53% | 1,36% | | 1,73% | 19,68% |
| 1-AMINO-2-PROPANOL | 614 | 56,7 | 0,7870 | 0,2577 | 0,7285 | 0,8890 | 2,0218 | -3,9786 | 0,84% | 2,62% | | 1,34% | 0,99% |
| 1-BROMOBUTANE | 570,4 | 40,41 | 0,3113 | 0,2687 | 0,2748 | 0,8651 | 2,3243 | -3,4850 | 2,59% | 3,57% | | 1,85% | 16,37% |
| 1-BROMODODECANE | 727,9 | 18,37 | 0,6823 | 0,2453 | 0,7202 | 0,8223 | 1,7055 | 22,4004 | 0,72% | 1,44% | | 1,97% | 22,72% |
| 1-BROMOHEPTANE | 646,1 | 28,97 | 0,4527 | 0,2654 | 0,4375 | 0,8776 | 2,1593 | -5,5956 | 0,95% | | | 2,85% | 19,42% |
| 1-BROMONAPHTHALENE | 824 | 37 | 0,3692 | 0,2545 | 1,2053 | 1,0000 | 0,7321 | 10,8624 | 0,65% | 1,04% | | 1,42% | 23,25% |
| 1-BROMOPROPANE | 535,5 | 45,78 | 0,2811 | 0,2646 | 0,2518 | 0,8666 | 2,3038 | -0,4317 | 4,18% | 4,53% | | 1,39% | 13,84% |
| 1-BUTANOL | 563,1 | 44,14 | 0,5883 | 0,2523 | 1,3851 | 1,0000 | 0,8538 | 1,5825 | 4,16% | 4,84% | 4,84% | 1,45% | 18,85% |
| 1-BUTENE | 419,5 | 40,2 | 0,1845 | 0,2743 | 0,2035 | 0,8532 | 2,0765 | -3,4679 | 2,15% | 2,01% | 1,77% | 1,64% | 12,11% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1-CHLORO-1,1-DIFLUOROETHANE | 410,29 | 40,41 | 0,2307 | 0,2665 | 0,3629 | 0,8278 | 1,4897 | 0,1103 | 0,40% | 0,95% | 2,28% | 1,39% | 15,28% |
| 1-CHLORO-2,4-DINITROBENZENE | 813,77 | 34,9 | 0,7319 | 0,2300 | 0,6049 | 0,8159 | 2,0625 | 27,7740 | 0,63% | 1,00% | | 1,89% | 18,87% |
| 1-CHLORONAPHTHALENE | 785 | 34 | 0,3827 | 0,2460 | 0,2255 | 0,8399 | 2,7185 | 20,7707 | 2,43% | 3,19% | | 1,45% | 31,18% |
| 1-CHLOROPENTANE | 571,2 | 33,52 | 0,2952 | 0,2561 | 0,3989 | 0,8335 | 1,6183 | 7,9390 | 1,01% | 2,17% | | 1,54% | 20,11% |
| 1-cis-2-trans-3-TRIMETHYLCYCLOPENTANE | 579,82 | 28,979 | 0,2800 | 0,2592 | 1,1351 | 1,0000 | 0,6742 | 5,8164 | 0,72% | 1,48% | | 1,74% | 21,24% |
| 1-cis-2-trans-4-TRIMETHYLCYCLOPENTANE | 579,26 | 28,779 | 0,2775 | 0,2592 | 1,1230 | 0,9998 | 0,6762 | 5,8010 | 0,84% | 1,70% | | 1,82% | 21,98% |
| 1-DECANOL | 688 | 23,08 | 0,6070 | 0,2484 | 2,4307 | 1,0000 | 0,4584 | 13,6732 | 1,78% | | 5,77% | 1,38% | 16,00% |
| 1-DECENE | 616,6 | 22,23 | 0,4805 | 0,2558 | 0,3362 | 0,8238 | 2,3809 | 6,3205 | 0,33% | 2,67% | 1,27% | 1,73% | 20,31% |
| 1-DECYNE | 619,85 | 23,7 | 0,5178 | 0,2580 | 0,2546 | 0,8267 | 2,9700 | 1,5141 | 1,65% | 1,91% | 6,07% | 1,78% | 20,82% |
| 1-DOCOSANOL | 824,4 | 10,35 | 0,8975 | 0,2245 | 0,3658 | 0,6070 | 2,2788 | 126,5383 | 0,57% | | | 1,49% | 24,88% |
| 1-DOCOSENE | 791,6 | 11,21 | 0,9481 | | 0,5254 | 0,8135 | 2,8000 | | 0,53% | 1,63% | | | |
| 1-DODECANOL | 718,7 | 19,54 | 0,6556 | 0,2443 | 0,2387 | 0,7525 | 2,8894 | 23,5152 | 3,70% | | 5,49% | 1,23% | 16,46% |
| 1-DODECENE | 657,1 | 18,88 | 0,5620 | 0,2490 | 0,4713 | 0,8055 | 2,0283 | 17,8443 | 0,41% | 2,16% | 3,02% | 1,62% | 20,23% |
| 1-EICOSANOL | 807,7 | 11,54 | 0,8789 | 0,2312 | 0,2477 | 0,7739 | 3,6907 | 88,3679 | 1,40% | | 1,35% | 2,06% | 23,23% |
| 1-EICOSENE | 771 | 12,2 | 0,8804 | 0,2405 | 0,4337 | 0,8115 | 3,0301 | 44,3180 | 0,93% | 2,04% | 1,15% | 3,02% | 20,84% |
| 1-ETHOXY-2-PROPANOL | 560,4 | 37,48 | 0,7581 | 0,2687 | 0,6369 | 0,8730 | 2,2175 | -13,4424 | 5,05% | | | 4,31% | 18,80% |
| 1-ETHYL-2-ISOPROPYLBENZENE | 666 | 26,7 | 0,4176 | 0,2561 | 0,5339 | 0,8228 | 1,5617 | 7,5474 | 0,32% | 0,45% | 0,26% | 1,42% | 18,86% |
| 1-ETHYLCYCLOHEXENE | 614,9 | 33,05 | 0,2922 | 0,2628 | 0,5469 | 0,8128 | 1,2347 | 2,3616 | 1,23% | 2,44% | | 1,49% | 16,26% |
| 1-ETHYLNAPHTHALENE | 776 | 33,2 | 0,4073 | 0,2565 | 0,5079 | 0,8201 | 1,5862 | 6,0442 | 2,05% | 2,43% | 2,02% | 1,34% | 13,72% |
| 1-ETHYLTETRALIN | 733 | 27,52 | 0,4292 | 0,2508 | 1,2329 | 1,0000 | 0,7817 | 15,7567 | 0,64% | 1,38% | | 1,63% | 19,82% |
| 1-HEPTADECANOL | 779,2 | 13,77 | 0,8123 | 0,2409 | 0,2431 | 0,7944 | 3,7696 | 49,1228 | 2,21% | | 3,23% | 2,92% | 20,44% |
| 1-HEPTADECENE | 736 | 14,1 | 0,7503 | 0,2433 | 0,3636 | 0,8197 | 3,0899 | 33,7770 | 1,90% | 1,94% | 1,60% | 2,43% | 20,40% |
| 1-HEPTANOL | 632,3 | 30,85 | 0,5621 | 0,2642 | 1,7829 | 1,0000 | 0,6175 | -4,3778 | 3,04% | | 8,28% | 2,96% | 18,97% |
| 1-HEPTENE | 537,4 | 29,2 | 0,3432 | 0,2648 | 0,3941 | 0,8352 | 1,7693 | -1,6608 | 1,77% | 2,56% | 1,90% | 1,55% | 17,42% |
| 1-HEPTYNE | 547 | 32,1 | 0,3778 | 0,2683 | 0,2893 | 0,8555 | 2,4634 | -5,6551 | 0,82% | 1,96% | 5,61% | 1,66% | 14,00% |
| 1-HEXACOSENE | 827,3 | 9,642 | 1,0757 | | 0,5208 | 0,8147 | 3,1264 | | 0,53% | 1,71% | | | |
| 1-HEXADECANOL | 768,6 | 14,68 | 0,7788 | 0,2375 | 0,2396 | 0,7965 | 3,7065 | 49,6106 | 3,10% | | 3,92% | 1,61% | 19,31% |
| 1-HEXADECENE | 722 | 14,8 | 0,7242 | 0,2435 | 0,4186 | 0,8094 | 2,6641 | 32,3289 | 1,51% | 1,64% | 0,80% | 2,21% | 20,49% |
| 1-HEXANOL | 611,3 | 34,46 | 0,5586 | 0,2515 | 1,5803 | 1,0000 | 0,7030 | 3,6961 | 2,99% | | 8,40% | 1,75% | 17,72% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1-HEXENE | 504 | 32,1 | 0,2851 | 0,2674 | 1,0769 | 1,0000 | 0,7257 | -2,1926 | 1,30% | 1,06% | 1,11% | 1,55% | 15,94% |
| 1-HEXYNE | 516,2 | 36,2 | 0,3327 | 0,2693 | 0,2358 | 0,8510 | 2,5334 | -5,2384 | 0,79% | 1,18% | 4,55% | 1,51% | 14,81% |
| 1-METHOXY-2-PROPANOL PROPANOATE | 611,7 | 26,02 | 0,5099 | 0,2490 | 1,6402 | 0,9999 | 0,6318 | 13,7912 | 0,74% | 1,40% | | 1,41% | 20,55% |
| 1-METHYL-1-ETHYLCYCLOPENTANE | 582 | 30,2 | 0,3298 | 0,2656 | 0,2068 | 0,8447 | 2,6362 | -2,0379 | 2,45% | | 2,13% | 1,87% | 15,56% |
| 1-METHYL-2-n-PROPYLBENZENE | 662 | 29,4 | 0,4070 | 0,2595 | 0,2629 | 0,8447 | 2,6367 | 3,1233 | 1,86% | 2,86% | 2,56% | 1,73% | 18,75% |
| 1-METHYL-3-(METHYLETHOXY)BENZENE | 670 | 28,4 | 0,4454 | 0,2601 | 0,2330 | 0,8317 | 2,8711 | 0,8407 | 1,87% | 3,68% | | 1,21% | 21,64% |
| 1-METHYL-3-HYDROXY-5-ISOPROPYL BENZENE | 726,8 | 34,08 | 0,5863 | | 1,5827 | 0,9927 | 0,7198 | | 0,52% | 0,98% | | | |
| 1-METHYL-3-HYDROXY-6-ISOPROPYL BENZENE | 722,5 | 34,08 | 0,5848 | | 0,3611 | 0,8358 | 2,6962 | | 0,49% | 1,36% | | | |
| 1-METHYL-3-n-PROPYLBENZENE | 654 | 28,1 | 0,4128 | 0,2599 | 0,2743 | 0,8367 | 2,5384 | 3,8987 | 1,03% | 2,40% | 2,15% | 2,75% | 22,60% |
| 1-METHYL-4-n-PROPYLBENZENE | 656 | 28,1 | 0,4134 | 0,2634 | 0,2579 | 0,8420 | 2,6815 | 0,5556 | 1,09% | 2,31% | 2,32% | 3,52% | 23,68% |
| 1-METHYL-4-VINYLCYCLOHEXENE | 626 | 31,2 | 0,3445 | 0,2620 | 0,7999 | 0,9075 | 1,0670 | 1,4001 | 1,05% | 1,92% | 1,27% | 1,57% | 17,03% |
| 1-METHYLCYCLOPENTENE | 542 | 41,3 | 0,2318 | 0,2728 | 1,1784 | 1,0000 | 0,5834 | -4,4727 | 0,54% | 1,80% | 1,73% | 1,38% | 12,18% |
| 1-METHYLINDAN | 694,1 | 34,37 | 0,3139 | 0,2626 | 1,0723 | 1,0000 | 0,7632 | 1,9179 | 0,50% | 1,32% | | 1,59% | 16,61% |
| 1-METHYLINDENE | 703 | 34,6 | 0,3349 | 0,2556 | 0,3677 | 0,8058 | 1,7236 | 9,5732 | 0,50% | 1,92% | 0,57% | 1,35% | 16,91% |
| 1-METHYLNAPHTHALENE | 772 | 36 | 0,3416 | 0,2561 | 1,0040 | 0,8943 | 0,8321 | 9,3901 | 0,90% | 2,21% | 0,47% | 1,44% | 15,85% |
| 1-METHYLTETRALIN | 719,3 | 30,57 | 0,3836 | 0,2539 | 1,2275 | 1,0000 | 0,7349 | 11,4144 | 0,53% | 1,36% | | 1,61% | 18,71% |
| 1-METHYLVINYL ACETATE | 552,2 | 41,81 | 0,4027 | 0,2801 | 0,2725 | 0,8471 | 2,5963 | -14,0912 | 1,98% | 2,79% | | 2,49% | 12,35% |
| 1-n-BUTYLNAPHTHALENE | 792 | 26,8 | 0,4951 | 0,2547 | 0,7785 | 0,8429 | 1,2975 | 8,1729 | 0,85% | 1,38% | 0,75% | 1,72% | 18,41% |
| 1-n-DECYLNAPHTHALENE | 844 | 15,23 | 0,7456 | | 0,7268 | 0,8284 | 1,8175 | | 0,64% | 1,64% | | | |
| 1-n-HEXYL-1,2,3,4-TETRAHYDRONAPHTHALENE | 779 | 18,9 | 0,5888 | 0,2398 | 0,6449 | 0,8044 | 1,6503 | 40,2048 | 0,59% | 1,63% | 0,76% | 2,09% | 31,42% |
| 1-n-HEXYLNAPHTHALENE | 813 | 22,5 | 0,5874 | 0,2531 | 0,6384 | 0,8111 | 1,6731 | 9,8127 | 0,45% | 0,73% | 0,68% | 2,54% | 23,31% |
| 1-NITROBUTANE | 623 | 37,6 | 0,4546 | 0,2472 | 0,3098 | 0,8486 | 2,5721 | 12,4014 | 5,79% | 4,04% | | 1,55% | 20,55% |
| 1-NITROPROPANE | 605 | 43,5 | 0,4128 | 0,2442 | 0,3397 | 0,8630 | 2,3535 | 13,1064 | 3,45% | 3,11% | 9,23% | 1,51% | 18,88% |
| 1-n-NONYLNAPHTHALENE | 835,1 | 16,43 | 0,7216 | 0,2272 | 0,6715 | 0,8262 | 1,8967 | 69,4737 | 0,67% | 1,65% | | 1,69% | 35,72% |
| 1-NONADECANOL | 798,8 | 12,2 | 0,8582 | 0,2349 | 0,3672 | 0,8111 | 3,2906 | 72,5458 | 1,79% | | | 2,86% | 22,21% |
| 1-NONADECENE | 760 | 12,8 | 0,8325 | 0,2417 | 0,3893 | 0,8170 | 3,1704 | 39,9849 | 1,95% | 1,98% | 1,49% | 2,82% | 20,52% |
| 1-NONANOL | 670,9 | 25,27 | 0,5841 | 0,2472 | 3,2674 | 1,0000 | 0,3260 | 13,2995 | 2,04% | | 5,65% | 2,15% | 15,50% |
| 1-NONENE | 593,1 | 24,28 | 0,4367 | 0,2592 | 0,3053 | 0,8302 | 2,4151 | 2,2587 | 0,33% | 3,16% | 1,87% | 1,67% | 18,72% |
| 1-NONYNE | 598,05 | 26,1 | 0,4710 | 0,2620 | 0,2603 | 0,8182 | 2,6813 | -2,1664 | 0,08% | 0,92% | 5,19% | 1,65% | 18,27% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1-n-PENTYLNAPHTHALENE | 803 | 24,4 | 0,5354 | 0,2516 | 0,8156 | 0,8389 | 1,3063 | 12,8659 | 1,05% | 1,43% | 0,67% | 1,83% | 20,74% |
| 1-OCTACOSENE | 842,2 | 9,011 | 1,1351 | | 0,5985 | 0,8263 | 2,9768 | | 0,62% | | | | |
| 1-OCTADECANOL | 789,3 | 12,95 | 0,8322 | 0,2344 | 0,2288 | 0,7907 | 3,8834 | 67,0476 | 2,57% | | 2,81% | 1,85% | 21,20% |
| 1-OCTADECENE | 748 | 13,4 | 0,7943 | 0,2427 | 0,4077 | 0,8123 | 2,9277 | 36,6056 | 1,85% | 1,91% | 1,29% | 2,62% | 20,56% |
| 1-OCTANOL | 652,3 | 27,83 | 0,5697 | 0,2550 | 2,2555 | 1,0000 | 0,4807 | 4,2322 | 1,94% | 4,16% | 9,03% | 1,34% | 16,86% |
| 1-OCTENE | 566,9 | 26,63 | 0,3921 | 0,2628 | 0,2493 | 0,8435 | 2,6575 | -0,9276 | 1,68% | 2,98% | 1,10% | 1,75% | 17,46% |
| 1-OCTYNE | 574 | 28,8 | 0,4233 | 0,2645 | 0,4099 | 0,8428 | 1,9983 | -3,7374 | 0,92% | 1,89% | 5,05% | 1,76% | 16,09% |
| 1-PENTADECANOL | 757,3 | 15,69 | 0,7507 | 0,2372 | 0,2288 | 0,7970 | 3,6930 | 45,0502 | 3,00% | | 4,09% | 1,41% | 17,68% |
| 1-PENTADECENE | 708 | 15,7 | 0,6815 | 0,2454 | 0,4179 | 0,8084 | 2,5458 | 27,0879 | 1,67% | 1,79% | 0,96% | 2,07% | 20,24% |
| 1-PENTANOL | 588,1 | 38,97 | 0,5748 | 0,2536 | 1,4595 | 1,0000 | 0,7878 | 1,1742 | 2,42% | 4,78% | 4,34% | 1,43% | 17,95% |
| 1-PENTENE | 464,8 | 35,6 | 0,2372 | 0,2705 | 0,9309 | 1,0000 | 0,7706 | -2,7711 | 0,44% | 1,11% | 1,82% | 1,66% | 14,68% |
| 1-PENTENE-4-YNE | 503 | 44 | 0,1786 | 0,2668 | 0,1413 | 0,8582 | 2,4235 | 1,3814 | 1,30% | 2,16% | 1,05% | 1,59% | 13,59% |
| 1-PENTYNE | 481,2 | 41,7 | 0,2899 | 0,2889 | 0,2208 | 0,8559 | 2,4580 | -12,1115 | 1,30% | 1,91% | 4,36% | 5,86% | 10,85% |
| 1-PHENYLNAPHTHALENE | 849 | 26,3 | 0,5309 | 0,2448 | 0,6986 | 0,8356 | 1,4898 | 25,9668 | 0,63% | 1,09% | | 1,45% | 21,81% |
| 1-PROPANOL | 536,8 | 51,69 | 0,6209 | 0,2471 | 1,1040 | 0,9376 | 1,1349 | 3,0740 | 3,61% | 2,84% | 5,64% | 1,75% | 19,80% |
| 1-tert-BUTOXY-2-[2-(HYDROXY)PROPOXY]PROPANE | 689,9 | 23 | 0,9350 | 0,2592 | 0,5710 | 0,8125 | 2,5859 | -17,6761 | 0,58% | 1,22% | | 2,72% | 24,89% |
| 1-tert-BUTOXY-2-[2-(tert-BUTOXY)PROPOXY]PROPANE | 729,4 | 15,27 | 0,6360 | | 0,6170 | 0,8213 | 1,8461 | | 0,63% | 1,74% | | | |
| 1-TETRACOSENE | 810,4 | 10,37 | 1,0139 | | 0,5235 | 0,8139 | 2,9640 | | 0,65% | 1,66% | | | |
| 1-TETRADECENE | 691 | 16,27 | 0,6503 | 0,2429 | 0,4827 | 0,8016 | 2,1964 | 31,8749 | 0,59% | 1,73% | 0,24% | 1,70% | 21,81% |
| 1-TRIACONTENE | 857 | 8,47 | 1,1817 | | 0,6820 | 0,8365 | 2,7810 | | 0,57% | | | | |
| 1-TRIDECANOL | 732,4 | 18,1 | 0,6881 | 0,2427 | 0,1773 | 0,7939 | 3,7845 | 29,6263 | 3,05% | | 5,28% | 1,28% | 16,81% |
| 1-TRIDECENE | 674,8 | 17,49 | 0,6074 | 0,2460 | 0,4309 | 0,8071 | 2,2863 | 24,1918 | 0,41% | 2,16% | 0,55% | 1,68% | 21,00% |
| 1-UNDECANOL | 703,9 | 21,19 | 0,6236 | 0,2486 | 0,3505 | 0,7194 | 2,2106 | 16,6819 | 4,28% | | 6,73% | 1,32% | 16,41% |
| 1-UNDECENE | 637,8 | 20,44 | 0,5225 | 0,2523 | 0,3936 | 0,8155 | 2,2277 | 11,6622 | 0,32% | 2,64% | 3,08% | 1,64% | 19,61% |
| 2-(2-HEXOXYETHOXY)ETHANOL | 684 | 24,1 | 1,1110 | 0,2669 | 1,8541 | 1,0000 | 0,9732 | -31,1801 | 4,57% | | 5,91% | 4,70% | 19,90% |
| 2-(2-PENTOXYETHOXY)ETHANOL | 705,3 | 25,03 | 0,7047 | 0,2563 | 0,2400 | 0,6927 | 2,5998 | -1,2956 | 0,52% | | | 2,22% | 20,25% |
| 2-(DIFLUOROMETHOXY)-1,1,1-TRIFLUOROETHANE | 444,03 | 34,2 | 0,3887 | 0,2635 | 1,2047 | 1,0000 | 0,7551 | -1,2321 | 0,49% | 0,93% | | 1,35% | 15,25% |
| 2-(N-MORPHOLINO)-2'-HYDROXYDIETHYLETHER | 728,4 | 28,93 | 0,7521 | | 0,5286 | 0,8241 | 2,3806 | | 0,62% | 1,39% | | | |
| 2,2',2"-NITRILOTRIS-ACETONITRILE | 823 | 26,4 | 0,9240 | | 0,4716 | 0,8087 | 2,9464 | | 0,53% | 1,44% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2,2,3,3-TETRAMETHYLBUTANE | 568 | 28,7 | 0,2450 | 0,2739 | 0,2444 | 0,8337 | 1,9789 | -9,1561 | 0,52% | 2,37% | 0,05% | 1,42% | 11,71% |
| 2,2,3,3-TETRAMETHYLHEXANE | 623 | 25,1 | 0,3659 | 0,2693 | 0,2633 | 0,8514 | 2,5277 | -10,0308 | 1,26% | 2,23% | 1,26% | 1,47% | 15,69% |
| 2,2,3,3-TETRAMETHYLPENTANE | 607,5 | 27,41 | 0,3051 | 0,2702 | 0,2049 | 0,8476 | 2,5879 | -8,4311 | 0,96% | 2,16% | 0,15% | 1,00% | 20,27% |
| 2,2,3,4-TETRAMETHYLPENTANE | 592,6 | 26 | 0,3138 | 0,2680 | 0,3948 | 0,8223 | 1,6372 | -5,8685 | 1,00% | 2,21% | 4,14% | 1,58% | 20,08% |
| 2,2,3-TRIMETHYLBUTANE | 531,1 | 29,5 | 0,2501 | 0,2704 | 0,1767 | 0,8497 | 2,5146 | -5,3936 | 0,27% | 1,12% | 0,35% | 1,45% | 16,97% |
| 2,2,3-TRIMETHYLPENTANE | 563,5 | 27,3 | 0,2971 | 0,2638 | 0,2606 | 0,8242 | 2,0622 | -1,4252 | 0,37% | 1,32% | 1,38% | 1,91% | 21,33% |
| 2,2,4,4,6,8,8-HEPTAMETHYLNONANE | 692 | 15,7 | 0,5482 | 0,2487 | 0,3566 | 0,8224 | 2,4990 | 17,7009 | 0,45% | 3,02% | 6,16% | 1,82% | 28,49% |
| 2,2,4,4-TETRAMETHYL-1,3-CYCLOBUTANEDIOL | 699,5 | 31,72 | 0,5711 | 0,2487 | 0,3107 | 0,7368 | 2,2701 | 11,6157 | 0,60% | 2,09% | | 1,25% | 21,06% |
| 2,2,4,4-TETRAMETHYLPENTANE | 574,6 | 24,9 | 0,3136 | 0,2692 | 0,3498 | 0,8368 | 1,8418 | -7,5300 | 0,92% | 1,76% | 0,70% | 1,20% | 18,52% |
| 2,2,4-TRIMETHYL-1,3-PENTANEDIOL | 697,9 | 27,04 | 0,5958 | 0,2331 | 0,1019 | 0,6777 | 2,7097 | 31,4458 | 0,42% | | | 3,94% | 24,89% |
| 2,2,4-TRIMETHYLPENTANE | 543,8 | 25,7 | 0,3035 | 0,2671 | 0,2817 | 0,8367 | 2,0767 | -4,0128 | 0,46% | 1,01% | 3,65% | 1,32% | 16,41% |
| 2,2,5,5-TETRAMETHYLHEXANE | 581,4 | 21,9 | 0,3767 | 0,2653 | 1,0410 | 0,8559 | 0,8407 | -3,8714 | 0,51% | 0,42% | 0,37% | 1,05% | 16,85% |
| 2,2,5-TRIMETHYLHEXANE | 569,8 | 23,3 | 0,3446 | 0,2632 | 1,5570 | 0,9992 | 0,5244 | 0,4517 | 0,84% | 1,89% | 0,87% | 1,48% | 20,34% |
| 2,2-DICHLORO-1,1,1-TRIFLUOROETHANE | 456,94 | 36,76 | 0,2825 | 0,2675 | 0,3364 | 0,8155 | 1,6897 | -1,6548 | 0,46% | 1,14% | 4,08% | 1,18% | 14,88% |
| 2,2-DICHLORO-1,1,2-TRIFLUOROETHANE | 462 | 36,1 | 0,2622 | | 0,8850 | 0,8786 | 0,8100 | | 0,55% | 2,15% | 4,12% | | |
| 2,2-DIMETHYL-1-PROPANOL | 552,7 | 40,78 | 0,5950 | | 0,1755 | 0,7513 | 2,9767 | | 0,48% | 1,44% | | | |
| 2,2-DIMETHYL-3-ETHYLPENTANE | 590 | 25,7 | 0,3353 | 0,2690 | 1,1634 | 1,0000 | 0,7204 | -7,1337 | 0,59% | 0,96% | | 1,59% | 16,22% |
| 2,2-DIMETHYLBUTANE | 489 | 31 | 0,2341 | 0,2731 | 0,2274 | 0,8329 | 2,0024 | -6,2766 | 0,90% | 1,99% | 1,11% | 1,19% | 14,37% |
| 2,2-DIMETHYLHEPTANE | 576,7 | 23,5 | 0,3911 | 0,2624 | 0,4739 | 0,8281 | 1,6508 | -1,0686 | 1,84% | 2,23% | 2,46% | 1,74% | 21,06% |
| 2,2-DIMETHYLHEXANE | 549,8 | 25,3 | 0,3378 | 0,2637 | 0,3112 | 0,8147 | 1,9547 | -0,6027 | 0,27% | 1,08% | 0,71% | 1,45% | 16,32% |
| 2,2-DIMETHYLOCTANE | 602 | 21,6 | 0,4288 | 0,2574 | 0,4076 | 0,8042 | 1,8665 | 4,7361 | 0,43% | 1,67% | 0,99% | 1,34% | 23,27% |
| 2,2-DIMETHYLPENTANE | 520,5 | 27,7 | 0,2871 | 0,2660 | 0,3147 | 0,8203 | 1,7937 | -1,8211 | 0,53% | 1,16% | 1,48% | 1,38% | 15,89% |
| 2,2'-IMINOBIS-ACETONITRILE | 731 | 35,4 | 0,7192 | | 0,3774 | 0,8100 | 2,8444 | | 0,59% | 1,46% | | | |
| 2,3,3,3-TETRAFLUOROPROPENE | 367,85 | 33,82 | 0,2820 | 0,2645 | 1,0265 | 1,0000 | 0,7569 | 0,4639 | 0,58% | 1,48% | | 1,30% | 16,32% |
| 2,3,3,4-TETRAMETHYLPENTANE | 607,5 | 27,2 | 0,3144 | 0,2700 | 0,3541 | 0,8278 | 1,7843 | -7,8307 | 0,23% | 2,21% | 0,84% | 1,57% | 17,38% |
| 2,3,3-TRIMETHYL-1-BUTENE | 531 | 31,4 | 0,2388 | 0,2771 | 0,1021 | 0,8351 | 2,8070 | -9,8520 | 1,31% | 4,26% | 2,72% | 1,38% | 16,03% |
| 2,3,3-TRIMETHYLPENTANE | 573,5 | 28,2 | 0,2903 | 0,2678 | 0,1805 | 0,8447 | 2,6366 | -4,5706 | 0,26% | 1,70% | 0,12% | 1,29% | 15,24% |
| 2,3,4,5,2',3',4',5'-OCTAHYDRO-BIFURYL-(3,3') | 738 | 37 | 0,3715 | | 0,5336 | 0,8400 | 1,4995 | | 0,94% | 2,35% | | | |
| 2,3,4-TRIMETHYLPENTANE | 566,4 | 27,3 | 0,3153 | 0,2650 | 0,2739 | 0,8303 | 2,1110 | -2,2772 | 0,35% | 1,16% | 0,82% | 1,36% | 15,77% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2,3,5-TRIMETHYLTHIOPHENE | 656,8 | 36,3 | 0,3238 | 0,2645 | 1,0758 | 1,0000 | 0,7724 | -0,5951 | 0,46% | 1,47% | | 1,35% | 16,34% |
| 2,3-DICHLOROBUTANE | 599 | 37,4 | 0,2682 | 0,2651 | 1,0986 | 1,0000 | 0,6780 | 2,0937 | 0,65% | 0,29% | | 1,69% | 18,73% |
| 2,3-DICHLOROPROPENE | 578 | 43,8 | 0,1945 | 0,2631 | 0,4622 | 0,8218 | 1,1962 | 5,5246 | 2,87% | | 0,17% | 1,88% | 19,77% |
| 2,3-DIHYDROFURAN | 524 | 55 | 0,2255 | 0,2675 | 1,0167 | 1,0000 | 0,6822 | -0,8361 | 0,57% | 1,22% | | 1,68% | 19,19% |
| 2,3-DIMETHYL-1,3-BUTADIENE | 526 | 35,2 | 0,2142 | 0,2612 | 1,2188 | 1,0000 | 0,5472 | 5,0840 | 1,41% | 1,18% | 0,40% | 2,16% | 19,63% |
| 2,3-DIMETHYL-1-BUTENE | 501 | 33,2 | 0,2333 | 0,2727 | 0,7848 | 0,9067 | 0,8794 | -5,1746 | 1,06% | 1,85% | 0,15% | 1,73% | 16,68% |
| 2,3-DIMETHYL-1-HEXENE | 561 | 27,6 | 0,3249 | 0,2668 | 0,3161 | 0,7731 | 1,7215 | -3,5385 | 0,41% | 3,01% | 2,40% | 1,36% | 17,54% |
| 2,3-DIMETHYL-2,3-DIPHENYLBUTANE | 805 | 19,9 | 0,5208 | | 0,2485 | 0,8248 | 3,0074 | | 0,32% | 1,34% | | | |
| 2,3-DIMETHYL-2-BUTENE | 528 | 33,2 | 0,2237 | 0,2590 | 1,3350 | 1,0000 | 0,5078 | 6,8361 | 1,89% | 1,39% | 2,45% | 2,49% | 19,29% |
| 2,3-DIMETHYLBENZOTHIOPHENE | 786 | 34,64 | 0,4205 | 0,2559 | 1,3021 | 1,0000 | 0,7259 | 7,2026 | 0,63% | 1,47% | | 1,34% | 25,56% |
| 2,3-DIMETHYLBUTANE | 500 | 31,5 | 0,2493 | 0,2701 | 0,1901 | 0,8436 | 2,3605 | -4,2239 | 0,38% | 1,37% | 0,97% | 1,30% | 13,55% |
| 2,3-DIMETHYLDECANE | 653,5 | 18,8 | 0,5159 | 0,2506 | 1,2202 | 0,9557 | 0,8864 | 16,6493 | 0,67% | 1,27% | | 1,95% | 20,41% |
| 2,3-DIMETHYLDODECANE | 689,7 | 16,56 | 0,6016 | 0,2464 | 0,8176 | 0,8506 | 1,4260 | 24,8099 | 0,66% | 1,44% | | 1,99% | 21,88% |
| 2,3-DIMETHYLHEPTANE | 588,8 | 23,9 | 0,3914 | 0,2604 | 0,3780 | 0,8214 | 1,9207 | 2,2761 | 1,95% | 2,79% | 1,50% | 1,79% | 17,71% |
| 2,3-DIMETHYLHEXANE | 563,5 | 26,3 | 0,3455 | 0,2617 | 0,2285 | 0,8287 | 2,4463 | 0,6507 | 0,25% | 0,87% | 0,50% | 1,38% | 16,87% |
| 2,3-DIMETHYLNONANE | 633,9 | 20,16 | 0,4703 | 0,2530 | 1,2811 | 1,0000 | 0,7921 | 12,8825 | 0,68% | 1,20% | | 2,08% | 19,63% |
| 2,3-DIMETHYLOCTANE | 613,1 | 21,73 | 0,4245 | 0,2553 | 0,6790 | 0,8417 | 1,3286 | 9,4731 | 0,82% | 2,09% | | 1,81% | 18,81% |
| 2,3-DIMETHYLPENTANE | 537,3 | 29,1 | 0,2964 | 0,2634 | 0,2151 | 0,8367 | 2,3741 | -0,7082 | 0,37% | 1,65% | 0,92% | 1,79% | 20,26% |
| 2,3-DIMETHYLTHIOPHENE | 637 | 40,5 | 0,2709 | 0,2582 | 1,1033 | 1,0000 | 0,6828 | 5,4278 | 0,64% | 1,73% | | 2,58% | 13,96% |
| 2,3-DIMETHYLUNDECANE | 671,4 | 17,61 | 0,5590 | 0,2482 | 0,8376 | 0,8624 | 1,3367 | 21,0037 | 0,66% | 1,42% | | 1,97% | 21,15% |
| 2,3-PENTADIENE | 497 | 38 | 0,2184 | 0,2578 | 1,3441 | 1,0000 | 0,4973 | 7,3873 | 1,79% | 0,96% | 1,53% | 2,00% | 10,81% |
| 2,3-XYLENOL | 722,95 | 49 | 0,5157 | 0,2930 | 0,3429 | 0,8459 | 2,6168 | -30,5656 | 1,07% | 1,29% | 2,44% | 1,80% | 13,24% |
| 2,4,4-TRIMETHYL-1-PENTENE | 550 | 26,8 | 0,3011 | 0,2656 | 0,2563 | 0,8298 | 2,1277 | -1,7339 | 1,73% | 1,87% | 1,52% | 1,29% | 20,70% |
| 2,4,4-TRIMETHYL-2-PENTENE | 555 | 26,8 | 0,2971 | 0,2632 | 1,4105 | 1,0000 | 0,5435 | 1,5770 | 0,73% | 1,28% | 1,02% | 1,46% | 21,04% |
| 2,4,4-TRIMETHYLHEXANE | 581 | 24,6 | 0,3522 | 0,2659 | 0,5061 | 0,8407 | 1,5041 | -4,1540 | 1,41% | 1,89% | 2,42% | 1,70% | 18,94% |
| 2,4,6-TRIMETHYLPYRIDINE | 653 | 33,3 | 0,3749 | 0,2499 | 1,3026 | 0,9997 | 0,6726 | 12,3214 | 0,58% | 0,79% | | 2,77% | 17,24% |
| 2,4-DIAMINOTOLUENE | 804 | 43,8 | 0,5794 | 0,2466 | 1,3203 | 1,0000 | 0,8777 | 11,3328 | 0,54% | 0,59% | | 1,14% | 21,76% |
| 2,4-DICHLOROBENZOTRIFLUORIDE | 646 | 28,1 | 0,4344 | | 1,2187 | 0,9883 | 0,7971 | | 0,58% | 1,06% | | | |
| 2,4-DICHLOROTOLUENE | 705 | 35,9 | 0,3590 | 0,2547 | 1,1837 | 1,0000 | 0,7340 | 9,5202 | 0,55% | 0,35% | | 1,33% | 21,88% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2,4-DIMETHYL-1,3-DIOXOLANE-2-METHANOL | 621,3 | 35,4 | 0,5507 | | 0,5963 | 0,8204 | 1,7165 | | 0,49% | 1,68% | | | |
| 2,4-DIMETHYL-3-ETHYLPENTANE | 591 | 25,3 | 0,3530 | 0,2659 | 0,6810 | 0,8674 | 1,2133 | -3,8184 | 0,94% | 1,37% | | 1,86% | 17,36% |
| 2,4-DIMETHYLHEXANE | 553,5 | 25,6 | 0,3436 | 0,2657 | 0,2681 | 0,8207 | 2,1839 | -3,0125 | 0,32% | 0,82% | 0,37% | 1,73% | 17,72% |
| 2,4-DIMETHYLOCTANE | 600 | 21,7 | 0,4345 | 0,2636 | 1,2942 | 0,9763 | 0,7434 | -1,9636 | 0,62% | 1,26% | 0,68% | 2,55% | 23,24% |
| 2,4-DIMETHYLPENTANE | 519,8 | 27,4 | 0,3022 | 0,2642 | 0,3283 | 0,8194 | 1,7978 | -0,9728 | 0,31% | 1,09% | 0,59% | 1,54% | 16,23% |
| 2,4-DINITROPHENOL | 766,9 | 38,88 | 0,8160 | 0,2444 | 0,4371 | 0,8092 | 2,8302 | 8,1085 | 0,61% | 1,77% | | 1,22% | 25,90% |
| 2,4-DIPHENYL-4-METHYLPENTENE-1 | 835 | 20 | 0,5467 | 0,2417 | 0,2706 | 0,8260 | 2,9829 | 38,3141 | 0,41% | 1,09% | | 1,38% | 22,62% |
| 2,4-TOLUENE DIISOCYANATE | 725 | 30,4 | 0,6582 | 0,2476 | 0,6146 | 0,8836 | 2,0851 | 12,9572 | 1,29% | | | 2,48% | 13,63% |
| 2,4-XYLENOL | 707,65 | 44 | 0,5136 | 0,2682 | 0,3002 | 0,8366 | 2,7778 | -10,3363 | 1,01% | 2,19% | 2,87% | 1,03% | 8,05% |
| 2,5-DIHYDROFURAN | 542 | 55 | 0,2197 | 0,2607 | 1,1981 | 1,0000 | 0,5624 | 3,2085 | 1,71% | 2,79% | 0,48% | 2,40% | 20,71% |
| 2,5-DIMETHYL-1,5-HEXADIENE | 567 | 27,4 | 0,3238 | 0,2588 | 0,5534 | 0,8026 | 1,2720 | 6,4382 | 0,42% | 1,60% | 0,22% | 1,33% | 17,41% |
| 2,5-DIMETHYL-2,4-HEXADIENE | 597 | 27,4 | 0,3218 | 0,2444 | 1,3538 | 1,0000 | 0,6083 | 21,5144 | 2,17% | 3,13% | 0,53% | 3,50% | 25,97% |
| 2,5-DIMETHYLHEXANE | 550 | 24,9 | 0,3576 | 0,2615 | 0,2415 | 0,8285 | 2,4260 | 1,2119 | 0,44% | 0,93% | 0,51% | 1,27% | 16,87% |
| 2,5-DIMETHYLOCTANE | 603 | 21,7 | 0,4403 | 0,2581 | 0,9469 | 0,8810 | 1,0203 | 4,1379 | 1,71% | 1,81% | 1,33% | 1,67% | 22,80% |
| 2,5-DIMETHYLTHIOPHENE | 629,9 | 44,62 | 0,3085 | | 0,2733 | 0,8647 | 2,3296 | | 0,39% | | | | |
| 2,5-XYLENOL | 707,05 | 49 | 0,5638 | 0,2877 | 0,5268 | 0,8794 | 2,1367 | -27,3815 | 0,45% | 1,30% | | 1,40% | 13,19% |
| 2,6,8-TRIMETHYL-4-NONANONE | 658 | 19,7 | 0,6490 | 0,2531 | 0,7449 | 0,8387 | 1,6241 | 2,5831 | 0,70% | 1,61% | | 2,15% | 25,16% |
| 2,6-DIETHYLNAPHTHALENE | 807 | 25,8 | 0,5118 | | 0,6836 | 0,8221 | 1,4547 | | 0,37% | 2,34% | 0,85% | | |
| 2,6-DIMETHYL-4-HEPTANOL | 603 | 25,5 | 0,8022 | 0,2684 | 0,7279 | 0,8580 | 1,9750 | -21,4162 | 1,01% | 2,40% | | 3,78% | 16,32% |
| 2,6-DIMETHYLHEPTANE | 579 | 23 | 0,3927 | 0,2582 | 0,6861 | 0,8162 | 1,2219 | 4,6810 | 0,71% | 0,27% | 1,34% | 1,51% | 22,83% |
| 2,6-DIMETHYLNAPHTHALENE | 777 | 31,7 | 0,4177 | 0,2612 | 0,9279 | 0,9105 | 1,0222 | 3,6570 | 0,34% | 0,95% | 0,47% | 2,31% | 19,77% |
| 2,6-DIMETHYLOCTANE | 606 | 21,7 | 0,4386 | 0,2616 | 0,8221 | 0,8489 | 1,1466 | 0,4775 | 0,36% | 1,49% | 0,97% | 1,95% | 24,05% |
| 2,6-DIMETHYLPYRIDINE | 623,75 | 37,5 | 0,3453 | 0,2562 | 0,4767 | 0,8137 | 1,5002 | 6,0990 | 1,11% | 0,42% | 0,75% | 1,92% | 12,34% |
| 2,6-DINITROPHENOL | 770,1 | 39,05 | 0,8220 | | 0,6389 | 0,7830 | 2,0572 | | 0,53% | 1,76% | | | |
| 2,6-NAPHTHALENEDICARBOXYLIC ACID | 904 | 30,5 | 1,1601 | | 0,5613 | 0,8182 | 3,1511 | | 0,62% | 0,93% | | | |
| 2,6-TOLUENE DIISOCYANATE | 749 | 29 | 0,4338 | 0,2366 | 2,0556 | 1,0000 | 0,4446 | 37,7440 | 1,25% | 1,55% | | 1,96% | 18,55% |
| 2,6-XYLENOL | 701,05 | 43 | 0,4554 | 0,2880 | 0,3068 | 0,8470 | 2,5988 | -27,2774 | 1,17% | 2,05% | 2,20% | 1,65% | 13,84% |
| 2,7-DIMETHYLBENZOTHIOPHENE | 772,4 | 34,64 | 0,4220 | | 0,5530 | 0,8377 | 1,5670 | | 0,58% | 1,81% | | | |
| 2,7-DIMETHYLNAPHTHALENE | 775 | 32,3 | 0,4477 | 0,2674 | 0,6905 | 0,8586 | 1,3665 | -3,4372 | 0,49% | 1,90% | 0,56% | 3,16% | 2,78% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2,7-DIMETHYLOCTANE | 604 | 21,3 | 0,4420 | 0,2559 | 0,3935 | 0,8145 | 1,9922 | 6,8782 | 0,70% | 0,52% | 1,64% | 1,36% | 24,85% |
| 2-ACETOACETOXY ETHYL METHACRYLATE | 724,2 | 22,57 | 0,8156 | 0,2399 | 1,1266 | 0,9380 | 1,3367 | 20,3462 | 0,23% | | | 2,25% | 28,78% |
| 2-AMINO-2-METHYL-1-PROPANOL | 619,8 | 38,621 | 0,6466 | 0,2362 | 1,4205 | 0,8503 | 0,8794 | 18,0865 | 0,55% | 1,79% | | 1,39% | 24,47% |
| 2-AMINOETHOXYETHANOL | 735 | 59 | 0,5598 | 0,2927 | 0,4234 | 0,7692 | 2,0275 | -23,1145 | 1,79% | 1,27% | 7,29% | 4,10% | 0,68% |
| 2-BROMOBUTANE | 567 | 46,3 | 0,2684 | 0,2868 | 1,2100 | 1,0000 | 0,6087 | -16,4396 | 0,54% | 1,66% | 0,62% | 1,20% | 2,95% |
| 2-BROMOPROPANE | 532 | 55,1 | 0,2432 | 0,3291 | 0,2040 | 0,8625 | 2,3610 | -31,9680 | 2,49% | 2,67% | 4,45% | 9,01% | 4,79% |
| 2-BUTANOL | 535,9 | 41,885 | 0,5808 | 0,2522 | 2,3032 | 1,0000 | 0,4725 | 3,0205 | 1,32% | 1,92% | | 1,59% | 20,00% |
| 2-BUTOXIME | 608,5 | 42,04 | 0,6071 | 0,2426 | 1,2094 | 0,8806 | 0,9878 | 10,0950 | 0,74% | 1,80% | 1,84% | 1,79% | 18,76% |
| 2-BUTOXYETHANOL | 633,9 | 32,7 | 0,5143 | 0,2535 | 0,2091 | 0,8151 | 3,1380 | 5,3933 | 1,08% | 2,43% | 3,05% | 1,47% | 15,70% |
| 2-BUTYL-1-DECANOL | 707,6 | 17,13 | 1,1142 | | 0,5220 | 0,8153 | 3,2152 | | 0,55% | 1,60% | | | |
| 2-BUTYL-2-ETHYL-1,3-PROPANEDIOL | 732 | 25,97 | 0,6907 | 0,2429 | 0,7518 | 0,7251 | 1,5286 | 19,8659 | 1,57% | | | 1,29% | 23,12% |
| 2-BUTYLBENZOTHIOPHENE | 818,7 | 28,41 | 0,5280 | | 0,2955 | 0,8126 | 2,6651 | | 0,57% | 1,72% | | | |
| 2-BUTYL-NONAN-1-OL | 681,5 | 18,26 | 1,0762 | 0,2508 | 0,5312 | 0,8136 | 3,0728 | -5,4199 | 0,61% | 1,50% | | 3,65% | 23,31% |
| 2-BUTYL-OCTAN-1-OL | 667,3 | 19,41 | 0,9889 | | 0,6623 | 0,8350 | 2,4719 | | 0,52% | | | | |
| 2-CHLORO-1,1,1,2-TETRAFLUOROETHANE | 395,65 | 36,6 | 0,2877 | 0,2697 | 0,2133 | 0,8457 | 2,4322 | -3,0896 | 0,58% | 1,72% | 3,90% | 1,95% | 14,59% |
| 2-CHLORO-1,1,1-TRIFLUOROETHANE | 430 | 38,4 | 0,2465 | 0,2551 | 0,1882 | 0,8552 | 2,4679 | 7,2401 | 0,51% | 1,93% | | 1,81% | 17,21% |
| 2-CHLORO-1,1-DIFLUOROETHYLENE | 400,55 | 44,583 | 0,2116 | 0,2657 | 0,3964 | 0,8605 | 1,4672 | 0,7633 | 2,91% | 2,44% | 0,11% | 1,30% | 16,17% |
| 2-CHLOROETHANOL | 585 | 59,2 | 0,6578 | 0,2393 | 0,6243 | 0,8863 | 2,0535 | 5,9787 | 1,41% | | | 2,41% | 16,31% |
| 2-CHLOROPROPENE | 478 | 47,1 | 0,1515 | 0,2792 | 0,9654 | 1,0000 | 0,6085 | -3,9326 | 0,66% | 1,34% | 1,64% | 2,76% | 12,53% |
| 2-CYCLOHEXENE-1-ONE | 684,2 | 45,35 | 0,3063 | | 1,0875 | 1,0000 | 0,7413 | | 0,64% | 1,69% | | | |
| 2-CYCLOHEXENYL CYCLOHEXANONE | 792,8 | 29,33 | 0,4284 | 0,2586 | 1,0192 | 0,8973 | 0,9423 | 3,9791 | 0,49% | 1,70% | | 1,39% | 18,22% |
| 2-ETHOXYETHYL ACETATE | 607,3 | 31,66 | 0,5522 | 0,2641 | 0,3319 | 0,8379 | 2,7547 | -4,8343 | 1,67% | 2,44% | | 2,95% | 9,29% |
| 2-ETHYL BUTYRIC ACID | 655 | 34,1 | 0,6326 | 0,2548 | 0,8190 | 0,8436 | 1,4667 | 2,5163 | 0,64% | 0,73% | | 2,30% | 25,56% |
| 2-ETHYL HEXANOIC ACID | 674,6 | 27,78 | 0,8013 | 0,2482 | 0,8616 | 0,8180 | 1,6291 | 4,2147 | 0,92% | 1,73% | | 2,72% | 16,75% |
| 2-ETHYL-1-BUTANOL | 591,2 | 35,35 | 0,6330 | 0,2634 | 0,1606 | 0,7312 | 2,9906 | -6,3070 | 0,48% | | | 1,73% | 18,51% |
| 2-ETHYL-1-BUTENE | 511 | 33 | 0,2523 | 0,2677 | 0,8675 | 0,8887 | 0,8182 | -1,0367 | 1,30% | 1,71% | 1,15% | 1,46% | 15,69% |
| 2-ETHYL-1-HEXANOL | 640,4 | 27,56 | 0,5498 | 0,2548 | 0,1410 | 0,6904 | 2,5299 | 5,3763 | 0,78% | | | 1,61% | 19,62% |
| 2-ETHYL-1-HEXENE | 569 | 26,7 | 0,3577 | 0,2603 | 1,0430 | 1,0000 | 0,8473 | 3,2454 | 0,93% | 0,82% | | 1,40% | 19,52% |
| 2-ETHYL-1-PENTENE | 543 | 29,5 | 0,3073 | 0,2644 | 0,3299 | 0,8779 | 2,1543 | -0,3730 | 1,92% | 4,94% | 1,09% | 1,63% | 18,30% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2-ETHYL-2-HEXENAL | 636 | 26,4 | 0,4535 | 0,2300 | 0,2330 | 0,8308 | 2,8882 | 40,7220 | 0,44% | 2,50% | 2,03% | 2,29% | 24,73% |
| 2-ETHYLBENZOTHIOPHENE | 774 | 35,26 | 0,4283 | 0,2626 | 0,6367 | 0,8294 | 1,3934 | -1,9560 | 0,59% | 1,60% | 0,32% | 1,41% | 21,34% |
| 2-ETHYLHEXANAL | 619,2 | 26,79 | 0,4539 | 0,2596 | 1,3001 | 1,0000 | 0,7621 | 3,5982 | 0,64% | 1,19% | | 3,12% | 21,56% |
| 2-ETHYLHEXYL ACRYLATE | 655 | 20,7 | 0,6730 | 0,2527 | 0,9075 | 0,9447 | 1,4884 | 4,3047 | 0,61% | | | 3,33% | 21,15% |
| 2-ETHYLHEXYL BENZOATE | 755,6 | 18,68 | 0,6858 | 0,2451 | 0,7974 | 0,8432 | 1,5935 | 22,8926 | 0,62% | 1,45% | | 2,84% | 22,69% |
| 2-ETHYL-m-XYLENE | 671 | 30,2 | 0,4066 | 0,2598 | 0,2567 | 0,8351 | 2,5940 | 3,0609 | 0,34% | 0,76% | 1,89% | 1,39% | 17,18% |
| 2-ETHYLNAPHTHALENE | 771 | 31,7 | 0,4213 | 0,2520 | 0,2832 | 0,8471 | 2,5964 | 10,9827 | 1,40% | 1,97% | 2,84% | 1,34% | 17,43% |
| 2-ETHYL-p-XYLENE | 663 | 28,8 | 0,4114 | 0,2554 | 0,5921 | 0,8108 | 1,4006 | 8,7178 | 0,35% | 3,39% | 0,69% | 1,47% | 20,26% |
| 2-ETHYL-TETRAHYDROTHIOPHENE | 657,8 | 38,1 | 0,2515 | 0,2643 | 1,5560 | 1,0000 | 0,4515 | 2,1529 | 0,80% | 2,20% | | 1,45% | 15,86% |
| 2-ETHYLTHIOPHENE | 626,6 | 44,09 | 0,2931 | | 1,0427 | 1,0000 | 0,7577 | | 0,46% | 1,20% | | | |
| 2-FORMYL BENZOIC ACID | 772 | 38,3 | 0,8188 | 0,2222 | 1,2323 | 0,9788 | 1,2204 | 33,4799 | 0,48% | 0,29% | | 1,29% | 29,49% |
| 2-HEPTANOL | 608,3 | 30 | 0,5677 | 0,2556 | 0,9444 | 0,1740 | 0,9932 | 2,7887 | 0,66% | | | 1,52% | 15,31% |
| 2-HEPTANONE | 611,4 | 29,4 | 0,4190 | 0,2550 | 0,3613 | 0,8181 | 2,0554 | 8,1904 | 0,98% | 1,80% | 0,22% | 1,32% | 20,58% |
| 2-HEXANOL | 585,3 | 33,11 | 0,5530 | 0,2554 | 1,5659 | 0,6023 | 0,7630 | 2,3682 | 3,80% | 4,52% | | 1,40% | 16,74% |
| 2-HEXANONE | 587,61 | 32,87 | 0,3846 | 0,2544 | 0,3537 | 0,8213 | 1,9841 | 7,7805 | 0,50% | 2,01% | 0,39% | 1,26% | 18,82% |
| 2-HEXYNE | 549 | 35,3 | 0,2214 | 0,2628 | 2,0437 | 1,0000 | 0,3150 | 5,9078 | 0,39% | 0,73% | | 1,33% | 18,31% |
| 2-HYDROXYPROPYL METHACRYLATE | 663 | 31,4 | 0,7544 | 0,2541 | 1,0308 | 0,8740 | 1,3530 | -0,2367 | 1,01% | 0,63% | 2,62% | 3,23% | 21,05% |
| 2-MERCAPTOBENZOTHIAZOLE | 749 | 40 | 0,3321 | | 0,1606 | 0,8327 | 2,8517 | | 0,40% | 1,89% | | | |
| 2-METHOXY PROPANOL-1 | 588,4 | 39,4 | 0,4727 | 0,2453 | 0,6442 | 0,8646 | 1,5315 | 12,2995 | 0,61% | 1,74% | | 1,35% | 21,11% |
| 2-METHOXYETHANOL | 597,6 | 52,85 | 0,4543 | 0,2512 | 0,4467 | 0,8464 | 1,9850 | 4,5282 | 0,71% | 2,05% | | 1,61% | 8,17% |
| 2-METHYL BENZOTHIOPHENE | 768,7 | 35 | 0,3302 | 0,2465 | 0,2539 | 0,8184 | 2,1848 | 21,7611 | 1,25% | 2,96% | 1,28% | 2,04% | 19,91% |
| 2-METHYL OCTANAL | 638,3 | 25 | 0,5483 | | 1,0050 | 0,8748 | 1,1117 | | 0,52% | 1,40% | | | |
| 2-METHYL THIAINDAN | 788,6 | 37,09 | 0,3023 | 0,2571 | 1,0828 | 1,0000 | 0,7395 | 9,2507 | 0,50% | 1,33% | | 1,39% | 17,40% |
| 2-METHYL-1,3-PROPANEDIOL | 697 | 53,5 | 0,7144 | 0,2663 | 0,8339 | 0,8450 | 1,5724 | -7,0012 | 0,32% | 0,57% | 3,07% | 5,60% | 16,43% |
| 2-METHYL-1-BUTANOL | 575,4 | 39,4 | 0,5877 | 0,2547 | 1,9933 | 1,0000 | 0,5599 | -0,4641 | 1,61% | 1,66% | | 1,79% | 13,59% |
| 2-METHYL-1-BUTENE | 465 | 34,47 | 0,2341 | 0,2617 | 1,1440 | 1,0000 | 0,6072 | 3,7100 | 0,77% | 0,97% | 0,24% | 1,74% | 16,81% |
| 2-METHYL-1-BUTENE-3-YNE | 492 | 43,8 | 0,1370 | 0,2752 | 0,2349 | 0,8182 | 1,5072 | -2,8682 | 0,67% | 0,83% | 1,20% | 1,20% | 16,92% |
| 2-METHYL-1-HEPTANOL | 608,5 | 28,57 | 0,7623 | 0,2708 | 0,5854 | 0,8178 | 2,1900 | -21,4100 | 0,64% | 1,18% | | 3,14% | 17,87% |
| 2-METHYL-1-HEPTENE | 567 | 26 | 0,3551 | 0,2584 | 0,8454 | 0,9090 | 1,0183 | 5,9295 | 0,43% | 1,51% | 2,11% | 1,43% | 21,73% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2-METHYL-1-HEXANOL | 595 | 30,3 | 0,7733 | 0,2561 | 0,6266 | 0,8117 | 2,0723 | -4,9766 | 0,46% | 0,98% | 9,63% | 1,86% | 17,33% |
| 2-METHYL-1-HEXENE | 538 | 28,7 | 0,3094 | 0,2612 | 0,3809 | 0,7995 | 1,5891 | 3,3967 | 0,32% | 1,53% | 0,16% | 1,36% | 19,53% |
| 2-METHYL-1-NONENE | 616 | 21,9 | 0,4527 | 0,2533 | 0,6949 | 0,8357 | 1,3491 | 11,4189 | 0,67% | 1,17% | 0,26% | 1,63% | 27,94% |
| 2-METHYL-1-OCTENE | 593 | 23,8 | 0,4051 | 0,2528 | 0,5174 | 0,8364 | 1,6047 | 11,1108 | 0,53% | 1,56% | 0,12% | 1,44% | 23,17% |
| 2-METHYL-1-PENTANOL | 604,4 | 34,5 | 0,5100 | 0,2544 | 0,1287 | 0,6591 | 2,2737 | 3,5847 | 0,29% | | | 2,03% | 16,89% |
| 2-METHYL-1-PENTENE | 505 | 31,9 | 0,2611 | 0,2641 | 0,3288 | 0,8092 | 1,6249 | 1,3637 | 0,38% | 0,76% | 0,17% | 1,46% | 17,56% |
| 2-METHYL-1-PROPANOL | 547,8 | 42,95 | 0,5857 | 0,2492 | 1,9959 | 1,0000 | 0,5560 | 3,4336 | 3,13% | 1,96% | 9,16% | 2,35% | 17,72% |
| 2-METHYL-1-TRIDECANOL | 707,7 | 17,13 | 1,1154 | | 0,5236 | 0,8155 | 3,2122 | | 0,73% | 1,59% | | | |
| 2-METHYL-1-UNDECANOL | 665,9 | 19,56 | 1,0345 | | 0,5248 | 0,8139 | 3,0065 | | 0,65% | 1,45% | | | |
| 2-METHYL-2-AMINOBUTANE | 526 | 36,6 | 0,3202 | 0,2819 | 1,1420 | 1,0000 | 0,7179 | -12,4634 | 0,60% | 1,23% | | 3,15% | 3,48% |
| 2-METHYL-2-BUTANOL | 543,7 | 37,1 | 0,4820 | 0,2592 | 4,7996 | 1,0000 | 0,1947 | 0,2939 | 3,16% | 2,23% | 6,57% | 1,68% | 15,51% |
| 2-METHYL-2-BUTENE | 470 | 34,2 | 0,2870 | 0,2538 | 0,3521 | 0,8413 | 1,7450 | 7,1782 | 1,51% | 2,00% | 0,99% | 3,12% | 17,83% |
| 2-METHYL-2-PENTENAL | 605 | 32,6 | 0,3494 | 0,2395 | 0,2298 | 0,8086 | 2,3025 | 24,4797 | 0,39% | 2,42% | 0,74% | 2,75% | 26,72% |
| 2-METHYL-2-PENTENE | 514 | 31,6 | 0,2445 | 0,2608 | 1,2262 | 1,0000 | 0,5820 | 5,3472 | 1,90% | 1,54% | 2,83% | 1,54% | 13,05% |
| 2-METHYL-2-PROPANOL | 506,2 | 39,72 | 0,6152 | 0,2557 | 3,1560 | 0,8906 | 0,3719 | 1,1488 | 1,43% | 3,11% | 4,62% | 1,28% | 18,03% |
| 2-METHYL-3-ETHYLPENTANE | 567,1 | 27 | 0,3297 | 0,2603 | 1,2649 | 0,9999 | 0,6450 | 1,8062 | 1,04% | 1,45% | 0,95% | 2,15% | 21,05% |
| 2-METHYLBENZOFURAN | 697 | 36,4 | 0,3752 | 0,2541 | 0,2495 | 0,8465 | 2,6061 | 8,9581 | 0,90% | 1,88% | | 1,13% | 18,05% |
| 2-METHYLBUTYRALDEHYDE | 543,2 | 38,29 | 0,3779 | 0,2634 | 0,2113 | 0,8374 | 2,7636 | -0,8780 | 1,10% | 4,10% | 1,00% | 1,14% | 16,87% |
| 2-METHYLBUTYRIC ACID | 643 | 38,9 | 0,5894 | 0,2524 | 0,9629 | 0,8828 | 1,2226 | 4,5224 | 0,63% | 0,69% | | 2,27% | 20,45% |
| 2-METHYLDECANE | 631,8 | 19,82 | 0,5230 | 0,2530 | 1,2549 | 0,9743 | 0,8691 | 10,6816 | 0,37% | 0,97% | | 1,57% | 20,01% |
| 2-METHYL-DODECAN-1-OL | 682,5 | 18,26 | 1,0722 | 0,2500 | 0,5314 | 0,8127 | 3,0568 | -3,6954 | 0,50% | 1,60% | | 3,59% | 23,58% |
| 2-METHYLDODECANE | 668 | 17,17 | 0,6188 | 0,2474 | 0,5841 | 0,8337 | 1,9302 | 19,8091 | 0,61% | 1,57% | | 1,76% | 21,82% |
| 2-METHYLHEPTANAL | 605,7 | 26,82 | 0,4869 | 0,2567 | 1,7744 | 1,0000 | 0,5626 | 4,1537 | 0,76% | 1,32% | | 1,21% | 18,89% |
| 2-METHYLHEPTANE | 559,7 | 25 | 0,3795 | 0,2585 | 0,4396 | 0,8205 | 1,6945 | 4,0482 | 0,39% | 0,76% | 1,77% | 1,41% | 16,43% |
| 2-METHYLHEXANAL | 592 | 28,5 | 0,4609 | 0,2539 | 0,4127 | 0,7966 | 1,9095 | 7,6025 | 0,38% | 1,79% | 0,53% | 1,25% | 19,20% |
| 2-METHYLHEXANE | 530,4 | 27,4 | 0,3280 | 0,2626 | 0,3983 | 0,8127 | 1,6391 | 0,7144 | 0,58% | 2,53% | 0,94% | 1,40% | 17,35% |
| 2-METHYLHEXANOIC ACID | 666 | 31,1 | 0,6957 | | 0,9648 | 0,8672 | 1,3594 | | 0,62% | 1,88% | | | |
| 2-METHYLINDENE | 711 | 34,6 | 0,3508 | 0,2538 | 0,3886 | 0,8043 | 1,7029 | 11,2220 | 0,28% | 0,99% | 0,51% | 1,36% | 17,89% |
| 2-METHYLNAPHTHALENE | 761 | 35 | 0,3781 | 0,2551 | 0,2741 | 0,8525 | 2,5103 | 8,5386 | 4,06% | 1,04% | 0,93% | 1,15% | 17,67% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2-METHYLNONANE | 610 | 21,2 | 0,4723 | 0,2547 | 0,4172 | 0,8095 | 1,9776 | 8,3349 | 0,86% | 2,04% | 1,03% | 1,71% | 24,71% |
| 2-METHYLOCTANE | 582,87 | 23,1 | 0,4602 | 0,2587 | 0,5764 | 0,8330 | 1,5877 | 1,9492 | 0,44% | 1,64% | 2,82% | 1,62% | 18,85% |
| 2-METHYLOCTANOIC ACID | 694 | 25,4 | 0,7913 | 0,2514 | 0,6340 | 0,8200 | 2,1155 | 2,3011 | 0,63% | 1,61% | | 2,90% | 21,68% |
| 2-METHYLPENTANE | 497,7 | 30,4 | 0,2791 | 0,2685 | 0,3496 | 0,8209 | 1,6593 | -3,0975 | 0,50% | 1,80% | 0,90% | 1,58% | 14,55% |
| 2-METHYLPROPANAL | 507 | 41 | 0,3622 | 0,2570 | 0,2863 | 0,8240 | 2,2010 | 4,1302 | 0,65% | 1,66% | | 1,15% | 18,60% |
| 2-METHYLPYRIDINE | 621 | 46 | 0,2990 | 0,2676 | 0,4600 | 0,8139 | 1,4063 | -1,1458 | 0,90% | 1,42% | 0,65% | 1,27% | 3,34% |
| 2-METHYLTETRAHYDROFURAN | 537 | 37,576 | 0,2816 | 0,2481 | 1,0306 | 1,0000 | 0,7529 | 12,0199 | 0,62% | 1,61% | | 3,40% | 32,29% |
| 2-METHYLTHIACYCLOPENTANE | 628,4 | 41,83 | 0,2489 | 0,2622 | 1,0973 | 1,0000 | 0,6596 | 3,5980 | 0,74% | 2,00% | | 1,47% | 15,96% |
| 2-METHYLTHIOPHENE | 609 | 49,1 | 0,2389 | 0,2780 | 0,3166 | 0,8135 | 1,5960 | -7,2943 | 1,02% | 1,99% | 0,79% | 1,74% | 17,93% |
| 2-METHYLTRIDECANE | 684,1 | 16,04 | 0,6649 | 0,2445 | 0,5742 | 0,8325 | 2,0586 | 26,1059 | 0,51% | 1,57% | | 1,94% | 22,72% |
| 2-METHYLUNDECANE | 650,7 | 18,42 | 0,5718 | 0,2502 | 0,7584 | 0,8452 | 1,4704 | 14,9021 | 0,63% | 1,46% | | 1,74% | 20,81% |
| 2-NITROPROPANE | 594 | 44,5 | 0,3836 | 0,2525 | 0,3013 | 0,8594 | 2,4048 | 7,6150 | 4,52% | 4,63% | 7,75% | 1,40% | 15,82% |
| 2-NONANOL | 649,5 | 25,408 | 0,6092 | 0,2613 | 0,2314 | 0,7364 | 2,6585 | -3,5733 | 0,71% | | | 2,29% | 13,85% |
| 2-NONANONE | 652,5 | 24,1 | 0,4979 | 0,2491 | 0,5871 | 0,7990 | 1,5721 | 16,2599 | 1,57% | 1,83% | 0,87% | 1,24% | 20,67% |
| 2-NORBORNENE | 583 | 39,3 | 0,1590 | | 0,2746 | 0,8231 | 1,4955 | | 0,68% | 2,55% | 0,06% | | |
| 2-n-PROPYLTHIOPHENE | 649,2 | 38,97 | 0,3407 | | 0,9352 | 0,9560 | 0,9179 | | 0,60% | 1,15% | | | |
| 2-OCTANOL | 629,8 | 27,49 | 0,5881 | 0,2523 | 0,1832 | 0,6765 | 2,4025 | 4,6120 | 0,12% | | | 1,79% | 13,46% |
| 2-OCTANONE | 632,7 | 26,4 | 0,4549 | 0,2528 | 1,3003 | 0,9712 | 0,7599 | 11,8530 | 0,58% | 1,34% | 1,91% | 1,33% | 20,86% |
| 2-OXAZOLIDONE | 930,5 | 54,88 | 0,3944 | | 1,1444 | 0,9897 | 0,8072 | | 0,63% | 2,67% | | | |
| 2-PENTANETHIOL | 584,3 | 35,36 | 0,2685 | 0,2709 | 1,1835 | 1,0000 | 0,6307 | -3,9347 | 0,70% | 1,27% | | 1,78% | 10,72% |
| 2-PENTANOL | 561 | 37 | 0,5550 | 0,2526 | 0,0000 | 0,2567 | 1,3025 | 3,8782 | 1,25% | | | 2,43% | 17,68% |
| 2-PENTANONE | 561,08 | 36,94 | 0,3433 | 0,2546 | 0,4364 | 0,8056 | 1,5599 | 7,4410 | 0,25% | 4,12% | 1,00% | 1,42% | 26,50% |
| 2-PENTOXYETHANOL | 641,2 | 30,36 | 0,6228 | 0,2606 | 0,2985 | 0,8061 | 2,9091 | -5,1742 | 0,44% | 3,22% | 4,32% | 2,44% | 18,99% |
| 2-PENTYNE | 519 | 40,3 | 0,1752 | 0,2631 | 1,1337 | 1,0000 | 0,5483 | 5,2022 | 1,58% | 4,33% | 0,53% | 1,34% | 17,37% |
| 2-PHENYL-2-PROPANOL | 660 | 34,9 | 0,6924 | 0,2641 | 0,6650 | 0,8894 | 2,0172 | -11,0999 | 0,93% | 1,70% | | 1,58% | 12,37% |
| 2-PHENYLBUTENE-1 | 666 | 30,1 | 0,3536 | 0,2562 | 1,2818 | 1,0000 | 0,6659 | 8,9603 | 0,68% | 0,91% | | 1,36% | 22,59% |
| 2-PHENYLETHANOL | 684 | 39,2 | 0,7429 | 0,2509 | 0,7213 | 0,8945 | 1,9606 | -0,6425 | 4,29% | 4,94% | | 1,42% | 15,40% |
| 2-PROPYLBENZOTHIOPHENE | 807,5 | 31,56 | 0,4782 | | 0,4455 | 0,8086 | 1,9069 | | 0,57% | 1,50% | | | |
| 2-PYRROLIDONE | 802 | 61,7 | 0,4324 | 0,2478 | 0,4158 | 0,8048 | 1,8518 | 10,6184 | 1,47% | 4,27% | 12,44% | 1,40% | 21,82% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 3-(METHYLMERCAPTO)PROPANAL | 650 | 40,2 | 0,4168 | 0,2418 | 1,2519 | 1,0000 | 0,7530 | 16,9534 | 0,43% | 1,31% | 2,68% | 2,31% | 26,21% |
| 3-(N,N-DIMETHYLAMINO) PROPYLAMINE | 593,3 | 35,86 | 0,4544 | 0,2679 | 0,6663 | 0,8747 | 1,4633 | -7,4648 | 0,48% | 1,30% | | 2,03% | 16,62% |
| 3,3,3-TRIFLUOROPROPENE | 378,59 | 36,09 | 0,2653 | | 0,5203 | 0,9457 | 1,4801 | | 0,82% | | | | |
| 3,3,5-TRIMETHYLHEPTANE | 609,5 | 23,2 | 0,3847 | 0,2643 | 0,3710 | 0,8097 | 1,8658 | -3,0052 | 1,47% | 1,64% | 1,81% | 1,79% | 16,89% |
| 3,3-DIETHYLPENTANE | 610,05 | 26,7498 | 0,3381 | 0,2644 | 0,2300 | 0,8482 | 2,5789 | -3,4339 | 0,92% | 2,32% | 2,18% | 1,20% | 23,96% |
| 3,3-DIMETHYL-1-BUTENE | 480 | 32,9 | 0,2285 | 0,2814 | 0,1590 | 0,8515 | 2,5245 | -12,2770 | 2,35% | 2,84% | 5,35% | 1,40% | 15,67% |
| 3,3-DIMETHYL-1-BUTYNE | 488,5 | 36,75 | 0,1615 | 0,2889 | 0,6740 | 0,8729 | 0,8385 | -15,7158 | 0,57% | 1,59% | | 0,96% | 11,43% |
| 3,3-DIMETHYL-2-BUTANONE | 564 | 33,2 | 0,3273 | 0,2604 | 0,2382 | 0,8364 | 2,3933 | 2,9509 | 0,88% | 1,51% | | 1,18% | 17,18% |
| 3,3-DIMETHYLHEXANE | 562 | 26,5 | 0,3202 | 0,2581 | 0,3043 | 0,8248 | 1,9717 | 3,3566 | 0,40% | 1,08% | 0,21% | 2,89% | 21,60% |
| 3,3-DIMETHYLPENTANE | 536,4 | 29,5 | 0,2679 | 0,2744 | 0,2606 | 0,8386 | 2,0363 | -8,3127 | 0,45% | 1,13% | 0,64% | 2,32% | 14,26% |
| 3,4-DICHLORO-1-BUTENE | 589 | 38,5 | 0,2959 | 0,2589 | 0,1179 | 0,7853 | 2,4756 | 5,5818 | 1,22% | | | 1,57% | 16,80% |
| 3,4-DICHLOROANILINE | 800 | 41,1 | 0,4678 | 0,2461 | 0,4002 | 0,8125 | 2,0379 | 15,3687 | 0,67% | 1,54% | | 1,23% | 17,88% |
| 3,4-DICHLOROPHENYL ISOCYANATE | 730,3 | 34,09 | 0,5050 | 0,2460 | 1,8795 | 1,0000 | 0,5407 | 16,0868 | 0,65% | 1,61% | | 1,49% | 20,51% |
| 3,4-DIMETHYLHEXANE | 568,8 | 26,9 | 0,3381 | 0,2626 | 0,2296 | 0,8299 | 2,4195 | -0,1076 | 0,17% | 1,12% | 0,43% | 1,36% | 16,00% |
| 3,4-DIMETHYLTHIOPHENE | 642,8 | 41,89 | 0,2786 | 0,2660 | 1,1079 | 1,0000 | 0,6896 | -0,5708 | 0,51% | 1,52% | | 1,27% | 15,18% |
| 3,4-XYLENOL | 729,95 | 50 | 0,5763 | 0,2826 | 0,3502 | 0,8388 | 2,7378 | -23,8056 | 1,40% | 1,56% | 3,19% | 1,25% | 13,41% |
| 3,5-DIISOPROPYL TOLUENE | 681,4 | 22,39 | 0,4887 | 0,2563 | 0,9657 | 0,8977 | 1,0824 | 5,1564 | 0,64% | 1,33% | | 1,75% | 19,98% |
| 3,5-DIMETHYLBENZOFURAN | 713,7 | 32,16 | 0,4222 | 0,2509 | 0,2861 | 0,8404 | 2,5380 | 12,7891 | 0,40% | | | 1,28% | 19,74% |
| 3,5-DIMETHYLBENZOTHIOPHENE | 784,8 | 34,64 | 0,4247 | 0,2573 | 0,3787 | 0,8680 | 2,2846 | 4,2663 | 1,57% | | | 1,61% | 18,51% |
| 3,5-XYLENOL | 715,65 | 36 | 0,4852 | 0,2375 | 1,7184 | 1,0000 | 0,5824 | 22,8991 | 1,36% | 2,25% | 2,16% | 3,52% | 1,08% |
| 3-AMINO-1-PROPANOL | 649 | 55 | 0,8273 | 0,2499 | 0,5584 | 0,8097 | 2,3860 | 1,6395 | 0,57% | 0,77% | | 2,06% | 22,43% |
| 3-CHLORO-o-XYLENE | 685,1 | 33,88 | 0,3424 | | 1,2264 | 1,0000 | 0,6877 | | 0,49% | 2,09% | | | |
| 3-CHLOROPROPENE | 514,15 | 47,1 | 0,1478 | 0,2604 | 1,1112 | 0,9940 | 0,5205 | 6,1897 | 1,21% | | 0,26% | 1,95% | 16,59% |
| 3-CHLOROPROPYLTRIMETHOXYSILANE | 647,3 | 21,34 | 0,5349 | 0,2415 | 0,7836 | 0,7628 | 1,2823 | 29,7112 | 3,28% | | 1,20% | 2,12% | 22,02% |
| 3-ETHYL HEPTANAL | 623,8 | 23,64 | 0,5671 | | 0,3749 | 0,8451 | 2,6298 | | 0,33% | | | | |
| 3-ETHYL-1-HEPTANOL | 636,7 | 25,46 | 0,8657 | 0,2582 | 1,3411 | 0,9867 | 1,1556 | -9,2568 | 1,39% | 2,13% | 6,58% | 3,18% | 20,75% |
| 3-ETHYL-1-HEXENE | 553,9 | 26,04 | 0,3600 | 0,2602 | 0,1826 | 0,8315 | 2,8176 | 2,6684 | 0,38% | 3,99% | 2,33% | 1,31% | 19,42% |
| 3-ETHYL-1-PENTENE | 530 | 30,3 | 0,3019 | 0,2736 | 0,2448 | 0,7990 | 1,9984 | -8,6886 | 0,54% | 3,61% | 1,39% | 1,75% | 14,51% |
| 3-ETHYL-2,5-DIMETHYLTHIOPHENE | 669 | 32,6 | 0,3794 | | 0,7939 | 0,8787 | 1,1087 | | 0,66% | 2,49% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c_{P,liq}^{sat}$ | $v_{liq}^{sat}$ | $v_c$ |
| 3-ETHYLBENZOTHIOPHENE | 776,5 | 35,26 | 0,4292 | 0,2607 | 0,7925 | 0,8924 | 1,2112 | 0,2842 | 0,62% | 1,42% | | 1,66% | 17,94% |
| 3-ETHYLDODECANE | 691,4 | 16,22 | 0,5995 | | 0,7128 | 0,8353 | 1,5913 | | 0,65% | 1,46% | | | |
| 3-ETHYLHEPTANE | 590 | 23,9 | 0,4080 | 0,2581 | 0,7439 | 0,8671 | 1,2209 | 3,8122 | 0,85% | 1,38% | | 1,60% | 18,78% |
| 3-ETHYLHEXANE | 565,5 | 26,1 | 0,3605 | 0,2575 | 0,2963 | 0,8175 | 2,1055 | 4,1357 | 0,35% | 1,17% | 0,76% | 1,88% | 20,80% |
| 3-ETHYL-o-XYLENE | 680 | 28,8 | 0,3621 | 0,2517 | 1,4100 | 1,0000 | 0,6062 | 16,5800 | 0,82% | 0,52% | 0,94% | 1,41% | 15,76% |
| 3-ETHYLPENTANE | 540,6 | 28,9 | 0,3091 | 0,2667 | 0,3854 | 0,8216 | 1,6497 | -2,1251 | 0,23% | 1,91% | 0,28% | 1,60% | 15,44% |
| 3-HEPTANOL | 605,4 | 30,73 | 0,5511 | 0,2624 | 0,3779 | 0,7427 | 2,0599 | -4,5292 | 2,62% | | | 2,03% | 17,06% |
| 3-HEPTANONE | 606,6 | 29,2 | 0,4076 | 0,2505 | 0,5913 | 0,8028 | 1,3950 | 12,4151 | 0,78% | 1,46% | 0,50% | 1,58% | 19,75% |
| 3-HEXANONE | 582,82 | 33,2 | 0,3801 | 0,2556 | 0,3481 | 0,8221 | 1,9949 | 6,4682 | 1,41% | 1,73% | 1,04% | 1,26% | 16,99% |
| 3-HEXYNE | 544 | 35,3 | 0,2183 | 0,2606 | 0,1380 | 0,3970 | 0,9137 | 6,8968 | 1,59% | | | 2,48% | 16,91% |
| 3-HYDROXY-2-METHYL PROPIONALDEHYDE | 615 | 45,9 | 0,7928 | | 1,4693 | 1,0000 | 0,9657 | | 1,83% | 1,60% | 2,85% | | |
| 3-HYDROXYBUTYROLACTONE | 830,6 | 53,97 | 0,6127 | 0,2324 | 0,3260 | 0,8213 | 2,8556 | 20,6187 | 0,30% | | | 1,84% | 25,50% |
| 3-MERCAPTOPROPIONIC ACID | 729 | 50,2 | 0,5885 | 0,2639 | 0,6634 | 0,8096 | 1,6149 | -0,5236 | 1,49% | | 1,90% | 5,83% | 32,27% |
| 3-METHOXYISOPROPYLAMINE | 548 | 40,9 | 0,4227 | 0,2772 | 0,3840 | 0,8049 | 1,9269 | -10,2631 | 0,45% | 1,24% | | 1,47% | 5,92% |
| 3-METHOXYPROPIONITRILE | 638 | 36,3 | 0,4597 | 0,2163 | 1,0513 | 0,9991 | 0,9837 | 40,9791 | 0,87% | 1,26% | | 4,82% | 26,00% |
| 3-METHYL SULFOLANE | 817 | 42,4 | 0,4191 | 0,2426 | 1,2133 | 0,9938 | 0,7839 | 19,6215 | 0,63% | 1,07% | | 1,71% | 33,96% |
| 3-METHYL-1,2-BUTADIENE | 490 | 38,3 | 0,1874 | 0,2650 | 1,4991 | 1,0000 | 0,4136 | 3,5776 | 1,97% | 1,27% | 1,41% | 1,27% | 11,14% |
| 3-METHYL-1,4-PENTADIENE | 497 | 34,9 | 0,2468 | 0,2730 | 0,6250 | 0,8909 | 1,1157 | -5,8053 | 0,95% | 1,73% | 0,84% | 1,53% | 14,48% |
| 3-METHYL-1-BUTANOL | 577,2 | 39,3 | 0,5900 | 0,2551 | 2,0991 | 1,0000 | 0,5272 | -0,7104 | 2,28% | 3,27% | | 1,79% | 14,31% |
| 3-METHYL-1-BUTENE | 452,7 | 35,3 | 0,2097 | 0,2748 | 0,4830 | 0,8810 | 1,2744 | -5,3180 | 0,69% | 3,00% | 0,41% | 1,59% | 9,21% |
| 3-METHYL-1-BUTYNE | 463,2 | 42 | 0,3081 | 0,2927 | 0,2065 | 0,8513 | 2,5283 | -16,1294 | 6,05% | 6,51% | 3,94% | 2,90% | 8,37% |
| 3-METHYL-1-HEXENE | 528 | 29,5 | 0,3057 | 0,2687 | 0,3028 | 0,8054 | 1,8355 | -4,7870 | 0,36% | 1,00% | 0,07% | 1,42% | 16,14% |
| 3-METHYL-1-PENTANOL | 588 | 34 | 0,7230 | 0,2505 | 0,2207 | 0,7981 | 3,6606 | -0,1472 | 3,04% | 3,71% | | 1,33% | 16,36% |
| 3-METHYL-1-PENTENE | 495 | 32,9 | 0,2640 | 0,2741 | 0,2085 | 0,8574 | 2,4350 | -7,5633 | 1,25% | 1,75% | 2,58% | 1,65% | 14,22% |
| 3-METHYL-2-BUTANOL | 556,1 | 38,7 | 0,5016 | 0,2611 | 3,7056 | 0,9998 | 0,2598 | -1,7866 | 3,05% | 3,90% | | 1,39% | 12,86% |
| 3-METHYL-2-PENTANONE | 573 | 33,2 | 0,3886 | 0,2586 | 0,3757 | 0,7838 | 1,7615 | 3,8186 | 0,87% | 7,40% | 1,23% | 1,52% | 18,51% |
| 3-METHYL-3-ETHYLPENTANE | 576,5 | 28,1 | 0,3050 | 0,2676 | 0,2453 | 0,8388 | 2,2650 | -4,4642 | 0,39% | 0,78% | 1,77% | 1,27% | 16,23% |
| 3-METHYL-3-PENTANOL | 575,6 | 35,2 | 0,4318 | 0,2662 | 0,3570 | 0,8069 | 2,0846 | -5,2879 | 2,67% | | | 1,05% | 11,38% |
| 3-METHYLBUTYRALDEHYDE | 543,2 | 38,29 | 0,3820 | 0,2651 | 0,7595 | 0,8840 | 1,1677 | -2,2158 | 0,56% | 1,46% | | 0,90% | 15,44% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 3-METHYL-cis-2-PENTENE | 515 | 32,902 | 0,2585 | 0,2644 | 0,5019 | 0,8076 | 1,2228 | 1,3355 | 1,03% | 0,99% | 0,65% | 1,46% | 16,25% |
| 3-METHYLCYCLOPENTENE | 526 | 41,3 | 0,2296 | 0,2774 | 1,1899 | 1,0000 | 0,5739 | -8,2822 | 0,58% | 1,62% | 1,54% | 1,25% | 10,16% |
| 3-METHYLDECANE | 634,1 | 19,89 | 0,5204 | 0,2520 | 0,2664 | 0,8286 | 2,9306 | 11,9422 | 0,26% | | | 1,88% | 20,19% |
| 3-METHYLDODECANE | 669 | 17,19 | 0,6156 | 0,2465 | 0,4069 | 0,8331 | 2,5497 | 21,7125 | 0,49% | | | 2,15% | 21,93% |
| 3-METHYLHEPTANE | 563,6 | 25,5 | 0,3723 | 0,2569 | 0,4268 | 0,8190 | 1,7037 | 4,9212 | 0,46% | 0,89% | 2,14% | 1,65% | 20,68% |
| 3-METHYLHEXANAL | 595 | 28,5 | 0,4570 | 0,2488 | 0,6454 | 0,8362 | 1,4378 | 12,6565 | 0,56% | | 0,96% | 1,40% | 23,74% |
| 3-METHYLHEXANE | 535,2 | 28,1 | 0,3204 | 0,2592 | 0,3594 | 0,8186 | 1,7541 | 2,8269 | 0,52% | 1,15% | 0,75% | 2,29% | 19,79% |
| 3-METHYLNONANE | 613 | 21,6 | 0,4649 | 0,2535 | 0,4565 | 0,8102 | 1,8397 | 9,4198 | 0,14% | 0,91% | 1,51% | 1,52% | 22,80% |
| 3-METHYLOCTANE | 590,15 | 23,4 | 0,4123 | 0,2578 | 0,4415 | 0,8210 | 1,7847 | 4,8546 | 1,22% | 1,79% | 1,61% | 1,72% | 20,93% |
| 3-METHYLPENTANE | 504,6 | 31,2 | 0,2702 | 0,2666 | 0,3066 | 0,8226 | 1,7779 | -1,6673 | 0,81% | 1,35% | 0,71% | 1,50% | 12,78% |
| 3-METHYLPYRIDINE | 645 | 46,6 | 0,2978 | 0,2613 | 0,2982 | 0,8283 | 1,9285 | 2,9912 | 0,69% | 1,64% | 0,60% | 1,24% | 9,62% |
| 3-METHYLTHIOPHENE | 613 | 49,1 | 0,2397 | 0,2741 | 0,4530 | 0,8040 | 1,2475 | -5,0694 | 0,78% | 1,46% | 0,31% | 1,31% | 17,45% |
| 3-METHYL-trans-2-PENTENE | 517 | 31,9 | 0,2627 | 0,2568 | 1,5197 | 1,0000 | 0,4684 | 7,9392 | 0,32% | 1,80% | 4,18% | 2,33% | 18,45% |
| 3-METHYLTRIDECANE | 684,7 | 16,06 | 0,6668 | 0,2438 | 0,6196 | 0,8337 | 1,9377 | 27,8981 | 0,66% | 1,55% | | 2,04% | 22,89% |
| 3-METHYLUNDECANE | 652,3 | 18,47 | 0,5690 | 0,2492 | 0,6013 | 0,8628 | 1,8491 | 16,3070 | 0,45% | | | 1,99% | 21,08% |
| 3-NITROBENZOTRIFLUORIDE | 667 | 28 | 0,5364 | 0,2322 | 0,3260 | 0,8389 | 2,7377 | 34,3510 | 1,22% | 2,57% | | 1,40% | 24,89% |
| 3-NONANONE | 648,1 | 24,53 | 0,4629 | 0,2519 | 1,6307 | 1,0000 | 0,5986 | 13,3428 | 0,59% | 1,08% | | 1,23% | 18,11% |
| 3-OCTANONE | 627,7 | 27,04 | 0,4406 | 0,2511 | 1,2328 | 0,9880 | 0,7943 | 11,7202 | 0,64% | 1,20% | | 1,54% | 17,03% |
| 3-PENTANOL | 559,6 | 37,14 | 0,5143 | 0,2530 | 0,5719 | 0,0001 | 0,9313 | 4,8042 | 3,30% | | | 2,30% | 17,01% |
| 3-PENTANONE | 560,95 | 37,4 | 0,3448 | 0,2578 | 0,3461 | 0,8156 | 1,8542 | 5,7013 | 0,93% | 6,01% | 0,41% | 1,08% | 12,39% |
| 4-((2-HYDROXYETHOXY)CARBONYL) BENZOIC ACID | 871,4 | 29,6 | 0,9669 | | 0,4173 | 0,8101 | 3,3401 | | 0,58% | 1,42% | | | |
| 4-(2-METHOXYETHYL)MORPHOLINE | 669,8 | 31,33 | 0,4696 | | 1,5166 | 1,0000 | 0,6551 | | 0,58% | 1,48% | | | |
| 4,4'-DIISOPROPYLBIPHENYL | 813,6 | 18,41 | 0,6164 | | 0,5761 | 0,8175 | 1,8997 | | 0,49% | 1,75% | | | |
| 4,4'-DINITRODIPHENYLAMINE | 926 | 26,2 | 1,0247 | | 0,4475 | 0,8104 | 3,3327 | | 0,71% | 0,79% | | | |
| 4,4'-DINITROTRIPHENYLAMINE | 946 | 20 | 1,0900 | | 0,4760 | 0,8099 | 3,3451 | | 0,62% | 0,80% | | | |
| 4,6-DIMETHYLDIBENZOTHIOPHENE | 939,4 | 29,81 | 0,4902 | | 0,5688 | 0,8195 | 1,6461 | | 0,62% | 2,03% | | | |
| 4,6-DINITRO-o-sec-BUTYLPHENOL | 793,9 | 27,5 | 1,0079 | | 0,5020 | 0,8208 | 3,0940 | | 0,61% | | | | |
| 4-[(TETRAHYDRO-2-FURANYL)OXY]-1-BUTANOL | 694,3 | 30,9 | 0,9319 | | 0,5283 | 0,8152 | 2,7607 | | 0,68% | 1,25% | | | |
| 4-[2-(2-AMINOETHOXY)ETHYL]MORPHOLINE | 706,9 | 28,5 | 0,6933 | | 0,8645 | 0,8485 | 1,4926 | | 0,91% | 1,20% | 1,17% | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 4-CARBOXYBENZALDEHYDE | 966 | 38,2 | 0,8174 | | 0,3690 | 0,8090 | 3,1685 | | 0,58% | 1,74% | | | |
| 4-CHLORO-3-NITROBENZOTRIFLUORIDE | 686 | 27,4 | 0,6038 | 0,2410 | 0,5363 | 0,8745 | 2,1974 | 21,5807 | 0,89% | | | 1,54% | 26,19% |
| 4-CHLORO-o-XYLENE | 689,1 | 33,22 | 0,3471 | | 1,2079 | 0,9999 | 0,7052 | | 0,49% | 1,89% | | | |
| 4-ETHYL-m-XYLENE | 665 | 28,8 | 0,4140 | 0,2555 | 0,3628 | 0,8192 | 2,0307 | 8,3252 | 0,44% | 3,07% | 1,58% | 1,61% | 20,71% |
| 4-ETHYL-o-XYLENE | 667 | 28,8 | 0,4114 | 0,2543 | 0,3633 | 0,8177 | 2,0137 | 9,5386 | 0,35% | 0,73% | 1,46% | 1,49% | 18,86% |
| 4-HEPTANONE | 602 | 29,2 | 0,4120 | 0,2553 | 0,2829 | 0,8274 | 2,4150 | 7,9448 | 0,22% | 1,22% | 2,20% | 1,23% | 19,58% |
| 4-HYDROXYACETOPHENONE | 860 | 44,5 | 0,6409 | 0,2480 | 0,6113 | 0,8859 | 2,0583 | 8,1126 | 4,00% | | | 1,52% | 23,31% |
| 4-HYDROXYBUTYRALDEHYDE | 599 | 44,8 | 0,8404 | 0,2382 | 0,4114 | 0,8008 | 2,9522 | 10,3755 | 0,57% | | 2,36% | 1,97% | 25,04% |
| 4-HYDROXYSTYRENE | 736 | 45,2 | 0,5090 | | 1,0403 | 0,9032 | 1,0295 | | 0,71% | 1,13% | 2,70% | | |
| 4-ISOBUTYLSTYRENE | 735 | 23,8 | 0,4631 | 0,2417 | 0,5532 | 0,8160 | 1,6089 | 32,3063 | 0,53% | 1,56% | 1,00% | 1,49% | 21,90% |
| 4-METHOXYPHENYLACETIC ACID | 768 | 39 | 0,8984 | | 0,6783 | 0,8363 | 2,2480 | | 0,37% | 0,37% | | | |
| 4-METHYL DIBENZOTHIOPHENE | 904,1 | 33,78 | 0,4414 | | 0,2222 | 0,8148 | 2,7518 | | 0,28% | | | | |
| 4-METHYL-1-HEPTENE | 557,3 | 26,04 | 0,3591 | 0,2591 | 1,0888 | 0,9873 | 0,8073 | 3,9780 | 0,47% | 1,40% | | 1,45% | 19,87% |
| 4-METHYL-1-HEXENE | 534 | 30,4 | 0,3024 | 0,2715 | 0,4952 | 0,8068 | 1,3356 | -7,1083 | 0,48% | 2,59% | 0,75% | 1,69% | 14,59% |
| 4-METHYL-1-OCTANOL | 631,7 | 24,84 | 0,8697 | 0,2564 | 0,6343 | 0,8586 | 2,4176 | -8,0930 | 0,94% | | | 3,27% | 22,32% |
| 4-METHYL-1-PENTENE | 496 | 32,2 | 0,2389 | 0,2716 | 1,1820 | 1,0000 | 0,5881 | -4,3644 | 0,38% | 1,52% | 1,94% | 1,53% | 15,38% |
| 4-METHYL-2-PENTANOL | 574,4 | 34,7 | 0,5730 | 0,2665 | 1,3913 | 1,0000 | 0,8191 | -9,1189 | 1,16% | 1,22% | | 2,01% | 13,74% |
| 4-METHYL-cis-2-PENTENE | 499 | 32,2 | 0,2442 | 0,2699 | 1,1862 | 1,0000 | 0,5952 | -2,9896 | 0,41% | 2,27% | 3,05% | 1,40% | 15,34% |
| 4-METHYL-CYCLOHEXANE-METHANOL | 647,6 | 32,43 | 0,6295 | 0,2792 | 1,7229 | 1,0000 | 0,6848 | -19,5963 | 0,56% | 0,84% | | 6,44% | 26,79% |
| 4-METHYLCYCLOPENTENE | 527 | 41,3 | 0,2357 | 0,2811 | 1,1708 | 1,0000 | 0,5907 | -9,8608 | 0,66% | 2,25% | 1,70% | 2,53% | 10,89% |
| 4-METHYLHEPTANE | 561,7 | 25,4 | 0,3707 | 0,2579 | 0,4228 | 0,8143 | 1,6964 | 4,4942 | 0,47% | 0,77% | 2,14% | 1,51% | 17,80% |
| 4-METHYLNONANE | 610 | 21,6 | 0,4651 | 0,2578 | 0,5791 | 0,8061 | 1,5388 | 4,6424 | 1,15% | 2,88% | 1,75% | 2,25% | 23,01% |
| 4-METHYLOCTANE | 587,65 | 23,4 | 0,4129 | 0,2575 | 0,4726 | 0,8154 | 1,6783 | 4,9267 | 1,33% | 1,97% | 2,04% | 1,67% | 21,78% |
| 4-METHYLPHENANTHRENE | 895,3 | 27,21 | 0,4401 | 0,2343 | 1,2221 | 1,0000 | 0,8058 | 48,8196 | 1,25% | 1,40% | | 2,03% | 23,58% |
| 4-METHYLPYRIDINE | 646,15 | 46,6 | 0,3010 | 0,2628 | 0,2640 | 0,8347 | 2,1275 | 2,0546 | 0,61% | 1,29% | 0,73% | 1,03% | 8,08% |
| 4-METHYL-trans-2-PENTENE | 501 | 32,2 | 0,2552 | 0,2696 | 1,2039 | 1,0000 | 0,5978 | -3,0848 | 0,36% | 2,04% | 1,54% | 1,46% | 15,82% |
| 4-NONANONE | 643,7 | 24,53 | 0,4988 | 0,2575 | 1,3527 | 0,9952 | 0,7738 | 5,9676 | 0,67% | 1,00% | | 2,10% | 18,61% |
| 4-OCTANONE | 623,8 | 27,04 | 0,4204 | 0,2562 | 1,7706 | 1,0000 | 0,5164 | 7,7275 | 0,70% | 0,97% | | 1,22% | 17,09% |
| 5-ETHYLIDENE-2-NORBORNENE | 629 | 34 | 0,3141 | 0,2657 | 0,6358 | 0,8416 | 1,1709 | -1,0675 | 0,22% | 0,75% | | 1,49% | 16,12% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 5-ETHYL-m-XYLENE | 655 | 27,5 | 0,4169 | 0,2510 | 0,2831 | 0,8322 | 2,4657 | 13,5611 | 0,25% | 1,05% | 2,00% | 1,57% | 23,49% |
| 5-HEXEN-2-ONE | 586,8 | 34,13 | 0,4174 | 0,2489 | 0,2862 | 0,8480 | 2,5809 | 10,4276 | 0,26% | | | 1,46% | 25,44% |
| 5-METHYL-1-HEXANOL | 605 | 30,3 | 0,7807 | 0,2700 | 0,7263 | 0,8173 | 1,8562 | -15,0797 | 0,60% | 0,53% | | 5,44% | 21,62% |
| 5-METHYL-1-HEXENE | 528 | 28,7 | 0,3105 | 0,2643 | 0,4583 | 0,8570 | 1,5782 | -0,9137 | 1,48% | 1,90% | 0,90% | 1,45% | 18,37% |
| 5-METHYL-2-HEXANONE | 601 | 29,7 | 0,4344 | 0,2568 | 0,2496 | 0,8370 | 2,7707 | 4,5386 | 0,49% | 1,22% | | 1,50% | 21,77% |
| 5-METHYLINDAN | 711,2 | 35,22 | 0,3262 | 0,2622 | 0,2709 | 0,8606 | 2,3880 | 1,6016 | 0,38% | | | 1,44% | 16,93% |
| 5-METHYLNONANE | 610 | 21,6 | 0,4562 | 0,2557 | 0,3924 | 0,8161 | 2,0458 | 6,8691 | 2,01% | 3,20% | 2,62% | 1,73% | 22,63% |
| 5-NONANONE | 640 | 23,2 | 0,5137 | 0,2423 | 0,3855 | 0,8185 | 2,2561 | 23,8364 | 1,11% | 2,31% | 0,46% | 1,51% | 21,65% |
| 5-o-TOLYL-2-PENTENE | 702,6 | 25,16 | 0,4794 | 0,2523 | 0,9576 | 0,8953 | 1,0771 | 12,0552 | 0,51% | 1,50% | | 1,44% | 22,46% |
| 6-AMINOHEXANAMIDE | 807,8 | 34,56 | 0,6975 | 0,2480 | 0,9432 | 0,8644 | 1,3914 | 9,2413 | 0,89% | 1,29% | 0,33% | 1,77% | 22,03% |
| 6-AMINOHEXANOL | 665 | 34,4 | 0,9689 | | 0,5131 | 0,7855 | 2,7418 | | 0,65% | 0,59% | | | |
| 6-METHYL-1-HEPTENE | 558 | 26 | 0,3555 | 0,2592 | 0,4059 | 0,8407 | 1,8123 | 3,2871 | 0,99% | 1,84% | 0,37% | 1,40% | 20,36% |
| 6-METHYL-1-OCTANOL | 633,4 | 24,84 | 0,8745 | 0,2555 | 0,5577 | 0,8435 | 2,6567 | -6,2128 | 0,72% | | | 3,37% | 22,29% |
| 7-METHYL-1-OCTENE | 579 | 23,8 | 0,4045 | | 0,5347 | 0,8348 | 1,5660 | | 0,90% | 1,34% | 0,35% | | |
| 8-HYDROXYQUINOLINE | 788 | 43,6 | 0,5223 | 0,2651 | 0,6589 | 0,8261 | 1,5332 | -4,0235 | 0,62% | 0,91% | | 2,05% | 12,55% |
| 8-METHYL-1-NONANOL | 676,7 | 23,93 | 0,6107 | 0,2551 | 0,0970 | 0,4980 | 1,8884 | 4,6738 | 0,57% | | | 1,69% | 20,08% |
| 8-METHYL-1-NONENE | 619 | 21,9 | 0,4523 | | 0,8716 | 0,8705 | 1,1254 | | 0,64% | 1,10% | 0,26% | | |
| 8-METHYLQUINOLINE | 787 | 43 | 0,3582 | 0,2736 | 0,3607 | 0,8344 | 1,9295 | -11,5235 | 2,06% | 2,87% | 2,44% | 1,73% | 9,16% |
| ACENAPHTHALENE | 792 | 32 | 0,3987 | | 1,4300 | 1,0000 | 0,6308 | | 0,57% | 1,36% | 2,36% | | |
| ACENAPHTHENE | 803,15 | 31 | 0,3811 | 0,2302 | 1,2012 | 1,0000 | 0,7537 | 44,7370 | 1,82% | 4,32% | 1,08% | 4,16% | 11,65% |
| ACETAL | 539,7 | 32,2 | 0,4869 | 0,2842 | 0,3750 | 0,8585 | 2,4192 | -23,8679 | 2,56% | 2,98% | 3,22% | 3,43% | 12,50% |
| ACETALDOL | 620 | 45,9 | 0,7966 | 0,2149 | 0,9720 | 0,9367 | 1,5550 | 21,6400 | 0,59% | | | 5,65% | 16,40% |
| ACETALDOXIME | 568 | 60,4 | 0,6384 | 0,2506 | 0,3800 | 0,8366 | 2,7789 | 4,6732 | 0,53% | 1,25% | | 1,30% | 10,65% |
| ACETAMIDE | 761 | 66 | 0,4210 | 0,2156 | 1,2132 | 0,8972 | 0,7825 | 28,2984 | 0,64% | 1,88% | 0,62% | 5,37% | 23,91% |
| ACETAMINOPHEN | 736 | 42,6 | 0,7997 | | 0,4710 | 0,7961 | 2,5669 | | 0,60% | 0,93% | 2,80% | | |
| ACETANILIDE | 825 | 37,3 | 0,5646 | 0,2364 | 1,2053 | 1,0000 | 0,9614 | 26,1003 | 0,40% | 0,78% | | 1,42% | 25,40% |
| ACETIC ANHYDRIDE | 606 | 40 | 0,4553 | 0,2446 | 0,3445 | 0,8167 | 2,2196 | 14,1733 | 0,61% | 3,36% | 1,94% | 1,54% | 22,71% |
| ACETOACETANILIDE | 879 | 30,3 | 0,7946 | 0,2337 | 0,5418 | 0,8125 | 2,3816 | 31,0280 | 0,63% | 1,01% | | 1,67% | 25,96% |
| ACETOACETIC ACID | 678,5 | 46,97 | 0,7073 | | 0,5681 | 0,8004 | 2,0676 | | 0,65% | 1,56% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ACETOIN | 607,4 | 44,63 | 0,5263 | 0,2469 | 0,5876 | 0,8035 | 1,6474 | 9,1289 | 0,63% | 1,87% | | 1,13% | 21,40% |
| ACETONE | 508,2 | 47,01 | 0,3065 | 0,2433 | 0,3663 | 0,8371 | 1,7519 | 12,5392 | 0,35% | 2,24% | 1,90% | 2,69% | 26,20% |
| ACETONE CYANOHYDRIN | 620 | 42,5 | 0,7673 | 0,2440 | 0,7529 | 0,8323 | 1,8042 | 7,8512 | 0,55% | 0,64% | | 1,88% | 23,31% |
| ACETONITRILE | 545,5 | 48,5 | 0,3419 | 0,1963 | 0,5432 | 0,9307 | 1,6066 | 38,9177 | 1,61% | 4,08% | | 8,91% | 28,78% |
| ACETOPHENONE | 709,6 | 40,1 | 0,3830 | 0,2572 | 0,3070 | 0,8345 | 2,2476 | 5,4852 | 0,55% | 1,10% | | 1,11% | 15,75% |
| ACETOVANILLONE | 786 | 36,5 | 0,7856 | | 0,4438 | 0,8042 | 2,6873 | | 0,48% | 0,76% | | | |
| ACETOXYACETIC ACID | 764 | 43,2 | 0,7104 | | 0,4790 | 0,8107 | 2,4037 | | 0,69% | 2,26% | | | |
| ACETYL CHLORIDE | 508 | 57,4 | 0,3340 | 0,2643 | 0,3288 | 0,8764 | 2,1738 | -1,4563 | 4,22% | 6,19% | | 1,36% | 16,15% |
| ACETYLENE | 308,3 | 61,38 | 0,1912 | 0,2708 | 0,1923 | 0,8685 | 2,2777 | -0,8748 | 0,35% | 2,23% | | 1,53% | 15,40% |
| ACETYLSALICYLIC ACID | 765 | 32,7 | 0,8327 | 0,2411 | 0,8496 | 0,8396 | 1,7260 | 14,7316 | 0,79% | 1,22% | 2,09% | 2,15% | 24,35% |
| ACRIDINE | 905 | 36,4 | 0,4400 | 0,2536 | 0,2754 | 0,8423 | 2,6769 | 8,3180 | 0,67% | 1,81% | 0,86% | 1,25% | 15,49% |
| ACROLEIN | 506 | 50 | 0,3198 | 0,2333 | 1,1861 | 1,0000 | 0,6578 | 16,2046 | 5,89% | 6,92% | 4,04% | 5,89% | 23,07% |
| ACROLEIN CYANOHYDRIN | 639 | 45,1 | 0,8435 | 0,2357 | 0,9806 | 0,9311 | 1,6035 | 12,7614 | 0,70% | | | 3,19% | 25,67% |
| ACRYLIC ACID | 615 | 56,6 | 0,5383 | 0,2447 | 1,3446 | 1,0000 | 0,8117 | 8,4231 | 1,82% | | 1,14% | 1,21% | 29,47% |
| ACRYLONITRILE | 540 | 46,6 | 0,3107 | 0,2256 | 0,3320 | 0,8517 | 1,9719 | 25,0317 | 0,91% | | | 3,89% | 25,53% |
| ACRYLOXY PROPIONIC ACID | 729,5 | 34,41 | 0,8018 | 0,2366 | 0,6019 | 0,8559 | 2,3695 | 18,7870 | 0,66% | | | 2,16% | 25,43% |
| ADAMANTANE | 703 | 29,2 | 0,1853 | | 0,1444 | 0,8570 | 2,4415 | | 0,31% | | 0,32% | | |
| ADIPIC ACID | 841 | 37 | 0,7778 | 0,2343 | 0,4923 | 0,7281 | 2,1918 | 25,3496 | 1,82% | 1,47% | | 1,12% | 27,14% |
| ADIPONITRILE | 781 | 28,3 | 0,6588 | 0,1925 | 0,9799 | 0,9616 | 1,3540 | 87,4935 | 0,23% | | | 6,55% | 52,18% |
| AIR | 132,45 | 37,74 | 0,0000 | 0,2943 | 0,0970 | 0,8966 | 1,9371 | -3,6643 | 1,27% | 5,80% | 3,04% | 1,05% | 2,07% |
| ALLYL ACETATE | 559 | 36,8 | 0,3879 | 0,2566 | 0,4789 | 0,8891 | 1,8319 | 4,4874 | 0,56% | 0,83% | | 1,98% | 18,81% |
| ALLYL ACRYLATE | 575,5 | 33,96 | 0,4264 | | 1,4569 | 1,0000 | 0,6467 | | 0,77% | 1,29% | | | |
| ALLYL ALCOHOL | 545,1 | 56,2 | 0,5697 | 0,2482 | 0,8476 | 0,8596 | 1,3362 | 3,9580 | 0,68% | 1,09% | | 1,61% | 17,28% |
| ALLYL ETHER | 550,6 | 31,99 | 0,2762 | 0,2555 | 1,3520 | 1,0000 | 0,5521 | 10,0389 | 0,74% | 1,66% | | 1,69% | 17,45% |
| ALLYL GLYCIDYL ETHER | 629 | 36,8 | 0,4087 | 0,2580 | 0,5806 | 0,8364 | 1,4759 | 3,4605 | 0,75% | 1,82% | | 1,35% | 18,41% |
| ALLYL METHACRYLATE | 600 | 30,2 | 0,3881 | 0,2542 | 0,5324 | 0,7716 | 1,4041 | 9,4307 | 1,25% | 2,87% | | 1,36% | 20,09% |
| ALLYLAMINE | 505 | 51,7 | 0,3265 | 0,2547 | 1,1593 | 1,0000 | 0,7129 | 3,6372 | 0,61% | 1,27% | | 3,64% | 0,40% |
| ALLYLIDENE DIACETATE | 639,1 | 28,64 | 0,5702 | 0,2526 | 1,0266 | 0,8653 | 1,1145 | 6,5549 | 0,54% | 1,35% | | 1,61% | 20,21% |
| ALLYL-TERT-BUTYLPEROXIDE | 563 | 28,8 | 0,4020 | 0,2747 | 0,3983 | 0,8177 | 1,8772 | -15,0722 | 1,07% | 2,07% | | 1,52% | 15,15% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| alpha-EPICHLOROHYDRIN | 615 | 49 | 0,2523 | 0,2409 | 0,1267 | 0,8378 | 2,7558 | 17,3383 | 2,28% | 2,63% | | 3,78% | 30,24% |
| alpha-HYDROXYISOBUTYRAMIDE | 771,7 | 53,42 | 0,6453 | | 0,4226 | 0,8211 | 2,5000 | | 0,57% | 1,46% | | | |
| alpha-HYDROXYISOBUTYRIC ACID | 664 | 49,2 | 0,9833 | | 0,4067 | 0,8071 | 3,4152 | | 0,72% | 0,73% | | | |
| alpha-METHYLBENZYL ALCOHOL | 699 | 37,7 | 0,4382 | 0,2522 | 1,8364 | 1,0000 | 0,5087 | 9,0208 | 0,83% | 1,50% | | 1,44% | 18,89% |
| alpha-METHYLBENZYL ALCOHOL FORMATE | 690 | 32,3 | 0,4377 | 0,2556 | 0,6561 | 0,8368 | 1,3842 | 5,9200 | 0,28% | 0,37% | | 1,38% | 20,28% |
| alpha-METHYLSTYRENE | 654 | 33,6 | 0,3230 | 0,2581 | 0,7793 | 0,8435 | 0,9988 | 7,8768 | 0,41% | 1,68% | 0,08% | 1,28% | 22,71% |
| alpha-PHELLANDRENE | 649 | 28,2 | 0,3807 | 0,2680 | 1,3816 | 0,9998 | 0,6361 | -4,3936 | 1,01% | 2,40% | 0,36% | 3,10% | 21,19% |
| alpha-PINENE | 644 | 27,6 | 0,2209 | 0,2528 | 0,6018 | 0,4168 | 0,7396 | 18,7273 | 0,25% | | | 3,94% | 27,23% |
| alpha-TERPINENE | 649 | 28 | 0,3721 | 0,2562 | 0,4443 | 0,8085 | 1,6257 | 6,5531 | 0,27% | 1,06% | 0,65% | 1,67% | 19,81% |
| alpha-TERPINEOL | 675 | 29,5 | 0,6992 | | 0,4023 | 0,8312 | 2,8116 | | 0,31% | | | | |
| alpha-TOCOPHEROL | 964,3 | 10,8 | 1,0314 | 0,2316 | 0,4861 | 0,8164 | 3,1919 | 85,1125 | 0,41% | | | 4,07% | 27,73% |
| AMINOACETONITRILE | 638 | 54,4 | 0,4657 | | 1,2942 | 1,0000 | 0,7766 | | 0,65% | 1,46% | 3,92% | | |
| AMINOCAPRONITRILE | 697 | 30,5 | 0,6532 | | 0,4212 | 0,8149 | 2,4849 | | 0,26% | 1,17% | 0,70% | | |
| AMMONIA | 405,65 | 112,8 | 0,2526 | 0,2460 | 0,2274 | 0,8645 | 2,3318 | 4,0306 | 0,87% | 2,17% | 8,48% | 2,66% | 21,27% |
| AMMONIUM SULFIDE | 479 | 31,54 | 0,1657 | 0,1904 | 0,2903 | 0,9025 | 1,8380 | 63,6892 | 0,39% | | | 8,99% | 35,20% |
| ANETHOLE | 723 | 29 | 0,4846 | 0,2428 | 0,5158 | 0,8186 | 1,7584 | 22,7380 | 0,61% | 1,26% | | 1,41% | 27,48% |
| ANILINE | 699 | 53,1 | 0,3775 | 0,2593 | 0,3471 | 0,8021 | 1,8984 | 1,4957 | 0,37% | 2,89% | 0,73% | 1,34% | 24,06% |
| ANISOLE | 645,6 | 42,5 | 0,3502 | 0,2639 | 0,3716 | 0,8264 | 1,8339 | -0,6140 | 0,14% | 0,79% | | 1,22% | 15,39% |
| ANTHRACENE | 873 | 29 | 0,4857 | 0,2289 | 0,2884 | 0,8387 | 2,7396 | 48,4969 | 3,63% | 5,94% | 2,96% | 2,81% | 30,13% |
| ANTHRAQUINONE | 900 | 31,5 | 0,6807 | 0,2390 | 0,6486 | 0,8908 | 2,0020 | 27,9989 | 2,92% | 4,85% | | 1,99% | 21,08% |
| ANTIMONY TRICHLORIDE | 794 | 48,2 | 0,1706 | 0,2188 | 0,1231 | 0,8532 | 2,4982 | 44,6417 | 1,06% | | | 7,22% | 39,40% |
| ARGON | 150,86 | 48,98 | 0,0000 | 0,2941 | 0,1227 | 0,9045 | 1,8541 | -3,2933 | 0,38% | 2,30% | 4,74% | 1,18% | 9,95% |
| ARSENIC (III) CHLORIDE | 629 | 52,6 | 0,3020 | 0,2599 | 0,2756 | 0,8287 | 2,0400 | 3,2752 | 0,50% | 2,76% | 2,32% | 1,24% | 17,19% |
| ARSENIC TRIOXIDE | 1200 | 40 | 0,0611 | | 0,1131 | 0,8728 | 2,0938 | | 0,51% | 2,32% | | | |
| ARSINE | 373 | 65,5 | 0,0105 | 0,2779 | 0,2810 | 0,8629 | 1,0129 | -1,2298 | 0,46% | 3,43% | 0,23% | 2,17% | 50,08% |
| AZELAIC ACID | 844 | 27,2 | 0,8923 | 0,2331 | 0,3619 | 0,6909 | 2,6172 | 29,2128 | 0,58% | | | 1,35% | 33,08% |
| BENZALDEHYDE | 695 | 46,5 | 0,3127 | 0,2597 | 0,4849 | 0,8272 | 1,4222 | 4,2219 | 0,18% | 0,59% | 0,99% | 1,37% | 16,60% |
| BENZAMIDE | 824 | 50,5 | 0,5585 | 0,2549 | 0,5355 | 0,8123 | 1,8633 | 2,7590 | 0,62% | 1,68% | | 1,03% | 19,73% |
| BENZANTHRACENE | 979 | 23,9 | 0,5692 | | 0,7917 | 0,8355 | 1,3983 | | 0,65% | 1,51% | 0,35% | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| BENZENE | 562,05 | 48,95 | 0,2103 | 0,2698 | 0,1348 | 0,8481 | 2,5791 | -1,4388 | 0,38% | 1,54% | 1,19% | 1,42% | 15,20% |
| BENZENE-1,2,4-TRICARBOXYLIC ACID TRIMETHYL ESTER | 821,7 | 23,34 | 0,8845 | 0,2400 | 0,6465 | 0,8580 | 2,4260 | 21,3489 | 2,83% | | | 3,60% | 24,96% |
| BENZIDINE | 929 | 33 | 0,7347 | | 0,5256 | 0,8105 | 2,2900 | | 0,62% | 0,84% | | | |
| BENZOIC ACID | 751 | 44,7 | 0,6028 | 0,2481 | 2,2106 | 1,0000 | 0,5033 | 8,9874 | 3,11% | 4,36% | 2,59% | 1,17% | 22,22% |
| BENZONITRILE | 702,3 | 42,15 | 0,3432 | 0,2467 | 0,5684 | 0,8426 | 1,3557 | 16,0973 | 0,20% | 2,04% | | 1,65% | 30,83% |
| BENZOPHENONE | 830 | 33,52 | 0,5019 | 0,2632 | 0,2934 | 0,8368 | 2,7743 | -5,0707 | 1,89% | 1,71% | | 1,77% | 12,37% |
| BENZOTHIOPHENE | 764 | 47,6 | 0,3071 | 0,2840 | 0,2388 | 0,8561 | 2,4542 | -13,3530 | 1,76% | 3,03% | | 4,34% | 11,76% |
| BENZOTRICHLORIDE | 737 | 33,4 | 0,2599 | 0,2539 | 1,0966 | 0,9999 | 0,6715 | 15,5020 | 0,59% | 1,45% | | 1,91% | 22,70% |
| BENZOTRIFLUORIDE | 559,9 | 32,1 | 0,2998 | 0,2522 | 0,7259 | 0,8258 | 1,0118 | 11,2754 | 0,74% | 2,54% | 0,50% | 2,76% | 22,06% |
| BENZOYL CHLORIDE | 697 | 40,6 | 0,4159 | 0,2610 | 0,9271 | 0,9959 | 1,0691 | 0,9460 | 0,66% | 0,54% | | 1,61% | 19,30% |
| BENZYL ACETATE | 699 | 31,8 | 0,4733 | 0,2593 | 0,6114 | 0,8318 | 1,5400 | 3,2464 | 0,81% | 1,66% | | 3,16% | 24,40% |
| BENZYL ALCOHOL | 720,15 | 43,74 | 0,3631 | 0,2450 | 0,0000 | 0,6216 | 2,0352 | 16,7227 | 0,64% | | | 4,09% | 5,78% |
| BENZYL CHLORIDE | 686 | 39,1 | 0,3136 | 0,2537 | 0,7299 | 0,7558 | 0,9746 | 11,1323 | 0,63% | 3,52% | 4,33% | 1,73% | 21,47% |
| BENZYL DICHLORIDE | 731 | 36,5 | 0,3264 | 0,2570 | 0,8189 | 0,9921 | 1,0630 | 8,7740 | 0,36% | 1,14% | | 1,62% | 24,53% |
| BENZYL ETHYL ETHER | 662 | 31,1 | 0,4332 | 0,2501 | 1,1065 | 0,9999 | 0,8904 | 10,4729 | 0,87% | 2,04% | | 2,19% | 20,72% |
| BENZYL FORMATE | 698 | 35,9 | 0,4203 | 0,2553 | 1,2609 | 1,0000 | 0,7502 | 7,6442 | 0,60% | 1,16% | 2,54% | 1,45% | 23,25% |
| BENZYL MERCAPTAN | 718 | 40,6 | 0,3126 | 0,2624 | 0,3965 | 0,8060 | 1,5837 | 3,4732 | 0,93% | 2,43% | 0,90% | 1,71% | 22,21% |
| BENZYLAMINE | 684 | 43,2 | 0,4011 | 0,2620 | 0,2205 | 0,8354 | 2,8002 | 0,3889 | 0,47% | 1,05% | | 1,51% | 8,39% |
| beta-PHELLANDRENE | 648 | 28,2 | 0,3766 | 0,2659 | 0,8020 | 0,8309 | 1,0562 | -2,8003 | 0,60% | 1,54% | 0,18% | 2,28% | 21,17% |
| beta-PINENE | 643 | 27,6 | 0,3249 | 0,2549 | 0,2156 | 0,8465 | 2,6058 | 11,8668 | 1,67% | 3,08% | | 1,31% | 18,13% |
| beta-TERPINEOL | 665,2 | 30,12 | 0,6872 | 0,2738 | 0,5184 | 0,8070 | 2,1909 | -24,3357 | 0,53% | 1,12% | | 2,02% | 17,06% |
| BICYCLO[2.2.1]HEPTANE | 594 | 36,96 | 0,1636 | | 0,1194 | 0,8446 | 2,3886 | | 0,52% | 3,05% | | | |
| BICYCLO[2.2.2]OCTANE | 625 | 34,2 | 0,2054 | 0,2417 | 0,1986 | 0,8663 | 2,3069 | 21,7338 | 0,55% | | 3,13% | 3,73% | 9,96% |
| BICYCLOHEXYL | 727 | 25,6 | 0,4276 | 0,2549 | 0,3155 | 0,8533 | 2,4966 | 8,4149 | 1,07% | 2,44% | | 1,19% | 19,97% |
| BIPHENYL | 773 | 33,8 | 0,4029 | 0,2551 | 0,2339 | 0,8327 | 2,7080 | 7,3452 | 0,83% | 1,69% | 0,15% | 1,34% | 16,13% |
| BIS-(2-AMINOETHYL)ETHER | 655,8 | 44,21 | 0,6152 | | 2,0161 | 1,0000 | 0,5650 | | 0,54% | 0,85% | | | |
| BIS(alpha-METHYLBENZYL) ETHER | 770,6 | 19,92 | 0,4834 | 0,2419 | 0,2061 | 0,7191 | 2,2825 | 40,0672 | 0,51% | | | 1,68% | 21,94% |
| BIS(CHLOROMETHYL)ETHER | 579 | 45,8 | 0,3239 | 0,2541 | 1,1521 | 0,9917 | 0,7138 | 7,2766 | 0,61% | 1,44% | | 1,51% | 22,42% |
| BIS(CYANOETHYL)ETHER | 783 | 28,3 | 0,7775 | 0,1978 | 0,4884 | 0,8412 | 2,6966 | 75,3673 | 0,51% | | | 3,96% | 67,58% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| BIS(DIFLUOROMETHYL)ETHER | 420,25 | 42,28 | 0,3676 | 0,2636 | 1,1959 | 1,0000 | 0,7363 | -0,8196 | 0,64% | 1,06% | | 1,24% | 14,29% |
| BIS(TRIFLUOROMETHYL)SULFIDE | 376,75 | 30,58 | 0,2638 | 0,2806 | 0,2677 | 0,8727 | 2,2209 | -11,1639 | 0,38% | | | 1,07% | 13,61% |
| BIS[3-(TRIMETHOXYSILYL)PROPYL]DISULFIDE | 736,2 | 13,09 | 1,1551 | 0,2452 | 0,6614 | 0,8348 | 2,8118 | -0,0419 | 0,85% | | | 4,08% | 29,50% |
| BORON TRIBROMIDE | 573,15 | 48,7 | 0,2599 | 0,2766 | 0,4084 | 0,9136 | 1,7635 | -7,7931 | 0,97% | | | 1,13% | 13,87% |
| BORON TRICHLORIDE | 451,95 | 38,706 | 0,1505 | 0,2436 | 0,0600 | 0,8404 | 2,7095 | 14,2446 | 0,57% | 1,90% | | 5,97% | 91,63% |
| BORON TRIFLUORIDE | 260,9 | 49,9 | 0,4337 | 0,2565 | 0,2342 | 0,8344 | 2,8200 | 0,1984 | 2,29% | 5,04% | 1,66% | 2,49% | 7,95% |
| BROMINE | 584,15 | 103 | 0,1290 | 0,3008 | 0,1358 | 0,8689 | 2,2719 | -9,9116 | 1,30% | 2,08% | 1,22% | 1,32% | 14,71% |
| BROMOBENZENE | 670,15 | 45,191 | 0,2506 | 0,2629 | 0,4417 | 0,8256 | 1,3456 | 2,7331 | 1,79% | 2,80% | 0,10% | 1,55% | 16,14% |
| BROMOCHLORODIFLUOROMETHANE | 426,15 | 42,54 | 0,1871 | 0,2749 | 1,4213 | 1,0000 | 0,4225 | -3,2746 | 2,05% | 4,91% | 1,77% | 1,34% | 5,41% |
| BROMOCHLOROMETHANE | 557 | 64,7 | 0,2064 | 0,2727 | 1,0407 | 1,0000 | 0,6379 | -1,8422 | 0,70% | 1,21% | | 1,30% | 8,76% |
| BROMODIFLUOROMETHANE | 411,98 | 51,32 | 0,2050 | 0,2665 | 0,2183 | 0,7928 | 1,7064 | -0,1783 | 0,56% | 5,88% | | 2,72% | 22,97% |
| BROMOETHANE | 503,8 | 55,65 | 0,2053 | 0,2750 | 0,2003 | 0,8673 | 2,2940 | -3,5853 | 1,79% | 2,95% | | 1,49% | 15,18% |
| BROMOMETHANE | 464 | 69,29 | 0,1534 | 0,2717 | 0,2956 | 0,8410 | 1,4581 | -0,7023 | 0,96% | 2,83% | 0,87% | 1,37% | 13,06% |
| BROMOTRICHLOROMETHANE | 606 | 49,7 | 0,1920 | 0,2800 | 0,2084 | 0,8324 | 1,9107 | -8,5558 | 0,41% | 1,99% | 0,84% | 1,01% | 12,75% |
| BROMOTRIFLUOROETHYLENE | 432 | 44,8 | 0,1754 | 0,2815 | 1,0711 | 1,0000 | 0,5724 | -5,3847 | 0,52% | 2,46% | 0,51% | 2,90% | 5,37% |
| BROMOTRIFLUOROMETHANE | 340,15 | 39,7 | 0,1704 | 0,2762 | 0,8682 | 1,0000 | 0,7202 | -3,6469 | 0,62% | 1,70% | | 1,21% | 11,32% |
| BUTANAL | 537,2 | 44,1 | 0,2826 | 0,2588 | 0,9865 | 1,0000 | 0,7914 | 4,1569 | 0,59% | 1,73% | | 1,50% | 19,06% |
| BUTYL VINYL ETHER | 536 | 31,2 | 0,3802 | 0,2620 | 0,5680 | 0,8316 | 1,4250 | 0,3397 | 0,75% | 1,50% | | 1,39% | 20,53% |
| BUTYRONITRILE | 585,4 | 38,8 | 0,3601 | 0,2303 | 0,3362 | 0,8702 | 2,2540 | 26,9023 | 1,33% | 2,89% | | 2,69% | 23,27% |
| CAMPHENE | 638 | 27,5 | 0,2957 | 0,2520 | 0,5139 | 0,8165 | 1,3020 | 15,9454 | 0,33% | 1,19% | | 2,70% | 15,63% |
| CAMPHOR | 709 | 29,9 | 0,3190 | 0,2560 | 0,1998 | 0,8438 | 2,6519 | 10,8238 | 0,80% | 2,68% | | 1,61% | 17,87% |
| CARBAMYL CHLORIDE | 517 | 73,8 | 0,4446 | | 0,2165 | 0,8128 | 2,7760 | | 0,43% | 0,89% | | | |
| CARBON DIOXIDE | 304,21 | 73,83 | 0,2236 | 0,2728 | 0,1784 | 0,8590 | 2,4107 | -1,1374 | 0,27% | 1,01% | 6,99% | 1,17% | 13,24% |
| CARBON DISULFIDE | 552 | 79 | 0,1107 | 0,2891 | 0,2523 | 0,8784 | 1,6011 | -7,0906 | 0,81% | 0,96% | 12,01% | 1,84% | 16,05% |
| CARBON MONOXIDE | 132,92 | 34,99 | 0,0482 | 0,2903 | 0,0997 | 0,8782 | 2,1509 | -3,6765 | 0,34% | 1,27% | 10,19% | 1,16% | 6,75% |
| CARBON TETRACHLORIDE | 556,35 | 45,6 | 0,1926 | 0,2721 | 0,2174 | 0,8228 | 1,8121 | -2,7606 | 0,53% | 1,80% | 3,53% | 1,46% | 13,98% |
| CARBON TETRAFLUORIDE | 227,51 | 37,45 | 0,1790 | 0,2811 | 0,4987 | 0,8428 | 1,0753 | -4,4212 | 0,66% | 1,85% | 0,64% | 1,03% | 11,67% |
| CARBONYL FLUORIDE | 297 | 57,6 | 0,2829 | 0,3291 | 0,1576 | 0,7500 | 2,0001 | -20,6636 | 1,82% | 3,80% | 0,50% | 0,86% | 8,12% |
| CARBONYL SULFIDE | 378,8 | 63,49 | 0,0970 | 0,2744 | 0,1557 | 0,8639 | 1,9347 | -1,3991 | 0,28% | 1,90% | 11,05% | 2,77% | 13,91% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| CELLOBIOSE | 1235 | 39,21 | 0,8442 | | 0,5382 | 0,8204 | 2,5420 | | 0,58% | 0,93% | | | |
| CHLORINE | 417,15 | 77,1 | 0,0688 | 0,2777 | 0,7775 | 0,8922 | 0,5817 | -1,4689 | 1,06% | 2,21% | 1,01% | 1,77% | 12,70% |
| CHLORINE TRIFLUORIDE | 433,7 | 45,78 | 0,3371 | 0,2040 | 0,6584 | 0,8418 | 1,2166 | 30,3732 | 3,69% | 1,66% | 0,69% | 6,62% | 31,53% |
| CHLOROACETALDEHYDE | 555 | 53,7 | 0,3297 | 0,2355 | 0,1537 | 0,8313 | 2,8787 | 16,5013 | 0,51% | 2,54% | | 2,96% | 23,21% |
| CHLOROACETIC ACID | 686 | 57,8 | 0,5461 | 0,2304 | 0,2388 | 0,8196 | 3,1206 | 17,5566 | 0,66% | 1,76% | | 2,26% | 29,31% |
| CHLOROACETYL CHLORIDE | 581 | 51,1 | 0,3540 | 0,2568 | 0,1495 | 0,8244 | 2,9349 | 4,2457 | 0,45% | | | 1,27% | 16,88% |
| CHLOROCYCLOHEXANE | 638 | 38,27 | 0,2611 | 0,2631 | 0,1855 | 0,8515 | 2,5262 | 2,6254 | 0,42% | 2,57% | | 1,22% | 16,02% |
| CHLORODIFLUOROMETHANE | 369,3 | 49,71 | 0,2192 | 0,2678 | 0,5065 | 0,8274 | 1,1425 | -0,0993 | 0,52% | 2,13% | 1,45% | 1,33% | 14,44% |
| CHLOROFLUOROMETHANE | 427 | 56,2 | 0,2108 | 0,2486 | 1,1809 | 1,0000 | 0,5370 | 9,0215 | 3,55% | 5,73% | 0,94% | 2,32% | 20,24% |
| CHLOROFORM | 536,4 | 54,72 | 0,2219 | 0,2765 | 0,8473 | 0,8716 | 0,7617 | -4,6795 | 1,93% | 2,95% | 0,19% | 1,02% | 6,79% |
| CHLOROMETHYL METHYL ETHER | 521 | 50,3 | 0,2698 | 0,2653 | 1,1220 | 1,0000 | 0,6676 | 2,0945 | 0,67% | 1,11% | | 2,82% | 22,73% |
| CHLOROPENTAFLUOROETHANE | 353,15 | 31,57 | 0,2514 | 0,2757 | 0,9683 | 0,9416 | 0,7413 | -6,1998 | 0,75% | 1,94% | 0,96% | 1,00% | 15,91% |
| CHLOROPRENE | 525 | 42,6 | 0,1974 | 0,2611 | 0,1736 | 0,8582 | 2,3346 | 5,2323 | 0,08% | 1,33% | | 1,84% | 13,46% |
| CHLOROTRIFLUOROETHYLENE | 379,15 | 40,53 | 0,2442 | 0,2735 | 0,3242 | 0,8472 | 1,7400 | -3,0626 | 0,74% | 1,95% | | 2,10% | 14,23% |
| CHLOROTRIFLUOROMETHANE | 302 | 38,7 | 0,1717 | 0,2775 | 0,1413 | 0,8584 | 2,4198 | -3,8903 | 0,47% | 1,64% | 1,72% | 1,18% | 12,79% |
| CHRYSENE | 979 | 23,9 | 0,6030 | | 0,3146 | 0,8046 | 2,7519 | | 0,49% | 1,80% | 0,20% | | |
| CINNAMIC ACID | 797 | 35,4 | 0,7121 | 0,2339 | 0,3765 | 0,7617 | 2,5362 | 23,5682 | 1,39% | | | 1,83% | 28,04% |
| cis,trans-2,4-HEXADIENE | 538 | 33,5 | 0,2754 | 0,2534 | 0,3258 | 0,8054 | 1,6660 | 10,9808 | 0,54% | 2,05% | 0,10% | 1,90% | 20,69% |
| cis-1,2-DICHLOROETHYLENE | 544 | 51,9 | 0,1349 | 0,2598 | 1,2711 | 0,5504 | 0,4557 | 7,2053 | 0,88% | 1,23% | | 2,34% | 16,38% |
| cis-1,2-DIMETHYLCYCLOHEXANE | 606,15 | 29,3843 | 0,2324 | 0,2544 | 1,4361 | 1,0000 | 0,4733 | 15,1714 | 1,06% | 0,79% | 1,87% | 2,54% | 11,32% |
| cis-1,2-DIMETHYLCYCLOPENTANE | 565,15 | 34,4505 | 0,2662 | 0,2698 | 0,3339 | 0,8212 | 1,6593 | -3,8161 | 0,92% | 1,67% | 1,70% | 1,11% | 14,35% |
| cis-1,3-DICHLOROPROPENE | 594,4 | 47,04 | 0,2278 | 0,2617 | 1,2217 | 1,0000 | 0,5603 | 3,9394 | 0,70% | 1,81% | | 1,69% | 16,01% |
| cis-1,3-DIMETHYLCYCLOHEXANE | 591,15 | 29,3843 | 0,2366 | 0,2639 | 1,2774 | 1,0000 | 0,5433 | 3,9578 | 1,04% | 0,91% | 0,62% | 1,34% | 13,38% |
| cis-1,3-DIMETHYLCYCLOPENTANE | 551 | 34,45 | 0,2743 | 0,2812 | 0,5287 | 0,8410 | 1,2580 | -13,8651 | 0,43% | 1,51% | 2,76% | 2,74% | 17,40% |
| cis-1,3-PENTADIENE | 499 | 37,4 | 0,1470 | 0,2559 | 1,4966 | 1,0000 | 0,3890 | 10,5278 | 3,86% | 3,23% | 0,48% | 2,77% | 19,74% |
| cis-1,4-DIMETHYLCYCLOHEXANE | 598,15 | 29,3843 | 0,2311 | 0,2598 | 1,3694 | 1,0000 | 0,4990 | 9,2041 | 1,34% | 0,73% | 0,96% | 1,51% | 11,10% |
| cis-1,8-TERPIN | 694,8 | 29,49 | 1,0801 | | 0,4535 | 0,8071 | 3,4152 | | 0,28% | 0,89% | | | |
| cis-1-PROPENYLBENZENE | 671 | 33,6 | 0,3411 | 0,2573 | 1,2311 | 1,0000 | 0,6767 | 9,1224 | 0,55% | 1,77% | 1,22% | 1,88% | 23,17% |
| cis-2-BUTENE | 435,5 | 42,1 | 0,2019 | 0,2702 | 0,4526 | 0,8193 | 1,1798 | -1,3959 | 0,53% | 1,32% | 0,84% | 1,40% | 13,58% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| cis-2-DECENE | 621 | 21,8 | 0,4752 | 0,2513 | 0,3857 | 0,7925 | 2,0170 | 13,5865 | 0,53% | 2,16% | 2,57% | 1,44% | 21,10% |
| cis-2-DODECENE | 663 | 18,9 | 0,5692 | | 0,4552 | 0,7910 | 2,0409 | | 0,53% | 1,83% | 3,82% | | |
| cis-2-HEPTENE | 543,7 | 28,4 | 0,3363 | 0,2568 | 0,2419 | 0,8464 | 2,4840 | 6,6447 | 0,38% | 3,92% | 1,31% | 1,44% | 20,06% |
| cis-2-HEXENE | 511,4 | 31,6 | 0,2874 | 0,2600 | 0,6893 | 0,8531 | 1,0505 | 4,4528 | 0,47% | 2,63% | 0,80% | 1,55% | 18,60% |
| cis-2-METHYLCYCLOHEXANOL | 614 | 37,9 | 0,6805 | 0,2658 | 0,3135 | 0,8192 | 3,1291 | -11,2656 | 5,51% | 1,49% | 2,38% | 1,33% | 13,72% |
| cis-2-NONENE | 598,1 | 23,7 | 0,4304 | | 1,0864 | 1,0000 | 0,9075 | | 0,28% | 1,28% | | | |
| cis-2-OCTENE | 572 | 25,9 | 0,3889 | 0,2549 | 0,2885 | 0,8536 | 2,4929 | 8,2419 | 0,28% | 0,85% | 4,81% | 1,43% | 20,39% |
| cis-2-PENTENE | 475 | 36,4 | 0,2454 | 0,2716 | 1,2515 | 0,9936 | 0,5580 | -2,5914 | 0,97% | 3,93% | 0,78% | 2,06% | 15,11% |
| cis-2-PHENYLBUTENE-2 | 685 | 30,1 | 0,3564 | 0,2482 | 0,5677 | 0,8210 | 1,3543 | 19,3095 | 0,71% | 1,53% | | 1,58% | 19,65% |
| cis-3-HEPTENE | 545 | 28,4 | 0,2949 | 0,2588 | 0,3901 | 0,7976 | 1,5218 | 6,9395 | 0,24% | 0,61% | 0,25% | 1,52% | 14,85% |
| cis-3-HEXENE | 509 | 31,7 | 0,2787 | 0,2634 | 0,4499 | 0,8116 | 1,3757 | 1,9649 | 0,18% | 1,25% | 0,62% | 1,46% | 16,36% |
| cis-3-METHYLCYCLOHEXANOL | 625 | 37,9 | 0,6943 | 0,2682 | 0,7222 | 0,7955 | 1,6712 | -13,4151 | 0,37% | 1,55% | 0,40% | 1,67% | 16,28% |
| cis-3-OCTENE | 569 | 25,9 | 0,3800 | 0,2551 | 0,2637 | 0,8484 | 2,5577 | 7,8424 | 0,22% | 1,93% | 4,26% | 1,51% | 20,10% |
| cis-4-METHYLCYCLOHEXANOL | 622 | 37,9 | 0,6880 | 0,2699 | 0,3345 | 0,8194 | 3,0433 | -14,3937 | 0,54% | 1,45% | 2,58% | 2,32% | 16,00% |
| cis-4-OCTENE | 568 | 25,9 | 0,3854 | 0,2551 | 0,2309 | 0,8407 | 2,7058 | 7,7225 | 0,59% | 5,66% | 2,27% | 1,46% | 19,91% |
| cis-CROTONALDEHYDE | 554 | 45,9 | 0,3241 | | 1,2297 | 1,0000 | 0,6622 | | 0,45% | 1,78% | 3,30% | | |
| cis-CROTONIC ACID | 647 | 47 | 0,5723 | 0,2403 | 0,2676 | 0,8097 | 2,9370 | 12,8363 | 0,43% | | | 1,28% | 25,56% |
| cis-CROTONITRILE | 568 | 38,8 | 0,3787 | 0,2225 | 0,4045 | 0,8452 | 1,8476 | 31,7709 | 3,24% | 2,17% | 3,58% | 4,52% | 29,20% |
| cis-DECAHYDRONAPHTHALENE | 703,6 | 32 | 0,2791 | 0,2640 | 1,4612 | 1,0000 | 0,4968 | 2,4814 | 1,69% | 1,38% | 0,96% | 1,39% | 16,56% |
| cis-DICYANO-1-BUTENE | 796 | 29,5 | 0,6639 | | 0,6512 | 0,8254 | 1,8265 | | 0,24% | 0,99% | | | |
| cis-STILBENE | 784 | 27,4 | 0,4758 | 0,2506 | 0,2816 | 0,8376 | 2,7603 | 14,5447 | 1,17% | 1,61% | | 1,43% | 20,26% |
| CITRACONIC ACID | 829 | 42,4 | 0,9269 | | 0,5223 | 0,8106 | 2,7486 | | 0,60% | 1,10% | | | |
| CROTYL GLYCOL ETHER | 643,9 | 33,87 | 0,5532 | 0,2518 | 0,1991 | 0,7947 | 3,1206 | 7,2547 | 0,43% | | | 1,81% | 20,87% |
| CUMENE | 631 | 32,09 | 0,3274 | 0,2626 | 1,2700 | 1,0000 | 0,6399 | 2,2429 | 1,05% | 1,54% | 2,17% | 1,56% | 15,28% |
| CYANOGEN | 400,15 | 59,24 | 0,2756 | 0,2615 | 0,9838 | 1,0000 | 0,7801 | 1,0004 | 0,25% | 2,53% | | 2,16% | 13,67% |
| CYANOGEN CHLORIDE | 449 | 59,9 | 0,3221 | 0,2363 | 0,8342 | 0,9984 | 1,0366 | 11,0036 | 0,80% | 1,52% | | 3,29% | 10,78% |
| CYCLOBUTANE | 459,93 | 49,8 | 0,1847 | 0,2701 | 0,2136 | 0,8638 | 2,0681 | -2,3923 | 0,11% | 1,80% | 1,51% | 3,12% | 13,54% |
| CYCLOHEPTANE | 604,2 | 38,2 | 0,2408 | 0,2725 | 0,2404 | 0,8471 | 2,0869 | -5,3516 | 0,66% | 1,65% | 0,80% | 0,96% | 16,04% |
| CYCLOHEPTENE | 598 | 40,1 | 0,2517 | 0,2786 | 1,2780 | 1,0000 | 0,5519 | -9,3040 | 0,81% | 2,33% | 2,96% | 1,76% | 16,21% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| CYCLOHEXANE | 553,8 | 40,8 | 0,2081 | 0,2730 | 0,3707 | 0,8119 | 1,3579 | -4,2349 | 0,38% | 0,92% | 0,44% | 1,43% | 14,01% |
| CYCLOHEXANECARBOXALDEHYDE | 639,4 | 35,79 | 0,3827 | 0,2552 | 0,2459 | 0,8445 | 2,6399 | 7,0878 | 0,62% | | 0,49% | 1,11% | 18,61% |
| CYCLOHEXANOL | 650,1 | 42,6 | 0,3690 | 0,2575 | 2,7410 | 0,6180 | 0,3960 | 4,3391 | 3,48% | 4,36% | 9,81% | 1,93% | 19,78% |
| CYCLOHEXANONE | 653 | 40 | 0,2990 | 0,2454 | 0,2645 | 0,8350 | 2,1232 | 16,9778 | 0,36% | 1,29% | | 2,64% | 28,70% |
| CYCLOHEXANONE OXIME | 715 | 46,9 | 0,4620 | | 0,2116 | 0,8209 | 2,9623 | | 0,45% | 1,20% | | | |
| CYCLOHEXENE | 560,4 | 43,5 | 0,2123 | 0,2723 | 0,8412 | 0,8782 | 0,7601 | -3,1784 | 1,17% | 2,14% | 0,97% | 1,29% | 14,24% |
| CYCLOHEXYL ACETATE | 648 | 31,2 | 0,4209 | 0,2622 | 0,7074 | 0,8154 | 1,2408 | -1,1693 | 0,35% | 2,34% | 0,31% | 1,80% | 22,02% |
| CYCLOHEXYL FORMATE | 645 | 35,2 | 0,3679 | 0,2629 | 0,2147 | 0,8397 | 2,7218 | 0,0662 | 0,83% | 1,34% | 1,62% | 1,67% | 21,94% |
| CYCLOHEXYL HYDROPEROXIDE | 685 | 42,1 | 0,7571 | 0,2632 | 0,8060 | 0,8370 | 1,6854 | -8,8687 | 0,64% | 0,52% | | 2,90% | 19,31% |
| CYCLOHEXYL ISOCYANATE | 633 | 34,7 | 0,5247 | 0,2514 | 1,0610 | 0,9135 | 1,0340 | 10,4129 | 0,75% | 0,63% | | 2,81% | 11,72% |
| CYCLOHEXYL MERCAPTAN | 664 | 39,7 | 0,2641 | 0,2695 | 0,1699 | 0,8472 | 2,5941 | -3,4152 | 0,60% | 2,13% | 0,26% | 1,57% | 21,38% |
| CYCLOHEXYLAMINE | 615 | 42 | 0,3604 | 0,2767 | 0,2284 | 0,8465 | 2,6036 | -10,8878 | 2,98% | 3,26% | 3,57% | 1,28% | 6,98% |
| CYCLOHEXYLBENZENE | 744 | 28,8 | 0,3783 | 0,2644 | 1,7813 | 1,0000 | 0,4806 | 0,5515 | 0,85% | 1,30% | | 2,02% | 24,71% |
| CYCLOOCTANE | 647,2 | 35,6 | 0,2524 | 0,2709 | 0,1321 | 0,8374 | 2,6993 | -4,1219 | 0,23% | 1,19% | 0,88% | 0,94% | 14,33% |
| CYCLOOCTENE | 632 | 36,8 | 0,2804 | 0,2711 | 1,0891 | 1,0000 | 0,7064 | -5,8729 | 1,29% | 1,01% | | 1,26% | 14,94% |
| CYCLOPENTADIENE | 507 | 51,5 | 0,2020 | 0,2741 | 0,4792 | 0,9532 | 1,4197 | -4,1502 | 0,73% | 2,91% | | 1,11% | 13,67% |
| CYCLOPENTANE | 511,7 | 45,1 | 0,1949 | 0,2691 | 0,3967 | 0,8269 | 1,2921 | -1,9877 | 0,25% | 2,80% | 0,93% | 3,00% | 12,30% |
| CYCLOPENTANONE | 624,5 | 46 | 0,2876 | 0,2469 | 1,2016 | 0,9943 | 0,6335 | 13,3171 | 1,12% | 2,03% | 1,54% | 2,99% | 29,33% |
| CYCLOPENTENE | 507 | 48 | 0,1961 | 0,2763 | 0,5816 | 0,8590 | 1,0079 | -4,8024 | 0,64% | 2,43% | 0,92% | 1,39% | 12,15% |
| CYCLOPENTYLACETIC ACID | 708 | 36,2 | 0,6144 | 0,2521 | 0,4908 | 0,7570 | 1,9453 | 5,1895 | 1,31% | | | 1,45% | 20,66% |
| CYCLOPENTYLAMINE | 584 | 46,4 | 0,3294 | 0,2702 | 1,0801 | 1,0000 | 0,7771 | -5,3222 | 1,08% | 1,29% | | 1,23% | 6,17% |
| CYCLOPROPANE | 398 | 55,4 | 0,1278 | 0,2776 | 0,2134 | 0,8571 | 1,7551 | -3,0579 | 0,74% | 1,23% | 2,66% | 1,19% | 15,23% |
| CYCLOPROPANE CARBOXYLIC ACID | 671 | 59,95 | 0,6048 | 0,2644 | 1,1531 | 0,9965 | 1,0623 | -4,6884 | 0,93% | | 2,04% | 1,85% | 17,24% |
| CYCLOPROPANECARBOXAMIDE | 779,1 | 57,39 | 0,5726 | | 0,4806 | 0,8081 | 2,0404 | | 0,48% | 2,42% | | | |
| CYCLOPROPYL CYANIDE | 621,9 | 44,62 | 0,3415 | 0,2202 | 0,9840 | 1,0000 | 0,8753 | 32,3084 | 1,74% | | 0,41% | 5,34% | 33,30% |
| CYCLOPROPYLAMINE | 508,6 | 57,48 | 0,3038 | 0,2649 | 0,2853 | 0,8688 | 2,2731 | -0,8204 | 0,39% | | | 1,18% | 19,46% |
| DECAFLUOROBUTANE | 386,35 | 23,23 | 0,3664 | 0,2710 | 0,4939 | 0,8180 | 1,5247 | -8,1146 | 0,75% | 1,47% | | 1,31% | 14,60% |
| DECAMETHYLCYCLOPENTASILOXANE | 617,4 | 10,35 | 0,6223 | 0,2485 | 1,4911 | 1,0000 | 0,7997 | 27,8266 | 1,42% | 1,10% | | 1,64% | 21,69% |
| DECAMETHYLTETRASILOXANE | 599,4 | 11,9 | 0,6596 | 0,2627 | 1,1940 | 0,9703 | 1,0775 | -20,3778 | 0,29% | 0,85% | | 2,72% | 18,89% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| DECAN-1,10-DIOL | 747 | 21,1 | 0,9194 | 0,2184 | 0,8601 | 0,8445 | 1,8442 | 54,3735 | 1,50% | | | 2,22% | 39,65% |
| DECANAL | 674 | 26 | 0,5201 | 0,2696 | 1,3952 | 1,0000 | 0,7673 | -16,7886 | 1,01% | 0,58% | | 1,38% | 18,15% |
| DEHYDROABIETIC ACID | 828 | 17,5 | 0,9154 | | 0,3941 | 0,8107 | 3,3255 | | 0,61% | 0,81% | | | |
| DEHYDROABIETYLAMINE | 863 | 17 | 0,7415 | | 0,6571 | 0,8208 | 1,9566 | | 0,53% | 1,07% | | | |
| DEUTERIUM OXIDE | 643,89 | 216,71 | 0,3658 | 0,2253 | 0,3802 | 0,8552 | 1,9806 | 5,5114 | 0,26% | 1,92% | 1,44% | 7,32% | 25,09% |
| DI-(2-CHLOROETHOXY)METHANE | 696,2 | 30,66 | 0,5230 | 0,2465 | 0,6788 | 0,8571 | 1,5498 | 15,5490 | 0,64% | 1,51% | | 1,55% | 21,47% |
| DI(2-CHLOROETHYL)ETHER | 666 | 35,9 | 0,3940 | 0,2470 | 0,2478 | 0,8030 | 2,3431 | 15,4778 | 0,47% | | 1,41% | 1,58% | 26,01% |
| DI-2-ETHYLHEXYLAMINE | 702 | 14,7 | 0,9179 | 0,2485 | 0,6327 | 0,8137 | 2,3444 | 6,3005 | 0,30% | 1,41% | | 2,61% | 23,27% |
| DIACETYL | 546,9 | 43,84 | 0,3641 | 0,2536 | 0,4723 | 0,7636 | 1,4466 | 6,7789 | 0,63% | 2,08% | | 1,66% | 18,65% |
| DIALLYL MALEATE | 693 | 23,3 | 0,7886 | 0,2450 | 0,7541 | 0,8318 | 1,8377 | 13,6260 | 0,58% | 0,78% | | 2,81% | 23,19% |
| DIALLYL PHTHALATE | 790,2 | 20,96 | 0,7345 | | 0,8631 | 0,8394 | 1,5500 | | 0,75% | 1,45% | | | |
| DIALLYL SULFIDE | 653,53 | 33,59 | 0,0824 | 0,2492 | 0,0000 | 0,2471 | 0,6192 | 24,8790 | 3,47% | | | 5,80% | 22,70% |
| DIALLYLAMINE | 556 | 33,2 | 0,4483 | 0,2768 | 1,2407 | 0,9959 | 0,7966 | -9,7753 | 0,65% | 0,69% | | 5,93% | 11,68% |
| DIAMANTANE | 791 | 22,6 | 0,1633 | | 0,1397 | 0,8596 | 2,4017 | | 0,46% | 3,75% | | | |
| DIAMYL KETONE | 678,5 | 20,52 | 0,5928 | 0,2479 | 0,2625 | 0,7891 | 2,8551 | 18,5170 | 0,45% | | | 1,29% | 19,45% |
| DIAMYLAMINE | 639 | 21,2 | 0,6767 | 0,2521 | 0,4228 | 0,8156 | 2,5539 | 3,3425 | 0,68% | 1,35% | | 1,74% | 21,94% |
| DIBENZOFURAN | 824 | 36,4 | 0,3988 | 0,2632 | 0,2618 | 0,8458 | 2,6172 | 0,8514 | 1,99% | 2,98% | 1,97% | 1,69% | 16,71% |
| DIBENZOPYRROLE | 899 | 32,6 | 0,4938 | | 0,3703 | 0,8543 | 2,4811 | | 1,86% | 4,63% | 0,27% | | |
| DIBENZOTHIOPHENE | 897 | 38,6 | 0,3983 | | 0,2730 | 0,8474 | 2,5723 | | 0,24% | 1,44% | | | |
| DIBORANE | 289,8 | 40,53 | 0,1311 | 0,2845 | 0,8825 | 0,9287 | 0,6115 | -5,5313 | 0,79% | 1,90% | 0,54% | 1,01% | 8,77% |
| DIBROMODIFLUOROMETHANE | 478 | 40,7 | 0,1085 | 0,2496 | 0,0614 | 0,8236 | 2,2200 | 12,0389 | 0,58% | | | 8,10% | 15,72% |
| DIBROMOMETHANE | 611 | 71,7 | 0,2095 | 0,2869 | 0,4694 | 0,8154 | 1,1474 | -8,5481 | 1,87% | 2,31% | 2,23% | 1,58% | 1,50% |
| DIBUTYL MALEATE | 716 | 19 | 0,8994 | 0,2450 | 0,6050 | 0,8137 | 2,4006 | 11,6923 | 0,53% | 0,86% | | 4,41% | 32,33% |
| DIBUTYL SEBACATE | 768 | 13,2 | 1,1245 | 0,2375 | 0,6603 | 0,8170 | 2,6713 | 27,5101 | 0,39% | 2,21% | 5,83% | 3,81% | 39,00% |
| DIBUTYL TEREPHTHALATE | 787,2 | 16,94 | 0,9642 | 0,2358 | 0,5423 | 0,8317 | 2,8709 | 31,0417 | 0,61% | | | 2,43% | 32,04% |
| DICHLOROACETALDEHYDE | 555 | 49,5 | 0,3437 | 0,2561 | 0,3218 | 0,8211 | 1,9750 | 4,6706 | 0,78% | 1,95% | | 1,24% | 17,95% |
| DICHLOROACETIC ACID | 686 | 51,7 | 0,5550 | 0,2531 | 0,5870 | 0,8156 | 1,7346 | 5,1209 | 0,66% | 1,03% | | 2,19% | 26,04% |
| DICHLOROACETYL CHLORIDE | 585 | 46,1 | 0,3089 | 0,2686 | 1,1517 | 1,0000 | 0,6959 | -3,0865 | 0,59% | 1,22% | | 1,12% | 15,70% |
| DICHLORODIETHYLSILANE | 595,75 | 30,6 | 0,3189 | 0,2733 | 1,5660 | 1,0000 | 0,5071 | -9,1447 | 1,02% | 1,65% | | 1,86% | 11,22% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| DICHLORODIFLUOROMETHANE | 384,95 | 41,25 | 0,1797 | 0,2765 | 0,1492 | 0,8586 | 2,4165 | -4,2188 | 0,34% | 1,37% | 5,74% | 1,20% | 11,86% |
| DICHLOROFLUOROMETHANE | 451,58 | 51,84 | 0,2048 | 0,2712 | 0,1506 | 0,8483 | 2,4453 | -1,7873 | 0,47% | 1,35% | 2,00% | 1,23% | 14,50% |
| DICHLOROMETHANE | 510 | 60,8 | 0,1986 | 0,2633 | 1,3448 | 1,0000 | 0,4642 | 2,8159 | 1,83% | 1,33% | 0,88% | 1,54% | 14,36% |
| DICHLOROSILANE | 451,5 | 45,99 | 0,1630 | 0,2781 | 0,1352 | 0,8186 | 2,0375 | -4,2688 | 0,45% | | | 1,14% | 7,67% |
| DICYANDIAMIDE | 834 | 53,4 | 0,6924 | | 0,3532 | 0,8052 | 2,8442 | | 0,48% | 1,07% | | | |
| DICYCLOHEXYL SULFIDE | 802 | 26,5 | 0,3955 | 0,2676 | 0,5048 | 0,8382 | 1,6281 | -7,1645 | 0,83% | 1,83% | 4,98% | 2,14% | 10,42% |
| DICYCLOPENTADIENE | 660 | 30,6 | 0,2880 | 0,2645 | 0,1239 | 0,8302 | 2,8525 | 8,7841 | 0,70% | 1,81% | 0,43% | 3,15% | 21,91% |
| DIETHANOLAMINE | 736,6 | 42,7 | 0,9529 | 0,2170 | 0,5721 | 0,8379 | 2,7540 | 24,8079 | 0,80% | 1,20% | | 3,01% | 19,22% |
| DIETHYL CARBONATE | 576 | 33,9 | 0,4857 | 0,2567 | 0,3533 | 0,8530 | 2,5019 | 1,6629 | 5,88% | 6,71% | | 1,26% | 21,52% |
| DIETHYL DISULFIDE | 642 | 38,7 | 0,3469 | 0,2695 | 0,5475 | -0,6196 | 2,0694 | 3,6899 | 2,30% | 2,62% | 2,59% | 2,67% | 17,40% |
| DIETHYL ETHER | 466,7 | 36,4 | 0,2811 | 0,2641 | 0,9137 | 0,8449 | 0,7998 | 0,8388 | 1,26% | 2,01% | 4,75% | 1,47% | 16,74% |
| DIETHYL MALEATE | 680 | 26,1 | 0,6658 | 0,2614 | 0,7521 | 0,9127 | 1,7721 | -9,5014 | 0,42% | | | 3,12% | 32,95% |
| DIETHYL MALONATE | 653 | 27,8 | 0,6155 | 0,2519 | 1,3575 | 1,0000 | 0,8830 | 7,0705 | 0,63% | | | 2,37% | 26,50% |
| DIETHYL PHTHALATE | 776 | 22,6 | 0,6249 | 0,2410 | 0,2833 | 0,8189 | 3,1361 | 29,2771 | 1,29% | 2,69% | | 1,67% | 23,30% |
| DIETHYL SUCCINATE | 663 | 25,3 | 0,6995 | 0,2525 | 0,3418 | 0,8230 | 3,0472 | 5,7045 | 4,89% | 3,58% | 3,89% | 2,68% | 17,04% |
| DIETHYL SULFATE | 749 | 64,8 | 0,3865 | 0,3829 | 1,1698 | 1,0000 | 0,7735 | -81,1483 | 0,58% | | 1,63% | 11,75% | 5,38% |
| DIETHYL SULFIDE | 557,15 | 39,6 | 0,2900 | 0,2665 | 0,6618 | 0,8320 | 1,0597 | -1,1574 | 0,96% | 2,61% | 0,71% | 1,33% | 13,44% |
| DIETHYLALUMINUM CHLORIDE | 723,15 | 30 | 0,3177 | | 1,5638 | 1,0000 | 0,5073 | | 1,15% | 2,00% | | | |
| DIETHYLAMINE | 496,6 | 37,1 | 0,3039 | 0,2611 | 1,0623 | 0,9023 | 0,7363 | 2,6822 | 0,47% | 2,44% | 0,61% | 1,72% | 12,77% |
| DIETHYLENE GLYCOL | 744,6 | 46 | 0,6221 | 0,2291 | 0,2641 | 0,8150 | 3,2231 | 20,2178 | 2,31% | | | 3,48% | 26,12% |
| DIETHYLENE GLYCOL DIETHYL ETHER | 624 | 23,7 | 0,6807 | 0,2550 | 0,4501 | 0,8369 | 2,5647 | -0,1768 | 0,59% | 1,61% | | 2,45% | 20,63% |
| DIETHYLENE GLYCOL DIMETHYL ETHER | 608 | 28,6 | 0,5775 | 0,2553 | 0,3217 | 0,8326 | 2,8529 | 3,4440 | 0,26% | 0,47% | | 2,93% | 27,94% |
| DIETHYLENE GLYCOL DI-n-BUTYL ETHER | 680 | 17,6 | 0,8455 | 0,2499 | 0,6358 | 0,8593 | 2,4070 | 3,0320 | 3,90% | | | 4,00% | 22,60% |
| DIETHYLENE GLYCOL ETHYL ETHER ACETATE | 660 | 24,2 | 0,7145 | 0,2490 | 0,7080 | 0,8953 | 1,9520 | 7,9192 | 1,50% | 3,00% | | 2,45% | 21,97% |
| DIETHYLENE GLYCOL MONOBUTYL ETHER ACETATE | 679 | 20,6 | 0,8420 | 0,2487 | 0,4196 | 0,8221 | 3,0660 | 6,0897 | 1,74% | | 1,95% | 3,07% | 22,63% |
| DIETHYLENE GLYCOL MONOPROPYL ETHER | 679,8 | 30,02 | 0,6114 | 0,2609 | 0,2802 | 0,8205 | 3,0996 | -4,1549 | 1,07% | 2,22% | 6,94% | 3,19% | 19,21% |
| DIETHYLSULFITE | 624 | 37,7 | 0,5065 | 0,2758 | 0,4407 | 0,8661 | 2,2449 | -15,8930 | 0,29% | 3,24% | | 3,22% | 17,68% |
| DIFLUOROMETHANE | 351,255 | 57,84 | 0,2771 | 0,2440 | 0,2968 | 0,8542 | 1,9991 | 7,2560 | 0,42% | 1,87% | 0,80% | 2,65% | 20,29% |
| DIFLUOROMETHYL TRIFLUOROMETHYL ETHER | 354,49 | 33,76 | 0,3253 | 0,2642 | 0,4436 | 0,8304 | 1,5745 | -2,1138 | 0,63% | 1,64% | 3,37% | 2,01% | 27,59% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| DIGLYCOLIC ACID | 820 | 44,2 | 1,0807 | | 0,4660 | 0,8090 | 3,3675 | | 0,57% | 0,99% | | | |
| DIHEXYL ADIPATE | 767 | 13,2 | 1,0935 | 0,2422 | 0,6460 | 0,8091 | 2,6442 | 18,2850 | 1,73% | 1,49% | 4,91% | 4,89% | 39,70% |
| DIIODOMETHANE | 747 | 54,7 | 0,1405 | 0,2379 | 0,0508 | 0,7806 | 2,0461 | 24,5608 | 1,06% | 2,72% | 4,47% | 6,51% | 19,29% |
| DIISOBUTYL ETHER | 562 | 25,3 | 0,4243 | 0,2703 | 0,2667 | 0,8183 | 2,4737 | -11,9423 | 0,27% | 4,47% | 0,71% | 1,95% | 19,03% |
| DIISOBUTYL KETONE | 615 | 24,8 | 0,5116 | 0,2581 | 0,3114 | 0,8393 | 2,7303 | -1,2414 | 2,66% | 2,97% | | 1,35% | 21,66% |
| DIISOBUTYL PHTHALATE | 762 | 17,8 | 0,9158 | 0,2503 | 0,6180 | 0,8176 | 2,4080 | 1,2277 | 0,88% | 1,43% | | 4,25% | 22,66% |
| DIISOBUTYLAMINE | 580 | 25,7 | 0,4854 | 0,2689 | 1,1536 | 1,0000 | 0,9089 | -12,3569 | 0,69% | | | 1,78% | 12,44% |
| DIISONONYL PHTHALATE | 835 | 10,8 | 1,0312 | | 0,6284 | 0,8167 | 2,6093 | | 1,19% | 1,24% | 1,54% | | |
| DIISOOCTYL PHTHALATE | 851 | 11,8 | 1,0880 | 0,2367 | 0,6976 | 0,8141 | 2,4790 | 45,7252 | 1,21% | 1,75% | 1,04% | 4,91% | 26,59% |
| DIISOPENTYLSULFIDE | 664,4 | 21,81 | 0,5971 | 0,2580 | 0,4902 | 0,8301 | 2,1524 | -3,0414 | 0,55% | | | 2,49% | 21,00% |
| DIISOPROPYL ETHER | 500,05 | 28,8 | 0,3387 | 0,2699 | 1,2730 | 1,0000 | 0,6465 | -6,1126 | 0,87% | 3,92% | 0,53% | 1,19% | 16,55% |
| DIISOPROPYL KETONE | 576 | 30,2 | 0,4044 | 0,2630 | 1,0546 | 1,0000 | 0,9023 | -2,2526 | 1,52% | 1,40% | | 1,32% | 17,72% |
| DIISOPROPYL SULFIDE | 585,2 | 32,25 | 0,3144 | 0,2782 | 0,2025 | 0,8443 | 2,6103 | -14,5108 | 0,88% | 2,51% | 0,40% | 1,89% | 15,25% |
| DIKETENE | 616 | 59,6 | 0,3821 | | 1,4817 | 1,0000 | 0,5843 | | 1,46% | | 1,05% | | |
| DILACTIC ACID | 660 | 34,8 | 0,9068 | | 0,5472 | 0,8186 | 2,6426 | | 0,33% | 0,43% | 2,54% | | |
| DIMERCAPTOETHYL ETHER | 720 | 36,9 | 0,4193 | 0,2454 | 0,7718 | 0,8629 | 1,1975 | 17,4319 | 0,83% | 1,31% | | 1,72% | 27,32% |
| DIMETHYL CARBONATE | 548 | 45 | 0,3846 | 0,2490 | 0,3088 | 0,8588 | 2,4135 | 8,1244 | 0,71% | 2,20% | | 1,85% | 20,77% |
| DIMETHYL DISULFIDE | 615 | 53,6 | 0,2059 | 0,2756 | 0,6400 | 0,8173 | 0,9152 | -4,7632 | 0,64% | 1,25% | 0,69% | 1,42% | 18,26% |
| DIMETHYL ETHER | 400,1 | 53,7 | 0,2002 | 0,2736 | 0,6020 | 0,8484 | 0,9760 | -2,1955 | 1,31% | 2,99% | 0,77% | 1,20% | 13,31% |
| DIMETHYL MALEATE | 675 | 32,2 | 0,5624 | 0,2391 | 0,3660 | 0,8146 | 2,4540 | 21,0954 | 0,47% | 1,89% | 2,01% | 1,38% | 27,71% |
| DIMETHYL PHTHALATE | 766 | 27,8 | 0,6568 | 0,2443 | 1,2643 | 0,9998 | 1,0064 | 17,8593 | 0,68% | | | 2,10% | 29,51% |
| DIMETHYL SILANE | 402 | 35,6 | 0,1300 | 0,2704 | 0,1636 | 0,8732 | 2,2150 | 0,0099 | 2,80% | 1,85% | | 1,30% | 11,86% |
| DIMETHYL SUCCINATE | 657 | 32,8 | 0,6223 | 0,2505 | 0,5841 | 0,8819 | 2,1054 | 5,7913 | 2,95% | | | 1,41% | 19,38% |
| DIMETHYL SULFIDE | 503,04 | 55,3 | 0,1943 | 0,2662 | 0,2563 | 0,8341 | 1,7208 | 0,4452 | 1,05% | 2,41% | 1,30% | 2,38% | 15,45% |
| DIMETHYL SULFOXIDE | 729 | 56,5 | 0,2806 | 0,2353 | 1,3438 | 1,0000 | 0,5655 | 22,0116 | 3,22% | 2,33% | 0,69% | 2,99% | 35,58% |
| DIMETHYL TEREPHTHALATE | 777,4 | 27,6 | 0,5807 | 0,2358 | 0,4147 | 0,8507 | 2,5160 | 30,7165 | 0,36% | | | 1,69% | 30,28% |
| DIMETHYL-1,4-CYCLOHEXANEDICARBOXYLATE | 736 | 24,9 | 0,6412 | 0,2420 | 0,2910 | 0,8190 | 3,1334 | 20,0964 | 1,00% | 1,49% | 6,73% | 1,18% | 29,24% |
| DIMETHYL-2,6-NAPHTHALENEDICARBOXYLATE | 883 | 24,85 | 0,6853 | | 0,3269 | 0,8182 | 3,0641 | | 0,30% | 1,02% | | | |
| DIMETHYLACETYLENE | 473,2 | 48,7 | 0,2385 | 0,2648 | 0,5053 | 0,8287 | 1,1969 | 1,0656 | 0,27% | 1,32% | 0,24% | 1,79% | 11,89% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| DIMETHYLALUMINUM CHLORIDE | 619 | 36,2 | 0,1834 | 0,2253 | 0,0000 | 0,3499 | 0,8754 | 42,0220 | 1,95% | | | 6,64% | 23,44% |
| DIMETHYLAMINE | 437,2 | 53,4 | 0,2999 | 0,2611 | 0,9960 | 0,7757 | 0,7533 | 0,8950 | 1,92% | 2,85% | 2,41% | 2,93% | 15,76% |
| DIMETHYLCHLOROSILANE | 472 | 36,2 | 0,2526 | 0,2677 | 0,4770 | 0,9247 | 1,5369 | -2,6073 | 1,34% | 2,04% | | 1,41% | 12,33% |
| DIMETHYLDICHLOROSILANE | 520,35 | 34,9 | 0,2675 | 0,2756 | 1,3160 | 1,0000 | 0,5521 | -6,9354 | 0,26% | 0,72% | 3,74% | 1,37% | 8,38% |
| DIMETHYLDIMETHOXYSILANE | 524 | 26,6 | 0,2629 | 0,2495 | 0,0000 | 0,2940 | 0,9297 | 18,4455 | 1,46% | | | 4,29% | 9,99% |
| DIMETHYLETHANOLAMINE | 571,82 | 41,4 | 0,7110 | 0,2612 | 0,5531 | 0,8113 | 2,1534 | -5,2996 | 0,92% | 1,03% | | 2,58% | 19,44% |
| DIMETHYLKETENE | 470,2 | 42,35 | 0,3112 | | 0,5875 | 0,9366 | 1,4159 | | 0,57% | | 7,30% | | |
| DI-n-BUTYL ETHER | 584,1 | 24,6 | 0,4476 | 0,2586 | 0,4528 | 0,8149 | 1,8238 | 1,8905 | 0,51% | 1,42% | 1,12% | 1,77% | 24,22% |
| DI-n-BUTYL PHTHALATE | 781 | 17,5 | 0,9569 | 0,2466 | 0,6494 | 0,8508 | 2,5372 | 7,6732 | 1,87% | | | 5,04% | 33,92% |
| DI-n-BUTYL SULFATE | 814 | 60 | 0,3651 | 0,4635 | 0,4329 | 0,7809 | 1,5602 | -168,9007 | 0,52% | | 3,60% | 18,50% | 15,33% |
| DI-n-BUTYL SULFIDE | 652 | 25,79 | 0,4665 | 0,2560 | 0,9777 | 0,9710 | 1,0710 | 3,7394 | 0,66% | | | 1,58% | 24,02% |
| DI-n-BUTYL SULFONE | 767 | 25,4 | 0,6877 | 0,2416 | 0,5841 | 0,8155 | 2,0251 | 21,8039 | 0,59% | 0,95% | | 1,53% | 31,81% |
| DI-n-BUTYLAMINE | 602,3 | 25,7 | 0,5296 | 0,2618 | 0,2751 | 0,8300 | 2,9028 | -5,1290 | 3,50% | 2,15% | 2,01% | 1,74% | 17,99% |
| DI-n-DECYL PHTHALATE | 905 | 9,95 | 0,8906 | 0,2194 | 0,4725 | 0,8242 | 2,9614 | 131,6393 | 1,10% | 2,75% | | 1,94% | 48,18% |
| DI-n-HEXYL ETHER | 658 | 18,16 | 0,7105 | 0,2486 | 0,5793 | 0,8037 | 2,0486 | 9,8182 | 0,48% | 1,29% | 2,01% | 2,07% | 31,27% |
| DI-n-HEXYL PHTHALATE | 793 | 14 | 1,1245 | 0,2377 | 0,9394 | 0,8412 | 1,9772 | 22,8279 | 0,53% | 0,63% | 1,42% | 3,51% | 34,42% |
| DI-n-NONYL PHTHALATE | 866 | 10,7 | 0,9961 | 0,2434 | 0,6061 | 0,7149 | 2,3262 | 35,5619 | 3,41% | | 5,61% | 7,23% | 48,40% |
| DI-n-OCTYL ETHER | 707 | 14,4 | 0,9336 | 0,2423 | 0,5295 | 0,8067 | 2,7115 | 17,4400 | 0,57% | 1,23% | 1,47% | 2,50% | 35,98% |
| DI-n-OCTYL TEREPHTHALATE | 855 | 11,6 | 1,0895 | 0,2342 | 0,6724 | 0,8084 | 2,5534 | 56,6243 | 1,14% | 1,77% | 0,75% | 3,36% | 26,89% |
| DI-n-OCTYLAMINE | 734 | 12,6 | 0,8187 | 0,2256 | 0,7506 | 0,8520 | 1,9446 | 85,8266 | 0,19% | | | 1,69% | 28,42% |
| DINONYL ETHER | 736 | 13 | 1,0021 | 0,2426 | 0,5557 | 0,8183 | 2,8189 | 19,6338 | 0,47% | | | 3,54% | 39,94% |
| DINONYLPHENOL | 902 | 12,4 | 1,1246 | | 0,5229 | 0,8147 | 3,2301 | | 0,71% | 1,35% | | | |
| DI-n-PENTYL ETHER | 622 | 20,9 | 0,6012 | 0,2534 | 0,3230 | 0,8300 | 2,9032 | 3,9977 | 1,02% | 6,51% | 2,62% | 2,09% | 27,60% |
| DI-n-PROPYL DISULFIDE | 675 | 30,3 | 0,4370 | 0,2649 | 0,4925 | 0,8207 | 1,6832 | -4,5118 | 1,02% | 2,58% | 1,80% | 2,55% | 23,95% |
| DI-n-PROPYL ETHER | 530,6 | 30,28 | 0,3688 | 0,2652 | 0,2793 | 0,8428 | 2,3806 | -3,9336 | 1,00% | 2,58% | 2,97% | 1,45% | 18,27% |
| DI-n-PROPYL SULFIDE | 608 | 30,8 | 0,3740 | 0,2600 | 0,2984 | 0,8338 | 2,2462 | 1,8904 | 1,06% | 2,54% | 1,21% | 1,54% | 22,00% |
| DI-n-PROPYL SULFONE | 763 | 31,1 | 0,5821 | 0,2415 | 0,9953 | 0,8872 | 1,1727 | 21,4609 | 0,30% | 0,35% | | 1,41% | 30,80% |
| DI-n-PROPYLAMINE | 550 | 31,4 | 0,4497 | 0,2689 | 0,2676 | 0,8390 | 2,7346 | -8,8980 | 1,43% | 1,13% | 2,17% | 1,51% | 13,58% |
| DIPHENYL DISULFIDE | 829,8 | 35,69 | 0,5697 | | 0,1552 | 0,6883 | 2,5166 | | 0,38% | | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c_{P,liq}^{sat}$ | $v_{liq}^{sat}$ | $v_c$ |
| DIPHENYL ETHER | 766,8 | 30,8 | 0,4389 | 0,2557 | 0,4108 | 0,8741 | 2,2038 | 7,1589 | 0,81% | 1,92% | | 1,62% | 25,08% |
| DIPHENYLACETYLENE | 832 | 29 | 0,3836 | | 0,8124 | 0,8724 | 1,0866 | | 0,60% | 1,24% | | | |
| DIPHENYLAMINE | 817 | 31,8 | 0,5297 | 0,2493 | 0,3500 | 0,8451 | 2,6287 | 13,3668 | 0,36% | 1,05% | | 1,38% | 19,35% |
| DIPHENYLDICHLOROSILANE | 814 | 23,3 | 0,4283 | 0,2423 | 1,8802 | 1,0000 | 0,4888 | 34,9370 | 1,57% | | 1,88% | 2,49% | 27,30% |
| DIPHENYLMETHANE | 760 | 27,1 | 0,4816 | 0,2424 | 0,2647 | 0,8336 | 2,8350 | 26,0760 | 0,46% | 0,67% | | 1,39% | 22,68% |
| DIPROPYL MALEATE | 691 | 22 | 0,7815 | 0,2468 | 0,3920 | 0,8170 | 3,0084 | 10,3533 | 0,72% | 1,53% | | 2,48% | 29,06% |
| DIPROPYLENE GLYCOL n-BUTYL ETHER | 647,1 | 20,96 | 1,0022 | 0,2563 | 0,6608 | 0,8465 | 2,6063 | -12,6706 | 3,73% | | | 5,26% | 21,29% |
| DIPROPYLENE GLYCOL t-BUTYL ETHER | 667 | 22,3 | 0,9966 | | 0,5322 | 0,8079 | 2,8506 | | 0,82% | 1,60% | 2,23% | | |
| DI-sec-BUTYL ETHER | 559 | 25,3 | 0,4319 | 0,2687 | 0,3206 | 0,8369 | 2,3740 | -10,3799 | 1,85% | 2,23% | 2,25% | 2,05% | 16,42% |
| DISILANE | 432 | 51,3 | 0,0939 | 0,3179 | 0,1252 | 0,8736 | 2,2094 | -24,2942 | 0,74% | 2,94% | | 1,35% | 7,41% |
| DI-t-BUTYL PEROXIDE | 547 | 24,8 | 0,4031 | 0,2794 | 0,2182 | 0,8315 | 2,7892 | -23,3983 | 0,74% | 1,65% | | 1,33% | 15,58% |
| DI-tert-BUTYL DISULFIDE | 689,7 | 31,59 | 0,4020 | | 0,3281 | 0,8606 | 2,3873 | | 0,40% | | | | |
| DI-tert-BUTYL ETHER | 550 | 23,23 | 0,2985 | 0,2555 | 1,5488 | 1,0000 | 0,4964 | 11,4707 | 1,53% | 1,39% | | 2,24% | 21,90% |
| DI-tert-BUTYL SULFIDE | 623,2 | 25,91 | 0,3008 | | 1,2943 | 0,9995 | 0,6025 | | 0,60% | 1,71% | | | |
| DIVINYL ETHER | 463 | 42,5 | 0,2911 | | 0,2084 | 0,8509 | 2,5343 | | 1,02% | 2,12% | | | |
| DODECAMETHYLCYCLOHEXASILOXANE | 645,8 | 9,005 | 0,7095 | 0,2488 | 1,5116 | 1,0000 | 0,8621 | 24,9833 | 0,29% | 1,04% | | 1,61% | 22,16% |
| DODECAMETHYLPENTASILOXANE | 628,4 | 9,45 | 0,7202 | 0,2560 | 1,1281 | 0,8621 | 1,1911 | 1,1205 | 0,80% | 1,10% | | 3,96% | 21,32% |
| DODECANAL | 705,1 | 23,2 | 0,6808 | | 1,2632 | 0,9982 | 1,0395 | | 0,62% | 1,82% | | | |
| DODECANEDIOIC ACID | 847 | 21,5 | 1,0418 | | 0,5025 | 0,8139 | 3,1141 | | 1,24% | | | | |
| EICOSAMETHYLNONASILOXANE | 707,2 | 5,75 | 1,0500 | 0,2430 | 0,8761 | 0,8057 | 1,9589 | 39,5104 | 0,91% | 1,43% | | 4,46% | 27,21% |
| epsilon-CAPROLACTAM | 818,2 | 46,21 | 0,3850 | 0,2504 | 1,7563 | 1,0000 | 0,4968 | 13,1771 | 1,06% | 1,41% | 0,78% | 1,33% | 16,23% |
| ERUCIC ACID | 809,9 | 10,21 | 1,2417 | 0,2247 | 0,6742 | 0,8300 | 2,9039 | 101,5677 | 0,75% | | | 4,39% | 24,25% |
| ETHANE | 305,32 | 48,72 | 0,0995 | 0,2817 | 0,3041 | 0,8694 | 1,3340 | -3,6754 | 0,41% | 1,30% | 7,25% | 1,18% | 12,61% |
| ETHANESULFONYL CHLORIDE | 682 | 47,4 | 0,3688 | 0,2541 | 0,2795 | 0,8544 | 2,4802 | 6,8643 | 1,08% | | | 1,45% | 18,71% |
| ETHANOL | 514 | 61,37 | 0,6436 | 0,2377 | 0,7770 | 0,9043 | 1,6691 | 5,9029 | 2,60% | 1,42% | 2,28% | 2,62% | 23,91% |
| ETHYL ACETATE | 523,3 | 38,8 | 0,3664 | 0,2549 | 1,0052 | 0,9200 | 0,8735 | 5,7372 | 0,92% | 1,71% | 0,36% | 1,45% | 18,52% |
| ETHYL ACETOACETATE | 642,9 | 32,7 | 0,5552 | 0,2461 | 0,4454 | 0,8406 | 2,2484 | 11,7107 | 0,50% | | | 1,32% | 19,70% |
| ETHYL ACRYLATE | 553 | 36,8 | 0,3718 | 0,2549 | 1,1573 | 1,0000 | 0,7703 | 5,5212 | 1,02% | 1,06% | | 1,82% | 17,20% |
| ETHYL ALUMINUM DICHLORIDE | 646,05 | 18,6 | 0,5338 | 0,1451 | 0,5960 | 0,8172 | 1,6742 | 183,0391 | 0,52% | 3,54% | | 22,33% | 130,30% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| ETHYL BENZOATE | 698 | 31,8 | 0,4771 | 0,2573 | 0,9128 | 0,9832 | 1,1851 | 4,4801 | 1,49% | 0,68% | | 2,27% | 13,81% |
| ETHYL CAPRATE | 688,1 | 17,88 | 0,6253 | 0,2427 | 1,8214 | 1,0000 | 0,6411 | 30,7178 | 0,70% | 1,15% | | 1,50% | 22,79% |
| ETHYL CAPRYLATE | 649 | 21,18 | 0,6114 | 0,2503 | 0,6941 | 0,8332 | 1,6478 | 11,0468 | 0,65% | 1,54% | | 1,90% | 21,02% |
| ETHYL CHLORIDE | 460,35 | 52,7 | 0,1886 | 0,2662 | 0,3689 | 0,8252 | 1,3384 | 1,0436 | 0,39% | 2,87% | 1,37% | 1,55% | 15,74% |
| ETHYL CHLOROFORMATE | 508,15 | 45 | 0,8350 | 0,2806 | 0,6293 | 0,8162 | 2,2036 | -17,6458 | 0,53% | 0,69% | | 4,31% | 11,77% |
| ETHYL CYANOACETATE | 679 | 33,4 | 0,5584 | 0,2184 | 0,7132 | 0,8321 | 1,5057 | 41,5131 | 0,22% | | | 4,10% | 33,54% |
| ETHYL ERUCATE | 808,2 | 8,817 | 1,1236 | | 0,6240 | 0,8316 | 2,8717 | | 0,61% | | | | |
| ETHYL FLUORIDE | 375,31 | 50,28 | 0,2179 | 0,2607 | 0,4165 | 0,8751 | 1,4524 | 2,5788 | 0,50% | 2,14% | 1,81% | 1,75% | 18,37% |
| ETHYL FORMATE | 508,4 | 47,4 | 0,2847 | 0,2579 | 1,0861 | 0,9039 | 0,6935 | 4,4451 | 0,82% | 1,61% | 0,68% | 1,97% | 17,77% |
| ETHYL HYDROGEN SULFATE | 857 | 89,8 | 0,4939 | | 1,2498 | 0,9860 | 0,8408 | | 0,68% | 0,52% | | | |
| ETHYL HYDROPEROXIDE | 560 | 65,81 | 0,4656 | | 1,6402 | 1,0000 | 0,5984 | | 0,94% | 0,98% | | | |
| ETHYL IODIDE | 554 | 47,11 | 0,1674 | 0,2501 | 1,0063 | 1,0000 | 0,6187 | 12,4872 | 2,16% | 1,35% | | 3,38% | 17,10% |
| ETHYL ISOAMYL KETONE | 617 | 27,27 | 0,4242 | 0,2568 | 0,1410 | 0,7159 | 2,3156 | 6,5935 | 0,47% | | | 1,32% | 18,36% |
| ETHYL ISOBUTYL ETHER | 519,2 | 30,41 | 0,3552 | 0,2719 | 1,1689 | 1,0000 | 0,7421 | -8,9089 | 0,63% | 1,09% | | 1,67% | 15,36% |
| ETHYL ISOBUTYRATE | 553,15 | 30,4 | 0,4264 | 0,2634 | 0,3068 | 0,8260 | 2,3377 | -1,3591 | 0,37% | 3,65% | 0,76% | 1,96% | 13,76% |
| ETHYL ISOPROPYL ETHER | 489 | 34,1 | 0,3056 | 0,2793 | 1,1995 | 0,9810 | 0,6562 | -11,2014 | 0,87% | 2,19% | 0,64% | 2,56% | 14,81% |
| ETHYL ISOPROPYL KETONE | 567 | 33,2 | 0,3891 | 0,2659 | 1,1295 | 1,0000 | 0,8123 | -1,5244 | 1,12% | 0,42% | | 2,48% | 18,71% |
| ETHYL ISOVALERATE | 587,95 | 28,4 | 0,4000 | 0,2636 | 1,4402 | 1,0000 | 0,6255 | -1,3388 | 2,58% | 4,46% | 0,76% | 1,91% | 20,01% |
| ETHYL LACTATE | 606,95 | 37,4006 | 0,6032 | 0,2601 | 0,3634 | 0,8379 | 2,7556 | -3,0179 | 0,48% | | | 2,01% | 18,02% |
| ETHYL LAURATE | 716,3 | 15,29 | 0,6992 | 0,2358 | 0,2339 | 0,7072 | 2,6944 | 51,6999 | 0,38% | | | 1,46% | 24,66% |
| ETHYL LEVULINATE | 666,1 | 29,24 | 0,6071 | 0,2463 | 0,3501 | 0,8346 | 2,8156 | 13,1006 | 0,30% | | | 1,78% | 21,87% |
| ETHYL LINOLEATE | 777,8 | 11,27 | 0,9443 | 0,2300 | 0,7308 | 0,8599 | 2,2459 | 85,7695 | 0,50% | | | 4,78% | 20,73% |
| ETHYL LINOLENATE | 779,8 | 11,5 | 0,9334 | 0,2313 | 0,6198 | 0,8146 | 2,4268 | 83,0256 | 0,64% | 1,75% | | 4,06% | 18,71% |
| ETHYL MERCAPTAN | 499,15 | 54,9 | 0,1878 | 0,2699 | 0,6890 | 0,8455 | 0,8462 | -0,7942 | 0,44% | 1,92% | 1,22% | 1,52% | 12,64% |
| ETHYL METHACRYLATE | 577 | 32,5 | 0,3432 | 0,2505 | 0,4879 | 0,8125 | 1,4591 | 10,8937 | 0,38% | 1,40% | | 3,18% | 18,10% |
| ETHYL METHYL DISULFIDE | 628,9 | 46,15 | 0,3010 | | 0,3039 | 0,8743 | 2,2012 | | 0,38% | | | | |
| ETHYL MYRISTATE | 738,7 | 13,23 | 0,7642 | 0,2296 | 1,8670 | 1,0000 | 0,7133 | 75,7691 | 0,73% | 1,36% | | 1,54% | 26,29% |
| ETHYL n-BUTYRATE | 571 | 29,5 | 0,4011 | 0,2503 | 0,2925 | 0,8370 | 2,3952 | 11,7841 | 0,45% | 3,07% | | 1,43% | 19,83% |
| ETHYL n-HEXYL ETHER | 583 | 24,6 | 0,4944 | 0,2576 | 0,4995 | 0,7980 | 1,7611 | 1,6514 | 0,67% | 2,17% | 0,67% | 1,76% | 24,04% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| ETHYL n-OCTYL SULFIDE | 700 | 24 | 0,5346 | 0,2725 | 0,2895 | 0,8318 | 2,8692 | -19,8829 | 1,81% | 1,35% | | 3,55% | 9,20% |
| ETHYL n-PENTYL SULFIDE | 633,2 | 27,97 | 0,4349 | | 1,2262 | 0,9951 | 0,7926 | | 0,63% | 1,37% | | | |
| ETHYL OLEATE | 772,1 | 10,98 | 0,9426 | 0,2245 | 0,6218 | 0,8481 | 2,5795 | 98,4175 | 0,58% | | | 2,86% | 29,68% |
| ETHYL PHENYL ACETATE | 702,1 | 28,53 | 0,5251 | 0,2525 | 0,7299 | 0,8539 | 1,4487 | 8,5486 | 0,51% | 1,47% | | 1,66% | 20,01% |
| ETHYL PROPIONATE | 546 | 33,62 | 0,3944 | 0,2539 | 0,5168 | 0,8085 | 1,5128 | 7,2820 | 0,64% | 1,92% | 0,31% | 1,34% | 18,20% |
| ETHYL PROPYL DISULFIDE | 660 | 36,12 | 0,3910 | 0,2746 | 0,2965 | 0,8538 | 2,4624 | -13,8892 | 0,38% | | | 2,59% | 15,33% |
| ETHYL PROPYL SULFIDE | 583,9 | 34,46 | 0,3331 | 0,2655 | 0,3716 | 0,8455 | 1,8703 | -1,9883 | 1,20% | 2,31% | | 1,71% | 16,33% |
| ETHYL STEARATE | 777,9 | 10,19 | 0,8985 | 0,2179 | 0,7954 | 0,7754 | 1,8341 | 140,2956 | 0,81% | 1,11% | | 1,73% | 31,22% |
| ETHYL t-BUTYL SULFIDE | 588 | 31,3 | 0,2861 | 0,2689 | 0,2056 | 0,8160 | 2,2183 | -4,7262 | 0,28% | 1,45% | 0,21% | 1,28% | 17,69% |
| ETHYL TERT-BUTYL DISULFIDE | 659,9 | 30,76 | 0,3471 | 0,2695 | 0,8691 | 0,9408 | 0,9968 | -7,9814 | 0,59% | 1,35% | | 1,61% | 15,65% |
| ETHYL tert-PENTYL ETHER | 546 | 27,4 | 0,3382 | 0,2654 | 1,2874 | 1,0000 | 0,6418 | -1,7431 | 0,82% | 1,94% | 3,89% | 1,25% | 13,06% |
| ETHYL THIOLACETATE | 590,55 | 40,75 | 0,3098 | 0,2641 | 1,1276 | 1,0000 | 0,7163 | 0,3117 | 0,53% | 0,88% | | 1,29% | 16,01% |
| ETHYL VANILLIN | 748 | 32,7 | 1,0728 | | 0,4974 | 0,8093 | 3,1919 | | 0,50% | 0,74% | | | |
| ETHYL VINYL ETHER | 475,15 | 40,7 | 0,2665 | 0,2698 | 0,4583 | 0,8394 | 1,3934 | -1,9761 | 0,72% | 1,32% | | 1,55% | 14,20% |
| ETHYL-3-ETHOXYPROPIONATE | 621 | 26,6 | 0,4975 | 0,2564 | 0,4970 | 0,7967 | 1,7717 | 6,2031 | 0,53% | 1,70% | 0,44% | 2,66% | 28,93% |
| ETHYLACETYLENE | 440 | 46 | 0,2470 | 0,2703 | 1,3229 | 1,0000 | 0,5247 | -2,0900 | 0,98% | 2,07% | 0,61% | 1,29% | 18,54% |
| ETHYLAL | 524 | 32,8 | 0,4297 | 0,2661 | 0,2128 | 0,8306 | 2,8912 | -5,4491 | 2,64% | 5,99% | 1,12% | 1,14% | 18,56% |
| ETHYLAMINE | 456,15 | 56,2 | 0,2848 | 0,2664 | 0,6667 | 0,7694 | 1,0012 | 0,2792 | 0,22% | 1,34% | 1,29% | 1,00% | 0,08% |
| ETHYLBENZENE | 617,15 | 36,09 | 0,3035 | 0,2620 | 0,4990 | 0,8222 | 1,3543 | 2,7030 | 0,81% | 0,88% | 0,49% | 1,41% | 16,14% |
| ETHYLBENZENE HYDROPEROXIDE | 737 | 37,9 | 0,8130 | 0,2573 | 0,8093 | 0,8375 | 1,7711 | -5,0889 | 1,30% | 1,03% | 2,86% | 2,94% | 20,70% |
| ETHYLCHLOROACETATE | 618 | 37,9 | 0,3932 | 0,2480 | 1,2938 | 1,0000 | 0,7016 | 12,5741 | 0,73% | 0,84% | | 1,77% | 23,60% |
| ETHYLCYCLOHEXANE | 609,15 | 30,4 | 0,2455 | 0,2590 | 1,2811 | 1,0000 | 0,5523 | 8,1470 | 1,25% | 0,99% | 0,89% | 1,87% | 17,21% |
| ETHYLCYCLOPENTANE | 569,5 | 34 | 0,2701 | 0,2668 | 0,8506 | 0,8661 | 0,8421 | -1,3241 | 1,14% | 1,55% | 1,31% | 1,52% | 14,51% |
| ETHYLENE | 282,34 | 50,41 | 0,0862 | 0,2825 | 0,2506 | 0,8535 | 1,3897 | -3,2910 | 0,29% | 1,25% | 3,15% | 1,10% | 11,79% |
| ETHYLENE CARBONATE | 806 | 67,7 | 0,4423 | 0,2235 | 0,4728 | 0,8909 | 2,0007 | 21,1394 | 4,33% | 4,69% | | 5,02% | 46,71% |
| ETHYLENE GLYCOL | 720 | 82 | 0,5068 | 0,2383 | 1,5389 | 1,0000 | 0,6793 | 8,3724 | 2,47% | 1,53% | 4,43% | 4,23% | 13,11% |
| ETHYLENE GLYCOL DIACETATE | 653 | 30,9 | 0,5595 | 0,2456 | 0,3083 | 0,8305 | 2,8940 | 13,9472 | 4,91% | 1,76% | | 1,52% | 26,48% |
| ETHYLENE GLYCOL DIACRYLATE | 689 | 27 | 0,6618 | 0,2441 | 0,9868 | 0,9625 | 1,3470 | 16,2182 | 0,50% | | | 2,01% | 22,78% |
| ETHYLENE GLYCOL DINITRATE | 654 | 40,4 | 0,7904 | 0,2500 | 0,7107 | 0,8471 | 1,9785 | 4,2455 | 0,42% | 0,57% | | 2,94% | 13,12% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| ETHYLENE OXIDE | 469,15 | 71,9 | 0,1974 | 0,2565 | 0,6207 | 0,8594 | 0,9605 | 4,1322 | 0,24% | 1,69% | 0,59% | 2,99% | 15,93% |
| ETHYLENEDIAMINE | 593 | 62,9 | 0,4724 | 0,2546 | 0,2359 | 0,8296 | 2,9106 | 2,3435 | 2,93% | 4,23% | 1,52% | 1,70% | 9,62% |
| ETHYLENEIMINE | 537 | 68,5 | 0,2007 | 0,2385 | 0,9526 | 0,2990 | 0,6035 | 12,6922 | 1,17% | 2,39% | | 6,53% | 8,48% |
| ETHYLIDENE DIACETATE | 627 | 31,4 | 0,5263 | 0,2537 | 1,3507 | 0,9993 | 0,8004 | 4,9029 | 0,91% | 1,02% | 2,44% | 1,13% | 21,50% |
| ETHYLNORBORNENE | 625 | 30,6 | 0,2605 | 0,2571 | 0,7447 | 0,8889 | 0,9618 | 10,4295 | 0,78% | 1,83% | | 1,55% | 17,07% |
| ETHYLTRICHLOROSILANE | 559,95 | 33,3 | 0,2698 | 0,2800 | 1,2855 | 1,0000 | 0,5744 | -11,0597 | 0,79% | 1,02% | | 3,19% | 9,39% |
| ETHYNYLBENZENE | 650 | 42,8 | 0,2264 | 0,2720 | 0,3910 | 0,7867 | 1,3031 | -2,6234 | 0,42% | 2,14% | 2,20% | 1,57% | 17,70% |
| FLUORANTHENE | 905 | 26,1 | 0,5875 | | 0,6418 | 0,9051 | 1,8482 | | 5,21% | 4,87% | | | |
| FLUORENE | 826 | 30 | 0,4042 | | 0,6058 | 0,8148 | 1,3732 | | 0,32% | 1,17% | 0,02% | | |
| FLUORINE | 144,12 | 51,724 | 0,0530 | 0,2876 | 0,3881 | 0,8851 | 0,9838 | -2,3318 | 0,19% | 1,59% | 0,66% | 1,24% | 10,52% |
| FLUOROBENZENE | 560,09 | 45,5051 | 0,2472 | 0,2654 | 0,6321 | 0,8681 | 1,0687 | 0,2844 | 0,60% | 1,84% | | 1,59% | 16,84% |
| FORMALDEHYDE | 420 | 65,9 | 0,1679 | 0,2068 | 1,2820 | 1,0000 | 0,4646 | 19,9111 | 0,58% | 1,23% | | 13,21% | 68,02% |
| FORMAMIDE | 771 | 78 | 0,4124 | 0,1913 | 0,9585 | 0,9283 | 0,9909 | 35,7512 | 0,50% | 2,75% | | 10,47% | 33,06% |
| FORMANILIDE | 787 | 41,1 | 0,5449 | | 0,6214 | 0,8238 | 1,6539 | | 0,63% | 1,13% | | | |
| FORMIC ACID | 588 | 58,1 | 0,3125 | 0,1673 | 0,2201 | 0,8517 | 2,5227 | 47,9845 | 1,94% | | 2,48% | 16,38% | 68,54% |
| FUMARIC ACID | 771 | 49,8 | 0,9885 | | 0,3492 | 0,7969 | 3,6944 | | 0,88% | 1,76% | 0,53% | | |
| FUMARONITRILE | 657 | 37,3 | 0,5566 | 0,1984 | 0,3494 | 0,7980 | 2,4066 | 55,6837 | 0,50% | 2,52% | 3,38% | 4,91% | 37,46% |
| FURAN | 490,15 | 55 | 0,2015 | 0,2698 | 0,9942 | 0,8696 | 0,6401 | -0,6332 | 0,45% | 0,83% | 0,31% | 1,44% | 4,77% |
| FURAN 2,5-DICARBOXYLIC ACID | 894,5 | 44,66 | 1,0134 | | 0,4812 | 0,8169 | 3,1793 | | 0,61% | | | | |
| FURFURAL | 670,15 | 56,6 | 0,3678 | 0,2633 | 0,5794 | 0,8397 | 1,3784 | -0,1773 | 0,72% | 1,23% | 0,52% | 1,44% | 20,16% |
| FURFURYL ALCOHOL | 632 | 53,5 | 0,7341 | 0,2581 | 0,4773 | 0,8322 | 2,5618 | -5,0498 | 0,88% | | 1,33% | 1,21% | 16,72% |
| GALLIUM TRICHLORIDE | 694 | 38,2 | 0,4577 | 0,1996 | 0,5536 | 0,9062 | 1,8371 | 55,6455 | 2,30% | | | 6,21% | 55,40% |
| gamma-BUTYROLACTONE | 731 | 51,3 | 0,3603 | | 0,5672 | 0,8553 | 1,4209 | | 1,31% | | 0,92% | | |
| gamma-TERPINENE | 661 | 28 | 0,3762 | 0,2621 | 0,7752 | 0,8297 | 1,0867 | 2,5011 | 0,55% | 1,99% | 0,05% | 1,94% | 22,88% |
| gamma-VALEROLACTONE | 727 | 48,4 | 0,4030 | 0,2547 | 0,4138 | 0,8823 | 2,1003 | 6,1503 | 1,23% | 2,01% | | 2,29% | 35,40% |
| GERMANIUM TETRACHLORIDE | 550 | 38,504 | 0,2411 | 0,2760 | 0,2688 | 0,8331 | 1,8701 | -7,2761 | 2,10% | 4,16% | 0,87% | 1,17% | 15,64% |
| GERMANIUM TETRAFLUORIDE | 352 | 46,04 | 0,2231 | 0,2627 | 0,2422 | 0,7999 | 1,7408 | 2,0189 | 0,90% | 2,87% | | 1,75% | 15,80% |
| GERMANIUM TETRAHYDRIDE | 308 | 55,5 | 0,1506 | 0,3025 | 0,4179 | 0,9579 | 1,3829 | -11,0988 | 4,37% | | | 1,33% | 9,24% |
| GLUTARALDEHYDE | 660 | 35,9 | 0,5373 | 0,2267 | 0,6368 | 0,8039 | 1,5646 | 32,4066 | 0,53% | 2,37% | 0,92% | 1,97% | 26,07% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| GLUTARIC ACID | 840 | 42,7 | 0,7526 | 0,2273 | 1,7646 | 1,0000 | 0,7524 | 27,8632 | 0,75% | 1,61% | 1,79% | 1,89% | 24,65% |
| GLUTARIC ANHYDRIDE | 838 | 58 | 0,5372 | 0,2556 | 0,5117 | 0,8810 | 2,1169 | 2,2350 | 1,81% | 2,65% | | 2,43% | 33,47% |
| GLUTARONITRILE | 782 | 31,5 | 0,6033 | 0,1852 | 0,4755 | 0,8630 | 2,3539 | 88,3300 | 4,44% | 7,16% | 3,51% | 8,93% | 55,16% |
| GLYCERYL TRIACETATE | 701,4 | 23,33 | 0,8758 | 0,2460 | 0,4708 | 0,8127 | 2,8568 | 7,5873 | 0,74% | 1,51% | | 2,18% | 21,93% |
| GLYCINE | 1021 | 67,4 | 0,6860 | | 0,5248 | 0,8076 | 2,1706 | | 0,56% | 1,77% | | | |
| GLYCOL ALDEHYDE | 609,3 | 66,44 | 0,7684 | | 0,3162 | 0,8037 | 3,2651 | | 0,50% | 2,71% | | | |
| GLYCOLIC ACID | 616 | 73,1 | 1,0592 | | 0,4464 | 0,8076 | 3,4036 | | 0,47% | 0,31% | | | |
| HALOTHANE | 496 | 39,2 | 0,2750 | 0,2751 | 0,1653 | 0,8452 | 2,6271 | -6,2739 | 3,71% | 2,16% | 0,31% | 1,54% | 11,37% |
| HEPTAFLUOROPROPYL METHYL ETHER | 437,7 | 24,81 | 0,4035 | 0,2584 | 1,1131 | 0,9758 | 0,8420 | 3,4261 | 0,62% | 1,45% | | 1,40% | 18,38% |
| HEPTANAL | 620 | 31,6 | 0,4058 | 0,2607 | 0,3894 | 0,8596 | 2,1085 | 1,5328 | 0,48% | 2,42% | | 1,56% | 15,19% |
| HEXACHLOROBENZENE | 825 | 28,5 | 0,4971 | | 0,3261 | 0,0001 | 0,9168 | | 2,24% | | | | |
| HEXACHLOROCYCLOPENTADIENE | 746 | 30,1 | 0,3834 | 0,2540 | 0,7766 | 0,8821 | 1,1416 | 11,7956 | 0,53% | 1,31% | | 1,27% | 18,18% |
| HEXACHLOROETHANE | 695 | 33,4 | 0,2386 | | 0,2205 | 0,7035 | 1,4742 | | 0,40% | 2,72% | | | |
| HEXACOSAMETHYLDODECASILOXANE | 751,3 | 4,7 | 1,3096 | 0,2464 | 0,6444 | 0,8197 | 3,1173 | -11,1598 | 0,74% | | | 6,53% | 25,28% |
| HEXADECAMETHYLCYCLOOCTASILOXANE | 689,2 | 6,92 | 0,8826 | 0,2445 | 0,4867 | 0,8112 | 2,7938 | 37,8779 | 0,63% | 1,51% | | 2,19% | 26,65% |
| HEXADECAMETHYLHEPTASILOXANE | 671,8 | 6,7685 | 0,8864 | 0,2407 | 1,5532 | 1,0000 | 0,9706 | 62,4423 | 1,43% | 1,35% | | 3,28% | 24,34% |
| HEXAETHYLBENZENE | 746 | 17,3 | 0,7534 | 0,2526 | 0,9872 | 0,9467 | 1,4719 | 4,6695 | 0,93% | 2,49% | 1,09% | 1,33% | 18,90% |
| HEXAFLUORO-1,3-BUTADIENE | 409,9 | 31,31 | 0,3510 | 0,2645 | 1,5047 | 1,0000 | 0,5572 | -0,8777 | 1,52% | 1,39% | | 1,31% | 17,30% |
| HEXAFLUOROACETONE | 357,14 | 28,371 | 0,3636 | 0,2652 | 0,1103 | 0,8170 | 3,1769 | -1,8817 | 0,72% | 4,55% | 1,53% | 1,50% | 1,64% |
| HEXAFLUOROBENZENE | 516,73 | 32,728 | 0,3953 | 0,2546 | 0,2073 | 0,8334 | 2,8374 | 6,0003 | 0,32% | 2,73% | 0,64% | 1,54% | 18,67% |
| HEXAFLUOROETHANE | 293,03 | 30,43 | 0,2549 | 0,2778 | 0,3898 | 0,8321 | 1,5057 | -6,6994 | 0,33% | 2,42% | 1,18% | 1,06% | 12,87% |
| HEXAMETHYLBENZENE | 758 | 27,7 | 0,4956 | 0,2475 | 1,1175 | 1,0000 | 0,9665 | 15,0911 | 1,05% | 2,28% | 0,85% | 2,07% | 15,40% |
| HEXAMETHYLCYCLOTRISILOXANE | 554,2 | 17,8 | 0,4962 | 0,2673 | 2,0029 | 1,0000 | 0,4938 | -13,3221 | 1,22% | 1,21% | | 0,87% | 16,92% |
| HEXAMETHYLDISILAZANE | 544 | 19,2 | 0,5101 | 0,2598 | 0,4274 | 0,8651 | 2,3238 | -2,1684 | 0,99% | 2,19% | | 0,88% | 18,49% |
| HEXAMETHYLDISILOXANE | 519 | 19,2 | 0,4142 | 0,2672 | 0,2165 | 0,8215 | 2,7335 | -9,1443 | 1,26% | 3,50% | 0,47% | 1,25% | 14,57% |
| HEXAMETHYLENEIMINE | 624 | 42,7 | 0,3454 | 0,2757 | 0,2221 | 0,8455 | 2,6233 | -9,7256 | 1,74% | 3,47% | | 1,52% | 6,16% |
| HEXAMETHYLENETETRAMINE | 837 | 36,8 | 0,2994 | | 0,1579 | 0,8376 | 2,7608 | | 0,39% | 2,20% | | | |
| HEXANAL | 594 | 34,6 | 0,3618 | 0,2606 | 0,7324 | 0,8940 | 1,1802 | 2,6937 | 0,60% | 1,30% | | 1,34% | 15,37% |
| HEXANENITRILE | 633,8 | 33 | 0,4343 | 0,2447 | 0,3839 | 0,8684 | 2,2788 | 17,1652 | 0,36% | 6,58% | | 1,50% | 21,15% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| HMX | 1030 | 25 | 1,1318 | | 0,5144 | 0,8129 | 3,2728 | | 0,57% | | | | |
| HYDRAZOBENZENE | 939 | 30,9 | 0,6718 | 0,2311 | 0,5231 | 0,8122 | 2,1596 | 42,6157 | 0,61% | 1,12% | | 1,34% | 22,55% |
| HYDROGEN BROMIDE | 363,15 | 85,52 | 0,0734 | 0,2832 | 0,8756 | 1,0000 | 0,5489 | -2,7161 | 1,43% | 1,24% | 0,26% | 1,67% | 11,25% |
| HYDROGEN CHLORIDE | 324,65 | 83,1 | 0,1315 | 0,2677 | 0,1704 | 0,8783 | 2,1502 | 0,8064 | 0,96% | 1,82% | 1,38% | 1,34% | 22,28% |
| HYDROGEN CYANIDE | 457 | 54 | 0,4043 | 0,1917 | 0,5467 | 0,9178 | 1,7240 | 31,3475 | 3,36% | | | 6,04% | 37,00% |
| HYDROGEN IODIDE | 423,85 | 83,1 | 0,0381 | 0,2883 | 0,7883 | 0,9215 | 0,5159 | -4,2880 | 0,69% | 1,14% | 0,60% | 1,74% | 10,46% |
| HYDROGEN PEROXIDE | 730,15 | 217 | 0,3582 | 0,2685 | 0,4006 | 0,8697 | 1,9445 | -0,8643 | 0,24% | 1,15% | | 1,82% | 11,79% |
| HYDROGEN SELENIDE | 411,15 | 89,2 | 0,0542 | 0,2876 | 0,0554 | 0,8613 | 2,3770 | -3,7756 | 1,16% | 3,78% | | 1,56% | 1,32% |
| HYDROGEN SULFIDE | 373,53 | 89,6291 | 0,0942 | 0,2825 | 0,1122 | 0,8688 | 2,2734 | -2,5075 | 0,57% | 1,44% | 9,75% | 1,19% | 10,68% |
| HYDROXYACETONITRILE | 664 | 59,3 | 0,8007 | 0,2097 | 1,0049 | 0,8702 | 1,4491 | 26,1022 | 0,44% | 0,74% | | 2,00% | 33,38% |
| HYDROXYCAPROIC ACID | 683 | 36,4 | 1,1375 | | 0,4979 | 0,8098 | 3,3489 | | 0,60% | 0,64% | | | |
| IBUPROFEN | 765 | 29,8 | 1,0101 | 0,3028 | 0,7292 | 0,8604 | 2,3907 | -71,3633 | 0,69% | | | 6,56% | 8,90% |
| IMIDAZOLE | 844,8 | 105,5 | 0,4138 | 0,2862 | 1,5194 | 1,0000 | 0,6037 | -11,7620 | 0,46% | 1,23% | | 1,36% | 13,31% |
| INDENE | 687 | 38,2 | 0,3338 | 0,2555 | 0,2353 | 0,8510 | 2,5334 | 9,4223 | 2,46% | 3,64% | 1,45% | 1,21% | 22,35% |
| INDOLE | 790 | 43 | 0,3763 | 0,2371 | 1,3128 | 1,0000 | 0,6724 | 25,8118 | 0,51% | 1,35% | 0,98% | 3,54% | 2,96% |
| IODINE | 819,15 | 116,54 | 0,1115 | 0,2988 | 0,1385 | 0,8728 | 2,2202 | -12,1665 | 1,34% | 3,57% | | 0,83% | 23,75% |
| IODOBENZENE | 721,15 | 45,191 | 0,2466 | 0,2652 | 0,3564 | 0,8209 | 1,5403 | 1,3282 | 0,42% | 0,96% | 0,86% | 1,26% | 15,82% |
| IRON PENTACARBONYL | 559,65 | 31,5307 | 0,2938 | 0,2669 | 1,6424 | 1,0000 | 0,4653 | -1,5628 | 2,96% | | 0,07% | 1,08% | 13,92% |
| ISOAGATHOLAL | 790 | 16,7 | 1,0832 | | 0,5095 | 0,8134 | 3,1867 | | 0,55% | 1,48% | | | |
| ISOBUTANE | 407,8 | 36,4 | 0,1835 | 0,2741 | 1,0649 | 0,9876 | 0,5812 | -3,8042 | 0,84% | 1,74% | 2,41% | 1,44% | 12,03% |
| ISOBUTENE | 417,9 | 40 | 0,1948 | 0,2723 | 0,3470 | 0,8375 | 1,4418 | -2,6428 | 0,76% | 1,22% | 2,29% | 1,28% | 12,83% |
| ISOBUTYL ACETATE | 560,8 | 30,1 | 0,4340 | 0,2542 | 1,4756 | 1,0000 | 0,6369 | 6,1666 | 0,76% | 3,66% | 3,03% | 1,57% | 20,83% |
| ISOBUTYL ACRYLATE | 587 | 29,5 | 0,4551 | 0,2617 | 0,7236 | 0,8707 | 1,3481 | -1,6040 | 0,60% | 0,87% | | 1,55% | 17,82% |
| ISOBUTYL CHLORIDE | 528 | 39 | 0,2416 | 0,2622 | 0,3052 | 0,8039 | 1,6007 | 2,1281 | 0,91% | 1,79% | 1,09% | 2,75% | 14,63% |
| ISOBUTYL FORMATE | 551,35 | 38,8075 | 0,3896 | 0,2779 | 0,5661 | 0,8166 | 1,4064 | -12,4500 | 0,85% | 2,05% | | 1,97% | 6,70% |
| ISOBUTYL ISOBUTYRATE | 601,89 | 26,1 | 0,4006 | 0,2680 | 1,6198 | 1,0000 | 0,5518 | -6,1391 | 0,60% | 2,37% | | 2,26% | 18,63% |
| ISOBUTYL MERCAPTAN | 559 | 40,6 | 0,2528 | 0,2723 | 0,3648 | 0,8191 | 1,5171 | -4,5703 | 1,80% | 2,01% | 1,29% | 1,79% | 16,12% |
| ISOBUTYL METHACRYLATE | 612 | 26,7 | 0,4205 | 0,2589 | 0,3064 | 0,8156 | 2,2566 | 3,1549 | 0,24% | 1,25% | 0,95% | 1,29% | 18,19% |
| ISOBUTYLAMINE | 513,73 | 42,15 | 0,3627 | 0,2701 | 0,1832 | 0,8337 | 2,8323 | -5,7232 | 1,65% | 3,80% | 0,46% | 1,07% | 1,48% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| ISOBUTYLBENZENE | 650 | 30,5 | 0,3817 | 0,2735 | 0,3306 | 0,8205 | 2,0472 | -12,0095 | 0,45% | 2,53% | 1,39% | 2,51% | 16,46% |
| iso-BUTYLCYCLOHEXANE | 642,1 | 25,85 | 0,3536 | 0,2669 | 1,2010 | 1,0000 | 0,7186 | -3,7552 | 0,54% | 1,11% | | 2,64% | 23,05% |
| ISOBUTYLENE GLYCOL | 626,3 | 50,33 | 0,8765 | 0,2681 | 0,5374 | 0,8240 | 2,6415 | -10,8430 | 0,51% | | | 5,05% | 15,00% |
| ISOBUTYL-tert-BUTYL ETHER | 558,3 | 25,61 | 0,3494 | 0,2781 | 1,2276 | 1,0000 | 0,6954 | -16,6692 | 0,52% | 1,04% | 0,56% | 2,78% | 17,83% |
| ISOBUTYRIC ACID | 605 | 37 | 0,6140 | 0,2213 | 0,2749 | 0,8185 | 3,1452 | 28,1981 | 1,49% | | | 3,81% | 33,47% |
| ISOBUTYRIC ANHYDRIDE | 631,5 | 27,19 | 0,5926 | 0,2712 | 0,5949 | 0,8901 | 2,0099 | -16,1833 | 1,14% | | | 5,06% | 25,47% |
| ISOBUTYRONITRILE | 565 | 37,6 | 0,3384 | 0,2333 | 0,9031 | 0,9124 | 0,9309 | 25,3378 | 0,65% | 1,50% | | 3,10% | 29,04% |
| ISOPENTANE | 460,4 | 33,8 | 0,2279 | 0,2710 | 0,2343 | 0,8384 | 1,9854 | -3,6084 | 0,23% | 1,51% | 1,11% | 1,41% | 14,95% |
| ISOPENTYL ISOVALERATE | 637 | 22 | 0,5785 | 0,2504 | 0,2857 | 0,8254 | 2,9969 | 5,7026 | 2,18% | 1,54% | 2,80% | 1,42% | 22,39% |
| ISOPHORONE | 707,6 | 30,9 | 0,4165 | 0,2543 | 0,4617 | 0,8908 | 1,9943 | 8,6709 | 0,04% | | | 1,33% | 19,13% |
| ISOPHORONE DIISOCYANATE | 765 | 25,2 | 0,6660 | | 0,6718 | 0,8320 | 1,8001 | | 0,74% | 1,50% | | | |
| ISOPHTHALIC ACID | 1007 | 39,5 | 1,0613 | | 0,4406 | 0,8065 | 3,4322 | | 0,56% | 1,13% | | | |
| ISOPHTHALOYL CHLORIDE | 768 | 33,3 | 0,6455 | 0,2501 | 0,7934 | 0,8434 | 1,5303 | 7,6850 | 0,30% | 0,11% | | 1,56% | 23,52% |
| ISOPRENE | 484 | 38,5003 | 0,1583 | 0,2649 | 1,4998 | 1,0000 | 0,3867 | 3,4430 | 1,88% | 1,37% | 1,16% | 1,91% | 15,17% |
| ISOPROPANOL | 508,3 | 47,65 | 0,6630 | 0,2454 | 1,3164 | 1,0000 | 0,9802 | 4,1020 | 3,96% | 4,23% | 7,09% | 1,51% | 20,96% |
| ISOPROPYL ACETATE | 532 | 32,9 | 0,3678 | 0,2554 | 1,2946 | 1,0000 | 0,6728 | 6,5278 | 1,47% | 1,58% | | 1,43% | 21,06% |
| ISOPROPYL ACRYLATE | 560 | 33,1 | 0,4051 | 0,2660 | 0,3621 | 0,8673 | 2,2719 | -4,6941 | 1,36% | | 2,70% | 1,74% | 16,25% |
| ISOPROPYL BUTYL ETHER | 549 | 27,4 | 0,4032 | 0,2702 | 0,3025 | 0,8042 | 2,1496 | -9,0155 | 0,57% | 4,53% | 0,10% | 2,18% | 19,80% |
| ISOPROPYL CHLORIDE | 489 | 45,4 | 0,1986 | 0,2736 | 1,1835 | 1,0000 | 0,5438 | -3,8464 | 0,62% | 1,60% | 0,69% | 1,43% | 13,01% |
| ISOPROPYL IODIDE | 578 | 51,2 | 0,2380 | 0,2987 | 0,2629 | 0,8790 | 2,1412 | -20,0979 | 1,95% | 2,85% | | 3,59% | 6,42% |
| ISOPROPYL ISOBUTYL ETHER | 537 | 27,9 | 0,3785 | 0,2786 | 0,4159 | 0,7970 | 1,6818 | -16,8334 | 0,50% | 4,48% | 0,69% | 2,56% | 16,96% |
| ISOPROPYL MERCAPTAN | 517 | 47,5 | 0,2138 | 0,2830 | 0,2177 | 0,8382 | 1,9951 | -9,5679 | 1,91% | 2,04% | 2,02% | 1,82% | 13,29% |
| ISOPROPYL PALMITATE | 766,2 | 10,9 | 0,8688 | 0,2223 | 0,8805 | 0,7916 | 1,6631 | 114,0388 | 0,76% | 1,52% | | 1,71% | 29,43% |
| ISOPROPYLAMINE | 471,85 | 45,4 | 0,2759 | 0,2677 | 1,8306 | 0,9816 | 0,3951 | -1,4235 | 0,24% | 0,81% | 1,92% | 1,43% | 20,84% |
| ISOPROPYLCYCLOHEXANE | 627 | 28,5 | 0,3295 | 0,2628 | 0,2458 | 0,8386 | 2,3693 | 0,9101 | 0,48% | 1,02% | | 1,51% | 20,99% |
| ISOPROPYLCYCLOPENTANE | 593 | 30,4 | 0,3030 | 0,2631 | 0,9998 | 0,9625 | 0,7951 | 0,8130 | 1,15% | 1,54% | 3,18% | 1,49% | 18,51% |
| ISOQUINOLINE | 803,15 | 51 | 0,3035 | 0,2827 | 0,2818 | 0,8320 | 2,0395 | -15,4484 | 0,45% | 1,53% | 1,53% | 2,06% | 11,75% |
| ISOVALERIC ACID | 629,09 | 36,88 | 0,6818 | 0,2406 | 0,4038 | 0,7898 | 2,4937 | 10,7908 | 0,42% | | | 1,50% | 36,45% |
| ISOXAZOLE | 590 | 61 | 0,2568 | 0,2472 | 0,2159 | 0,8595 | 2,4041 | 9,7260 | 1,49% | 1,22% | | 2,75% | 24,37% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| ITACONIC ACID | 821 | 42,4 | 0,9247 | | 0,3887 | 0,8090 | 3,3687 | | 0,51% | 1,13% | | | |
| KETENE | 370 | 58,1 | 0,1257 | 0,2720 | 0,8185 | 0,7937 | 0,6251 | -0,4681 | 1,63% | 3,05% | | 1,85% | 13,36% |
| KRYPTON | 209,35 | 55,0195 | 0,0000 | 0,2906 | 0,1015 | 0,8955 | 1,9494 | -3,3328 | 0,26% | 1,59% | | 1,50% | 10,29% |
| LACTONITRILE | 643 | 50,3 | 0,7886 | 0,2195 | 1,1221 | 0,9273 | 1,3041 | 20,2612 | 0,32% | 0,61% | | 3,41% | 26,12% |
| LEVULINIC ACID | 738 | 40,2 | 0,7557 | 0,2172 | 0,3726 | 0,8179 | 3,0346 | 29,9904 | 0,26% | 0,89% | | 4,57% | 28,05% |
| LINOLEIC ACID | 775 | 14,1 | 1,1801 | 0,2288 | 0,6086 | 0,8164 | 2,9787 | 41,9217 | 0,69% | 1,35% | | 2,38% | 37,67% |
| LINOLENIC ACID | 780 | 14,4 | 1,1870 | 0,2373 | 0,5624 | 0,8162 | 3,1960 | 28,1374 | 0,78% | 1,74% | | 4,53% | 26,76% |
| L-MENTHOL | 658 | 27,1 | 0,7796 | 0,2567 | 0,6858 | 0,8806 | 2,1212 | -9,9981 | 2,24% | 3,14% | | 1,07% | 18,31% |
| L-PHENYLALANINE | 854 | 34,7 | 0,8516 | | 0,3441 | 0,8079 | 3,3964 | | 0,66% | 1,16% | 1,83% | | |
| LYSINE | 821 | 35,3 | 1,0127 | | 0,5849 | 0,8120 | 2,7010 | | 0,70% | 0,70% | | | |
| MALEIC ACID | 773 | 49,9 | 0,9976 | | 0,4229 | 0,8086 | 3,3780 | | 0,54% | 0,86% | | | |
| MALEONITRILE | 704 | 37,3 | 0,5575 | | 1,4995 | 1,0000 | 0,7348 | | 2,64% | 4,34% | 3,10% | | |
| MALONIC ACID | 834 | 61 | 0,7383 | | 0,6082 | 0,7605 | 1,9167 | | 0,63% | | | | |
| MALONONITRILE | 715 | 40,4 | 0,5016 | 0,1742 | 0,2883 | 0,8229 | 2,6852 | 74,9703 | 0,26% | 2,01% | | 12,24% | 52,16% |
| m-CHLOROANILINE | 751 | 45,9 | 0,4198 | 0,2661 | 0,4926 | 0,8356 | 1,7022 | -0,6933 | 0,75% | 0,89% | | 3,86% | 15,08% |
| m-CHLOROBENZOYL CHLORIDE | 724 | 36,8 | 0,4542 | | 1,0513 | 1,0000 | 0,9769 | | 0,91% | 0,41% | | | |
| m-CHLORONITROBENZENE | 742 | 39,8 | 0,4919 | 0,2458 | 0,3237 | 0,8454 | 2,6238 | 14,0166 | 1,35% | 4,09% | 3,63% | 1,20% | 7,06% |
| m-CHLOROPHENOL | 729 | 53,2 | 0,4856 | 0,2800 | 0,6070 | 0,9152 | 1,7489 | -14,3897 | 2,51% | 3,48% | | 3,45% | 13,94% |
| m-CRESOL | 705,85 | 45,6 | 0,4480 | 0,2513 | 0,9416 | 0,7674 | 0,9938 | 6,0176 | 1,39% | 2,25% | 1,72% | 2,57% | 24,87% |
| m-CYMENE | 649 | 28,1 | 0,3780 | 0,2552 | 1,0609 | 0,9319 | 0,8407 | 9,6400 | 0,30% | 1,63% | 1,43% | 1,41% | 17,54% |
| m-DIBROMOBENZENE | 761 | 46,6 | 0,2932 | 0,2742 | 0,2803 | 0,8573 | 2,1606 | -9,1717 | 0,66% | 2,00% | 1,83% | 1,30% | 14,67% |
| m-DICHLOROBENZENE | 683,95 | 40,7 | 0,2790 | 0,2624 | 0,3681 | 0,8298 | 1,6428 | 3,8309 | 0,70% | 1,38% | 0,51% | 1,35% | 21,27% |
| m-DIETHYLBENZENE | 663 | 28,8 | 0,3540 | 0,2582 | 1,2816 | 0,9994 | 0,6664 | 7,3383 | 0,67% | 1,17% | | 1,65% | 19,07% |
| m-DIISOPROPYLBENZENE | 684 | 24,5 | 0,3587 | 0,2813 | 1,6539 | 1,0000 | 0,5061 | -18,8244 | 2,59% | 3,41% | | 7,79% | 22,06% |
| m-DIVINYLBENZENE | 692 | 31,2 | 0,3734 | 0,2497 | 1,1058 | 0,9924 | 0,8112 | 16,4047 | 0,70% | 0,44% | | 1,57% | 25,11% |
| MELAMINE | 1008 | 58,58 | 0,6973 | | 0,4260 | 0,8386 | 2,7426 | | 0,50% | | | | |
| MERCURY | 1735 | 1608,03 | -0,1645 | 0,3906 | 0,0763 | 0,9749 | 1,2008 | -7,762 | 1,75% | 8,40% | 1,00% | 0,86% | 21,14% |
| MERCURY DICHLORIDE | 972 | 115,21 | 0,2563 | 0,2548 | 0,1743 | 0,8495 | 2,5577 | 4,9516 | 0,21% | 2,56% | | 2,41% | 20,69% |
| MESITYL OXIDE | 600 | 34,1 | 0,3254 | 0,2464 | 1,3605 | 0,9974 | 0,5948 | 17,3261 | 0,80% | 1,21% | 0,57% | 2,49% | 21,80% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| MESITYLENE | 637,3 | 31,27 | 0,3985 | 0,2550 | 0,4215 | 0,8389 | 1,8658 | 7,2930 | 0,04% | 0,88% | 0,92% | 1,27% | 18,62% |
| METHACROLEIN | 530 | 42,5 | 0,2456 | 0,2459 | 0,8130 | 0,9054 | 0,8676 | 14,6800 | 0,63% | 1,77% | | 2,76% | 19,24% |
| METHACRYLONITRILE | 554 | 38,8 | 0,3013 | 0,2306 | 0,1689 | 0,8425 | 2,6746 | 27,5459 | 4,15% | 7,64% | 0,74% | 3,79% | 27,32% |
| METHANE | 190,564 | 45,99 | 0,0115 | 0,2894 | 0,1473 | 0,9075 | 1,8243 | -3,5604 | 0,31% | 1,73% | 7,17% | 1,53% | 11,02% |
| METHANOL | 512,5 | 80,84 | 0,5658 | 0,2263 | 0,6650 | 0,9116 | 1,7833 | 9,1802 | 0,94% | 4,22% | 6,84% | 3,98% | 30,64% |
| METHOXYACETONE | 584,1 | 42,13 | 0,3805 | 0,2493 | 0,9399 | 1,0000 | 0,9930 | 10,2638 | 0,15% | | | 1,31% | 19,89% |
| METHOXYDIHYDROPYRAN | 599 | 39,3 | 0,3669 | 0,2659 | 0,8319 | 0,8751 | 1,0360 | -3,3408 | 0,59% | 1,28% | | 1,10% | 18,70% |
| METHYL ACETATE | 506,55 | 47,5 | 0,3313 | 0,2564 | 1,2447 | 0,9825 | 0,6548 | 4,4328 | 1,99% | 3,12% | 0,30% | 1,64% | 17,60% |
| METHYL ACRYLATE | 536 | 42,5 | 0,3423 | 0,2495 | 0,3797 | 0,8485 | 1,8745 | 8,3029 | 0,42% | 0,62% | | 2,97% | 16,31% |
| METHYL alpha-HYDROXYISOBUTYRATE | 585,1 | 34,88 | 0,5444 | 0,2533 | 0,5032 | 0,8464 | 2,0395 | 4,4484 | 0,46% | 1,64% | | 1,43% | 20,20% |
| METHYL alpha-METHOXYISOBUTYRATE | 589,3 | 29,35 | 0,4212 | | 0,7962 | 0,8693 | 1,1727 | | 0,51% | 1,79% | | | |
| METHYL BENZOATE | 693 | 35,9 | 0,4205 | 0,2567 | 0,2297 | 0,8353 | 2,8032 | 7,0269 | 2,85% | 3,69% | 1,40% | 1,51% | 11,55% |
| METHYL CAPRYLATE | 650,7 | 23,84 | 0,4947 | 0,2558 | 1,5533 | 1,0000 | 0,6564 | 7,4314 | 1,99% | 1,66% | | 1,74% | 20,87% |
| METHYL CHLORIDE | 416,25 | 66,8 | 0,1510 | 0,2686 | 0,3125 | 0,8460 | 1,4296 | 0,5047 | 0,54% | 2,19% | 0,71% | 1,59% | 12,59% |
| METHYL CHLOROACETATE | 600 | 45 | 0,4340 | 0,2524 | 0,5854 | 0,8276 | 1,5023 | 7,2231 | 1,28% | 2,06% | 0,70% | 1,38% | 23,54% |
| METHYL CHLOROFORMATE | 525 | 53,6 | 0,3921 | 0,2680 | 1,2124 | 1,0000 | 0,7535 | -3,5743 | 0,64% | 0,96% | | 1,29% | 14,89% |
| METHYL CYANOACETATE | 687 | 38,1 | 0,5413 | 0,2266 | 0,3213 | 0,8210 | 2,6401 | 34,1008 | 0,38% | 1,35% | | 2,03% | 39,92% |
| METHYL DECANOATE | 686,9 | 19,42 | 0,5491 | 0,2429 | 1,7128 | 1,0000 | 0,6306 | 31,0741 | 1,37% | 1,22% | | 1,43% | 22,26% |
| METHYL DICHLOROSILANE | 483 | 39,5 | 0,2758 | 0,2658 | 0,1891 | 0,8522 | 2,5151 | -2,7834 | 3,34% | 5,10% | 7,82% | 3,41% | 9,10% |
| METHYL DIETHANOLAMINE | 741,9 | 41,6 | 0,6286 | 0,2489 | 0,8133 | 0,8398 | 1,4669 | 5,9551 | 0,68% | 1,37% | | 1,48% | 18,70% |
| METHYL DODECANOATE | 712 | 16,5 | 0,6644 | 0,2370 | 1,5183 | 0,9680 | 0,8235 | 45,7165 | 0,54% | 1,11% | | 1,45% | 24,37% |
| METHYL EICOSANOATE | 797,9 | 9,591 | 0,9021 | | 1,3224 | 0,8191 | 1,1878 | | 0,83% | 1,47% | | | |
| METHYL ERUCATE | 806,2 | 9,375 | 1,0984 | 0,2199 | 0,5993 | 0,8101 | 2,8186 | 137,1782 | 0,81% | 1,91% | | 3,54% | 27,21% |
| METHYL ETHYL ETHER | 437,8 | 44 | 0,2314 | 0,2678 | 1,0839 | 1,0000 | 0,6430 | -1,1444 | 2,48% | 1,54% | | 1,87% | 15,59% |
| METHYL ETHYL KETONE | 535,5 | 41,5 | 0,3234 | 0,2531 | 0,3361 | 0,8295 | 1,8817 | 8,5961 | 0,31% | 1,88% | 1,30% | 1,31% | 20,30% |
| METHYL ETHYL SULFIDE | 533 | 42,6 | 0,2091 | 0,2552 | 0,7348 | 0,8302 | 0,8439 | 8,6285 | 0,91% | 1,19% | 0,01% | 2,67% | 22,50% |
| METHYL FLUORIDE | 317,42 | 58,7511 | 0,1947 | 0,2474 | 0,2537 | 0,8739 | 1,9972 | 6,1328 | 0,65% | 2,54% | 3,65% | 3,28% | 16,77% |
| METHYL FORMATE | 487,2 | 60 | 0,2556 | 0,2570 | 0,7820 | 0,8656 | 0,8912 | 4,0763 | 0,31% | 1,19% | 1,69% | 2,16% | 18,29% |
| METHYL HYDROPEROXIDE | 566,1 | 92,44 | 0,4827 | | 0,6977 | 0,8658 | 1,4446 | | 0,50% | 1,19% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| METHYL IODIDE | 528,2 | 66 | 0,1567 | 0,2669 | 0,3833 | 0,8174 | 1,1315 | 1,6218 | 3,40% | 4,51% | 0,96% | 2,17% | 15,96% |
| METHYL ISOBUTYL ETHER | 497 | 34,1 | 0,3078 | 0,2706 | 0,1688 | 0,8387 | 2,7400 | -5,9539 | 0,53% | 4,06% | 0,13% | 1,11% | 15,03% |
| METHYL ISOBUTYL KETONE | 574,6 | 32,7 | 0,3557 | 0,2575 | 0,2070 | 0,8389 | 2,7372 | 4,9942 | 2,30% | 1,50% | | 1,30% | 20,36% |
| METHYL ISOBUTYRATE | 540,7 | 34,32 | 0,3637 | 0,2579 | 0,3892 | 0,7981 | 1,7207 | 4,3139 | 0,74% | 1,79% | 0,27% | 1,30% | 17,51% |
| METHYL ISOCYANATE | 488 | 54,8 | 0,3007 | 0,2484 | 0,1632 | 0,8370 | 2,7325 | 9,8111 | 0,49% | 1,93% | | 0,96% | 7,82% |
| METHYL ISOPROPENYL KETONE | 566 | 38,9 | 0,2862 | 0,2509 | 1,1422 | 1,0000 | 0,6747 | 11,9487 | 0,59% | 1,38% | | 2,01% | 19,18% |
| METHYL ISOPROPYL ETHER | 464,48 | 37,62 | 0,2656 | 0,2705 | 1,1587 | 0,9935 | 0,6348 | -3,1785 | 0,59% | 1,89% | 0,34% | 1,50% | 15,49% |
| METHYL ISOPROPYL KETONE | 553,4 | 38 | 0,3208 | 0,2596 | 1,4870 | 0,9633 | 0,5315 | 3,6482 | 0,90% | 7,97% | 0,88% | 1,61% | 18,89% |
| METHYL ISOPROPYL SULFIDE | 553,1 | 40,21 | 0,2461 | 0,2711 | 1,0940 | 1,0000 | 0,6544 | -3,8166 | 0,44% | 2,04% | | 1,26% | 8,35% |
| METHYL LACTATE | 607,3 | 42,3492 | 0,5297 | 0,2476 | 0,6567 | 0,8578 | 1,6126 | 7,6794 | 0,50% | 1,57% | | 1,39% | 18,82% |
| METHYL MERCAPTAN | 469,95 | 72,3 | 0,1582 | 0,2722 | 0,4578 | 0,8357 | 1,0623 | -1,1008 | 2,72% | 3,69% | 1,03% | 1,73% | 15,33% |
| METHYL METHACRYLATE | 566 | 36,8 | 0,2802 | 0,2552 | 0,3087 | 0,7035 | 1,4126 | 10,0667 | 0,43% | 1,60% | | 1,61% | 18,59% |
| METHYL MYRISTATE | 741,2 | 14,21 | 0,6979 | 0,2335 | 1,8451 | 1,0000 | 0,6744 | 66,9719 | 2,16% | 1,92% | | 1,61% | 27,51% |
| METHYL n-BUTYL ETHER | 512,74 | 33,71 | 0,3130 | 0,2624 | 0,2096 | 0,8200 | 2,3406 | 0,6024 | 0,40% | 3,55% | 0,04% | 1,51% | 17,98% |
| METHYL n-BUTYL SULFIDE | 593 | 34,7 | 0,3229 | 0,2610 | 0,3126 | 0,8180 | 1,9120 | 2,5060 | 0,59% | 1,30% | 0,70% | 1,40% | 20,63% |
| METHYL n-BUTYRATE | 554,5 | 34,73 | 0,3775 | 0,2533 | 1,1073 | 0,9105 | 0,7996 | 7,4788 | 1,35% | 2,32% | 3,45% | 1,88% | 17,82% |
| METHYL NONAFLUORO-N-BUTYL ETHER | 468,45 | 22,3 | 0,4322 | 0,2597 | 0,6533 | 0,8032 | 1,3250 | 1,8641 | 3,60% | | 0,61% | 1,69% | 17,85% |
| METHYL n-PENTYL ETHER | 546,49 | 30,42 | 0,3442 | 0,2633 | 0,2420 | 0,8162 | 2,2785 | 0,1801 | 0,39% | 2,50% | 0,06% | 1,44% | 20,78% |
| METHYL n-PROPYL ETHER | 476,25 | 38,01 | 0,2770 | 0,2692 | 0,1764 | 0,8461 | 2,6121 | -2,2683 | 1,90% | 2,62% | 1,05% | 1,75% | 16,85% |
| METHYL n-PROPYL SULFIDE | 565 | 39,7 | 0,2737 | 0,2671 | 0,3016 | 0,8158 | 1,7743 | -0,8316 | 0,28% | 1,50% | 0,47% | 1,57% | 18,75% |
| METHYL OLEATE | 764 | 12,8 | 1,0494 | 0,2397 | 0,4888 | 0,8152 | 3,2202 | 28,1117 | 0,31% | 0,31% | | 3,88% | 41,27% |
| METHYL PALMITATE | 762,2 | 12,35 | 0,7765 | 0,2264 | 1,8632 | 1,0000 | 0,7160 | 96,5217 | 2,32% | 2,10% | | 1,57% | 28,77% |
| METHYL PALMITOLEATE | 744,4 | 14,15 | 0,9974 | 0,2404 | 0,5432 | 0,8159 | 2,8534 | 26,5128 | 0,65% | 1,70% | | 3,17% | 37,87% |
| METHYL para-TOLUATE | 718,4 | 31,78 | 0,3662 | | 0,0291 | 0,7445 | 2,8492 | | 0,47% | | | | |
| METHYL PENTYL SULFIDE | 611,9 | 30,81 | 0,3653 | 0,2594 | 0,5059 | 0,7996 | 1,4653 | 3,5846 | 1,21% | 1,63% | 0,69% | 1,49% | 18,31% |
| METHYL PHENYL SULFIDE | 712,8 | 42,06 | 0,3080 | 0,2666 | 0,1175 | 0,8266 | 2,9693 | -0,5365 | 0,30% | | | 1,29% | 10,63% |
| METHYL PROPIONATE | 530,6 | 40,04 | 0,3466 | 0,2558 | 0,4961 | 0,8059 | 1,4408 | 5,4025 | 0,87% | 1,88% | 0,24% | 1,50% | 18,19% |
| METHYL sec-BUTYL ETHER | 498 | 34,1 | 0,3062 | 0,2670 | 0,8017 | 0,8601 | 0,9560 | -3,1120 | 0,53% | 3,88% | 0,27% | 1,47% | 14,40% |
| METHYL SILANE | 352,5 | 47 | 0,1314 | 0,3066 | 0,6715 | 1,0000 | 0,8654 | -15,6471 | 0,39% | | | 2,69% | 1,14% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| METHYL SILICATE | 562,8 | 28,73 | 0,4442 | 0,2674 | 0,3738 | 0,8297 | 2,1383 | -6,9406 | 0,38% | 1,92% | 1,86% | 1,08% | 14,07% |
| METHYL STEARATE | 781,1 | 10,84 | 0,8595 | 0,2181 | 1,8170 | 1,0000 | 0,7894 | 134,9957 | 2,62% | 2,41% | | 1,65% | 30,28% |
| METHYL t-BUTYL SULFIDE | 570 | 35,4 | 0,2334 | 0,2722 | 0,3777 | 0,7868 | 1,3523 | -4,9399 | 0,33% | 1,03% | 0,09% | 1,22% | 15,69% |
| METHYL tert-BUTYL ETHER | 497,1 | 32,86 | 0,2465 | 0,2642 | 1,3385 | 1,0000 | 0,5286 | 1,7479 | 1,06% | 1,45% | | 1,51% | 16,99% |
| METHYL tert-PENTYL ETHER | 534 | 30,4 | 0,2981 | 0,2606 | 0,2027 | 0,8479 | 2,5831 | 2,9760 | 1,01% | 1,43% | 3,26% | 1,52% | 15,54% |
| METHYL t-PENTYL SULFIDE | 632 | 31,3 | 0,2836 | 0,2592 | 0,1756 | 0,8378 | 2,5693 | 7,0107 | 0,57% | 2,73% | 1,55% | 1,36% | 17,03% |
| METHYL TRICHLOROSILANE | 517 | 35,3 | 0,2634 | 0,2705 | 0,2014 | 0,8450 | 2,3518 | -3,7311 | 1,01% | | 3,93% | 1,06% | 11,19% |
| METHYL VINYL DICHLOROSILANE | 544,1 | 29,4 | 0,2928 | 0,2505 | 1,1925 | 0,9996 | 0,6502 | 14,2866 | 0,59% | 1,63% | | 2,93% | 12,16% |
| METHYL VINYL ETHER | 437 | 46,7 | 0,2416 | 0,2603 | 1,1166 | 1,0000 | 0,6353 | 2,7501 | 0,87% | 1,15% | | 2,64% | 12,58% |
| METHYL-3-MERCAPTOPROPIONATE | 644 | 39,26 | 0,3990 | | 1,2513 | 1,0000 | 0,7361 | | 0,65% | 1,40% | | | |
| METHYL-4-FORMYLBENZOATE | 759,5 | 31,69 | 0,6107 | 0,2282 | 0,5992 | 0,8880 | 2,0335 | 31,7990 | 1,30% | | | 3,19% | 19,01% |
| METHYLACETYLENE | 402,4 | 56,3 | 0,2115 | 0,2706 | 0,4325 | 0,8088 | 1,2275 | -1,1612 | 0,47% | 1,61% | 0,30% | 1,30% | 12,10% |
| METHYLAL | 480,6 | 39,5 | 0,2856 | 0,2463 | 0,0853 | 0,8231 | 3,0448 | 11,6371 | 0,53% | 3,34% | 0,66% | 4,00% | 40,53% |
| METHYLAMINE | 430,05 | 74,6 | 0,2814 | 0,2593 | 1,3034 | 1,0000 | 0,5781 | 2,1726 | 0,83% | 0,38% | 0,59% | 1,94% | 5,74% |
| METHYLCYCLOHEXANE | 572,1 | 34,8 | 0,2361 | 0,2715 | 0,6890 | 0,8442 | 0,9392 | -4,0869 | 0,95% | 2,05% | 0,94% | 1,53% | 14,98% |
| METHYLCYCLOPENTADIENE | 541 | 44,3 | 0,2376 | 0,2743 | 0,9073 | 0,9191 | 0,7688 | -5,4847 | 0,63% | 0,98% | | 1,10% | 13,84% |
| METHYLCYCLOPENTADIENE DIMER | 675 | 26,4 | 0,4229 | | 1,2281 | 1,0000 | 0,7782 | | 0,65% | 1,34% | | | |
| METHYLCYCLOPENTANE | 532,7 | 37,9 | 0,2288 | 0,2712 | 0,8731 | 0,8789 | 0,7645 | -3,3528 | 0,46% | 1,42% | 1,41% | 1,46% | 13,66% |
| METHYLETHANOLAMINE | 630 | 52,2 | 0,5855 | 0,2523 | 0,4431 | 0,8109 | 2,2058 | 3,3297 | 0,67% | 1,20% | | 1,35% | 20,61% |
| METHYLGERMANIUM TRICHLORIDE | 595,4 | 39,51 | 0,2243 | 0,2684 | 1,2179 | 1,0000 | 0,5654 | -1,2674 | 1,46% | 1,59% | 2,14% | 1,29% | 15,01% |
| METHYLGLUTARONITRILE | 742 | 28,8 | 0,6381 | 0,2143 | 0,7735 | 0,8428 | 1,5559 | 60,9805 | 0,68% | 1,19% | | 2,26% | 47,90% |
| METHYLNORBORNENE | 600 | 34,4 | 0,2108 | 0,2601 | 1,0268 | 1,0000 | 0,6540 | 7,6594 | 0,64% | 1,71% | | 1,70% | 16,21% |
| m-ETHYLSTYRENE | 670,7 | 29,36 | 0,3955 | 0,2531 | 1,2333 | 1,0000 | 0,7437 | 12,2771 | 0,64% | 1,64% | | 2,00% | 23,72% |
| m-ETHYLTOLUENE | 637,15 | 31,5 | 0,3649 | 0,2585 | 1,2438 | 1,0000 | 0,6968 | 5,5607 | 0,41% | 2,14% | 1,70% | 1,66% | 19,77% |
| m-METHYLSTYRENE | 657 | 32,9 | 0,3487 | 0,2504 | 1,1658 | 1,0000 | 0,7358 | 14,4554 | 0,63% | 1,09% | | 1,60% | 21,85% |
| m-NITROANILINE | 815 | 44,2 | 0,7297 | | 0,3283 | 0,8169 | 3,1809 | | 1,81% | 0,40% | | | |
| MONOBUTYL SULFATE | 889,2 | 76,1 | 0,4390 | | 1,3031 | 1,0000 | 0,7433 | | 0,64% | 1,93% | | | |
| MONOCHLOROBENZENE | 632,35 | 45,191 | 0,2499 | 0,2641 | 0,3599 | 0,8253 | 1,5543 | 1,3868 | 0,43% | 1,98% | 2,35% | 1,50% | 15,67% |
| MONOCHLOROSILANE | 399,2 | 53,01 | 0,1327 | | 0,5308 | 0,8567 | 0,9538 | | 1,24% | 1,79% | 0,95% | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| MONOMETHYL TEREPHTHALATE | 797,8 | 31,08 | 0,8770 | | 0,4911 | 0,8038 | 2,7175 | | 0,47% | | | | |
| MONOMETHYL UREA | 836,5 | 63,53 | 0,5690 | | 0,1186 | 0,6698 | 2,5233 | | 0,55% | | | | |
| MONOOLEIN | 856,9 | 12,01 | 1,0985 | 0,2316 | 0,5577 | 0,8226 | 3,0542 | 63,9944 | 0,58% | | | 3,52% | 28,44% |
| MONO-TERT-BUTYLHYDROQUINONE | 805,5 | 37,65 | 0,7321 | | 0,6286 | 0,8755 | 2,1849 | | 1,02% | | | | |
| MORPHOLINE | 618 | 53,4 | 0,3579 | 0,2693 | 0,2295 | 0,8446 | 2,6385 | -4,4486 | 1,30% | 2,84% | | 1,02% | 15,92% |
| m-PHENYLENEDIAMINE | 824 | 51,8 | 0,5464 | 0,2486 | 0,7887 | 0,9433 | 1,5000 | 9,4283 | 1,07% | 1,23% | | 1,44% | 5,34% |
| m-TERPHENYL | 883 | 24,8 | 0,6509 | 0,2451 | 0,5270 | 0,8400 | 2,2042 | 18,7008 | 0,49% | 1,06% | | 1,34% | 23,11% |
| m-TOLUALCOHOL | 681 | 39,1 | 0,7508 | 0,2736 | 0,3874 | 0,8175 | 2,9386 | -21,5164 | 0,27% | 0,43% | 4,34% | 2,89% | 20,59% |
| m-TOLUALDEHYDE | 691 | 36,7 | 0,4332 | 0,2458 | 1,2580 | 1,0000 | 0,7687 | 15,5122 | 0,58% | 0,78% | | 1,63% | 23,86% |
| m-TOLUIC ACID | 754 | 39,01 | 0,6809 | | 0,9867 | 0,7533 | 1,2509 | | 0,71% | 1,96% | | | |
| m-TOLUIDINE | 707 | 42,8 | 0,4348 | 0,2536 | 1,6546 | 1,0000 | 0,5579 | 6,8306 | 3,93% | 2,69% | 0,66% | 1,45% | 24,73% |
| m-XYLENE | 617 | 35,41 | 0,3265 | 0,2581 | 0,3606 | 0,8335 | 1,8255 | 5,1486 | 0,35% | 1,04% | 0,86% | 1,40% | 17,39% |
| N-(2-HYDROXYETHYL)PIPERAZINE | 780 | 49,37 | 0,4203 | 0,2863 | 1,4104 | 1,0000 | 0,6645 | -22,4950 | 2,43% | 2,60% | | 2,99% | 15,53% |
| N,N'-BIS(2-HYDROXYETHYL)ETHYLENEDIAMINE | 781,8 | 38,04 | 1,1400 | 0,2584 | 0,7896 | 0,8579 | 2,4268 | -13,0498 | 0,26% | | | 3,06% | 21,79% |
| N,N'-DI(2-HYDROXYETHYL)PIPERAZINE | 825,3 | 38,8 | 0,6303 | | 1,2352 | 0,8983 | 0,9954 | | 0,57% | 1,30% | 3,46% | | |
| N,N-DIETHYLANILINE | 702 | 28,5 | 0,4262 | 0,2523 | 1,5350 | 1,0000 | 0,6089 | 12,8577 | 2,41% | 2,34% | 0,46% | 1,41% | 10,92% |
| N,N-DIETHYLHYDROXYLAMINE | 567 | 41,3 | 0,7154 | 0,2712 | 1,3040 | 0,9984 | 1,0377 | -10,7228 | 0,87% | 2,00% | | 3,26% | 9,25% |
| N,N-DIETHYLMETHYLAMINE | 506,1 | 33,43 | 0,3051 | 0,2725 | 0,2147 | 0,8408 | 2,4536 | -7,1981 | 0,40% | | | 1,75% | 14,91% |
| N,N-DIMETHYLACETAMIDE | 658 | 40,3 | 0,3635 | 0,2310 | 1,2046 | 1,0000 | 0,7280 | 28,5732 | 1,44% | 0,67% | | 3,81% | 21,10% |
| N,N-DIMETHYLANILINE | 687,15 | 36,3 | 0,4022 | 0,2540 | 1,0981 | 1,0000 | 0,8570 | 7,9324 | 1,55% | 2,97% | | 1,51% | 2,34% |
| N,N-DIMETHYLFORMAMIDE | 649,6 | 44,2 | 0,3177 | 0,2200 | 0,3779 | 0,8324 | 1,7570 | 34,8754 | 1,00% | 2,50% | 0,89% | 5,70% | 30,06% |
| N,N-DIMETHYL-n-BUTYLAMINE | 538 | 29,3 | 0,3403 | 0,2666 | 0,7319 | 0,8573 | 1,1028 | -2,6053 | 0,63% | 1,29% | | 1,18% | 12,90% |
| N,N'-DI-tert-BUTYLETHYLENEDIAMINE | 625 | 21,6 | 0,6278 | | 1,0423 | 0,9781 | 1,2256 | | 0,68% | 1,18% | 7,71% | | |
| N-AMINOETHYL ETHANOLAMINE | 698 | 44,6 | 1,0473 | 0,2524 | 0,6011 | 0,8148 | 2,7271 | -3,2670 | 0,65% | 1,02% | | 4,22% | 22,95% |
| N-AMINOETHYL PIPERAZINE | 710,7 | 37,87 | 0,5271 | 0,2618 | 0,3102 | 0,8369 | 2,7722 | -4,7888 | 0,41% | | | 1,53% | 16,73% |
| NAPHTHACENE | 987 | 23,9 | 0,5653 | | 0,2865 | 0,7998 | 2,7330 | | 0,48% | 2,92% | | | |
| NAPHTHALENE | 748,4 | 40,5 | 0,3020 | 0,2603 | 0,2701 | 0,8209 | 2,0158 | 4,5164 | 0,98% | 5,07% | 3,02% | 1,47% | 14,93% |
| n-BUTANE | 425,12 | 37,96 | 0,2002 | 0,2732 | 0,4120 | 0,8488 | 1,3282 | -3,4371 | 0,35% | 1,16% | 2,67% | 1,22% | 13,60% |
| n-BUTYL ACETATE | 575,4 | 30,9 | 0,4394 | 0,2574 | 0,2283 | 0,8317 | 2,8709 | 3,2972 | 0,69% | 1,03% | 1,29% | 1,44% | 21,50% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| n-BUTYL ACRYLATE | 598 | 29,1 | 0,4817 | 0,2620 | 0,2744 | 0,8357 | 2,7944 | -0,6540 | 1,87% | 1,85% | | 3,05% | 22,87% |
| n-BUTYL BENZOATE | 724 | 25,9 | 0,5767 | 0,2518 | 1,0814 | 0,9922 | 1,1067 | 8,7877 | 0,22% | | | 2,18% | 27,15% |
| n-BUTYL CHLORIDE | 539,2 | 37,21 | 0,2472 | 0,2561 | 1,2537 | 0,9975 | 0,5644 | 8,5231 | 1,19% | 2,12% | | 1,91% | 18,25% |
| n-BUTYL FORMATE | 559 | 35,1 | 0,3878 | 0,2559 | 0,4658 | 0,7949 | 1,5689 | 5,0674 | 0,75% | 2,17% | 0,39% | 1,47% | 19,64% |
| n-BUTYL ISOCYANATE | 568 | 34,4 | 0,4145 | 0,2438 | 1,2232 | 1,0000 | 0,7715 | 14,1958 | 0,62% | 0,70% | | 3,35% | 13,28% |
| n-BUTYL MERCAPTAN | 570,1 | 39,7 | 0,2714 | 0,2628 | 0,3022 | 0,8313 | 1,8319 | 1,6506 | 1,75% | 1,71% | 1,46% | 1,48% | 19,02% |
| n-BUTYL METHACRYLATE | 619 | 26,3 | 0,4467 | 0,2519 | 1,3401 | 1,0000 | 0,7274 | 10,8162 | 1,61% | 1,22% | | 1,49% | 22,81% |
| n-BUTYL n-BUTYRATE | 616 | 25,4 | 0,4815 | 0,2535 | 0,2895 | 0,8296 | 2,6554 | 7,0282 | 0,24% | 1,57% | 1,89% | 1,63% | 24,05% |
| n-BUTYL PROPIONATE | 594,6 | 28 | 0,4644 | 0,2558 | 1,3082 | 1,0000 | 0,7666 | 4,6712 | 0,47% | 0,64% | 0,77% | 1,57% | 21,74% |
| n-BUTYL STEARATE | 764 | 11,1 | 1,0246 | 0,2496 | 0,4503 | 0,8106 | 3,3286 | 5,7899 | 0,72% | 2,28% | 7,76% | 5,68% | 42,55% |
| n-BUTYL VALERATE | 629 | 23,3 | 0,5955 | 0,2539 | 0,4791 | 0,8095 | 2,0961 | 3,9271 | 0,56% | | 0,19% | 2,41% | 25,42% |
| n-BUTYLAMINE | 531,9 | 42 | 0,3292 | 0,2650 | 0,1877 | 0,8113 | 2,4556 | -1,4344 | 0,57% | 2,32% | 2,60% | 1,63% | 4,88% |
| n-BUTYLBENZENE | 660,5 | 28,9 | 0,3941 | 0,2606 | 0,4682 | 0,8213 | 1,6558 | 3,1642 | 0,75% | 1,26% | 1,54% | 2,08% | 16,90% |
| n-BUTYLBENZENE HYDROPEROXIDE | 762,5 | 29,44 | 0,9570 | | 0,5801 | 0,8162 | 2,6227 | | 0,72% | 1,54% | | | |
| n-BUTYLCYCLOHEXANE | 667 | 25,7 | 0,2743 | 0,2579 | 1,5567 | 1,0000 | 0,4774 | 11,5341 | 3,26% | 2,79% | 4,69% | 1,53% | 22,06% |
| n-BUTYLCYCLOPENTANE | 621 | 27,2 | 0,3719 | 0,2592 | 0,4520 | 0,8104 | 1,6090 | 4,0952 | 1,47% | 3,39% | 0,83% | 1,59% | 19,96% |
| n-BUTYLHYDROPEROXIDE | 565 | 52,1 | 0,8658 | 0,3040 | 0,5584 | 0,8130 | 2,4826 | -31,4488 | 0,27% | 0,74% | | 5,94% | 4,97% |
| n-BUTYRIC ACID | 615,7 | 40,6 | 0,6750 | 0,2297 | 0,4405 | 0,8431 | 2,6374 | 17,8529 | 0,52% | | | 2,53% | 26,19% |
| n-CROTYL ACETATE | 585,4 | 33,14 | 0,4383 | 0,2578 | 1,2062 | 0,9862 | 0,8112 | 3,1313 | 0,63% | 1,30% | | 1,47% | 18,30% |
| n-DECANE | 617,7 | 21,1 | 0,4923 | 0,2517 | 0,3784 | 0,8105 | 2,1713 | 12,8329 | 0,44% | 1,22% | 0,66% | 1,26% | 19,19% |
| n-DECYL FORMATE | 672 | 19,9 | 0,7118 | 0,2481 | 0,3353 | 0,8200 | 3,1107 | 12,1297 | 1,00% | | 1,51% | 2,15% | 22,09% |
| n-DECYL MERCAPTAN | 696 | 21,3 | 0,5874 | 0,2417 | 0,5681 | -0,8025 | 2,3285 | 41,3308 | 1,98% | 2,37% | 2,68% | 5,39% | 27,22% |
| n-DECYLAMINE | 663 | 21,8 | 0,6664 | 0,2477 | 0,3196 | 0,8216 | 3,0771 | 10,3406 | 2,53% | 4,23% | 2,65% | 1,15% | 21,93% |
| n-DECYLBENZENE | 753 | 17,7 | 0,6797 | 0,2468 | 0,3636 | 0,8280 | 2,9432 | 19,7540 | 2,85% | 3,07% | 1,96% | 2,80% | 31,31% |
| n-DECYLCYCLOHEXANE | 751,25 | 16,5 | 0,6627 | 0,2471 | 0,6069 | 0,8158 | 1,9413 | 21,2530 | 1,83% | 4,03% | 0,61% | 2,46% | 33,15% |
| n-DODECANE | 658 | 18,2 | 0,5764 | 0,2466 | 0,4577 | 0,8011 | 2,0899 | 22,2261 | 0,62% | 1,22% | 2,35% | 1,34% | 19,45% |
| n-DODECANOIC ACID | 743 | 19,3 | 0,8983 | 0,2406 | 1,8223 | 1,0000 | 0,8217 | 23,5008 | 0,64% | 1,01% | 6,22% | 1,77% | 25,22% |
| n-DODECYLAMINE | 696 | 18,8 | 0,7638 | 0,2440 | 0,3783 | 0,8217 | 3,0734 | 14,6555 | 5,29% | 6,85% | 3,90% | 1,29% | 26,74% |
| n-DODECYLBENZENE | 780 | 15,6 | 0,7333 | 0,2446 | 0,5888 | 0,8077 | 2,0826 | 29,0028 | 0,70% | 2,24% | 0,17% | 3,14% | 35,31% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| n-EICOSANE | 768 | 11,6 | 0,9069 | 0,2335 | 0,4688 | 0,8098 | 2,9217 | 63,8215 | 0,43% | 1,98% | 1,04% | 2,14% | 21,52% |
| NEOABIETIC ACID | 812 | 16,7 | 0,8598 | | 0,3622 | 0,8102 | 3,3382 | | 0,53% | 0,88% | | | |
| NEOHEXANOIC ACID | 653 | 34,1 | 0,5671 | 0,2396 | 0,9083 | 0,8360 | 1,2276 | 15,0973 | 0,36% | 1,69% | 2,10% | 3,37% | 21,94% |
| NEOPENTANE | 433,8 | 31,96 | 0,1957 | 0,2756 | 0,1268 | 0,8494 | 2,5589 | -5,9635 | 0,21% | 1,66% | 1,17% | 1,37% | 14,94% |
| N-ETHYL-2-METHYLALLYLAMINE | 556 | 31,8 | 0,3550 | 0,2673 | 0,8721 | 0,8639 | 0,9627 | -2,6759 | 0,59% | 1,68% | 3,05% | 1,26% | 11,00% |
| N-ETHYLANILINE | 698,55 | 35,8 | 0,4149 | 0,2522 | 0,2958 | 0,7728 | 2,0549 | 10,6883 | 0,32% | 1,02% | | 1,45% | 14,56% |
| N-ETHYLMORPHOLINE | 617 | 36,83 | 0,3327 | | 0,9249 | 0,9169 | 0,9018 | | 0,69% | 1,46% | | | |
| n-HENEICOSANE | 778 | 11,1 | 0,9420 | 0,2315 | 0,4695 | 0,8115 | 3,0185 | 72,6911 | 1,48% | 2,04% | 1,33% | 2,22% | 21,89% |
| n-HEPTACOSANE | 826 | 8,83 | 1,2136 | 0,2265 | 0,5930 | 0,8189 | 3,1353 | 101,2761 | 1,40% | | 1,30% | 3,22% | 23,10% |
| n-HEPTADECANE | 736 | 13,4 | 0,7697 | 0,2364 | 0,5607 | 0,7924 | 2,1874 | 52,5854 | 0,25% | 0,40% | 0,41% | 1,64% | 21,73% |
| n-HEPTADECYLBENZENE | 826 | 12,1 | 0,9195 | 0,2374 | 0,6564 | 0,8170 | 2,2955 | 51,2232 | 1,13% | 1,04% | 0,74% | 3,69% | 41,13% |
| n-HEPTANE | 540,2 | 27,4 | 0,3495 | 0,2602 | 0,3643 | 0,8200 | 1,8313 | 3,1112 | 0,41% | 1,52% | 2,76% | 1,28% | 17,01% |
| n-HEPTANOIC ACID | 677,3 | 30,43 | 0,7599 | 0,2495 | 0,9347 | 0,8294 | 1,4521 | 5,8003 | 1,01% | 2,07% | | 2,01% | 20,83% |
| n-HEPTYL ACETATE | 637 | 23,3 | 0,5943 | 0,2552 | 0,3494 | 0,8203 | 2,6649 | 3,4761 | 0,27% | 2,72% | 1,96% | 2,57% | 27,11% |
| n-HEPTYL FORMATE | 628 | 25,4 | 0,5337 | 0,2525 | 0,2691 | 0,8277 | 2,9492 | 7,8674 | 1,71% | 1,42% | 1,87% | 1,69% | 26,33% |
| n-HEPTYL MERCAPTAN | 645 | 27,7 | 0,4226 | 0,2534 | 0,3282 | 0,8281 | 2,2458 | 8,9332 | 1,96% | 1,89% | 2,04% | 1,32% | 26,07% |
| n-HEPTYLAMINE | 607 | 28,5 | 0,5077 | 0,2553 | 0,2411 | 0,8258 | 2,9880 | 3,5786 | 2,06% | 3,34% | 2,41% | 1,08% | 14,81% |
| n-HEPTYLBENZENE | 714 | 21,8 | 0,5272 | 0,2504 | 0,2997 | 0,8344 | 2,8190 | 14,9158 | 3,75% | 4,17% | 1,91% | 2,15% | 26,88% |
| n-HEXACOSANE | 819 | 9,1 | 1,1544 | 0,2267 | 0,5134 | 0,8105 | 3,3319 | 99,9368 | 1,68% | | 1,28% | 2,95% | 23,61% |
| n-HEXADECANE | 723 | 14 | 0,7174 | 0,2366 | 0,6147 | 0,7868 | 1,9249 | 52,1490 | 0,28% | 0,47% | 0,76% | 1,47% | 21,90% |
| n-HEXADECANOIC ACID | 785 | 14,9 | 0,9919 | 0,2348 | 2,0243 | 1,0000 | 0,7942 | 43,5908 | 4,17% | | 8,48% | 1,85% | 28,37% |
| n-HEXADECYLBENZENE | 818 | 12,7 | 0,8996 | 0,2414 | 0,7145 | 0,8174 | 2,0924 | 38,7214 | 0,26% | 1,08% | 0,61% | 4,07% | 41,01% |
| n-HEXANE | 507,6 | 30,25 | 0,3013 | 0,2633 | 0,2806 | 0,8357 | 2,0600 | 0,7940 | 0,80% | 1,48% | 2,32% | 1,25% | 15,39% |
| n-HEXANOIC ACID | 660,2 | 33,08 | 0,7330 | 0,2397 | 1,8838 | 1,0000 | 0,6836 | 13,7839 | 0,43% | | | 1,76% | 21,64% |
| n-HEXYL ACETATE | 618 | 25,4 | 0,5396 | 0,2550 | 0,2921 | 0,8314 | 2,8759 | 4,0691 | 0,53% | 2,95% | 2,27% | 2,25% | 25,06% |
| n-HEXYL FORMATE | 607 | 28 | 0,4830 | 0,2504 | 0,2527 | 0,8024 | 2,6348 | 9,3240 | 0,42% | 2,89% | 0,49% | 1,48% | 23,25% |
| n-HEXYL MERCAPTAN | 623 | 30,8 | 0,3681 | 0,2559 | 0,3764 | 0,8257 | 1,8689 | 6,7750 | 1,38% | 1,90% | 1,79% | 1,44% | 23,84% |
| n-HEXYLAMINE | 584 | 31,8 | 0,4577 | 0,2570 | 0,1969 | 0,8229 | 3,0476 | 2,2567 | 1,67% | 4,33% | 1,17% | 1,30% | 11,75% |
| n-HEXYLBENZENE | 698 | 23,8 | 0,4790 | 0,2518 | 0,3542 | 0,8311 | 2,3499 | 12,3922 | 1,71% | 2,75% | 1,96% | 1,78% | 24,31% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| NIACIN | 760 | 46,4 | 0,5958 | | 0,2409 | 0,8146 | 3,2331 | | 0,40% | 1,43% | | | |
| NICKEL CARBONYL | 452,55 | 30,398 | 0,4631 | 0,2738 | 0,2936 | 0,8430 | 2,6643 | -12,4558 | 3,77% | | 0,24% | 0,75% | 12,27% |
| NICOTINONITRILE | 703 | 41,2 | 0,4215 | 0,2272 | 0,4594 | 0,8434 | 1,8495 | 30,4773 | 1,53% | 1,92% | 3,26% | 3,90% | 17,92% |
| NITROETHANE | 593 | 51,6 | 0,3803 | 0,2412 | 0,3078 | 0,8615 | 2,3754 | 13,7392 | 5,00% | 5,05% | 3,86% | 1,58% | 18,64% |
| NITROGEN | 126,2 | 34 | 0,0377 | 0,2908 | 0,1242 | 0,8898 | 2,0130 | -3,6428 | 0,27% | 1,44% | 3,26% | 1,07% | 10,43% |
| NITROGEN TRIFLUORIDE | 234 | 44,607 | 0,1200 | 0,2779 | 0,6463 | 0,8859 | 0,7859 | -2,1633 | 0,62% | 0,57% | | 1,31% | 14,73% |
| NITROGEN TRIOXIDE | 425 | 69,9 | 0,4312 | | 0,3313 | 0,8046 | 2,1335 | | 0,46% | | | | |
| NITROMETHANE | 588,15 | 63,1 | 0,3480 | 0,2310 | 0,2923 | 0,8638 | 2,3416 | 16,7596 | 3,22% | 4,84% | 2,06% | 2,92% | 28,02% |
| NITROSYL CHLORIDE | 440,65 | 91,2 | 0,3005 | 0,3061 | 0,5168 | 0,9352 | 1,5683 | -12,1333 | 0,83% | 1,32% | | 1,30% | 2,43% |
| NITROUS OXIDE | 309,57 | 72,45 | 0,1409 | 0,2753 | 1,2023 | 0,9324 | 0,4689 | -1,2290 | 1,36% | 1,94% | 0,13% | 1,68% | 13,39% |
| N-METHYL-2-PYRROLIDONE | 721,6 | 45,2 | 0,3732 | 0,2407 | 0,2742 | 0,8518 | 2,5206 | 18,2102 | 1,02% | 4,53% | | 2,33% | 25,75% |
| N-METHYLACETAMIDE | 718 | 49,8 | 0,4351 | 0,2239 | 0,3634 | 0,8051 | 2,0400 | 28,5063 | 0,76% | 1,95% | | 4,07% | 27,34% |
| N-METHYLANILINE | 701,55 | 52 | 0,4750 | 0,2883 | 0,4323 | 0,8735 | 2,2106 | -21,4403 | 1,85% | 1,93% | | 3,78% | 1,81% |
| N-METHYLCYCLOHEXYLAMINE | 622 | 34,9 | 0,3855 | 0,2654 | 0,3953 | 0,8162 | 1,8318 | -3,4116 | 0,67% | 1,54% | | 1,07% | 16,78% |
| N-METHYLFORMAMIDE | 721 | 56,2 | 0,4100 | 0,2062 | 1,2134 | 1,0000 | 0,7745 | 37,4037 | 0,62% | 1,66% | | 7,13% | 35,11% |
| N-METHYLPYRROLE | 610 | 47,7 | 0,2128 | 0,2710 | 1,5715 | 1,0000 | 0,4157 | 0,5256 | 1,82% | 1,61% | 0,48% | 2,80% | 15,31% |
| N-METHYLPYRROLIDINE | 550 | 42 | 0,2258 | 0,2755 | 1,0691 | 1,0000 | 0,6445 | -6,5026 | 0,63% | 1,21% | | 1,21% | 13,73% |
| N-METHYLTHIOPYRROLIDONE | 869 | 43,2 | 0,2381 | | 0,8070 | 0,9179 | 0,8639 | | 0,34% | 1,63% | | | |
| N-NITROSODIETHANOLAMINE | 887,1 | 48,36 | 0,9833 | 0,2424 | 0,4405 | 0,8126 | 3,2796 | 7,4143 | 0,42% | | | 3,82% | 24,71% |
| N-NITROSODIMETHYLAMINE | 661 | 48,9 | 0,2738 | 0,2284 | 1,3471 | 1,0000 | 0,5525 | 28,1929 | 0,91% | 2,23% | 1,01% | 4,62% | 23,46% |
| n-NONADECANE | 758 | 12,1 | 0,8522 | 0,2334 | 0,4715 | 0,7926 | 2,6734 | 64,7870 | 0,28% | 0,83% | 1,11% | 1,82% | 21,93% |
| n-NONANE | 594,6 | 22,9 | 0,4435 | 0,2544 | 0,4171 | 0,8081 | 1,8918 | 9,3455 | 0,13% | 0,94% | 0,53% | 1,30% | 18,75% |
| n-NONANOIC ACID | 710,7 | 25,14 | 0,7787 | 0,2507 | 1,8354 | 1,0000 | 0,7324 | 7,2173 | 1,06% | 0,48% | | 2,44% | 22,49% |
| n-NONYL ACETATE | 661 | 19,9 | 0,7036 | 0,2553 | 0,4740 | 0,8050 | 2,3655 | 1,0823 | 0,26% | 0,65% | 1,47% | 3,34% | 29,84% |
| n-NONYL FORMATE | 656 | 21,4 | 0,6504 | 0,2507 | 0,3039 | 0,8208 | 3,0936 | 8,7559 | 1,02% | | 1,28% | 1,99% | 21,24% |
| n-NONYL MERCAPTAN | 681 | 23,1 | 0,5260 | 0,2491 | 0,4090 | 0,8095 | 2,1576 | 13,9664 | 3,96% | 4,35% | 2,13% | 1,40% | 29,51% |
| n-NONYL n-UNDECYL PHTHALATE | 914,6 | 9,951 | 0,9080 | | 0,4599 | 0,8154 | 2,9972 | | 0,39% | | | | |
| n-NONYLAMINE | 648 | 23,6 | 0,6171 | 0,2530 | 0,2976 | 0,8231 | 3,0431 | 5,3140 | 2,37% | 5,09% | 2,60% | 1,52% | 20,70% |
| n-OCTACOSANE | 832 | 8,5 | 1,2375 | 0,2256 | 0,5473 | 0,8091 | 3,3648 | 108,0359 | 2,52% | 2,56% | 0,92% | 3,27% | 24,03% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| n-OCTADECANE | 747 | 12,7 | 0,8114 | 0,2347 | 0,5802 | 0,7925 | 2,2165 | 59,1697 | 0,35% | 0,45% | 0,36% | 1,70% | 21,36% |
| n-OCTADECYLBENZENE | 834 | 11,6 | 0,9505 | 0,2346 | 0,6788 | 0,8159 | 2,2901 | 60,2534 | 1,59% | 1,14% | 0,54% | 3,17% | 42,19% |
| n-OCTANE | 568,7 | 24,9 | 0,3996 | 0,2569 | 0,3573 | 0,8171 | 1,9988 | 6,4292 | 0,41% | 1,11% | 0,63% | 1,21% | 18,79% |
| n-OCTANOIC ACID | 694,26 | 27,79 | 0,7734 | 0,2466 | 0,7739 | 0,7962 | 1,6970 | 8,3895 | 1,10% | 1,47% | | 1,37% | 20,48% |
| n-OCTYL ACETATE | 652 | 21,5 | 0,6558 | 0,2525 | 0,4070 | 0,8075 | 2,5134 | 5,4093 | 0,89% | | 1,31% | 2,38% | 28,28% |
| n-OCTYL FORMATE | 645 | 23,3 | 0,5871 | 0,2520 | 0,2842 | 0,8232 | 3,0421 | 7,6634 | 5,40% | | 1,03% | 2,05% | 27,95% |
| n-OCTYL MERCAPTAN | 667,3 | 25,2 | 0,4497 | 0,2509 | 0,3724 | 0,8186 | 2,1050 | 12,8726 | 1,18% | 1,48% | 2,00% | 1,42% | 28,17% |
| n-OCTYLAMINE | 627 | 25,8 | 0,5694 | 0,2552 | 0,2682 | 0,8230 | 3,0461 | 3,1326 | 1,85% | 4,59% | 1,98% | 1,26% | 17,94% |
| n-OCTYLBENZENE | 729 | 20,2 | 0,5670 | 0,2482 | 0,3121 | 0,8317 | 2,8709 | 18,6277 | 2,40% | 3,21% | 2,04% | 2,15% | 28,56% |
| NONANAL | 658,5 | 26,8 | 0,4733 | 0,2627 | 1,3055 | 1,0000 | 0,7803 | -3,2922 | 0,71% | 2,26% | | 1,40% | 16,26% |
| NONYLPHENOL | 770 | 20,7 | 0,8795 | 0,2446 | 0,3346 | 0,8036 | 3,5074 | 9,5033 | 1,38% | 1,10% | | 1,92% | 24,34% |
| n-PENTADECANE | 708 | 14,8 | 0,6863 | 0,2384 | 0,5798 | 0,7877 | 1,9485 | 45,3502 | 0,34% | 1,75% | 0,66% | 1,44% | 21,50% |
| n-PENTADECANOIC ACID | 774 | 15,7 | 0,9639 | 0,2345 | 1,8947 | 1,0000 | 0,8382 | 42,2353 | 4,54% | | 7,81% | 2,19% | 27,92% |
| n-PENTADECYLBENZENE | 809 | 13,3 | 0,8567 | 0,2421 | 0,6214 | 0,8155 | 2,2673 | 36,5473 | 0,39% | 1,30% | 0,89% | 3,88% | 39,28% |
| n-PENTANE | 469,7 | 33,7 | 0,2515 | 0,2679 | 0,2933 | 0,8366 | 1,8242 | -1,5965 | 0,41% | 1,04% | 1,22% | 1,28% | 14,32% |
| n-PENTANOIC ACID | 639,16 | 36,3 | 0,7066 | 0,2357 | 0,3020 | 0,7954 | 3,0643 | 15,7760 | 0,17% | | | 1,73% | 24,07% |
| n-PENTYL ACETATE | 599,9 | 27,7 | 0,4478 | 0,2540 | 0,2245 | 0,8296 | 2,9105 | 7,2925 | 1,21% | 2,09% | 1,29% | 1,40% | 23,58% |
| n-PENTYL MERCAPTAN | 598 | 34,7 | 0,3207 | 0,2624 | 0,3776 | -0,7241 | 1,2186 | 11,8497 | 1,59% | 1,82% | 1,29% | 3,38% | 19,39% |
| n-PENTYLAMINE | 555 | 35,8 | 0,4070 | 0,2607 | 0,1743 | 0,8250 | 3,0041 | 0,3550 | 1,30% | 4,29% | 0,76% | 1,18% | 8,46% |
| n-PENTYLBENZENE | 679,9 | 26,04 | 0,4378 | 0,2534 | 0,3968 | 0,8305 | 2,0377 | 10,1432 | 2,42% | | 2,12% | 1,55% | 19,49% |
| n-PENTYLCYCLOHEXANE | 669,2 | 23,85 | 0,4612 | 0,2586 | 0,5843 | 0,8640 | 1,6444 | 2,1826 | 0,58% | 1,70% | | 1,81% | 18,57% |
| n-PROPYL ACETATE | 549,73 | 33,6 | 0,3889 | 0,2531 | 0,6462 | 0,8114 | 1,2670 | 8,2270 | 0,67% | 1,17% | 0,66% | 1,46% | 18,82% |
| n-PROPYL ACRYLATE | 569 | 32,5 | 0,4315 | 0,2597 | 1,0527 | 0,9212 | 0,9211 | 1,3971 | 0,67% | 1,03% | | 1,39% | 18,64% |
| n-PROPYL FORMATE | 538 | 40,2 | 0,3088 | 0,2567 | 1,5662 | 1,0000 | 0,4908 | 5,9223 | 0,98% | 1,61% | 0,52% | 1,83% | 17,94% |
| n-PROPYL IODIDE | 586,3 | 41,52 | 0,2230 | 0,2521 | 0,9407 | 1,0000 | 0,7438 | 11,5647 | 0,53% | 1,71% | | 2,83% | 16,06% |
| n-PROPYL ISOBUTYRATE | 579,4 | 28,4 | 0,4838 | 0,2650 | 0,3461 | 0,7942 | 2,1835 | -5,8466 | 0,45% | 2,28% | 1,57% | 2,00% | 19,29% |
| n-PROPYL MERCAPTAN | 536,6 | 46,3 | 0,2318 | 0,2689 | 0,3346 | 0,8206 | 1,5408 | -1,2347 | 1,87% | 1,97% | 1,19% | 1,33% | 17,11% |
| n-PROPYL METHACRYLATE | 599 | 29,1 | 0,3966 | 0,2582 | 0,1929 | 0,8302 | 2,8988 | 5,2489 | 1,19% | 2,05% | | 1,79% | 21,69% |
| n-PROPYL n-BUTYRATE | 593,7 | 27,2 | 0,4335 | 0,2535 | 0,6250 | 0,7986 | 1,3705 | 9,1573 | 0,64% | 3,68% | 0,45% | 1,58% | 24,14% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c_{P,liq}^{sat}$ | $v_{liq}^{sat}$ | $v_c$ |
| n-PROPYL PROPIONATE | 568,6 | 30,6 | 0,4487 | 0,2564 | 0,3312 | 0,8081 | 2,1964 | 4,0784 | 0,40% | 3,52% | 5,49% | 1,39% | 21,04% |
| n-PROPYLAMINE | 496,95 | 47,4 | 0,2798 | 0,2636 | 1,7704 | 1,0000 | 0,4131 | 1,1989 | 1,77% | 3,79% | 1,25% | 1,79% | 2,60% |
| n-PROPYLBENZENE | 638,35 | 32 | 0,3444 | 0,2634 | 0,4895 | 0,8240 | 1,4833 | 1,4607 | 0,39% | 1,00% | 1,18% | 2,11% | 15,54% |
| n-PROPYLBENZENE HYDROPEROXIDE | 746,8 | 32,9 | 0,9058 | | 0,6204 | 0,8178 | 2,3817 | | 0,56% | 1,39% | | | |
| n-PROPYLCYCLOHEXANE | 639,15 | 28,07 | 0,2595 | 0,2608 | 1,3406 | 1,0000 | 0,5431 | 7,0001 | 2,29% | 2,10% | 0,80% | 1,51% | 20,54% |
| n-PROPYLCYCLOPENTANE | 596 | 30,2 | 0,3266 | 0,2623 | 0,5976 | 0,8305 | 1,2408 | 1,3381 | 0,92% | 1,48% | 1,28% | 1,50% | 17,54% |
| n-TETRACOSANE | 804 | 9,8 | 1,0710 | 0,2284 | 0,4691 | 0,8103 | 3,3371 | 89,6456 | 0,50% | 2,06% | 0,96% | 2,63% | 23,14% |
| n-TETRADECANE | 693 | 15,7 | 0,6430 | 0,2401 | 0,5704 | 0,7890 | 1,8888 | 39,9098 | 0,23% | 0,86% | 0,88% | 1,37% | 21,32% |
| n-TETRADECANOIC ACID | 763 | 16,4 | 0,9535 | 0,2334 | 1,9269 | 1,0000 | 0,8157 | 42,6388 | 4,20% | | 7,09% | 1,65% | 28,82% |
| n-TETRADECYLAMINE | 722 | 16,6 | 0,8609 | 0,2415 | 0,4067 | 0,8153 | 3,2179 | 19,1666 | 5,48% | | 4,22% | 1,95% | 30,06% |
| n-TETRADECYLBENZENE | 800 | 14 | 0,8130 | 0,2428 | 0,6318 | 0,8154 | 2,1490 | 34,1963 | 0,63% | 1,34% | 0,86% | 3,63% | 38,48% |
| n-TRICOSANE | 796 | 10,2 | 1,0262 | 0,2293 | 0,4779 | 0,8096 | 3,1734 | 84,6520 | 0,48% | 2,12% | 1,44% | 2,46% | 22,43% |
| n-TRIDECANE | 675 | 16,8 | 0,6174 | 0,2433 | 0,4772 | 0,7990 | 2,1208 | 30,1374 | 0,26% | 0,82% | 0,42% | 1,40% | 20,67% |
| n-TRIDECANOIC ACID | 754 | 17,9 | 0,9134 | 0,2380 | 1,8617 | 1,0000 | 0,8165 | 30,6685 | 2,53% | 2,65% | 6,54% | 2,05% | 26,32% |
| n-TRIDECYLBENZENE | 790 | 14,8 | 0,7799 | 0,2440 | 0,5491 | 0,8101 | 2,3162 | 29,7965 | 1,31% | 1,94% | 0,85% | 3,41% | 36,45% |
| n-UNDECANE | 639 | 19,5 | 0,5303 | 0,2488 | 0,4799 | 0,8001 | 1,9060 | 18,3288 | 0,63% | 1,30% | 0,32% | 1,33% | 19,59% |
| n-UNDECANOIC ACID | 732 | 20,9 | 0,8531 | 0,2426 | 1,8323 | 1,0000 | 0,7876 | 19,3172 | 0,68% | 0,99% | 5,64% | 1,82% | 24,23% |
| n-UNDECYLBENZENE | 764 | 16,72 | 0,7287 | 0,2469 | 0,3880 | 0,8267 | 2,9697 | 18,8639 | 4,04% | 3,43% | 2,44% | 3,21% | 32,37% |
| o-ANISIDINE | 736 | 42,4 | 0,4447 | 0,2547 | 0,2233 | 0,8293 | 2,9166 | 5,6815 | 1,79% | 3,10% | | 1,24% | 19,02% |
| o-CHLOROANILINE | 722 | 45,9 | 0,4213 | 0,2578 | 0,3173 | 0,8552 | 2,4688 | 2,9202 | 2,50% | 3,41% | | 1,18% | 9,65% |
| o-CHLOROBENZOIC ACID | 792 | 40,3 | 0,6637 | | 0,4185 | 0,8005 | 2,4492 | | 0,55% | | | | |
| o-CHLORONITROBENZENE | 757 | 39,8 | 0,4864 | 0,2497 | 0,6195 | 0,8269 | 1,5293 | 12,7561 | 3,85% | | 1,59% | 1,30% | 9,58% |
| o-CHLOROPHENOL | 675 | 50 | 0,4372 | 0,2744 | 0,4292 | 0,8839 | 2,0816 | -10,1749 | 4,74% | 6,62% | | 1,57% | 9,30% |
| o-CHLOROTOLUENE | 656 | 39,1 | 0,3044 | 0,2587 | 0,4391 | 0,8295 | 1,5165 | 4,9461 | 0,40% | 0,80% | | 1,56% | 19,74% |
| o-CRESOL | 697,55 | 50,1 | 0,4339 | 0,2688 | 0,1860 | 0,8237 | 3,0314 | -7,5829 | 1,00% | 1,51% | 1,80% | 1,01% | 28,88% |
| OCTADECAMETHYLOCTASILOXANE | 688,9 | 6,2416 | 0,9837 | 0,2533 | 1,2135 | 0,9100 | 1,4005 | 2,5898 | 0,58% | 0,91% | | 7,09% | 14,29% |
| OCTAFLUORO-2-BUTENE | 392 | 23,3 | 0,2922 | 0,2417 | 0,2160 | 0,8523 | 2,5134 | 18,0868 | 1,41% | 1,72% | 1,53% | 5,44% | 18,71% |
| OCTAFLUOROCYCLOBUTANE | 388,37 | 27,775 | 0,3558 | 0,2719 | 0,2733 | 0,7999 | 2,0802 | -6,9005 | 0,19% | 1,45% | 0,04% | 0,91% | 12,15% |
| OCTAFLUOROPROPANE | 345,05 | 26,8 | 0,3280 | 0,2780 | 1,0245 | 1,0000 | 0,8170 | -10,6238 | 0,48% | | | 1,45% | 13,61% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| OCTAHYDRO-PENTALENE-1-CARBOXYLIC ACID | 799,5 | 33,37 | 0,6928 | | 0,4155 | 0,8370 | 2,7710 | | 0,51% | | | | |
| OCTAMETHYLCYCLOTETRASILOXANE | 586,5 | 13,172 | 0,5837 | 0,2572 | 1,8359 | 0,9979 | 0,6066 | 2,5270 | 0,55% | 1,46% | | 0,99% | 15,40% |
| OCTAMETHYLTRISILOXANE | 564,4 | 14,6 | 0,5377 | 0,2667 | 0,2860 | 0,8265 | 2,8698 | -16,9603 | 0,98% | 2,18% | | 2,76% | 15,78% |
| OCTANAL | 638,9 | 29,6 | 0,4420 | 0,2667 | 1,1777 | 1,0000 | 0,8440 | -6,6507 | 0,83% | 1,17% | | 1,60% | 14,41% |
| o-CYMENE | 657 | 29 | 0,3662 | 0,2566 | 1,1266 | 1,0000 | 0,7854 | 8,2233 | 1,41% | 0,93% | | 1,45% | 16,49% |
| o-DICHLOROBENZENE | 705 | 40,7 | 0,2192 | 0,2553 | 1,5967 | 0,7780 | 0,4377 | 12,8329 | 1,26% | 1,44% | | 2,15% | 22,48% |
| o-DIETHYLBENZENE | 668 | 28,8 | 0,3395 | 0,2534 | 1,3185 | 1,0000 | 0,6342 | 13,6248 | 0,94% | 1,67% | 0,63% | 1,47% | 15,38% |
| o-ETHYLANILINE | 704 | 37,4 | 0,4620 | 0,2594 | 1,2479 | 1,0000 | 0,8077 | 2,9312 | 0,56% | 0,49% | | 2,34% | 12,25% |
| o-ETHYLPHENOL | 703 | 42,9 | 0,4763 | 0,2770 | 0,2112 | 0,8235 | 3,0350 | -14,6774 | 2,78% | 3,57% | 3,18% | 3,17% | 23,51% |
| o-ETHYLSTYRENE | 666,7 | 29,36 | 0,3962 | 0,2497 | 1,1978 | 1,0000 | 0,7700 | 15,7032 | 0,64% | 1,00% | | 1,56% | 22,22% |
| o-ETHYLTOLUENE | 650 | 32,9 | 0,3353 | 0,2605 | 0,6803 | 0,8347 | 1,1400 | 4,3034 | 0,24% | 0,70% | | 1,54% | 17,25% |
| OLEIC ACID | 781 | 13,9 | 1,1822 | 0,2349 | 0,7864 | 0,8242 | 2,3973 | 30,8313 | 0,47% | 0,10% | | 3,35% | 40,52% |
| o-METHYLSTYRENE | 659 | 34,7 | 0,3412 | 0,2594 | 1,0763 | 0,9088 | 0,7785 | 5,2208 | 0,33% | 0,38% | | 1,47% | 17,98% |
| o-NITROANISOLE | 782 | 37,6 | 0,5613 | 0,2444 | 0,7580 | 0,8437 | 1,4505 | 16,0895 | 0,64% | 0,96% | | 1,55% | 22,15% |
| o-NITRODIPHENYLAMINE | 835 | 28,7 | 0,7669 | | 0,9445 | 0,9362 | 1,5593 | | 0,88% | | | | |
| o-NITROTOLUENE | 720 | 38 | 0,4878 | 0,2536 | 0,4245 | 0,8690 | 2,2702 | 8,6822 | 2,60% | 3,00% | | 2,07% | 7,84% |
| o-PHENYLENEDIAMINE | 781 | 51,8 | 0,5389 | 0,2509 | 0,7891 | 0,8624 | 1,3795 | 6,3499 | 0,46% | 1,04% | | 1,04% | 20,32% |
| o-TERPHENYL | 857 | 29,9 | 0,5513 | 0,2889 | 0,2654 | 0,8250 | 3,0052 | -46,1500 | 3,89% | 4,24% | | 4,06% | 6,53% |
| o-TOLUALDEHYDE | 694 | 36,7 | 0,4346 | 0,2453 | 0,3877 | 0,8490 | 2,1501 | 16,5372 | 0,26% | | | 1,38% | 20,93% |
| o-TOLUIC ACID | 751 | 38,6 | 0,6572 | 0,2468 | 0,3529 | 0,8072 | 2,7566 | 9,6476 | 0,58% | 1,16% | | 1,04% | 22,83% |
| o-TOLUIDINE | 716,5 | 47 | 0,3842 | 0,2691 | 0,2666 | 0,8176 | 2,3042 | -4,7145 | 2,15% | 1,38% | 2,32% | 1,84% | 13,45% |
| OXAZOLE | 554 | 63,2 | 0,2310 | | 0,9150 | 0,9888 | 0,7744 | | 1,67% | 3,09% | | | |
| OXYGEN | 154,58 | 50,43 | 0,0222 | 0,2899 | 0,2337 | 0,8896 | 1,3060 | -2,7621 | 0,35% | 1,38% | 4,38% | 1,14% | 10,50% |
| o-XYLENE | 630,3 | 37,32 | 0,3101 | 0,2611 | 0,3300 | 0,8425 | 1,9311 | 2,5506 | 0,37% | 1,51% | 1,04% | 1,29% | 15,98% |
| OZONE | 261 | 55,7 | 0,2119 | 0,2505 | 0,2606 | 0,8077 | 1,6250 | 3,9988 | 2,47% | 6,20% | 9,85% | 4,73% | 30,07% |
| p,alpha-DIMETHYLBENZYL ALCOHOL | 695,9 | 34,92 | 0,5945 | 0,2614 | 0,7169 | 0,8404 | 1,5821 | -5,0165 | 0,65% | 1,79% | | 2,29% | 18,79% |
| p-AMINOAZOBENZENE | 877 | 29 | 0,6345 | | 0,5835 | 0,8142 | 1,9087 | | 0,61% | 0,95% | | | |
| p-AMINODIPHENYL | 867 | 32,9 | 0,5419 | | 1,0512 | 0,9760 | 1,0871 | | 0,44% | | | | |
| p-AMINODIPHENYLAMINE | 867 | 31,9 | 0,6940 | | 0,6732 | 0,8223 | 1,8286 | | 0,57% | 0,70% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| PARALDEHYDE | 579 | 35 | 0,4368 | 0,2792 | 0,1193 | 0,8099 | 3,3466 | -17,0285 | 1,77% | 3,35% | 1,96% | 1,15% | 20,50% |
| p-BROMOTOLUENE | 699 | 43,7 | 0,3179 | 0,2813 | 1,0348 | 1,0000 | 0,7962 | -14,5903 | 1,32% | 1,90% | | 1,72% | 11,72% |
| p-CHLOROANILINE | 754 | 45,9 | 0,4210 | 0,2561 | 0,4555 | 0,8258 | 1,7839 | 6,1374 | 0,53% | 1,35% | | 1,08% | 13,66% |
| p-CHLOROBENZOTRIFLUORIDE | 601 | 30,1 | 0,3715 | 0,2495 | 1,1930 | 1,0000 | 0,7431 | 13,5724 | 0,58% | 1,10% | | 2,11% | 24,50% |
| p-CHLORONITROBENZENE | 751 | 39,8 | 0,4874 | 0,2407 | 1,2953 | 1,0000 | 0,8005 | 18,0484 | 0,83% | 1,63% | 0,49% | 2,95% | 7,46% |
| p-CHLOROPHENOL | 738 | 53,2 | 0,4849 | 0,2743 | 0,6048 | 0,9141 | 1,7592 | -10,3441 | 2,08% | 2,59% | | 2,62% | 12,28% |
| p-CHLOROTOLUENE | 660 | 39,1 | 0,3123 | 0,2610 | 0,1847 | 0,8418 | 2,6862 | 2,7111 | 0,36% | 1,27% | | 1,27% | 19,09% |
| p-CRESOL | 704,65 | 51,5 | 0,5072 | 0,2697 | 0,2386 | 0,8250 | 3,0043 | -11,3407 | 4,76% | 4,85% | 3,05% | 1,06% | 30,34% |
| p-CUMYLPHENOL | 834 | 28,6 | 0,6888 | 0,2679 | 0,3053 | 0,8166 | 3,1875 | -18,0934 | 0,47% | 1,46% | 1,75% | 2,95% | 8,59% |
| p-CYMENE | 652 | 28 | 0,3738 | 0,2559 | 0,5425 | 0,8337 | 1,4651 | 8,9738 | 0,81% | 2,58% | 1,97% | 1,44% | 17,94% |
| p-DICHLOROBENZENE | 684,75 | 40,7 | 0,2846 | 0,2607 | 0,5452 | 0,8121 | 1,2117 | 5,1202 | 0,33% | 1,39% | 3,33% | 1,17% | 21,05% |
| p-DIETHYLBENZENE | 657,9 | 28,03 | 0,4028 | 0,2550 | 1,3300 | 1,0000 | 0,6844 | 9,9876 | 1,64% | 2,67% | 0,90% | 1,37% | 18,69% |
| p-DIISOPROPYLBENZENE | 689 | 24,5 | 0,3900 | 0,2577 | 1,8430 | 1,0000 | 0,4702 | 7,8325 | 1,00% | 1,42% | | 1,31% | 18,89% |
| p-DIISOPROPYLBENZENE HYDROPEROXIDE | 810 | 24,9 | 0,9279 | 0,2472 | 0,7608 | 0,8243 | 2,0487 | 6,4038 | 1,03% | 0,89% | 2,23% | 3,22% | 23,32% |
| p-DIMETHYLAMINOBENZALDEHYDE | 832 | 30,7 | 0,5272 | 0,2258 | 0,6342 | 0,9119 | 1,7806 | 48,5626 | 0,83% | 2,84% | | 1,70% | 36,75% |
| p-DIVINYLBENZENE | 691,5 | 30,77 | 0,3830 | 0,2473 | 0,5722 | 0,8440 | 1,4475 | 19,0921 | 0,60% | 2,07% | | 1,53% | 20,19% |
| PENTACHLOROETHANE | 665 | 36,8 | 0,2455 | 0,2523 | 0,1756 | 0,8516 | 2,5240 | 13,6116 | 0,80% | | | 2,58% | 21,48% |
| PENTACHLOROFLUOROETHANE | 624 | 33,4 | 0,2450 | 0,2522 | 0,1030 | 0,8332 | 2,8411 | 14,6746 | 0,63% | 2,72% | | 2,58% | 21,16% |
| PENTAETHYLENE GLYCOL DIMETHYL ETHER | 769,8 | 16,67 | 1,1388 | 0,2420 | 0,6103 | 0,8280 | 2,9438 | 16,1594 | 0,43% | | | 6,06% | 41,79% |
| PENTAFLUORO(TRIFLUOROMETHYL)SULFUR | 381,3 | 33,71 | 0,2796 | 0,2973 | 0,8907 | 1,0000 | 0,8852 | -21,1626 | 0,33% | 0,95% | | 1,29% | 6,99% |
| PENTAFLUOROETHANE | 339,165 | 36,199 | 0,3053 | 0,2669 | 0,2569 | 0,8429 | 2,2482 | -1,5351 | 0,80% | 1,35% | 5,55% | 1,08% | 14,06% |
| PENTAFLUOROETHYL METHYL ETHER | 406,83 | 28,87 | 0,3535 | 0,2568 | 1,0932 | 0,9874 | 0,7963 | 5,1094 | 0,50% | 1,74% | | 1,28% | 18,08% |
| PENTAFLUOROETHYL TRIFLUOROVINYL ETHER | 401 | 28 | 0,4493 | | 1,2257 | 0,9891 | 0,8086 | | 0,62% | 1,16% | | | |
| PENTAFLUOROPHENOL | 609 | 40 | 0,5030 | 0,2630 | 0,2740 | 0,8321 | 2,8629 | -2,7200 | 2,04% | 3,95% | | 1,07% | 14,91% |
| PENTAMETHYLBENZENE | 719,15 | 28,7 | 0,4637 | 0,2561 | 0,9527 | 0,9573 | 1,0911 | 7,1881 | 0,56% | 0,79% | 1,91% | 1,50% | 17,70% |
| PENTANAL | 566,1 | 38,45 | 0,3132 | 0,2567 | 1,0201 | 1,0000 | 0,8276 | 5,1063 | 4,63% | 1,45% | | 1,71% | 18,59% |
| PERCHLORIC ACID | 631 | 38,6 | 0,0498 | 0,1701 | 0,0189 | 0,8464 | 2,4381 | 87,0211 | 0,57% | | | 27,46% | 96,90% |
| PERCHLORYL FLUORIDE | 368,4 | 53,7 | 0,1726 | 0,2822 | 0,2797 | 0,8393 | 1,5772 | -4,9858 | 0,29% | 1,42% | 7,13% | 1,32% | 12,00% |
| PERFLUOROBUTANOIC ACID | 530 | 26,5 | 0,7925 | 0,2413 | 0,6492 | 0,7813 | 1,9674 | 13,5434 | 0,59% | | | 1,25% | 24,10% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| PERFLUOROMETHYLCYCLOPENTANE | 451,437 | 21,717 | 0,4111 | 0,2667 | 0,2598 | 0,8051 | 2,3747 | -6,2960 | 0,60% | 1,82% | | 0,88% | 16,61% |
| PERFLUORO-n-DODECANE | 570,5 | 9,723 | 0,6209 | | 0,4437 | 0,8111 | 2,2924 | | 0,52% | | | | |
| PERFLUORO-n-HEPTANE | 475,65 | 16,1 | 0,5429 | 0,2557 | 1,3467 | 1,0000 | 0,8201 | 4,7168 | 0,74% | 1,15% | | 1,04% | 14,09% |
| PERFLUORO-n-HEXADECANE | 620,8 | 6,354 | 0,6461 | 0,1964 | 0,3508 | 0,8107 | 2,7491 | 308,0624 | 0,33% | | | 3,84% | 36,82% |
| PERFLUORO-n-HEXANE | 449,55 | 18,02 | 0,4965 | 0,2628 | 0,9150 | 0,8603 | 1,1297 | -3,3707 | 0,14% | 1,72% | | 1,56% | 13,85% |
| PERFLUORO-n-NONANE | 523,9 | 12,96 | 0,5253 | 0,2448 | 0,2129 | 0,8172 | 3,1724 | 31,6578 | 0,39% | | | 1,13% | 21,69% |
| PERFLUORO-n-OCTANE | 502,2 | 14,78 | 0,5084 | 0,2536 | 0,1637 | 0,8089 | 3,3700 | 10,6434 | 1,23% | 3,32% | | 0,98% | 19,40% |
| PERFLUORO-n-PENTANE | 423,1 | 20,466 | 0,4016 | 0,2663 | 1,4924 | 1,0000 | 0,6055 | -5,2243 | 0,69% | 1,11% | | 1,41% | 15,75% |
| p-ETHYLPHENOL | 716,45 | 42,9 | 0,5154 | 0,2691 | 1,7497 | 1,0000 | 0,5859 | -9,4710 | 0,97% | 2,91% | 1,14% | 1,20% | 16,66% |
| p-ETHYLSTYRENE | 674 | 29,36 | 0,3965 | 0,2529 | 1,1736 | 1,0000 | 0,7885 | 12,8608 | 0,59% | 1,04% | | 1,67% | 25,30% |
| p-ETHYLTOLUENE | 640,2 | 32,3 | 0,3666 | 0,2670 | 1,2752 | 1,0000 | 0,6733 | -2,2727 | 2,82% | 3,15% | 1,63% | 2,31% | 19,17% |
| PHENANTHRENE | 869 | 29 | 0,4707 | 0,2221 | 0,3681 | 0,8495 | 2,3700 | 56,0051 | 1,13% | 2,08% | 1,10% | 4,84% | 28,14% |
| PHENETOLE | 647,15 | 34,2 | 0,4179 | 0,2546 | 0,2490 | 0,8390 | 2,7355 | 6,9208 | 1,11% | 2,37% | | 1,26% | 22,23% |
| PHENOL | 694,25 | 61,3 | 0,4435 | 0,2754 | 0,1991 | 0,8256 | 2,9911 | -10,9341 | 3,59% | 3,90% | 4,60% | 1,15% | 31,18% |
| PHENOTHIAZINE | 923 | 40,01 | 0,5796 | | 0,3416 | 0,8080 | 2,5762 | | 0,54% | 1,24% | | | |
| PHENYL ISOCYANATE | 653 | 40,6 | 0,4123 | 0,2615 | 0,4346 | 0,8859 | 2,0581 | 1,7393 | 1,51% | 2,66% | | 2,19% | 10,63% |
| PHENYL MERCAPTAN | 689 | 47,4 | 0,2628 | 0,2675 | 0,2927 | 0,8019 | 1,7338 | -0,6020 | 2,00% | 2,09% | 0,79% | 1,25% | 18,13% |
| PHENYLACETONITRILE | 732 | 34,6 | 0,4715 | 0,2273 | 1,0452 | 0,9998 | 1,0090 | 36,3803 | 2,00% | 1,40% | | 3,21% | 28,99% |
| PHENYLHYDRAZINE | 761 | 49,1 | 0,5351 | 0,2583 | 0,5860 | 0,8999 | 1,9025 | 2,7944 | 5,70% | | | 2,30% | 5,90% |
| PHENYLMETHYLDICHLOROSILANE | 689 | 28,7 | 0,4022 | 0,2664 | 0,5232 | 0,8305 | 1,5677 | -2,9274 | 0,29% | 0,54% | | 3,22% | 21,36% |
| PHENYLTRICHLOROSILANE | 688 | 29,6 | 0,3956 | 0,2637 | 0,6191 | 0,8573 | 1,3992 | -1,3447 | 0,35% | 0,86% | | 1,90% | 19,32% |
| PHOSGENE | 455 | 56,742 | 0,2013 | 0,2788 | 0,3624 | 0,8156 | 1,3444 | -5,1141 | 1,28% | 1,94% | 0,67% | 1,17% | 10,56% |
| PHOSPHINE | 324,75 | 65,4 | 0,0452 | 0,3001 | 0,1762 | 0,9066 | 1,8325 | -7,2264 | 1,10% | 2,76% | | 2,02% | 18,71% |
| PHOSPHORUS (RED) | 993,75 | 83,2891 | 0,0051 | | 0,2623 | 0,9676 | 1,3073 | | 0,09% | | | | |
| PHOSPHORUS OXYCHLORIDE | 602,15 | 34,4 | 0,0832 | 0,2108 | 1,2225 | 0,7088 | 0,4262 | 54,9744 | 4,41% | | 0,32% | 10,27% | 95,23% |
| PHOSPHORUS TRICHLORIDE | 563,15 | 56,7 | 0,2344 | 0,2971 | 0,2007 | 0,8647 | 2,3288 | -16,0226 | 4,07% | 3,94% | 1,56% | 3,39% | 3,80% |
| PHOSPHORUS TRIFLUORIDE | 271,1 | 43,266 | 0,2121 | 0,2804 | 0,1374 | 0,8497 | 2,5548 | -4,5602 | 1,96% | 4,76% | 2,50% | 0,86% | 10,92% |
| PHTHALAN | 700 | 42,85 | 0,3715 | 0,2598 | 0,2863 | 0,8308 | 2,2767 | 2,7910 | 0,62% | 3,41% | | 1,14% | 16,43% |
| PHTHALIC ACID | 800 | 39,5 | 1,0585 | | 0,4384 | 0,8064 | 3,4341 | | 0,50% | 0,64% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| PHTHALIDE | 830,9 | 50,95 | 0,5360 | 0,2665 | 0,5861 | 0,8993 | 1,9083 | -6,3795 | 3,98% | | | 2,40% | 12,85% |
| p-HYDROQUINONE | 838,8 | 58,91 | 0,4858 | 0,2455 | 0,1064 | 0,6884 | 2,4519 | 12,1189 | 0,41% | | | 2,07% | 20,89% |
| p-HYDROXYBENZALDEHYDE | 844 | 49,9 | 0,6172 | 0,2395 | 1,0061 | 0,9741 | 1,2571 | 13,8071 | 0,88% | 1,01% | | 1,83% | 15,92% |
| PIMELIC ACID | 842 | 32,8 | 0,8114 | 0,2459 | 0,3655 | 0,7015 | 2,4893 | 17,1331 | 0,59% | | | 3,40% | 32,02% |
| PIPERAZINE | 638 | 55,3 | 0,4138 | | 0,3886 | 0,8008 | 1,8691 | | 0,53% | 1,38% | | | |
| PIPERIDINE | 594,05 | 46,5082 | 0,2428 | 0,2730 | 1,1275 | 1,0000 | 0,6322 | -4,4548 | 1,34% | 1,00% | 2,85% | 0,98% | 7,44% |
| p-ISOPROPENYL PHENOL | 742,7 | 39,36 | 0,5236 | | 0,6645 | 0,7801 | 1,4577 | | 0,68% | 1,73% | | | |
| p-MENTHANE HYDROPEROXIDE | 711 | 29,5 | 0,9007 | 0,2794 | 0,5643 | 0,8126 | 2,5382 | -40,0082 | 0,66% | 0,79% | | 3,60% | 18,63% |
| p-METHYLSTYRENE | 665 | 33,6 | 0,3175 | 0,2664 | 1,3231 | 1,0000 | 0,6028 | 3,3157 | 0,31% | 0,72% | 0,55% | 3,66% | 16,60% |
| p-NITROANILINE | 851 | 44,2 | 0,7824 | | 0,3522 | 0,8154 | 3,2138 | | 1,07% | 0,51% | | | |
| p-NITROTOLUENE | 743 | 32,07 | 0,4252 | 0,2205 | 0,4860 | 0,8942 | 1,9642 | 49,3312 | 2,42% | | | 3,91% | 23,09% |
| p-PHENETIDINE | 754 | 35,7 | 0,5351 | 0,2573 | 0,4999 | 0,8158 | 1,9113 | 5,2814 | 0,30% | 2,12% | | 3,35% | 19,85% |
| p-PHENYLENEDIAMINE | 796 | 51,8 | 0,5386 | 0,2480 | 0,4385 | 0,8055 | 2,0724 | 9,0429 | 0,53% | 1,43% | | 1,03% | 21,04% |
| PROPADIENE | 394 | 52,5 | 0,1041 | 0,2682 | 1,9507 | 0,8298 | 0,2743 | 1,8231 | 1,09% | 1,30% | | 2,03% | 15,14% |
| PROPANAL | 503,6 | 50,38 | 0,2813 | 0,2549 | 0,9688 | 1,0000 | 0,8039 | 5,9752 | 0,59% | 3,90% | | 1,46% | 22,31% |
| PROPANE | 369,83 | 42,48 | 0,1523 | 0,2774 | 0,7212 | 0,9076 | 0,7830 | -3,7399 | 0,42% | 1,22% | 4,35% | 1,49% | 13,13% |
| PROPARGYL ALCOHOL | 588,8 | 61,9 | 0,4567 | 0,2405 | 0,3924 | 0,8636 | 2,2901 | 10,4454 | 0,29% | | | 1,32% | 22,46% |
| PROPARGYL CHLORIDE | 541 | 53 | 0,1500 | 0,2444 | 1,0067 | 0,9989 | 0,5787 | 12,8417 | 0,67% | 2,28% | | 6,79% | 17,56% |
| PROPENYL CYCLOHEXENE | 636 | 31,2 | 0,3420 | 0,2612 | 1,2597 | 1,0000 | 0,6648 | 2,3737 | 0,52% | 1,15% | 3,19% | 1,40% | 18,68% |
| PROPIONIC ACID | 600,81 | 46,68 | 0,5796 | 0,2254 | 1,2117 | 1,0000 | 0,9675 | 20,7991 | 0,55% | | | 3,47% | 31,13% |
| PROPIONIC ANHYDRIDE | 623 | 32,7 | 0,5599 | 0,2586 | 0,3352 | 0,8378 | 2,7562 | 0,4300 | 1,13% | 2,49% | 1,12% | 2,82% | 22,86% |
| PROPIONITRILE | 561,3 | 42,6 | 0,3501 | 0,2165 | 0,3483 | 0,8764 | 2,1740 | 32,8820 | 2,35% | 3,86% | | 5,44% | 25,57% |
| PROPYL CHLORIDE | 503,15 | 44,25 | 0,2150 | 0,2621 | 0,2752 | 0,8165 | 1,6682 | 3,1458 | 1,02% | 2,58% | 1,12% | 1,89% | 18,30% |
| PROPYLENE | 364,85 | 46 | 0,1376 | 0,2782 | 0,4902 | 0,8457 | 1,0060 | -3,5465 | 0,79% | 1,86% | 2,15% | 1,41% | 11,49% |
| PROPYLENE GLYCOL 1-tert-BUTYL ETHER | 600,7 | 27,2 | 0,4863 | 0,2553 | 1,0406 | 0,9233 | 1,0078 | 5,4491 | 0,57% | 1,42% | | 1,38% | 19,19% |
| PROPYLENE GLYCOL 2-tert-BUTYL ETHER | 600,6 | 27,2 | 0,4867 | 0,2554 | 0,6412 | 0,8299 | 1,5055 | 5,3292 | 0,49% | 1,63% | | 1,19% | 19,20% |
| PROPYLENE GLYCOL MONOALLYL ETHER | 616,6 | 33,76 | 0,4797 | 0,2571 | 1,6151 | 1,0000 | 0,6190 | 3,1209 | 0,65% | 1,28% | | 1,50% | 18,89% |
| PROPYLENE GLYCOL MONOMETHYL ETHER | 579,8 | 41,13 | 0,4427 | 0,2520 | 1,2018 | 1,0000 | 0,8256 | 5,9428 | 2,21% | 1,46% | | 1,53% | 24,77% |
| PROPYLENE GLYCOL MONOMETHYL ETHER ACETATE | 597,9 | 30,09 | 0,4807 | 0,2548 | 1,3420 | 1,0000 | 0,7606 | 5,8149 | 1,49% | 0,88% | 2,18% | 1,52% | 19,25% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| PROPYLENE GLYCOL n-BUTYL ETHER | 624,9 | 27,39 | 0,5008 | 0,2485 | 1,4088 | 1,0000 | 0,7424 | 12,6298 | 0,88% | 1,02% | | 1,57% | 24,83% |
| PROPYLENEIMINE | 539,9 | 54,79 | 0,2295 | 0,2572 | 0,8255 | 0,4104 | 0,6777 | 6,0264 | 0,51% | | | 2,69% | 16,51% |
| p-TERPHENYL | 908 | 29,9 | 0,6426 | 0,2753 | 0,2908 | 0,8187 | 3,1388 | -30,9638 | 0,60% | 1,20% | 0,97% | 1,67% | 10,72% |
| p-tert-AMYLPHENOL | 752 | 29,8 | 0,5635 | | 0,3054 | 0,8167 | 2,7600 | | 0,29% | 0,49% | | | |
| p-tert-BUTYL ETHYLBENZENE | 684 | 23,8 | 0,4347 | 0,2533 | 0,5717 | 0,8091 | 1,4905 | 12,7611 | 0,29% | 0,95% | 0,50% | 1,39% | 19,30% |
| p-tert-BUTYLCATECHOL | 776 | 37,7 | 0,7344 | 0,2829 | 0,4654 | 0,8105 | 2,5069 | -31,5520 | 0,86% | 0,81% | | 3,69% | 9,13% |
| p-tert-BUTYLPHENOL | 734 | 33,4 | 0,5094 | 0,2652 | 0,1914 | 0,8143 | 3,2397 | -8,0032 | 1,72% | 3,62% | | 0,92% | 15,55% |
| p-tert-BUTYLSTYRENE | 709 | 24,8 | 0,4216 | 0,2499 | 0,2518 | 0,8395 | 2,7257 | 18,2276 | 1,28% | 2,17% | 1,90% | 1,36% | 19,94% |
| p-tert-OCTYLPHENOL | 765 | 22,8 | 0,6326 | | 0,2924 | 0,8169 | 3,0742 | | 0,27% | 0,49% | | | |
| p-TOLUALDEHYDE | 715,8 | 39,22 | 0,3827 | 0,2540 | 0,3623 | 0,8384 | 2,0386 | 8,5065 | 0,68% | 2,12% | | 1,23% | 18,95% |
| p-TOLUIC ACID | 775 | 38 | 0,6291 | | 0,4275 | 0,7617 | 2,1573 | | 0,55% | 2,40% | | | |
| p-TOLUIDINE | 693,15 | 40 | 0,4722 | 0,2444 | 0,2824 | 0,8385 | 2,7441 | 13,5783 | 1,74% | 3,28% | 1,33% | 1,68% | 24,08% |
| p-XYLENE | 616,2 | 35,11 | 0,3218 | 0,2581 | 0,2243 | 0,8496 | 2,5557 | 5,3664 | 0,44% | 0,86% | 5,48% | 1,45% | 17,25% |
| PYRAZINE | 626 | 54,9 | 0,2030 | 0,2496 | 0,1365 | 0,8489 | 2,5663 | 12,0445 | 1,79% | 2,43% | | 2,83% | 1,97% |
| PYRAZOLE | 734 | 66 | 0,2868 | 0,2352 | 0,2284 | 0,8276 | 2,2063 | 18,3442 | 0,64% | 1,61% | | 3,93% | 13,15% |
| PYRENE | 936 | 26,1 | 0,5074 | | 0,3707 | 0,8530 | 2,5016 | | 1,92% | 3,17% | 1,51% | | |
| PYRIDAZINE | 774 | 54,9 | 0,2035 | 0,2242 | 0,7406 | 0,8586 | 0,8452 | 34,0376 | 1,14% | | 1,61% | 6,61% | 19,09% |
| PYRIDINE | 619,95 | 56,3 | 0,2386 | 0,2697 | 0,5362 | 0,8088 | 1,1171 | -0,8471 | 0,30% | 1,07% | 0,31% | 1,20% | 11,14% |
| PYRIMIDINE | 638 | 54,9 | 0,2105 | 0,2458 | 0,1032 | 0,8404 | 2,7103 | 14,1518 | 0,89% | | 0,41% | 4,05% | 3,24% |
| PYRROLE | 639,75 | 65,3 | 0,2976 | 0,2584 | 1,2799 | 1,0000 | 0,6072 | 3,2543 | 0,82% | 0,89% | 0,20% | 2,27% | 7,45% |
| PYRROLIDINE | 568,55 | 56,1 | 0,2668 | 0,2767 | 1,4160 | 1,0000 | 0,5105 | -6,4105 | 0,24% | 0,58% | | 1,08% | 6,60% |
| QUINALDINE | 769 | 33,5 | 0,3591 | 0,2426 | 1,5327 | 1,0000 | 0,5515 | 26,9970 | 2,39% | 2,48% | | 2,45% | 14,23% |
| QUINOLINE | 782,15 | 48,6 | 0,3465 | 0,2768 | 0,2825 | 0,8527 | 2,3413 | -12,2038 | 0,68% | 2,34% | 2,67% | 2,19% | 14,16% |
| QUINONE | 683 | 59,6 | 0,4945 | 0,2796 | 0,5641 | 0,8476 | 1,7204 | -14,1206 | 0,65% | 0,80% | 10,01% | 0,67% | 5,50% |
| RADON | 377,5 | 62,8 | 0,0000 | 0,2806 | 0,1563 | 0,0000 | 0,2808 | -0,8068 | 1,83% | | | 2,73% | 12,20% |
| RDX | 895,2 | 41,6 | 1,0118 | | 0,5757 | 0,8094 | 2,7219 | | 0,86% | 1,17% | 1,16% | | |
| SACCHARIN | 968 | 57,25 | 0,6157 | | 1,1061 | 0,9149 | 1,1021 | | 0,89% | 0,82% | 0,66% | | |
| SALICYLIC ACID | 739 | 51,8 | 0,8512 | 0,2752 | 0,3647 | 0,8111 | 3,3170 | -19,5143 | 1,14% | 1,15% | | 1,39% | 17,84% |
| SEBACIC ACID | 845 | 25 | 0,9608 | 0,2338 | 0,6816 | 0,6761 | 1,9555 | 27,5417 | 0,66% | | | 1,28% | 34,46% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| sec-BUTENYL ACETATE | 563,5 | 33,07 | 0,3922 | 0,2636 | 1,3918 | 1,0000 | 0,6470 | -1,4440 | 0,73% | 1,20% | | 1,34% | 16,83% |
| sec-BUTYL ACETATE | 561 | 31,7 | 0,3954 | 0,2675 | 1,3282 | 1,0000 | 0,6810 | -4,6660 | 1,14% | 3,59% | 0,18% | 2,07% | 17,48% |
| sec-BUTYL ACRYLATE | 580 | 29,7 | 0,4418 | 0,2636 | 1,3415 | 1,0000 | 0,7249 | -3,1400 | 1,14% | 1,19% | | 1,47% | 17,08% |
| sec-BUTYL CHLORIDE | 520,6 | 39 | 0,2907 | 0,2682 | 0,2168 | 0,8550 | 2,4713 | -2,7749 | 1,10% | 2,77% | 0,93% | 1,38% | 14,65% |
| sec-BUTYL FORMATE | 546 | 35,8 | 0,3489 | 0,2636 | 1,3683 | 1,0000 | 0,6114 | -0,4638 | 0,75% | 2,23% | 2,58% | 1,45% | 16,15% |
| sec-BUTYL MERCAPTAN | 554 | 40,6 | 0,2506 | 0,2743 | 0,3249 | 0,8256 | 1,6494 | -6,0639 | 1,80% | 2,03% | 1,19% | 1,80% | 15,58% |
| sec-BUTYLAMINE | 514,3 | 40 | 0,2815 | 0,2642 | 0,5057 | 0,8049 | 1,2627 | 0,3295 | 0,31% | 2,00% | 0,29% | 1,75% | 5,90% |
| sec-BUTYLBENZENE | 664,54 | 29,5 | 0,2791 | 0,2605 | 1,2505 | 1,0000 | 0,6094 | 6,5217 | 1,13% | 4,23% | 1,64% | 1,42% | 14,53% |
| sec-BUTYLCYCLOHEXANE | 654 | 25,85 | 0,3516 | 0,2589 | 1,1977 | 1,0000 | 0,7189 | 6,6855 | 0,69% | 1,20% | | 2,03% | 24,26% |
| sec-BUTYL-tert-BUTYL ETHER | 559,4 | 25,61 | 0,3489 | 0,2728 | 1,1879 | 1,0000 | 0,7202 | -11,3662 | 0,58% | 1,36% | 0,47% | 1,42% | 16,97% |
| SILANE | 269,7 | 48,4 | 0,0938 | 0,3138 | 0,3757 | 0,9627 | 1,3457 | -12,8044 | 3,10% | | | 5,65% | 16,97% |
| SITOSTEROL | 953 | 11,2 | 1,0543 | | 0,4877 | 0,8123 | 3,2139 | | 0,51% | 1,25% | | | |
| STIGMASTEROL | 953,6 | 11,38 | 1,0631 | | 0,4812 | 0,8128 | 3,2767 | | 0,61% | 1,75% | | | |
| STYRENE | 636 | 38,4 | 0,2971 | 0,2612 | 0,3391 | 0,8164 | 1,7254 | 4,1190 | 1,29% | 1,40% | 1,98% | 1,18% | 19,09% |
| STYRENE GLYCOL | 776,4 | 39,24 | 0,6159 | | 0,5014 | 0,8121 | 2,0970 | | 0,64% | 1,62% | | | |
| SUBERIC ACID | 843 | 29,7 | 0,8514 | 0,2317 | 0,2467 | 0,6582 | 2,7155 | 31,4460 | 0,54% | | | 1,61% | 31,19% |
| SUCCINIC ANHYDRIDE | 811 | 67,3 | 0,5322 | | 0,5992 | 0,9042 | 1,8574 | | 3,95% | 4,89% | | | |
| SUCCINIMIDE | 858 | 59,7 | 0,4834 | 0,2250 | 0,2075 | 0,8060 | 2,9202 | 26,3508 | 0,48% | | | 3,67% | 25,82% |
| SUCCINONITRILE | 770 | 35,4 | 0,5587 | 0,1781 | 0,4509 | 0,8104 | 2,1089 | 86,1566 | 0,67% | 2,08% | | 10,76% | 56,59% |
| SUCROSE | 1086 | 26,9 | 0,3653 | 0,2213 | 0,6660 | 0,8422 | 1,2332 | 78,5403 | 0,57% | 1,88% | | 9,69% | 25,27% |
| SULFOLANE | 853 | 50,3 | 0,3823 | 0,2355 | 0,2527 | 0,8448 | 2,6046 | 23,8418 | 0,26% | 1,34% | | 2,81% | 36,53% |
| SULFUR DIOXIDE | 430,75 | 78,841 | 0,2454 | 0,2671 | 0,3949 | 0,8240 | 1,4643 | -0,0517 | 2,03% | 1,14% | 4,05% | 1,02% | 14,50% |
| SULFUR HEXAFLUORIDE | 318,69 | 37,6 | 0,2151 | 0,2796 | 0,3620 | 0,8049 | 1,3725 | -5,6658 | 1,04% | 1,80% | | 1,10% | 11,98% |
| SULFUR TRIOXIDE | 490,85 | 82,1 | 0,4240 | 0,2726 | 0,0000 | 0,3050 | 1,2510 | -0,0539 | 5,01% | 5,81% | | 3,41% | 20,36% |
| SULFURYL CHLORIDE | 545 | 46,1 | 0,1764 | 0,2491 | 1,3947 | 0,5856 | 0,4704 | 13,4150 | 1,22% | 1,71% | | 3,94% | 23,39% |
| SYRINGOL | 752,2 | 37,85 | 0,6551 | 0,2570 | 0,5070 | 0,8245 | 2,2217 | -1,6616 | 0,60% | 1,48% | | 1,69% | 19,90% |
| t-BUTYL ACETOACETATE | 636,5 | 27,73 | 0,5832 | | 0,6893 | 0,8429 | 1,6217 | | 0,64% | 1,27% | | | |
| t-BUTYL HYDROPEROXIDE | 552 | 43,4 | 0,6623 | 0,2720 | 1,3697 | 0,9935 | 0,9228 | -12,1170 | 0,47% | 0,46% | | 1,43% | 16,27% |
| TEREPHTHALDEHYDE | 739 | 36,7 | 0,5832 | | 0,3513 | 0,8006 | 2,4948 | | 0,51% | 1,71% | 0,66% | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| TEREPHTHALIC ACID | 883,6 | 34,86 | 0,9469 | | 0,6124 | 0,8475 | 2,5903 | | 0,32% | | | | |
| TEREPHTHALOYL CHLORIDE | 755,4 | 38,2 | 0,6730 | 0,2701 | 0,4341 | 0,8269 | 2,5628 | -17,3226 | 0,57% | 1,39% | | 1,88% | 10,99% |
| TERPINOLENE | 667 | 28,2 | 0,3762 | 0,2572 | 0,9683 | 0,8671 | 0,9050 | 8,0086 | 0,66% | 1,15% | 0,08% | 1,44% | 21,00% |
| tert-BUTYL ACETATE | 545 | 31,7 | 0,3396 | 0,2667 | 1,3717 | 1,0000 | 0,6113 | -4,0778 | 1,77% | 2,47% | | 1,25% | 14,01% |
| tert-BUTYL CHLORIDE | 507 | 39 | 0,1914 | 0,2796 | 0,1480 | 0,8472 | 2,3778 | -8,1791 | 0,61% | 3,25% | 0,30% | 0,81% | 13,48% |
| tert-BUTYL ETHYL ETHER | 509,4 | 29,34 | 0,3162 | 0,2689 | 1,2429 | 0,9987 | 0,6473 | -4,1529 | 0,56% | 1,70% | | 1,31% | 13,68% |
| tert-BUTYL FORMATE | 537 | 35,8 | 0,2944 | 0,2748 | 0,3191 | 0,7935 | 1,6955 | -6,1669 | 0,59% | 2,01% | 3,69% | 1,45% | 16,63% |
| tert-BUTYL MERCAPTAN | 530 | 40,6 | 0,1914 | 0,2879 | 0,1162 | 0,8339 | 2,4491 | -14,0514 | 0,82% | 2,45% | 0,25% | 0,82% | 13,26% |
| tert-BUTYL METHACRYLATE | 588,3 | 27,27 | 0,3977 | 0,2672 | 1,4867 | 1,0000 | 0,6055 | -6,5005 | 0,57% | 1,22% | | 1,25% | 15,98% |
| tert-BUTYLAMINE | 483,9 | 38,4 | 0,2748 | 0,2689 | 1,6973 | 0,8302 | 0,4451 | -3,1773 | 1,04% | 3,15% | 1,62% | 2,47% | 11,01% |
| tert-BUTYLBENZENE | 660 | 29,7 | 0,2674 | 0,2663 | 1,4331 | 1,0000 | 0,5120 | 1,4661 | 2,03% | 2,17% | 0,51% | 1,64% | 15,14% |
| tert-BUTYLCYCLOHEXANE | 652 | 26,6 | 0,2991 | 0,2669 | 0,4896 | 0,7783 | 1,2845 | -0,8934 | 0,75% | 4,88% | | 1,64% | 23,01% |
| tert-BUTYLFORMAMIDE | 692 | 35,6 | 0,4491 | 0,2371 | 0,5645 | 0,8194 | 1,5636 | 25,6791 | 0,64% | 1,45% | | 1,87% | 23,01% |
| tert-DODECYL MERCAPTAN | 691 | 18,6 | 0,6098 | 0,2498 | 0,7686 | 0,8384 | 1,5075 | 14,8093 | 0,84% | 1,00% | 1,81% | 1,71% | 21,23% |
| tert-NONYL MERCAPTAN | 659 | 23,4 | 0,4514 | 0,2476 | 0,5079 | 0,7809 | 1,5995 | 21,0079 | 0,35% | 2,60% | 0,93% | 1,40% | 20,48% |
| tert-OCTYL MERCAPTAN | 627 | 25,9 | 0,3001 | 0,2629 | 0,5244 | 0,8099 | 1,2812 | 2,7719 | 0,46% | 2,09% | 0,19% | 1,34% | 16,44% |
| TETRACHLOROETHYLENE | 620 | 44,9 | 0,2138 | 0,2646 | 1,2026 | 1,0000 | 0,5578 | 0,8955 | 1,94% | 1,34% | 1,38% | 2,09% | 41,95% |
| TETRACHLOROSILANE | 507 | 35,9 | 0,2318 | 0,2710 | 1,3947 | 0,9710 | 0,4835 | -3,0903 | 0,65% | 1,91% | 0,38% | 1,34% | 11,67% |
| TETRADECAMETHYLHEXASILOXANE | 653,2 | 8,0351 | 0,7769 | 0,2481 | 1,5812 | 0,9987 | 0,8737 | 25,8390 | 0,71% | 0,94% | | 2,65% | 22,14% |
| TETRAETHYL LEAD | 655 | 21,25 | 0,4812 | 0,2366 | 0,5041 | 0,8196 | 1,7846 | 33,1483 | 1,71% | 2,09% | 1,32% | 3,82% | 18,64% |
| TETRAETHYL SILANE | 606 | 24 | 0,4002 | 0,2673 | 0,6572 | 0,8510 | 1,3199 | -7,6875 | 0,42% | 1,53% | 6,01% | 1,61% | 11,25% |
| TETRAETHYLENE GLYCOL | 795 | 25,9 | 0,9174 | 0,2294 | 0,4426 | 0,8185 | 3,1435 | 30,0710 | 1,16% | 1,96% | | 1,67% | 33,77% |
| TETRAETHYLENE GLYCOL DIMETHYL ETHER | 705 | 19,4 | 0,9652 | 0,2508 | 0,8040 | 0,8796 | 2,1344 | 1,3344 | 0,83% | | | 5,97% | 37,61% |
| TETRAETHYLENE GLYCOL MONOETHYL ETHER | 732 | 23,6 | 0,9045 | 0,2630 | 0,5458 | 0,8108 | 2,6065 | -21,4580 | 0,64% | 1,28% | | 3,31% | 20,09% |
| TETRAETHYLENE GLYCOL MONOMETHYL ETHER | 720 | 26,01 | 0,9717 | 0,2660 | 0,5178 | 0,8132 | 2,8862 | -25,7852 | 0,62% | 1,28% | | 3,57% | 19,82% |
| TETRAFLUOROETHYLENE | 306,45 | 39,44 | 0,2265 | 0,2702 | 0,2950 | 0,8162 | 1,6400 | -1,3926 | 0,39% | 1,38% | 0,35% | 1,25% | 16,27% |
| TETRAFLUOROHYDRAZINE | 309,35 | 37,1 | 0,2233 | 0,2776 | 0,4809 | 0,9523 | 1,4271 | -5,0829 | 3,95% | 6,55% | | 1,13% | 2,44% |
| TETRAHYDROFURAN | 540,15 | 51,9 | 0,2254 | 0,2676 | 0,5172 | 0,8287 | 1,1418 | -0,6084 | 1,01% | 2,48% | 0,87% | 1,48% | 19,02% |
| TETRAHYDROPYRAN | 572,04 | 47,712 | 0,2162 | 0,2744 | 1,0475 | 1,0000 | 0,6469 | -5,9254 | 0,46% | 1,74% | | 1,63% | 18,90% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| TETRAHYDROTHIOPHENE | 631,95 | 51,6 | 0,1996 | 0,2596 | 0,6056 | 0,8264 | 0,9587 | 4,8990 | 0,55% | 1,24% | 0,50% | 3,09% | 23,74% |
| TETRAMANTANE | 867,7 | 15,51 | 0,2726 | | 0,3735 | 0,8141 | 1,5549 | | 0,54% | 3,43% | | | |
| TETRAMETHYLETHYLENEDIAMINE | 569 | 28,2 | 0,3915 | 0,2642 | 0,3221 | 0,8048 | 2,0425 | -2,4523 | 0,53% | 1,72% | 0,40% | 1,21% | 16,97% |
| TETRAMETHYLSILANE | 450,4 | 28,14 | 0,2240 | 0,2722 | 0,8272 | 0,8391 | 0,7839 | -4,2442 | 0,69% | 0,57% | 0,53% | 1,12% | 15,78% |
| TETRAPHENYLETHYLENE | 996 | 17,1 | 0,7285 | | 0,4448 | 0,8065 | 2,5493 | | 0,50% | 1,43% | | | |
| TETRAPHENYLMETHANE | 983 | 17,9 | 0,6794 | | 0,4643 | 0,7959 | 2,3027 | | 0,61% | 1,89% | 1,13% | | |
| THIACYCLOPROPANE | 547 | 67,8 | 0,1610 | 0,2599 | 0,2366 | 0,8359 | 1,6825 | 4,2711 | 0,40% | 1,55% | | 2,35% | 20,92% |
| THIAINDAN | 759,8 | 37,07 | 0,3327 | 0,2425 | 1,0847 | 1,0000 | 0,7768 | 24,7587 | 0,46% | 1,65% | | 2,15% | 20,85% |
| THIOGLYCOLIC ACID | 733 | 61 | 0,5598 | 0,2394 | 1,1010 | 0,9967 | 1,0591 | 12,4575 | 0,67% | | | 1,54% | 23,29% |
| THIONYL CHLORIDE | 567 | 44,3 | 0,0946 | 0,2221 | 1,3093 | 1,0000 | 0,3991 | 33,9521 | 4,55% | 1,91% | | 9,60% | 40,95% |
| THIOPHENE | 579,35 | 56,9 | 0,1970 | 0,2722 | 0,3234 | 0,7975 | 1,3835 | -2,2421 | 1,07% | 1,84% | 0,68% | 1,20% | 19,85% |
| THIOUREA | 854 | 82,3 | 0,3586 | | 0,4246 | 0,8057 | 1,6354 | | 0,51% | 1,49% | | | |
| THYMOL | 698,25 | 34,08 | 0,7226 | 0,2646 | 0,6248 | 0,8760 | 2,1786 | -18,2163 | 1,33% | | | 1,16% | 24,28% |
| TIN(IV) CHLORIDE | 591,85 | 37,436 | 0,2613 | 0,2668 | 0,4205 | 0,7875 | 1,3372 | -0,1157 | 0,48% | 1,68% | 1,00% | 1,13% | 15,15% |
| TOLUENE | 591,75 | 41,08 | 0,2640 | 0,2641 | 0,3172 | 0,8302 | 1,7523 | 1,2382 | 0,39% | 1,39% | 0,50% | 1,35% | 16,12% |
| trans,trans-2,4-HEXADIENE | 535 | 33,5 | 0,2821 | 0,2540 | 0,1857 | 0,8327 | 2,4513 | 9,4781 | 0,49% | 1,73% | 0,29% | 2,34% | 20,45% |
| trans-1,2-DICHLOROETHYLENE | 516,5 | 55,1 | 0,2234 | 0,2768 | 0,2048 | 0,8451 | 2,0956 | -4,4260 | 3,53% | 1,38% | 1,89% | 0,92% | 8,93% |
| trans-1,2-DIMETHYLCYCLOHEXANE | 596,15 | 29,3843 | 0,2379 | 0,2590 | 1,2389 | 1,0000 | 0,5616 | 8,9640 | 0,67% | 0,86% | 0,43% | 2,00% | 10,78% |
| trans-1,2-DIMETHYLCYCLOPENTANE | 553,15 | 34,4505 | 0,2698 | 0,2789 | 0,1992 | 0,8532 | 2,4987 | -12,0184 | 0,56% | 1,30% | | 2,30% | 17,33% |
| trans-1,3,3,3-TETRAFLUOROPROPENE | 382,51 | 36,62 | 0,3238 | 0,2662 | 0,2065 | 0,8072 | 2,3128 | -1,4445 | 1,03% | 2,80% | | 1,23% | 14,22% |
| trans-1,3-DICHLOROPROPENE | 606,5 | 47,04 | 0,2234 | 0,2596 | 1,6930 | 0,9985 | 0,3896 | 5,8801 | 0,69% | 2,06% | | 2,22% | 16,42% |
| trans-1,3-DIMETHYLCYCLOHEXANE | 598 | 29,3843 | 0,2335 | 0,2598 | 1,3855 | 1,0000 | 0,4950 | 9,2856 | 1,33% | 0,77% | 1,20% | 1,47% | 11,06% |
| trans-1,3-DIMETHYLCYCLOPENTANE | 553 | 34,45 | 0,2699 | 0,2785 | 1,2632 | 1,0000 | 0,5758 | -11,3865 | 2,03% | 2,46% | 0,74% | 2,08% | 17,13% |
| trans-1,3-HEXADIENE | 521,1 | 33,54 | 0,2783 | 0,2595 | 0,3865 | 0,8307 | 1,5917 | 4,7891 | 0,52% | 2,15% | | 1,56% | 18,52% |
| trans-1,3-PENTADIENE | 500 | 37,4 | 0,1162 | 0,2595 | 1,7636 | 1,0000 | 0,3047 | 8,7234 | 4,46% | 3,75% | 1,18% | 2,72% | 20,64% |
| trans-1,4-DIETHYLCYCLOHEXANE | 649,9 | 28,17 | 0,3846 | 0,2731 | 1,1972 | 1,0000 | 0,7573 | -14,6970 | 0,67% | 0,96% | | 1,84% | 14,68% |
| trans-1,4-DIMETHYLCYCLOHEXANE | 587,7 | 29,4 | 0,2548 | 0,2647 | 0,7137 | 0,8390 | 0,9475 | 2,2398 | 0,29% | 1,02% | 0,22% | 1,29% | 13,04% |
| trans-1,8-TERPIN | 702,7 | 29,49 | 1,0818 | | 0,4536 | 0,8070 | 3,4188 | | 0,56% | 1,29% | | | |
| trans-1-PROPENYLBENZENE | 670 | 33,6 | 0,3393 | 0,2553 | 1,2639 | 1,0000 | 0,6589 | 10,5794 | 0,61% | 1,52% | 0,70% | 1,34% | 22,62% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| trans-2,2,4,6,6-PENTAMETHYL-3-HEPTENE | 637,8 | 19,64 | 0,3619 | | 1,1809 | 1,0000 | 0,7411 | | 0,49% | 1,73% | | | |
| trans-2,n-HEXYL-DECAHYDRONAPHTHALENE | 777,2 | 18,14 | 0,4668 | | 0,3286 | 0,8084 | 2,2779 | | 0,50% | 3,40% | 5,15% | | |
| trans-2-BUTENE | 428,6 | 41 | 0,2176 | 0,2720 | 0,3114 | 0,8502 | 1,6777 | -2,8797 | 0,90% | 1,02% | 0,83% | 1,12% | 13,47% |
| trans-2-DECENE | 619 | 21,8 | 0,4820 | 0,2509 | 0,5182 | 0,7972 | 1,6870 | 14,2461 | 0,56% | 1,62% | 1,85% | 1,38% | 20,59% |
| trans-2-DODECENE | 663 | 18,9 | 0,5693 | | 0,5440 | 0,7955 | 1,8156 | | 0,57% | 1,50% | 3,33% | | |
| trans-2-EICOSENE | 741,8 | 12,21 | 0,8784 | | 0,4590 | 0,8121 | 2,9102 | | 0,53% | 2,11% | 7,32% | | |
| trans-2-HEPTENE | 543,1 | 28,5 | 0,3366 | 0,2586 | 0,2308 | 0,8388 | 2,4882 | 4,6414 | 0,43% | 3,22% | 0,18% | 1,37% | 20,00% |
| trans-2-HEXENE | 509,8 | 31,68 | 0,2886 | 0,2623 | 0,6213 | 0,8513 | 1,1545 | 2,0502 | 0,40% | 1,89% | 0,52% | 1,47% | 18,62% |
| trans-2-METHYL-1,3-PENTADIENE | 530,3 | 33,8 | 0,2477 | 0,2574 | 1,2764 | 1,0000 | 0,5552 | 8,2250 | 0,54% | 2,05% | | 1,95% | 16,90% |
| trans-2-NONENE | 597,1 | 23,7 | 0,4304 | | 1,0958 | 1,0000 | 0,9001 | | 0,76% | 1,09% | | | |
| trans-2-OCTENE | 571,6 | 25,89 | 0,3840 | 0,2556 | 0,2307 | 0,8407 | 2,7042 | 7,5383 | 0,44% | 4,40% | 0,70% | 1,33% | 20,51% |
| trans-2-PENTADECENE | 701,6 | 15,67 | 0,6894 | | 0,5947 | 0,8229 | 2,0209 | | 0,47% | 1,82% | | | |
| trans-2-PENTENE | 474,2 | 36,6 | 0,2484 | 0,2709 | 0,4710 | 0,8384 | 1,3073 | -3,4350 | 0,45% | 1,25% | 1,24% | 1,38% | 14,19% |
| trans-2-PHENYLBUTENE-2 | 654 | 30,1 | 0,3610 | 0,2570 | 0,7383 | 0,8469 | 1,1241 | 7,4600 | 0,70% | 1,60% | | 1,27% | 18,07% |
| trans-3-HEPTENE | 540 | 28,5 | 0,3341 | 0,2604 | 0,3723 | 0,8292 | 1,7944 | 3,1812 | 0,85% | 2,39% | 2,16% | 1,57% | 18,49% |
| trans-3-HEXENE | 509 | 31,7 | 0,2854 | 0,2654 | 0,4171 | 0,8173 | 1,4861 | 0,3305 | 0,80% | 0,61% | 0,79% | 1,41% | 16,83% |
| trans-3-METHYLCYCLOHEXANOL | 627 | 37,9 | 0,6806 | 0,2605 | 0,4211 | 0,8027 | 2,4951 | -8,4099 | 0,62% | 1,22% | 1,74% | 1,05% | 15,30% |
| trans-3-OCTENE | 574 | 25,8 | 0,3438 | 0,2569 | 0,3207 | 0,8186 | 1,9599 | 8,3484 | 0,84% | 2,30% | 0,95% | 1,46% | 16,73% |
| trans-4-METHYLCYCLOHEXANOL | 622 | 37,9 | 0,6940 | 0,2679 | 0,4610 | 0,7978 | 2,3558 | -13,7784 | 0,74% | 1,16% | 1,45% | 1,57% | 15,84% |
| trans-4-OCTENE | 573 | 25,8 | 0,3393 | 0,2573 | 0,2720 | 0,8286 | 2,2123 | 7,8095 | 1,08% | 1,92% | 1,12% | 1,36% | 16,63% |
| trans-CROTONALDEHYDE | 565 | 38,7 | 0,3435 | | 0,2903 | 0,8616 | 2,3738 | | 2,70% | | 5,72% | | |
| trans-CROTONIC ACID | 666 | 47 | 0,5708 | 0,2514 | 0,1832 | 0,8063 | 3,4372 | 8,5195 | 0,67% | 1,73% | | 2,11% | 30,98% |
| trans-CROTONITRILE | 586 | 38,8 | 0,3977 | 0,2243 | 0,4074 | 0,8814 | 2,1120 | 31,1022 | 0,32% | 1,64% | | 2,93% | 25,86% |
| trans-DECAHYDRONAPHTHALENE | 687 | 32 | 0,2993 | 0,2713 | 0,2893 | 0,8348 | 2,0054 | -8,3627 | 0,77% | 2,19% | 1,95% | 1,25% | 16,06% |
| trans-STILBENE | 820 | 27,4 | 0,4874 | 0,2438 | 1,8978 | 1,0000 | 0,5183 | 27,7304 | 1,27% | 2,21% | | 1,77% | 21,44% |
| TRIALLYLAMINE | 592 | 24,6 | 0,4987 | 0,2605 | 0,6933 | 0,8344 | 1,4314 | -1,5939 | 1,49% | 1,71% | 3,73% | 1,79% | 18,36% |
| TRIAMANTANE | 834,5 | 18,39 | 0,1869 | | 0,2660 | 0,8154 | 1,5852 | | 0,44% | | | | |
| TRIAMYLAMINE | 660 | 15 | 0,8526 | 0,2488 | 0,8548 | 0,8440 | 1,7525 | 4,3449 | 0,44% | 0,32% | | 2,06% | 25,45% |
| TRIBROMOMETHANE | 696 | 60,9 | 0,1561 | 0,2856 | 1,0701 | 0,7536 | 0,5325 | -8,7536 | 0,83% | 2,02% | 2,25% | 1,41% | 5,19% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| TRICAPRIN | 876,6 | 4,546 | 1,3974 | 0,1719 | 0,6510 | 0,8127 | 3,2769 | 686,3760 | 1,43% | | | 2,60% | 50,43% |
| TRICAPRYLIN | 850,7 | 5,932 | 1,2174 | 0,1822 | 0,6451 | 0,8262 | 2,9801 | 463,3649 | 1,16% | | | 2,26% | 44,89% |
| TRICHLOROACETALDEHYDE | 565 | 44,1 | 0,3323 | 0,2668 | 1,1769 | 1,0000 | 0,7077 | -2,4221 | 0,61% | 1,19% | | 1,16% | 14,54% |
| TRICHLOROACETIC ACID | 688 | 48,1 | 0,5490 | 0,2630 | 1,3798 | 1,0000 | 0,8055 | -3,2413 | 0,87% | 0,72% | | 1,32% | 19,36% |
| TRICHLOROACETYL CHLORIDE | 604 | 43,2 | 0,2824 | 0,2821 | 0,2396 | 0,8611 | 2,3811 | -13,0537 | 1,39% | 2,57% | | 1,93% | 8,69% |
| TRICHLOROETHYLENE | 571 | 49,1 | 0,2166 | 0,2707 | 0,6971 | 0,8571 | 0,9100 | -2,0093 | 1,25% | 1,57% | 0,14% | 1,25% | 16,89% |
| TRICHLOROFLUOROMETHANE | 471,2 | 44,08 | 0,1894 | 0,2763 | 0,3599 | 0,8296 | 1,3654 | -4,7380 | 0,69% | 0,73% | 0,97% | 1,13% | 12,08% |
| TRICHLOROSILANE | 479 | 41,7 | 0,2031 | 0,2784 | 1,2549 | 1,0000 | 0,5106 | -7,2617 | 0,52% | 2,57% | | 1,26% | 12,26% |
| TRIDECAFLUOROHEPTANOIC ACID | 583 | 20,75 | 0,9562 | 0,2612 | 0,4223 | 0,7242 | 2,7263 | -16,7576 | 0,59% | | | 1,80% | 20,47% |
| TRIDECANAL | 720 | 22,38 | 0,7452 | 0,2631 | 0,5079 | 0,8488 | 2,5682 | -17,0924 | 0,46% | 1,27% | | 2,40% | 18,22% |
| TRIETHYL ALUMINUM | 678,15 | 89,3 | 0,8418 | 0,4531 | 1,2515 | 0,9407 | 1,2091 | -106,3511 | 1,25% | 0,99% | | 8,79% | 30,63% |
| TRIETHYL ESTER PHOSPHOROUS ACID | 664,4 | 53,77 | 0,3308 | 0,3805 | 1,0897 | 1,0000 | 0,7699 | -95,5918 | 0,61% | 1,28% | | 4,69% | 5,22% |
| TRIETHYL GALLIUM | 581,2 | 25 | 0,4957 | 0,2420 | 2,2985 | 0,4384 | 0,6011 | 23,9098 | 5,47% | | 8,72% | 1,87% | 21,85% |
| TRIETHYL ORTHOFORMATE | 585 | 26,76 | 0,5447 | 0,2714 | 0,6387 | 0,8565 | 1,6827 | -15,6482 | 0,62% | 1,24% | | 3,35% | 18,67% |
| TRIETHYL PHOSPHATE | 757 | 68,4 | 0,4145 | 0,4800 | 0,9738 | 1,0000 | 1,0000 | -148,9122 | 1,11% | | | 18,31% | 26,32% |
| TRIETHYLAMINE | 535,15 | 30,4 | 0,3162 | 0,2690 | 0,6306 | 0,8435 | 1,1857 | -5,2167 | 0,53% | 1,94% | 2,47% | 1,46% | 16,70% |
| TRIETHYLENE GLYCOL BIS(2-ETHYLHEXANOATE) | 820,7 | 10,94 | 1,0371 | 0,2277 | 0,7132 | 0,8509 | 2,4490 | 69,2799 | 0,65% | | | 2,58% | 42,05% |
| TRIETHYLENE GLYCOL DIMETHYL ETHER | 651 | 23,1 | 0,7915 | 0,2650 | 0,7393 | 0,8280 | 1,8682 | -10,8522 | 0,53% | 0,62% | | 7,49% | 33,42% |
| TRIETHYLENEDIAMINE | 655 | 39,1 | 0,4602 | | 0,2181 | 0,8267 | 2,9702 | | 0,40% | 1,03% | | | |
| TRIETHYLENETETRAMINE | 718 | 31,7 | 0,9735 | 0,2557 | 0,4541 | 0,8143 | 3,1972 | -7,7182 | 0,77% | 1,23% | | 3,41% | 21,70% |
| TRIFLUOROACETAMIDE | 648 | 50,59 | 0,4814 | | 0,1398 | 0,8080 | 3,3930 | | 1,10% | 3,97% | 5,85% | | |
| TRIFLUOROACETIC ACID | 491,25 | 32,58 | 0,5238 | 0,1972 | 0,2281 | 0,8205 | 3,1005 | 45,7598 | 1,72% | | 0,23% | 6,93% | 66,48% |
| TRIFLUOROIODOMETHANE | 396,44 | 39,53 | 0,1763 | 0,2762 | 0,4745 | 0,8816 | 1,1941 | -3,3910 | 0,47% | 1,91% | | 0,88% | 15,28% |
| TRIFLUOROMETHANE | 299,01 | 48,162 | 0,2641 | 0,2569 | 0,3870 | 0,8427 | 1,5748 | 2,9427 | 0,28% | 1,97% | 1,50% | 2,11% | 17,98% |
| TRIFLUOROMETHYL TRIFLUOROVINYL ETHER | 363 | 31,1 | 0,3497 | | 1,1746 | 1,0000 | 0,7303 | | 0,60% | 1,23% | | | |
| TRIISOBUTYL ALUMINUM | 690,1 | 17,59 | 0,4304 | 0,2519 | 0,3899 | 0,8671 | 2,2308 | 19,5685 | 0,33% | | | 1,19% | 19,61% |
| TRIMETHYL BORATE | 501,7 | 35,87 | 0,4161 | 0,2550 | 0,3426 | 0,8616 | 2,3737 | -0,5695 | 0,41% | | | 3,33% | 43,79% |
| TRIMETHYL SILANE | 432 | 31,9 | 0,1751 | 0,2738 | 1,0052 | 1,0000 | 0,6166 | -3,3422 | 0,66% | 1,35% | | 1,24% | 12,37% |
| TRIMETHYL SILANOL | 526,5 | 38,09 | 0,6341 | 0,2741 | 0,2372 | 0,6424 | 2,1984 | -12,5994 | 0,53% | | | 1,10% | 12,23% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| TRIMETHYLALUMINUM | 620 | 40 | 0,2179 | 0,2347 | 0,1660 | 0,0003 | 0,6092 | 27,0899 | 2,56% | 4,63% | | 6,41% | 36,19% |
| TRIMETHYLAMINE | 433,25 | 40,7 | 0,2062 | 0,2714 | 0,1977 | 0,8531 | 2,1837 | -2,1551 | 0,80% | 3,22% | 1,82% | 1,12% | 7,96% |
| TRIMETHYLCHLOROSILANE | 497,75 | 32 | 0,2701 | 0,2750 | 1,0592 | 1,0000 | 0,7094 | -6,4300 | 0,61% | 1,73% | 2,36% | 1,36% | 10,38% |
| TRIMETHYLENE SULFIDE | 602 | 58,6 | 0,1731 | 0,2533 | 0,5796 | 0,8343 | 0,9454 | 8,1800 | 0,66% | 1,46% | 0,05% | 4,55% | 16,69% |
| TRI-n-BUTYL BORATE | 743,15 | 19,8901 | 0,1887 | 0,2929 | 0,9876 | 1,0000 | 0,6488 | -40,9280 | 0,61% | 0,97% | | 7,67% | 15,36% |
| TRI-n-BUTYLAMINE | 644 | 18 | 0,6943 | 0,2492 | 0,7494 | 0,8352 | 1,6885 | 7,9992 | 0,66% | 0,86% | | 1,88% | 23,32% |
| TRI-n-OCTYLAMINE | 782 | 10,1 | 0,9688 | 0,2432 | 0,5373 | 0,8312 | 2,8800 | 32,7099 | 1,52% | | | 5,95% | 42,06% |
| TRIOXANE | 604 | 58,2 | 0,3337 | 0,2594 | 0,1664 | 0,8336 | 2,8349 | 2,5442 | 0,55% | 2,24% | | 1,42% | 17,28% |
| TRIPHENYLENE | 990,8 | 28,7 | 0,6733 | 0,2402 | 0,4648 | 0,8408 | 2,5084 | 28,8052 | 0,40% | | | 1,18% | 23,88% |
| TRIPHENYLETHYLENE | 908 | 21 | 0,5998 | | 0,5760 | 0,8122 | 1,8472 | | 0,58% | 1,18% | 0,58% | | |
| TRIPHENYLMETHANE | 865 | 22 | 0,5735 | 0,2426 | 0,2708 | 0,7916 | 2,7684 | 31,0653 | 0,38% | 2,01% | 6,05% | 1,31% | 29,33% |
| TRIPHENYLPHOSPHINE | 1008 | 78,4 | 0,4517 | 0,5378 | 0,3577 | 0,8167 | 2,1613 | -242,8642 | 0,77% | | | 14,98% | 3,15% |
| TRIPROPYLENE GLYCOL MONOETHYL ETHER | 664 | 20,2 | 1,1610 | 0,2616 | 2,0514 | 1,0000 | 0,8977 | -28,8882 | 3,99% | | 11,00% | 3,82% | 23,44% |
| TRIPROPYLENE GLYCOL MONOMETHYL ETHER | 657 | 21,8 | 1,1254 | 0,2625 | 0,5845 | 0,8010 | 2,9234 | -26,0516 | 1,59% | | 1,66% | 4,88% | 22,14% |
| TRIS(2-METHOXYETHOXY)VINYLSILANE | 723,9 | 17,79 | 0,7150 | 0,2570 | 0,3530 | 0,8135 | 2,9776 | -6,1069 | 0,47% | | | 4,48% | 20,24% |
| UNDECANAL | 690 | 23,93 | 0,6352 | 0,2659 | 1,1432 | 0,9534 | 1,1027 | -16,4860 | 0,77% | 1,28% | | 1,78% | 18,47% |
| UNDECYL MERCAPTAN | 710 | 19,8 | 0,6388 | 0,2405 | 0,5868 | -0,8567 | 2,2913 | 44,1498 | 3,34% | 1,84% | 1,78% | 4,86% | 29,05% |
| UNDECYLAMINE | 682 | 20,2 | 0,7043 | 0,2437 | 0,3339 | 0,8184 | 3,1452 | 15,5900 | 5,80% | | 2,91% | 1,19% | 24,24% |
| VALERONITRILE | 610,3 | 35,8 | 0,4069 | 0,2381 | 0,3849 | 0,8730 | 2,2169 | 21,4095 | 2,10% | 4,01% | | 1,75% | 21,14% |
| VANADIUM OXYTRICHLORIDE | 636 | 37,4 | 0,1305 | 0,2388 | 1,5370 | 1,0000 | 0,3455 | 29,4144 | 0,17% | | | 6,49% | 39,73% |
| VANADIUM TETRACHLORIDE | 697 | 60,3 | 0,1858 | 0,3025 | 0,7542 | 1,0000 | 0,8703 | -24,8634 | 0,77% | | | 1,35% | 19,51% |
| VANILLIC ACID | 825,1 | 37,98 | 0,8503 | | 0,3730 | 0,8103 | 3,2578 | | 0,44% | 1,74% | | | |
| VANILLIN | 777 | 40,1 | 0,7573 | | 0,4161 | 0,8123 | 2,7858 | | 0,59% | 0,99% | | | |
| VINYL ACETATE | 519,13 | 39,58 | 0,3513 | 0,2487 | 1,5912 | 1,0000 | 0,5178 | 10,3625 | 1,13% | 3,32% | 3,87% | 2,61% | 20,32% |
| VINYL CHLORIDE | 432 | 56,7 | 0,1001 | 0,2745 | 1,0721 | 0,3534 | 0,4585 | -1,1912 | 0,63% | 1,55% | | 2,54% | 9,45% |
| VINYL FLUORIDE | 327,8 | 52,4 | 0,1429 | 0,2727 | 0,1457 | 0,8631 | 2,3515 | -1,8564 | 2,64% | | 1,25% | 2,56% | 12,32% |
| VINYL FORMATE | 498 | 50,2 | 0,2849 | 0,2614 | 1,7272 | 1,0000 | 0,4273 | 2,9074 | 1,24% | 2,03% | | 1,25% | 15,50% |
| VINYL PIVALATE | 556 | 29,5 | 0,3913 | 0,2698 | 1,2119 | 1,0000 | 0,7513 | -8,5009 | 0,54% | 0,96% | | 1,49% | 15,89% |
| VINYL PROPIONATE | 546 | 36,8 | 0,3802 | 0,2606 | 1,2023 | 1,0000 | 0,7466 | 1,7187 | 0,61% | 0,99% | | 1,35% | 16,87% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| VINYLACETONITRILE | 584 | 38,8 | 0,3782 | 0,2183 | 1,0664 | 1,0000 | 0,8456 | 35,6597 | 2,17% | 3,51% | 2,00% | 5,28% | 34,76% |
| VINYLACETYLENE | 454 | 48,6 | 0,1069 | 0,2656 | 1,0009 | 1,0000 | 0,5625 | 2,9006 | 5,90% | 3,99% | 0,44% | 1,61% | 15,05% |
| VINYLCYCLOHEXANE | 599,4 | 32,7 | 0,2902 | 0,2671 | 0,3349 | 0,8055 | 1,6950 | -2,3023 | 0,77% | 2,64% | 1,37% | 1,60% | 15,68% |
| VINYLETHYLENE CARBONATE | 759,1 | 48 | 0,4733 | 0,2388 | 1,3651 | 1,0000 | 0,7431 | 16,0215 | 0,66% | 1,31% | 0,10% | 2,96% | 36,20% |
| VINYLNORBORNENE | 626 | 32,1 | 0,2487 | 0,2814 | 1,0612 | 1,0000 | 0,6815 | -9,1857 | 0,64% | 1,35% | | 7,53% | 18,88% |
| VINYLTRICHLOROSILANE | 543,15 | 30,6 | 0,2815 | 0,2535 | 1,0792 | 1,0000 | 0,7129 | 11,2670 | 0,58% | 1,17% | | 2,58% | 8,43% |
| VINYLTRIMETHOXYSILANE | 553,7 | 26,85 | 0,5514 | 0,2606 | 0,4849 | 0,8659 | 2,2059 | -4,5259 | 1,48% | | 3,69% | 2,28% | 21,09% |
| WATER | 647,096 | 220,64 | 0,3449 | 0,2289 | 0,3872 | 0,8720 | 1,9668 | 5,2711 | 0,36% | 1,69% | 3,09% | 6,44% | 24,56% |
| XENON | 289,74 | 58,4037 | 0,0000 | 0,2880 | 0,1785 | 0,9199 | 1,7045 | -3,7740 | 0,15% | 1,67% | | 1,49% | 10,65% |
| XYLITOL | 941,8 | 59,37 | 0,9066 | | 0,5792 | 0,8065 | 2,4743 | | 0,54% | 1,33% | | | |
| DEUTERIUM | 38,35 | 16,62 | -0,1449 | 0,315 | 0,1486 | 0,9968 | 1,0587 | -4,5555 | 1,06% | 5,52% | | 1,61% | 2,41% |
| HELIUM-4 | 5,2 | 2,27 | -0,3900 | 0,3355 | 0,0063 | 1,2175 | 1,0909 | -4,8915 | 1,75% | 7,00% | | 6,16% | 1,13% |
| HYDROGEN | 33,19 | 13,13 | -0,2160 | 0,3192 | 1,5147 | -3,7959 | -0,1377 | -5,3386 | 2,16% | 4,66% | | 2,50% | 0,24% |
| NEON | 44,4 | 26,53 | -0,0396 | 0,3004 | 0,1887 | 0,9470 | 1,4698 | -2,3573 | 0,28% | 1,89% | | 1,71% | 2,81% |

# Annexe A-2

# Modélisation des corps purs Paramètres et déviations du modèle tc-RK

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| (3-METHYLACRYLOXYPROPYL)TRICHLOROSILANE | 708,1 | 21,13 | 0,6267 | 0,2457 | 0,6853 | 0,8223 | 1,8942 | 58,3785 | 0,72% | 1,30% | | 3,18% | 31,08% |
| (Z)-1,3-DICHLORO-2-BUTENE | 617 | 37,80 | 0,2370 | 0,2508 | 1,2265 | 1,0000 | 0,6707 | 35,8987 | 1,37% | | 0,79% | 6,15% | 26,21% |
| [3-(2,3-EPOXYPROXY)PROPYL]TRIMETHOXYSILANE | 701,4 | 18,12 | 0,7605 | 0,2336 | 0,7512 | 0,8299 | 2,0118 | 86,7044 | 1,03% | 1,82% | 1,06% | 2,87% | 34,71% |
| [3-(MERCAPTO)PROPYL]TRIETHOXYSILANE | 647,5 | 18,63 | 0,8370 | 0,2587 | 0,6611 | 0,8518 | 2,5206 | 25,3744 | 2,13% | | | 1,74% | 27,43% |
| 1-(4-ETHYLPHENYL)-2-(4-ETHYLPHENYL)ETHANE | 780,9 | 19,17 | 0,5860 | | 0,3928 | 0,8247 | 2,8158 | | 0,65% | 2,08% | | | |
| 1-(4-ETHYLPHENYL)-2-PHENYLETHANE | 771 | 21,70 | 0,5782 | | 0,8081 | 0,8448 | 1,5803 | | 1,12% | 1,11% | 3,74% | | |
| 1,1,1,2,2,3,4,5,5,5-DECAFLUOROPENTANE | 454,2 | 22,88 | 0,5000 | 0,2605 | 1,3001 | 1,0000 | 0,9201 | 23,2572 | 1,96% | 2,60% | | 2,63% | 22,54% |
| 1,1,1,2,2-PENTAFLUOROPROPANE | 380,11 | 31,37 | 0,3046 | 0,2658 | 0,6653 | 0,8738 | 1,3376 | 14,5421 | 0,63% | 1,33% | | 3,59% | 17,59% |
| 1,1,1,2,3,3,3-HEPTAFLUOROPROPANE | 374,83 | 29,12 | 0,3552 | 0,2650 | 0,7157 | 0,8700 | 1,3513 | 14,4877 | 0,46% | 1,06% | | 3,29% | 24,93% |
| 1,1,1,2,3,3-HEXAFLUOROPROPANE | 412,38 | 34,12 | 0,3688 | 0,2649 | 0,2624 | 0,8353 | 2,8025 | 13,1684 | 0,47% | 0,93% | | 3,28% | 19,20% |
| 1,1,1,2-TETRACHLORODIFLUOROETHANE | 552 | 33,40 | 0,2570 | 0,2615 | 0,2674 | 0,8058 | 2,1097 | 24,9922 | 1,01% | 3,28% | | 3,92% | 23,38% |
| 1,1,1,2-TETRACHLOROETHANE | 624 | 40,20 | 0,2422 | 0,2615 | 0,2061 | 0,8434 | 2,6591 | 24,7234 | 1,57% | 2,50% | | 4,08% | 24,76% |
| 1,1,1,2-TETRAFLUOROETHANE | 374,18 | 40,56 | 0,3269 | 0,2590 | 0,2829 | 0,8469 | 2,6001 | 13,8865 | 0,29% | 0,80% | 4,26% | 3,88% | 21,63% |
| 1,1,1,3,3,3-HEXAFLUOROPROPANE | 398,07 | 32,19 | 0,3905 | 0,2645 | 0,4659 | 0,8182 | 1,9067 | 13,1112 | 0,69% | 1,57% | | 3,33% | 23,91% |
| 1,1,1,3,3-PENTACHLOROPROPANE | 670,9 | 32,96 | 0,3241 | 0,2568 | 0,5745 | 0,7982 | 1,4341 | 34,5325 | 0,71% | 1,70% | | 4,34% | 21,75% |
| 1,1,1,3,3-PENTAFLUOROBUTANE | 473,7 | 33,92 | 0,2571 | 0,2742 | 1,4359 | 0,4498 | 0,6382 | 13,2022 | 0,89% | | | 3,10% | 20,59% |
| 1,1,1,3,3-PENTAFLUOROPROPANE | 427,2 | 36,40 | 0,3755 | 0,2630 | 0,4168 | 0,7873 | 1,9006 | 14,1028 | 0,67% | 1,50% | | 3,73% | 20,14% |
| 1,1,1-TRICHLOROETHANE | 545 | 43,00 | 0,2183 | 0,2707 | 0,2091 | 0,8500 | 2,5488 | 13,9665 | 0,91% | 1,97% | 1,42% | 3,55% | 20,04% |
| 1,1,1-TRICHLOROFLUOROETHANE | 565 | 39,90 | 0,2501 | | 0,7724 | 0,9114 | 1,0871 | | 0,72% | 1,35% | | | |
| 1,1,1-TRICHLOROTRIFLUOROETHANE | 483 | 33,20 | 0,2667 | 0,2655 | 0,2462 | 0,8504 | 2,5434 | 17,6245 | 4,03% | 1,80% | 0,55% | 3,52% | 20,12% |
| 1,1,1-TRIFLUOROETHANE | 345,88 | 37,64 | 0,2614 | 0,2565 | 0,2780 | 0,8581 | 2,4241 | 16,5559 | 0,47% | 1,52% | 1,40% | 4,36% | 22,11% |
| 1,1,2,2,3-PENTAFLUOROPROPANE | 447,57 | 39,25 | 0,3531 | 0,2665 | 0,4482 | 0,8459 | 1,9559 | 11,7840 | 0,58% | 1,36% | | 3,16% | 18,85% |
| 1,1,2,2-TETRACHLOROETHANE | 645 | 40,90 | 0,2467 | 0,2545 | 1,9804 | 0,6276 | 0,4698 | 32,2350 | 1,38% | | | 6,25% | 24,56% |
| 1,1,2,2-TETRAFLUOROETHANE | 391,8 | 46,40 | 0,2660 | 0,2691 | 0,2740 | 0,8571 | 2,4388 | 9,1038 | 4,11% | 2,07% | | 3,38% | 17,76% |
| 1,1,2,2-TETRAPHENYLETHANE | 827 | 16,70 | 0,7322 | | 0,3721 | 0,8103 | 3,2718 | | 0,60% | 1,13% | 1,48% | | |
| 1,1,2-TRICHLOROETHANE | 602 | 44,80 | 0,2591 | 0,2591 | 0,1983 | 0,8391 | 2,7339 | 23,4636 | 0,51% | 2,02% | 0,07% | 3,70% | 24,18% |
| 1,1,2-TRICHLOROTRIFLUOROETHANE | 487,25 | 34,10 | 0,2515 | 0,2719 | 0,4158 | 0,8447 | 1,7364 | 13,3944 | 0,70% | 1,63% | 0,43% | 3,30% | 17,73% |
| 1,1,2-TRIFLUOROETHANE | 429,8 | 52,41 | 0,3265 | 0,2622 | 1,1727 | 1,0000 | 0,8156 | 11,1295 | 0,37% | 0,97% | | 3,91% | 20,75% |
| 1,1,2-TRIMETHYLCYCLOPENTANE | 579,54 | 29,39 | 0,2523 | 0,2613 | 0,2132 | 0,8433 | 2,6597 | 29,7354 | 0,64% | 2,09% | | 4,61% | 23,95% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1,1,2-TRIPHENYLETHANE | 840 | 20,40 | 0,6116 | | 0,6677 | 0,8255 | 1,9107 | | 0,96% | 1,11% | 1,63% | | |
| 1,1,3-TRIMETHYLCYCLOHEXANE | 611,3 | 29,78 | 0,2753 | 0,2783 | 0,2728 | 0,8533 | 2,4969 | 10,9472 | 1,07% | 2,19% | | 1,96% | 18,97% |
| 1,1,3-TRIMETHYLCYCLOPENTANE | 569,54 | 28,27 | 0,2119 | 0,2608 | 1,2333 | 1,0000 | 0,6350 | 32,6060 | 0,93% | 1,20% | | 6,49% | 26,09% |
| 1,1-DIBROMOETHANE | 628 | 60,30 | 0,1250 | 0,3016 | 2,7303 | 0,2381 | 0,4259 | -4,1161 | 2,66% | 6,49% | | 1,34% | 6,07% |
| 1,1-DICHLORO-1-FLUOROETHANE | 478,85 | 43,40 | 0,2211 | 0,2756 | 0,2354 | 0,8553 | 2,4661 | 8,8559 | 0,63% | 1,32% | 1,92% | 3,08% | 17,36% |
| 1,1-DICHLOROETHANE | 523 | 50,70 | 0,2339 | 0,2751 | 0,4346 | 0,8279 | 1,5561 | 8,7766 | 0,56% | 1,73% | 1,33% | 3,11% | 15,47% |
| 1,1-DICHLOROPROPANE | 560 | 42,40 | 0,2529 | 0,2572 | 0,3170 | 0,8296 | 2,0121 | 21,6289 | 0,54% | 1,14% | 2,31% | 7,14% | 18,36% |
| 1,1-DICHLOROTETRAFLUOROETHANE | 418,55 | 33,00 | 0,2533 | 0,2748 | 0,2384 | 0,8502 | 2,5463 | 9,8082 | 0,49% | 1,73% | 5,25% | 2,89% | 16,23% |
| 1,1-DIETHYLCYCLOHEXANE | 643 | 25,70 | 0,4036 | 0,2567 | 0,6928 | 0,8714 | 1,5080 | 38,2682 | 0,83% | 1,54% | 2,64% | 3,22% | 22,69% |
| 1,1-DIFLUOROETHANE | 386,44 | 45,20 | 0,2751 | 0,2534 | 0,2955 | 0,8587 | 2,3956 | 16,5622 | 0,44% | 1,18% | 5,38% | 4,89% | 23,13% |
| 1,1-DIFLUOROETHYLENE | 302,8 | 44,60 | 0,1362 | 0,2725 | 0,2022 | 0,8634 | 2,3480 | 8,2885 | 2,44% | | 2,69% | 3,38% | 16,80% |
| 1,1-DIMETHOXYETHANE | 507,8 | 37,73 | 0,3277 | 0,2660 | 0,2078 | 0,8306 | 2,8911 | 15,5184 | 1,78% | 6,01% | 2,53% | 3,42% | 20,37% |
| 1,1-DIMETHYLCYCLOHEXANE | 591,15 | 29,38 | 0,2326 | 0,2605 | 0,6078 | 0,8246 | 1,2010 | 34,0689 | 0,42% | 1,07% | 0,64% | 4,77% | 16,33% |
| 1,1-DIMETHYLCYCLOPENTANE | 547 | 34,45 | 0,2724 | 0,2786 | 0,5960 | 0,8414 | 1,3012 | 9,3273 | 3,21% | 1,24% | 1,82% | 2,52% | 19,65% |
| 1,1-DIPHENYLETHANE | 775 | 26,80 | 0,4566 | 0,2559 | 0,5531 | 0,8270 | 1,8559 | 45,0492 | 0,84% | 1,35% | | 2,23% | 25,23% |
| 1,2,3,4-TETRAHYDRONAPHTHALENE | 720 | 36,50 | 0,3353 | 0,2597 | 0,3915 | 0,8388 | 2,0567 | 28,1565 | 0,97% | 3,36% | 0,82% | 4,36% | 27,09% |
| 1,2,3,4-TETRAMETHYLBENZENE | 693 | 31,10 | 0,4172 | 0,2564 | 0,3283 | 0,8424 | 2,6757 | 33,8521 | 2,56% | 2,88% | | 3,15% | 22,89% |
| 1,2,3,4-TETRAMETHYLCYCLOHEXANE | 642 | 25,70 | 0,4016 | 0,2564 | 0,5002 | 0,8215 | 1,8436 | 38,6531 | 0,71% | 1,60% | 2,91% | 3,72% | 23,80% |
| 1,2,3,5-TETRAETHYLBENZENE | 708 | 20,70 | 0,5940 | 0,2494 | 1,0616 | 0,9319 | 1,2881 | 56,3498 | 1,25% | 4,04% | 2,51% | 2,48% | 26,82% |
| 1,2,3,5-TETRAMETHYLBENZENE | 679 | 29,70 | 0,4242 | 0,2543 | 0,4643 | 0,8495 | 2,1342 | 37,1886 | 1,17% | 1,90% | 0,75% | 3,26% | 23,74% |
| 1,2,3,6-TETRAHYDROBENZALDEHYDE | 655 | 40,30 | 0,3638 | 0,2607 | 0,2953 | 0,8307 | 2,5554 | 21,6425 | 0,54% | 3,38% | 3,31% | 3,78% | 24,29% |
| 1,2,3-BENZENETRIOL | 830 | 88,10 | 0,9452 | | 0,7111 | 0,8495 | 2,5573 | | 6,84% | | | | |
| 1,2,3-TRICHLOROBENZENE | 734 | 45,10 | 0,4263 | 0,2848 | 0,3905 | 0,8530 | 2,4535 | 0,0413 | 0,56% | 1,83% | 1,24% | 1,16% | 14,18% |
| 1,2,3-TRICHLOROPROPANE | 652 | 38,70 | 0,3056 | 0,2393 | 0,2819 | 0,8262 | 2,3555 | 43,1918 | 0,53% | 2,30% | 2,88% | 7,77% | 26,87% |
| 1,2,3-TRIETHYLBENZENE | 683 | 23,80 | 0,5054 | | 0,5681 | 0,8542 | 2,0312 | | 1,05% | 1,75% | 0,99% | | |
| 1,2,3-TRIMETHYL-4-ETHYLBENZENE | 702,7 | 27,95 | 0,4574 | 0,2543 | 0,5299 | 0,8353 | 1,9562 | 39,6218 | 0,73% | 1,59% | | 3,13% | 23,76% |
| 1,2,3-TRIMETHYLBENZENE | 664,5 | 34,54 | 0,3666 | 0,2560 | 0,4191 | 0,8532 | 2,1354 | 29,3233 | 0,29% | 0,97% | 1,06% | 4,83% | 21,71% |
| 1,2,3-TRIMETHYLINDENE | 726 | 27,70 | 0,4419 | 0,2427 | 0,9759 | 0,9817 | 1,1969 | 58,9975 | 1,06% | 0,75% | 6,49% | 4,08% | 26,16% |
| 1,2,4,5-TETRAISOPROPYLBENZENE | 703 | 15,56 | 0,6360 | | 0,2698 | 0,8041 | 3,4951 | | 0,31% | 1,10% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1,2,4,5-TETRAMETHYLBENZENE | 676 | 29,00 | 0,4217 | 0,2481 | 0,5624 | 0,8625 | 1,8464 | 44,1802 | 0,48% | 0,99% | 2,20% | 4,27% | 24,87% |
| 1,2,4-TRICHLOROBENZENE | 725 | 37,20 | 0,3581 | 0,2524 | 0,5177 | 0,8323 | 1,6961 | 36,7163 | 1,00% | 1,77% | 0,32% | 4,35% | 27,45% |
| 1,2,4-TRIETHYLBENZENE | 684 | 23,80 | 0,5011 | 0,2513 | 0,4315 | 0,8512 | 2,5304 | 47,5737 | 0,75% | 3,33% | 0,51% | 2,50% | 24,82% |
| 1,2,4-TRIMETHYL-3-ETHYLBENZENE | 697,3 | 27,95 | 0,4569 | 0,2562 | 0,5923 | 0,8955 | 1,9499 | 36,2530 | 1,03% | | | 2,52% | 23,39% |
| 1,2,4-TRIMETHYL-5-ETHYLBENZENE | 687,3 | 26,78 | 0,4638 | 0,2531 | 0,4464 | 0,8479 | 2,3232 | 41,5549 | 0,54% | 1,79% | | 2,97% | 24,02% |
| 1,2,4-TRIMETHYLBENZENE | 649,1 | 32,32 | 0,3787 | 0,2557 | 0,4102 | 0,8508 | 2,1979 | 31,9729 | 0,43% | 0,82% | 1,26% | 3,95% | 22,01% |
| 1,2-BENZENE DICARBOXYLIC ACID, HEPTYL, UNDECYL ESTER | 878 | 10,70 | 1,0205 | 0,2217 | 0,6663 | 0,8345 | 2,8168 | 195,1602 | 1,33% | | | 3,35% | 51,75% |
| 1,2-BENZENEDICARBOXYLIC ACID, HEPTYL, NONYL ESTER | 841 | 11,60 | 1,0944 | 0,2275 | 0,6780 | 0,8298 | 2,9077 | 148,2866 | 1,30% | | | 2,07% | 46,54% |
| 1,2-BENZENEDIOL | 764 | 74,90 | 0,6937 | 0,3102 | 0,6914 | 0,8801 | 2,1272 | -19,0418 | 7,33% | 5,75% | | 2,08% | 0,58% |
| 1,2-BUTADIENE | 452 | 43,60 | 0,1659 | 0,2627 | 0,7627 | 0,8646 | 0,8971 | 18,1073 | 1,10% | 2,57% | 0,57% | 4,92% | 22,37% |
| 1,2-BUTANEDIOL | 680 | 52,10 | 0,6305 | 0,2557 | 1,3354 | 0,9214 | 1,0321 | 15,4984 | 0,73% | 0,67% | | 3,14% | 14,27% |
| 1,2-DIBROMOETHANE | 650,15 | 54,77 | 0,2067 | 0,2663 | 0,6398 | 0,8415 | 1,1033 | 16,6860 | 1,06% | 1,46% | 0,66% | 4,44% | 19,38% |
| 1,2-DIBROMOTETRAFLUOROETHANE | 487,8 | 33,93 | 0,2431 | 0,2710 | 0,2022 | 0,8429 | 2,6675 | 14,4440 | 0,62% | 1,04% | | 4,01% | 12,61% |
| 1,2-DICHLORO-1,1,2-TRIFLUOROETHANE | 461,6 | 36,10 | 0,2410 | 0,2642 | 0,2718 | 0,8450 | 2,2632 | 18,1727 | 0,44% | 1,38% | 5,71% | 3,98% | 20,94% |
| 1,2-DICHLORO-4-NITROBENZENE | 758 | 36,00 | 0,5385 | 0,2438 | 0,4750 | 0,8252 | 2,3183 | 42,4080 | 0,72% | 1,18% | | 3,79% | 24,11% |
| 1,2-DICHLOROBUTANE | 600 | 36,80 | 0,2988 | 0,2503 | 0,3430 | 0,8460 | 2,1750 | 31,8649 | 0,42% | 1,05% | | 6,66% | 22,45% |
| 1,2-DICHLOROETHANE | 561,6 | 53,70 | 0,2866 | 0,2659 | 0,2803 | 0,8557 | 2,4607 | 12,8718 | 2,71% | 3,09% | 2,76% | 3,33% | 25,90% |
| 1,2-DICHLOROHEXAFLUOROCYCLOBUTANE | 497 | 27,30 | 0,2330 | | 0,3663 | 0,8485 | 1,8495 | | 0,49% | 1,82% | | | |
| 1,2-DICHLOROPROPANE | 572 | 42,40 | 0,2564 | 0,2604 | 0,2198 | 0,8450 | 2,6306 | 21,7256 | 0,39% | 3,71% | 1,49% | 4,58% | 21,02% |
| 1,2-DICHLOROTETRAFLUOROETHANE | 418,85 | 32,60 | 0,2520 | 0,2725 | 0,2315 | 0,8483 | 2,5774 | 11,3686 | 0,68% | 1,85% | 4,94% | 3,46% | 17,25% |
| 1,2-DIETHOXYETHANE | 561 | 29,30 | 0,4818 | 0,2535 | 0,4681 | 0,7605 | 1,9194 | 27,7487 | 3,50% | 6,86% | 4,94% | 5,43% | 25,10% |
| 1,2-DIFLUOROBENZENE | 566 | 42,99 | 0,2792 | 0,2646 | 0,2828 | 0,8552 | 2,4676 | 17,1510 | 0,94% | 2,16% | | 3,51% | 19,91% |
| 1,2-DIFLUOROETHANE | 445 | 43,40 | 0,2224 | 0,2286 | 0,2699 | 0,8639 | 2,3404 | 35,3368 | 0,75% | 2,93% | | 8,20% | 27,61% |
| 1,2-DIMETHOXYETHANE | 536,15 | 38,71 | 0,3475 | 0,2587 | 0,9804 | 0,9285 | 1,0108 | 19,6520 | 0,46% | 0,97% | | 4,68% | 34,59% |
| 1,2-DIMETHOXYPROPANE | 543 | 34,46 | 0,3522 | 0,2674 | 0,4121 | 0,8353 | 2,0365 | 15,7918 | 0,65% | 1,23% | | 2,90% | 20,26% |
| 1,2-DIMETHYL-3-PROPYLBENZENE | 687,7 | 27,24 | 0,4531 | 0,2615 | 0,4595 | 0,8520 | 2,2564 | 32,8700 | 0,70% | 1,44% | | 1,31% | 13,79% |
| 1,2-DIPHENYLETHANE | 780 | 26,50 | 0,4885 | 0,2518 | 0,3594 | 0,8383 | 2,7470 | 48,8602 | 0,75% | 1,09% | | 2,98% | 24,50% |
| 1,2-EPOXY-2-METHYLPROPANE | 521 | 46,60 | 0,1709 | 0,2674 | 0,1994 | 0,8554 | 2,4269 | 15,0631 | 0,48% | 4,42% | 0,22% | 5,05% | 21,82% |
| 1,2-EPOXY-3-PHENOXYPROPANE | 720 | 29,50 | 0,5943 | 0,2317 | 0,3225 | 0,8176 | 3,1641 | 63,1577 | 1,72% | 2,09% | | 4,61% | 32,17% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1,2-EPOXYBUTANE | 526 | 43,90 | 0,2345 | 0,2570 | 0,4555 | 0,8206 | 1,4940 | 22,3921 | 0,51% | 2,86% | 0,65% | 5,51% | 20,03% |
| 1,2-ETHANEDITHIOL | 663 | 53,60 | 0,2570 | 0,2566 | 0,6877 | 0,8825 | 1,2039 | 21,6588 | 0,71% | 1,44% | | 4,66% | 53,66% |
| 1,2-HEXADIENE | 526 | 33,50 | 0,2762 | 0,2564 | 0,3242 | 0,8233 | 2,0408 | 27,9917 | 0,59% | 2,90% | 0,16% | 5,18% | 23,01% |
| 1,2-PENTADIENE | 500 | 38,00 | 0,1542 | 0,2570 | 1,0966 | 1,0000 | 0,6588 | 26,3032 | 3,52% | 4,41% | 0,61% | 6,60% | 22,60% |
| 1,2-PROPANEDIAMINE | 587 | 52,70 | 0,4738 | 0,2798 | 0,4508 | 0,8360 | 2,2671 | 3,3597 | 0,15% | 0,97% | | 1,22% | 3,37% |
| 1,2-PROPYLENE OXIDE | 482,25 | 49,20 | 0,2683 | 0,2456 | 0,3479 | 0,8417 | 1,9903 | 22,9958 | 2,06% | 2,62% | 0,96% | 7,01% | 33,69% |
| 1,3,5,7-CYCLOOCTATETRAENE | 641,4 | 44,20 | 0,2870 | | 0,2583 | 0,8487 | 2,5698 | | 1,00% | 2,48% | 0,83% | | |
| 1,3,5-TRICHLOROBENZENE | 718 | 37,20 | 0,3596 | 0,2566 | 0,9663 | 0,9955 | 1,0738 | 32,0834 | 0,76% | 1,55% | | 3,32% | 18,32% |
| 1,3,5-TRIETHYLBENZENE | 678 | 23,00 | 0,5077 | 0,2476 | 0,5614 | 0,8515 | 2,0456 | 53,4642 | 0,65% | 2,70% | 0,39% | 3,54% | 28,75% |
| 1,3,5-TRIISOPROPYLBENZENE | 696,6 | 19,50 | 0,5324 | | 0,5614 | 0,8005 | 1,9439 | | 0,77% | 1,35% | | | |
| 1,3,5-TRI-tert-BUTYLBENZENE | 717,8 | 16,56 | 0,4865 | | 0,3762 | 0,7504 | 2,1766 | | 0,58% | 1,71% | | | |
| 1,3-BENZENEDIOL | 810 | 74,90 | 0,6767 | 0,2911 | 0,6911 | 0,8329 | 2,0011 | -9,6602 | 1,79% | 1,77% | 2,27% | 0,92% | 3,13% |
| 1,3-BUTADIENE | 425 | 43,20 | 0,1950 | 0,2708 | 0,2225 | 0,8585 | 2,4186 | 11,2082 | 1,12% | 1,81% | 1,59% | 3,97% | 18,30% |
| 1,3-BUTANEDIOL | 676 | 40,20 | 0,7043 | 0,2106 | 1,6658 | 1,0000 | 0,8563 | 55,6564 | 0,72% | 2,22% | 9,20% | 11,16% | 34,55% |
| 1,3-CYCLOHEXADIENE | 558 | 47,30 | 0,2308 | 0,2823 | 0,3331 | 0,8483 | 1,9417 | 6,3389 | 1,56% | 1,66% | 2,57% | 1,30% | 15,74% |
| 1,3-DICHLOROHEXAFLUOROPROPANE | 449 | 25,70 | 0,3286 | 0,2570 | 0,6063 | 0,8592 | 1,4906 | 26,9532 | 0,71% | 1,22% | | 5,49% | 23,91% |
| 1,3-DICHLOROPROPANE | 603 | 41,50 | 0,2916 | 0,2456 | 0,9765 | 0,8756 | 0,8848 | 34,3897 | 3,66% | 3,97% | 0,22% | 7,45% | 26,57% |
| 1,3-DIFLUOROBENZENE | 548,4 | 42,99 | 0,2862 | 0,2710 | 0,3064 | 0,8598 | 2,3996 | 12,0059 | 1,16% | 2,36% | | 2,66% | 16,96% |
| 1,3-DIMETHYL UREA | 787,1 | 48,70 | 0,5900 | | 0,3779 | 0,8189 | 2,8531 | | 0,43% | 1,33% | | | |
| 1,3-DIMETHYL-2-IMIDAZOLIDINONE | 749,9 | 42,75 | 0,3701 | 0,2485 | 0,4512 | 0,8532 | 2,0314 | 36,0255 | 0,70% | 1,71% | | 4,34% | 24,35% |
| 1,3-DIMETHYL-5-NITROBENZENE | 787,7 | 33,13 | 0,4745 | | 0,3997 | 0,8270 | 2,4399 | | 0,69% | 1,93% | | | |
| 1,3-DIMETHYLADAMANTANE | 708 | 30,00 | 0,2935 | 0,2785 | 0,2701 | 0,8500 | 2,5500 | 11,0475 | 0,53% | 2,22% | 1,12% | 2,43% | 12,81% |
| 1,3-DIOXANE | 590 | 51,50 | 0,2891 | 0,2703 | 0,5735 | 0,8427 | 1,4255 | 11,9898 | 0,79% | 1,83% | 2,45% | 2,22% | 27,83% |
| 1,3-DIPHENYLTRIAZENE | 845 | 28,30 | 0,6173 | | 0,4261 | 0,8201 | 2,7210 | | 0,66% | 1,02% | | | |
| 1,3-DI-TERT-BUTYL GLYCERIN | 667,1 | 21,86 | 0,6502 | 0,2721 | 0,4652 | 0,8279 | 2,6925 | 7,3052 | 0,58% | 1,24% | | 1,17% | 21,52% |
| 1,3-PROPANEDIAMINE | 608 | 51,20 | 0,5063 | 0,2737 | 0,4785 | 0,8603 | 2,3923 | 8,8145 | 1,24% | | | 2,06% | 1,36% |
| 1,3-PROPYLENE GLYCOL | 724 | 95,00 | 0,7385 | 0,3022 | 0,5770 | 0,8499 | 2,5508 | -14,6580 | 5,82% | 2,03% | | 1,18% | 4,09% |
| 1,3-PROPYLENE OXIDE | 520 | 57,50 | 0,2005 | 0,2535 | 0,1889 | 0,8482 | 2,5777 | 19,3453 | 0,80% | 2,12% | 0,46% | 5,97% | 23,03% |
| 1,4-BENZENEDICARBOXYLIC ACID, 2-HYDROXYETHYL METHYL ESTER | 832 | 26,75 | 0,8033 | | 0,4703 | 0,8219 | 3,0707 | | 0,81% | 1,32% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1,4-BIS(3-AMINOPROPYL)PIPERAZINE | 750,3 | 22,66 | 0,8314 | 0,2553 | 0,5182 | 0,8088 | 2,8512 | 38,3757 | 2,12% | | 1,90% | 1,74% | 18,18% |
| 1,4-BUTANEDIISOCYANATE | 724,3 | 29,47 | 0,4258 | 0,2245 | 0,4569 | 0,8508 | 2,1785 | 80,0338 | 0,60% | 1,96% | 0,45% | 7,02% | 30,96% |
| 1,4-CYCLOHEXANEDICARBOXYLIC ACID | 819,8 | 37,36 | 1,0050 | | 0,6414 | 0,8319 | 2,8664 | | 0,92% | 2,42% | | | |
| 1,4-DIBROMOBENZENE | 738,15 | 44,72 | 0,4257 | 0,2748 | 0,5888 | 0,9023 | 1,8768 | 7,8983 | 4,52% | | | 1,26% | 21,18% |
| 1,4-DICHLOROBUTANE | 641 | 36,10 | 0,3260 | 0,2414 | 0,3384 | 0,8131 | 2,1110 | 43,7910 | 0,51% | 2,05% | 1,10% | 6,92% | 30,70% |
| 1,4-DICHLORO-cis-2-BUTENE | 640 | 37,80 | 0,3299 | 0,2434 | 0,4046 | 0,8216 | 1,9268 | 41,2222 | 0,67% | 2,04% | 0,96% | 5,76% | 24,79% |
| 1,4-DICHLORO-trans-2-BUTENE | 646 | 37,80 | 0,3282 | 0,2432 | 0,4086 | 0,8207 | 1,9047 | 41,8006 | 0,65% | 1,91% | 0,94% | 5,44% | 24,81% |
| 1,4-DICYANO-2-BUTENE | 755 | 29,50 | 0,6668 | 0,2004 | 0,3952 | 0,8228 | 3,0502 | 105,4566 | 0,68% | 1,47% | | 7,53% | 41,75% |
| 1,4-DIFLUOROBENZENE | 556,9 | 44,00 | 0,2985 | 0,2722 | 0,3101 | 0,8586 | 2,4173 | 11,5642 | 1,33% | 2,65% | | 2,03% | 13,11% |
| 1,4-DIOXANE | 587 | 52,08 | 0,2793 | 0,2679 | 0,2161 | 0,8403 | 2,7120 | 12,5746 | 0,65% | 1,44% | 7,69% | 3,31% | 25,96% |
| 1,4-DI-tert-BUTYLBENZENE | 708 | 23,00 | 0,5023 | 0,2705 | 0,3377 | 0,8319 | 2,8673 | 19,7462 | 2,31% | 1,77% | 0,99% | 1,31% | 13,85% |
| 1,4-HEXADIENE | 510 | 33,50 | 0,2800 | 0,2636 | 1,2116 | 1,0000 | 0,7142 | 21,5351 | 2,78% | 2,93% | 3,30% | 4,28% | 20,96% |
| 1,4-PENTADIENE | 479 | 37,40 | 0,0837 | 0,2770 | 1,6703 | 1,0000 | 0,3558 | 16,2922 | 4,11% | 4,73% | 1,67% | 1,38% | 11,77% |
| 1,5,9-CYCLODODECATRIENE | 745 | 29,90 | 0,4031 | 0,2717 | 0,6407 | 0,9187 | 1,7155 | 15,9497 | 0,57% | | | 1,66% | 19,82% |
| 1,5-CYCLOOCTADIENE | 645 | 39,00 | 0,2858 | 0,2803 | 0,4247 | 0,8329 | 1,7741 | 9,5999 | 1,12% | 1,45% | | 1,65% | 22,61% |
| 1,5-DICHLOROPENTANE | 668 | 31,90 | 0,3766 | 0,2406 | 0,4552 | 0,8044 | 1,8444 | 51,0101 | 0,41% | 3,20% | 3,35% | 6,55% | 33,67% |
| 1,5-HEXADIENE | 508 | 33,50 | 0,2259 | 0,2633 | 0,8240 | 0,9337 | 0,9852 | 22,3059 | 0,74% | 1,00% | | 5,44% | 17,39% |
| 1,5-NAPHTHALENE DIISOCYANATE | 818 | 27,20 | 0,7301 | | 0,4264 | 0,8217 | 3,0731 | | 1,04% | 1,55% | | | |
| 1,5-PENTANEDIAMINE | 642 | 37,35 | 0,5874 | 0,2647 | 0,6290 | 0,8806 | 2,1215 | 17,4708 | 2,13% | | | 1,46% | 8,75% |
| 1,5-PENTANEDIOL | 673 | 41,50 | 1,2216 | 0,2260 | 1,0260 | 0,8743 | 2,2004 | 26,5534 | 5,91% | | 11,74% | 5,16% | 22,58% |
| 1,9-DECADIENE | 606,8 | 22,67 | 0,5110 | 0,2538 | 0,5610 | 0,8425 | 2,0229 | 40,4972 | 0,63% | 1,36% | | 2,57% | 24,13% |
| 1-AMINO-2-PROPANOL | 614 | 56,70 | 0,7870 | 0,2577 | 0,7389 | 0,8743 | 2,2011 | 8,8653 | 1,81% | 3,84% | | 1,82% | 4,77% |
| 1-BROMOBUTANE | 570,4 | 40,41 | 0,3113 | 0,2687 | 0,3468 | 0,8661 | 2,3101 | 14,5119 | 3,22% | 3,66% | | 2,44% | 20,35% |
| 1-BROMODODECANE | 727,9 | 18,37 | 0,6823 | 0,2453 | 0,5248 | 0,8200 | 2,4952 | 69,4538 | 0,79% | 1,47% | | 2,05% | 27,48% |
| 1-BROMOHEPTANE | 646,1 | 28,97 | 0,4527 | 0,2654 | 0,5745 | 0,8919 | 1,9895 | 22,1412 | 1,53% | | | 1,37% | 23,64% |
| 1-BROMONAPHTHALENE | 824 | 37,00 | 0,3692 | 0,2545 | 0,6728 | 0,8594 | 1,4471 | 38,7730 | 0,79% | 1,15% | | 3,70% | 27,69% |
| 1-BROMOPROPANE | 535,5 | 45,78 | 0,2811 | 0,2646 | 0,3217 | 0,8671 | 2,2963 | 14,5664 | 4,85% | 4,63% | | 4,51% | 17,73% |
| 1-BUTANOL | 563,1 | 44,14 | 0,5883 | 0,2523 | 1,4358 | 1,0000 | 0,9184 | 17,2551 | 2,90% | 4,09% | 4,83% | 4,12% | 23,19% |
| 1-BUTENE | 419,5 | 40,20 | 0,1845 | 0,2743 | 0,2331 | 0,8619 | 2,3697 | 10,0884 | 1,88% | 2,20% | 1,98% | 3,35% | 15,82% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1-CHLORO-1,1-DIFLUOROETHANE | 410,29 | 40,41 | 0,2307 | 0,2665 | 0,3375 | 0,8452 | 1,9263 | 13,1752 | 0,60% | 1,05% | 2,72% | 4,34% | 19,21% |
| 1-CHLORO-2,4-DINITROBENZENE | 813,77 | 34,90 | 0,7319 | 0,2300 | 0,5054 | 0,8219 | 2,7114 | 55,2914 | 0,75% | 1,09% | | 4,87% | 23,63% |
| 1-CHLORONAPHTHALENE | 785 | 34,00 | 0,3827 | 0,2460 | 0,2854 | 0,8389 | 2,7373 | 49,8042 | 3,05% | 3,21% | | 4,55% | 35,96% |
| 1-CHLOROPENTANE | 571,2 | 33,52 | 0,2952 | 0,2561 | 0,3193 | 0,8496 | 2,3069 | 29,4596 | 1,09% | 2,14% | | 4,71% | 24,39% |
| 1-cis-2-trans-3-TRIMETHYLCYCLOPENTANE | 579,82 | 28,98 | 0,2800 | 0,2592 | 0,8716 | 0,9187 | 1,0191 | 31,4925 | 0,73% | 1,37% | | 5,24% | 25,43% |
| 1-cis-2-trans-4-TRIMETHYLCYCLOPENTANE | 579,26 | 28,78 | 0,2775 | 0,2592 | 0,6082 | 0,8677 | 1,3772 | 31,4268 | 1,00% | 1,78% | | 5,33% | 26,24% |
| 1-DECANOL | 688 | 23,08 | 0,6070 | 0,2484 | 2,1934 | 1,0000 | 0,5738 | 50,1049 | 2,15% | | 5,17% | 4,21% | 20,32% |
| 1-DECENE | 616,6 | 22,23 | 0,4805 | 0,2558 | 0,3475 | 0,8369 | 2,7728 | 40,3286 | 0,47% | 2,34% | 1,69% | 2,42% | 24,73% |
| 1-DECYNE | 619,85 | 23,70 | 0,5178 | 0,2580 | 0,3208 | 0,8269 | 2,9659 | 33,6276 | 2,25% | 2,12% | 6,20% | 2,04% | 25,22% |
| 1-DOCOSANOL | 824,4 | 10,35 | 0,8975 | 0,2245 | 0,3960 | 0,6822 | 2,7439 | 219,3129 | 0,71% | | | 3,83% | 30,05% |
| 1-DOCOSENE | 791,6 | 11,21 | 0,9481 | | 0,5482 | 0,8216 | 3,0766 | | 0,84% | 1,57% | | | |
| 1-DODECANOL | 718,7 | 19,54 | 0,6556 | 0,2443 | 1,3647 | 0,7364 | 1,0430 | 68,6593 | 5,77% | | 3,63% | 4,05% | 20,80% |
| 1-DODECENE | 657,1 | 18,88 | 0,5620 | 0,2490 | 0,4328 | 0,8212 | 2,5309 | 59,9893 | 0,56% | 1,84% | 3,44% | 2,62% | 24,77% |
| 1-EICOSANOL | 807,7 | 11,54 | 0,8789 | 0,2312 | 0,2864 | 0,7853 | 3,9920 | 169,8267 | 1,59% | | 1,47% | 1,89% | 28,26% |
| 1-EICOSENE | 771 | 12,20 | 0,8804 | 0,2405 | 0,4845 | 0,8171 | 3,1749 | 117,8119 | 1,46% | 2,27% | 1,25% | 1,40% | 25,67% |
| 1-ETHOXY-2-PROPANOL | 560,4 | 37,48 | 0,7581 | 0,2687 | 0,6718 | 0,8636 | 2,3442 | 4,3018 | 6,27% | | | 2,05% | 23,15% |
| 1-ETHYL-2-ISOPROPYLBENZENE | 666 | 26,70 | 0,4176 | 0,2561 | 0,4541 | 0,8314 | 2,0665 | 38,5250 | 0,26% | 0,52% | 0,29% | 3,31% | 23,17% |
| 1-ETHYLCYCLOHEXENE | 614,9 | 33,05 | 0,2922 | 0,2628 | 0,3746 | 0,8307 | 1,9574 | 25,8927 | 1,35% | 2,52% | | 3,91% | 20,33% |
| 1-ETHYLNAPHTHALENE | 776 | 33,20 | 0,4073 | 0,2565 | 0,4174 | 0,8337 | 2,1744 | 35,0427 | 2,12% | 2,45% | 2,63% | 4,00% | 17,84% |
| 1-ETHYLTETRALIN | 733 | 27,52 | 0,4292 | 0,2508 | 0,6804 | 0,8578 | 1,5617 | 48,7148 | 0,78% | 1,43% | | 3,72% | 24,23% |
| 1-HEPTADECANOL | 779,2 | 13,77 | 0,8123 | 0,2409 | 0,2921 | 0,7921 | 3,8411 | 115,7287 | 2,85% | | 2,94% | 1,32% | 25,22% |
| 1-HEPTADECENE | 736 | 14,10 | 0,7503 | 0,2433 | 0,4408 | 0,8221 | 3,0654 | 95,6628 | 2,48% | 2,12% | 1,59% | 1,48% | 25,09% |
| 1-HEPTANOL | 632,3 | 30,85 | 0,5621 | 0,2642 | 1,7500 | 1,0000 | 0,7107 | 20,7602 | 2,58% | | 7,51% | 1,40% | 23,26% |
| 1-HEPTENE | 537,4 | 29,20 | 0,3432 | 0,2648 | 0,2966 | 0,8476 | 2,5874 | 21,4378 | 1,84% | 2,93% | 2,03% | 3,06% | 21,55% |
| 1-HEPTYNE | 547 | 32,10 | 0,3778 | 0,2683 | 0,3692 | 0,8583 | 2,4216 | 15,7757 | 1,32% | 2,11% | 5,93% | 2,08% | 17,96% |
| 1-HEXACOSENE | 827,3 | 9,64 | 1,0757 | | 0,6109 | 0,8205 | 3,0999 | | 1,18% | 1,59% | | | |
| 1-HEXADECANOL | 768,6 | 14,68 | 0,7788 | 0,2375 | 0,2798 | 0,7927 | 3,8221 | 111,5111 | 3,89% | | 3,29% | 2,44% | 24,03% |
| 1-HEXADECENE | 722 | 14,80 | 0,7242 | 0,2435 | 0,4402 | 0,8200 | 2,9710 | 90,1474 | 1,82% | 1,86% | 1,09% | 1,63% | 25,19% |
| 1-HEXANOL | 611,3 | 34,46 | 0,5586 | 0,2515 | 1,5800 | 1,0000 | 0,7946 | 25,4396 | 2,26% | | 7,50% | 4,79% | 22,04% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1-HEXENE | 504 | 32,10 | 0,2851 | 0,2674 | 1,0614 | 1,0000 | 0,8585 | 17,9573 | 0,66% | 0,63% | 1,51% | 3,55% | 19,88% |
| 1-HEXYNE | 516,2 | 36,20 | 0,3327 | 0,2693 | 0,3018 | 0,8510 | 2,5330 | 12,8435 | 1,38% | 1,39% | 4,58% | 3,07% | 18,75% |
| 1-METHOXY-2-PROPANOL PROPANOATE | 611,7 | 26,02 | 0,5099 | 0,2490 | 0,9179 | 0,8225 | 1,2816 | 42,7416 | 0,78% | 1,32% | | 3,69% | 25,01% |
| 1-METHYL-1-ETHYLCYCLOPENTANE | 582 | 30,20 | 0,3298 | 0,2656 | 0,2638 | 0,8429 | 2,6677 | 22,4107 | 3,09% | | 1,95% | 3,07% | 19,55% |
| 1-METHYL-2-n-PROPYLBENZENE | 662 | 29,40 | 0,4070 | 0,2595 | 0,3302 | 0,8450 | 2,6317 | 31,3306 | 2,53% | 3,10% | 2,72% | 2,57% | 22,97% |
| 1-METHYL-3-(METHYLETHOXY)BENZENE | 670 | 28,40 | 0,4454 | 0,2601 | 0,3034 | 0,8329 | 2,8477 | 30,1343 | 2,30% | 3,80% | | 2,48% | 26,00% |
| 1-METHYL-3-HYDROXY-5-ISOPROPYL BENZENE | 726,8 | 34,08 | 0,5863 | | 0,5872 | 0,7898 | 1,9671 | | 0,64% | 1,00% | | | |
| 1-METHYL-3-HYDROXY-6-ISOPROPYL BENZENE | 722,5 | 34,08 | 0,5848 | | 0,4548 | 0,8443 | 2,6432 | | 0,73% | 1,36% | | | |
| 1-METHYL-3-n-PROPYLBENZENE | 654 | 28,10 | 0,4128 | 0,2599 | 0,3234 | 0,8419 | 2,6839 | 32,9028 | 1,35% | 2,49% | 2,36% | 1,65% | 27,00% |
| 1-METHYL-4-n-PROPYLBENZENE | 656 | 28,10 | 0,4134 | 0,2634 | 0,3301 | 0,8434 | 2,6579 | 29,7203 | 1,56% | 2,36% | 2,61% | 1,47% | 28,07% |
| 1-METHYL-4-VINYLCYCLOHEXENE | 626 | 31,20 | 0,3445 | 0,2620 | 0,5638 | 0,8656 | 1,6558 | 26,6230 | 0,99% | 1,98% | 0,86% | 3,24% | 21,16% |
| 1-METHYLCYCLOPENTENE | 542 | 41,30 | 0,2318 | 0,2728 | 0,9664 | 0,9316 | 0,8350 | 12,6121 | 1,17% | 2,25% | 1,62% | 3,96% | 15,88% |
| 1-METHYLINDAN | 694,1 | 34,37 | 0,3139 | 0,2626 | 0,6757 | 0,8866 | 1,3599 | 27,4956 | 0,62% | 1,35% | | 3,58% | 20,68% |
| 1-METHYLINDENE | 703 | 34,60 | 0,3349 | 0,2556 | 0,3230 | 0,8307 | 2,3083 | 35,1067 | 0,62% | 1,76% | 1,10% | 4,11% | 21,10% |
| 1-METHYLNAPHTHALENE | 772 | 36,00 | 0,3416 | 0,2561 | 0,7256 | 0,8461 | 1,2701 | 36,6109 | 0,53% | 2,31% | 0,11% | 4,46% | 19,94% |
| 1-METHYLTETRALIN | 719,3 | 30,57 | 0,3836 | 0,2539 | 0,7779 | 0,8745 | 1,3097 | 40,9078 | 0,66% | 1,35% | | 3,94% | 22,98% |
| 1-METHYLVINYL ACETATE | 552,2 | 41,81 | 0,4027 | 0,2801 | 0,3460 | 0,8487 | 2,5704 | 2,4533 | 2,48% | 2,89% | | 1,25% | 16,16% |
| 1-n-BUTYLNAPHTHALENE | 792 | 26,80 | 0,4951 | 0,2547 | 0,7175 | 0,8400 | 1,5877 | 44,6226 | 1,45% | 1,48% | 0,79% | 2,87% | 22,73% |
| 1-n-DECYLNAPHTHALENE | 844 | 15,23 | 0,7456 | | 0,5568 | 0,8251 | 2,5578 | | 0,67% | 1,73% | | | |
| 1-n-HEXYL-1,2,3,4-TETRAHYDRONAPHTHALENE | 779 | 18,90 | 0,5888 | 0,2398 | 0,5695 | 0,8153 | 2,0952 | 90,0449 | 0,80% | 1,56% | 1,19% | 3,19% | 36,48% |
| 1-n-HEXYLNAPHTHALENE | 813 | 22,50 | 0,5874 | 0,2531 | 0,5783 | 0,8190 | 2,0764 | 53,5698 | 0,80% | 0,82% | 1,05% | 1,79% | 27,92% |
| 1-NITROBUTANE | 623 | 37,60 | 0,4546 | 0,2472 | 0,3787 | 0,8489 | 2,5663 | 33,0409 | 6,57% | 4,23% | | 3,58% | 24,98% |
| 1-NITROPROPANE | 605 | 43,50 | 0,4128 | 0,2442 | 0,4123 | 0,8638 | 2,3423 | 30,5741 | 4,33% | 3,48% | 9,34% | 4,87% | 23,22% |
| 1-n-NONYLNAPHTHALENE | 835,1 | 16,43 | 0,7216 | 0,2272 | 0,5307 | 0,8277 | 2,6124 | 129,4616 | 0,72% | 1,73% | | 4,66% | 41,19% |
| 1-NONADECANOL | 798,8 | 12,20 | 0,8582 | 0,2349 | 0,4675 | 0,8169 | 3,1798 | 148,8349 | 2,03% | | | 1,37% | 27,16% |
| 1-NONADECENE | 760 | 12,80 | 0,8325 | 0,2417 | 0,4711 | 0,8193 | 3,1270 | 109,5755 | 2,54% | 2,21% | 1,45% | 1,39% | 25,28% |
| 1-NONANOL | 670,9 | 25,27 | 0,5841 | 0,2472 | 2,6200 | 1,0000 | 0,4615 | 45,8731 | 2,47% | | 5,15% | 5,23% | 19,78% |
| 1-NONENE | 593,1 | 24,28 | 0,4367 | 0,2592 | 0,3878 | 0,8424 | 2,4505 | 32,4892 | 0,56% | 2,35% | 3,04% | 2,55% | 23,00% |
| 1-NONYNE | 598,05 | 26,10 | 0,4710 | 0,2620 | 0,3004 | 0,8287 | 2,9299 | 26,0308 | 0,23% | 0,89% | 5,58% | 2,05% | 22,54% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 1-n-PENTYLNAPHTHALENE | 803 | 24,40 | 0,5354 | 0,2516 | 0,6647 | 0,8304 | 1,7659 | 53,0722 | 1,40% | 1,53% | 1,09% | 2,81% | 25,22% |
| 1-OCTACOSENE | 842,2 | 9,01 | 1,1351 | | 0,6742 | 0,8255 | 2,9938 | | 1,46% | | | | |
| 1-OCTADECANOL | 789,3 | 12,95 | 0,8322 | 0,2344 | 0,2885 | 0,7900 | 3,9058 | 138,3976 | 3,11% | | 2,83% | 2,08% | 26,08% |
| 1-OCTADECENE | 748 | 13,40 | 0,7943 | 0,2427 | 0,4564 | 0,8204 | 3,1015 | 102,1290 | 2,22% | 2,13% | 1,52% | 1,40% | 25,32% |
| 1-OCTANOL | 652,3 | 27,83 | 0,5697 | 0,2550 | 2,0999 | 1,0000 | 0,5827 | 33,0536 | 1,53% | 3,76% | 8,20% | 3,14% | 21,13% |
| 1-OCTENE | 566,9 | 26,63 | 0,3921 | 0,2628 | 0,3337 | 0,8474 | 2,5914 | 25,6825 | 2,06% | 2,83% | 1,85% | 2,50% | 21,62% |
| 1-OCTYNE | 574 | 28,80 | 0,4233 | 0,2645 | 0,4090 | 0,8515 | 2,3614 | 20,9630 | 1,14% | 1,93% | 5,58% | 2,09% | 20,23% |
| 1-PENTADECANOL | 757,3 | 15,69 | 0,7507 | 0,2372 | 0,2817 | 0,7954 | 3,7394 | 102,3866 | 3,54% | | 3,96% | 2,89% | 22,31% |
| 1-PENTADECENE | 708 | 15,70 | 0,6815 | 0,2454 | 0,4215 | 0,8213 | 2,9485 | 80,7445 | 1,87% | 1,88% | 1,37% | 1,74% | 24,90% |
| 1-PENTANOL | 588,1 | 38,97 | 0,5748 | 0,2536 | 1,5032 | 1,0000 | 0,8572 | 19,6994 | 1,52% | 4,08% | 4,06% | 4,17% | 22,25% |
| 1-PENTENE | 464,8 | 35,60 | 0,2372 | 0,2705 | 0,7399 | 0,9337 | 1,1261 | 14,0580 | 0,64% | 1,34% | 2,07% | 3,38% | 18,54% |
| 1-PENTENE-4-YNE | 503 | 44,00 | 0,1786 | 0,2668 | 0,1869 | 0,8540 | 2,4863 | 16,4093 | 2,04% | 2,71% | 0,16% | 4,73% | 17,35% |
| 1-PENTYNE | 481,2 | 41,70 | 0,2899 | 0,2889 | 0,2806 | 0,8546 | 2,4773 | 2,6772 | 1,97% | 2,30% | 4,31% | 3,17% | 14,49% |
| 1-PHENYLNAPHTHALENE | 849 | 26,30 | 0,5309 | 0,2448 | 0,4784 | 0,8281 | 2,2984 | 65,1737 | 0,73% | 1,20% | | 3,14% | 26,45% |
| 1-PROPANOL | 536,8 | 51,69 | 0,6209 | 0,2471 | 1,0602 | 0,9168 | 1,3265 | 15,6881 | 2,69% | 2,42% | 5,11% | 5,00% | 24,26% |
| 1-tert-BUTOXY-2-[2-(HYDROXY)PROPOXY]PROPANE | 689,9 | 23,00 | 0,9350 | 0,2592 | 0,5316 | 0,8201 | 3,1078 | 16,8535 | 0,73% | 1,24% | | 1,34% | 29,69% |
| 1-tert-BUTOXY-2-[2-(tert-BUTOXY)PROPOXY]PROPANE | 729,4 | 15,27 | 0,6360 | | 0,4943 | 0,8257 | 2,5191 | | 0,75% | 1,54% | | | |
| 1-TETRACOSENE | 810,4 | 10,37 | 1,0139 | | 0,5798 | 0,8208 | 3,0927 | | 1,12% | 1,56% | | | |
| 1-TETRADECENE | 691 | 16,27 | 0,6503 | 0,2429 | 0,4776 | 0,8137 | 2,5587 | 82,8101 | 0,74% | 1,57% | 0,41% | 2,55% | 26,50% |
| 1-TRIACONTENE | 857 | 8,47 | 1,1817 | | 0,6752 | 0,8220 | 3,0680 | | 1,43% | | | | |
| 1-TRIDECANOL | 732,4 | 18,10 | 0,6881 | 0,2427 | 0,3836 | 0,7296 | 2,5798 | 78,7290 | 4,73% | | 4,27% | 3,33% | 21,25% |
| 1-TRIDECENE | 674,8 | 17,49 | 0,6074 | 0,2460 | 0,4219 | 0,8220 | 2,7213 | 70,6006 | 0,56% | 1,84% | 0,96% | 2,48% | 25,62% |
| 1-UNDECANOL | 703,9 | 21,19 | 0,6236 | 0,2486 | 2,1398 | 0,9126 | 0,6252 | 57,6129 | 6,32% | | 4,76% | 3,36% | 20,70% |
| 1-UNDECENE | 637,8 | 20,44 | 0,5225 | 0,2523 | 0,3734 | 0,8317 | 2,7479 | 49,6045 | 0,43% | 2,25% | 3,53% | 2,53% | 24,08% |
| 2-(2-HEXOXYETHOXY)ETHANOL | 684 | 24,10 | 1,1110 | 0,2669 | 1,8516 | 0,9868 | 1,0778 | 1,1257 | 5,69% | | 5,19% | 2,59% | 24,48% |
| 2-(2-PENTOXYETHOXY)ETHANOL | 705,3 | 25,03 | 0,7047 | 0,2563 | 0,4310 | 0,7107 | 2,3726 | 32,3338 | 0,74% | | | 1,89% | 24,77% |
| 2-(DIFLUOROMETHOXY)-1,1,1-TRIFLUOROETHANE | 444,03 | 34,20 | 0,3887 | 0,2635 | 0,6183 | 0,8520 | 1,5938 | 14,9469 | 0,63% | 1,09% | | 3,17% | 19,34% |
| 2-(N-MORPHOLINO)-2'-HYDROXYDIETHYLETHER | 728,4 | 28,93 | 0,7521 | | 0,4939 | 0,8314 | 2,8763 | | 0,75% | 1,36% | | | |
| 2,2',2"-NITRILOTRIS-ACETONITRILE | 823 | 26,40 | 0,9240 | | 0,5077 | 0,8171 | 3,1759 | | 0,76% | 1,37% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2,2,3,3-TETRAMETHYLBUTANE | 568 | 28,70 | 0,2450 | 0,2739 | 0,2299 | 0,8487 | 2,5469 | 16,1957 | 0,52% | 2,35% | 0,08% | 2,54% | 15,47% |
| 2,2,3,3-TETRAMETHYLHEXANE | 623 | 25,10 | 0,3659 | 0,2693 | 0,3297 | 0,8514 | 2,5268 | 21,3030 | 1,86% | 2,44% | 1,35% | 2,41% | 19,68% |
| 2,2,3,3-TETRAMETHYLPENTANE | 607,5 | 27,41 | 0,3051 | 0,2702 | 0,2743 | 0,8487 | 2,5704 | 19,7560 | 1,22% | 2,26% | 0,57% | 3,07% | 24,37% |
| 2,2,3,4-TETRAMETHYLPENTANE | 592,6 | 26,00 | 0,3138 | 0,2680 | 0,3966 | 0,8397 | 1,9751 | 22,9910 | 1,25% | 2,15% | 4,73% | 3,39% | 24,22% |
| 2,2,3-TRIMETHYLBUTANE | 531,1 | 29,50 | 0,2501 | 0,2704 | 0,2367 | 0,8501 | 2,5469 | 17,7466 | 0,37% | 1,36% | 0,41% | 3,72% | 20,91% |
| 2,2,3-TRIMETHYLPENTANE | 563,5 | 27,30 | 0,2971 | 0,2638 | 0,2786 | 0,8415 | 2,4489 | 24,7301 | 0,51% | 1,30% | 1,80% | 5,18% | 25,53% |
| 2,2,4,4,6,8,8-HEPTAMETHYLNONANE | 692 | 15,70 | 0,5482 | 0,2487 | 0,3779 | 0,8339 | 2,8287 | 71,1996 | 0,66% | 3,20% | 6,41% | 3,59% | 33,30% |
| 2,2,4,4-TETRAMETHYL-1,3-CYCLOBUTANEDIOL | 699,5 | 31,72 | 0,5711 | 0,2487 | 0,2600 | 0,7795 | 3,0779 | 38,4021 | 0,59% | 1,86% | | 3,04% | 25,61% |
| 2,2,4,4-TETRAMETHYLPENTANE | 574,6 | 24,90 | 0,3136 | 0,2692 | 0,3641 | 0,8475 | 2,1477 | 21,7113 | 1,14% | 1,83% | 0,87% | 3,15% | 22,59% |
| 2,2,4-TRIMETHYL-1,3-PENTANEDIOL | 697,9 | 27,04 | 0,5958 | 0,2331 | 0,2712 | 0,6814 | 2,4509 | 62,7583 | 0,53% | | | 6,65% | 29,73% |
| 2,2,4-TRIMETHYLPENTANE | 543,8 | 25,70 | 0,3035 | 0,2671 | 0,2897 | 0,8524 | 2,5116 | 22,7063 | 0,52% | 1,11% | 3,61% | 3,46% | 20,45% |
| 2,2,5,5-TETRAMETHYLHEXANE | 581,4 | 21,90 | 0,3767 | 0,2653 | 0,5899 | 0,8062 | 1,5299 | 29,4315 | 0,20% | 0,78% | 0,32% | 3,18% | 20,95% |
| 2,2,5-TRIMETHYLHEXANE | 569,8 | 23,30 | 0,3446 | 0,2632 | 0,5754 | 0,8077 | 1,4853 | 31,1929 | 0,89% | 1,47% | 2,21% | 3,70% | 24,58% |
| 2,2-DICHLORO-1,1,1-TRIFLUOROETHANE | 456,94 | 36,76 | 0,2825 | 0,2675 | 0,3219 | 0,8360 | 2,1408 | 14,1630 | 0,64% | 1,20% | 4,78% | 3,68% | 18,83% |
| 2,2-DICHLORO-1,1,2-TRIFLUOROETHANE | 462 | 36,10 | 0,2622 | | 0,4509 | 0,8288 | 1,6054 | | 0,79% | 2,21% | 4,58% | | |
| 2,2-DIMETHYL-1-PROPANOL | 552,7 | 40,78 | 0,5950 | | 0,2690 | 0,7600 | 2,9454 | | 0,59% | 1,45% | | | |
| 2,2-DIMETHYL-3-ETHYLPENTANE | 590 | 25,70 | 0,3353 | 0,2690 | 0,8437 | 0,9040 | 1,1440 | 21,9287 | 0,76% | 1,07% | | 2,92% | 20,22% |
| 2,2-DIMETHYLBUTANE | 489 | 31,00 | 0,2341 | 0,2731 | 0,2316 | 0,8523 | 2,5126 | 13,9389 | 1,01% | 1,86% | 1,64% | 3,75% | 18,22% |
| 2,2-DIMETHYLHEPTANE | 576,7 | 23,50 | 0,3911 | 0,2624 | 0,4736 | 0,8407 | 1,9529 | 29,6112 | 2,18% | 2,25% | 3,01% | 2,94% | 25,34% |
| 2,2-DIMETHYLHEXANE | 549,8 | 25,30 | 0,3378 | 0,2637 | 0,3054 | 0,8337 | 2,4200 | 26,7431 | 0,42% | 1,17% | 0,97% | 3,59% | 20,40% |
| 2,2-DIMETHYLOCTANE | 602 | 21,60 | 0,4288 | 0,2574 | 0,3894 | 0,8230 | 2,3031 | 39,2700 | 0,46% | 1,62% | 1,22% | 3,42% | 27,73% |
| 2,2-DIMETHYLPENTANE | 520,5 | 27,70 | 0,2871 | 0,2660 | 0,3043 | 0,8410 | 2,2702 | 22,0237 | 0,67% | 1,18% | 1,95% | 4,13% | 19,89% |
| 2,2'-IMINOBIS-ACETONITRILE | 731 | 35,40 | 0,7192 | | 0,4133 | 0,8205 | 3,0999 | | 0,69% | 1,35% | | | |
| 2,3,3,3-TETRAFLUOROPROPENE | 367,85 | 33,82 | 0,2820 | 0,2645 | 0,6863 | 0,8978 | 1,2821 | 14,3435 | 0,65% | 1,37% | | 3,77% | 20,33% |
| 2,3,3,4-TETRAMETHYLPENTANE | 607,5 | 27,20 | 0,3144 | 0,2700 | 0,3518 | 0,8443 | 2,1810 | 20,3858 | 0,39% | 2,20% | 1,27% | 2,92% | 21,42% |
| 2,3,3-TRIMETHYL-1-BUTENE | 531 | 31,40 | 0,2388 | 0,2771 | 0,1528 | 0,8329 | 2,8470 | 12,0088 | 1,81% | 4,61% | 2,63% | 2,99% | 19,86% |
| 2,3,3-TRIMETHYLPENTANE | 573,5 | 28,20 | 0,2903 | 0,2678 | 0,2382 | 0,8433 | 2,6598 | 21,4209 | 0,74% | 2,08% | 0,12% | 4,09% | 19,17% |
| 2,3,4,5,2',3',4',5'-OCTAHYDRO-BIFURYL-(3,3') | 738 | 37,00 | 0,3715 | | 0,3728 | 0,8463 | 2,3321 | | 1,03% | 2,16% | | | |
| 2,3,4-TRIMETHYLPENTANE | 566,4 | 27,30 | 0,3153 | 0,2650 | 0,2981 | 0,8450 | 2,4506 | 23,9088 | 0,41% | 1,14% | 1,18% | 4,18% | 19,80% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2,3,5-TRIMETHYLTHIOPHENE | 656,8 | 36,30 | 0,3238 | 0,2645 | 0,5870 | 0,8700 | 1,5446 | 22,2110 | 0,59% | 1,43% | | 3,32% | 20,41% |
| 2,3-DICHLOROBUTANE | 599 | 37,40 | 0,2682 | 0,2651 | 0,5764 | 0,8648 | 1,4087 | 22,5460 | 0,85% | 0,53% | | 2,66% | 22,84% |
| 2,3-DICHLOROPROPENE | 578 | 43,80 | 0,1945 | 0,2631 | 1,1576 | 1,0000 | 0,6678 | 22,8714 | 2,62% | | 0,90% | 2,83% | 23,78% |
| 2,3-DIHYDROFURAN | 524 | 55,00 | 0,2255 | 0,2675 | 0,6035 | 0,8853 | 1,2853 | 11,4395 | 0,66% | 1,26% | | 4,73% | 23,22% |
| 2,3-DIMETHYL-1,3-BUTADIENE | 526 | 35,20 | 0,2142 | 0,2612 | 1,1625 | 1,0000 | 0,6766 | 24,5821 | 0,65% | 1,07% | 0,58% | 5,32% | 23,67% |
| 2,3-DIMETHYL-1-BUTENE | 501 | 33,20 | 0,2333 | 0,2727 | 0,5585 | 0,8627 | 1,3585 | 14,3326 | 1,21% | 1,73% | 0,61% | 3,26% | 20,56% |
| 2,3-DIMETHYL-1-HEXENE | 561 | 27,60 | 0,3249 | 0,2668 | 0,2711 | 0,8110 | 2,3753 | 22,1092 | 0,51% | 3,15% | 2,78% | 3,62% | 21,62% |
| 2,3-DIMETHYL-2,3-DIPHENYLBUTANE | 805 | 19,90 | 0,5208 | | 0,3385 | 0,8296 | 2,9116 | | 0,61% | 1,50% | | | |
| 2,3-DIMETHYL-2-BUTENE | 528 | 33,20 | 0,2237 | 0,2590 | 1,2721 | 1,0000 | 0,6248 | 27,5915 | 1,09% | 1,12% | 2,90% | 5,70% | 23,34% |
| 2,3-DIMETHYLBENZOTHIOPHENE | 786 | 34,64 | 0,4205 | 0,2559 | 0,6493 | 0,8394 | 1,5752 | 35,3647 | 0,76% | 1,43% | | 3,45% | 30,11% |
| 2,3-DIMETHYLBUTANE | 500 | 31,50 | 0,2493 | 0,2701 | 0,2391 | 0,8510 | 2,5337 | 16,1281 | 0,60% | 1,48% | 1,36% | 4,11% | 17,39% |
| 2,3-DIMETHYLDECANE | 653,5 | 18,80 | 0,5159 | 0,2506 | 0,6845 | 0,8424 | 1,7097 | 59,0147 | 0,81% | 1,41% | | 2,88% | 24,91% |
| 2,3-DIMETHYLDODECANE | 689,7 | 16,56 | 0,6016 | 0,2464 | 0,5868 | 0,8332 | 2,1358 | 74,8718 | 0,77% | 1,53% | | 2,50% | 26,54% |
| 2,3-DIMETHYLHEPTANE | 588,8 | 23,90 | 0,3914 | 0,2604 | 0,3766 | 0,8409 | 2,3377 | 32,8713 | 2,02% | 2,87% | 2,22% | 2,88% | 21,93% |
| 2,3-DIMETHYLHEXANE | 563,5 | 26,30 | 0,3455 | 0,2617 | 0,2642 | 0,8396 | 2,7253 | 27,5965 | 0,40% | 0,87% | 0,74% | 4,23% | 20,99% |
| 2,3-DIMETHYLNONANE | 633,9 | 20,16 | 0,4703 | 0,2530 | 0,7207 | 0,8577 | 1,5649 | 51,5033 | 0,83% | 1,39% | | 2,95% | 24,05% |
| 2,3-DIMETHYLOCTANE | 613,1 | 21,73 | 0,4245 | 0,2553 | 0,4779 | 0,8386 | 2,0443 | 44,2778 | 0,91% | 2,24% | | 3,11% | 23,15% |
| 2,3-DIMETHYLPENTANE | 537,3 | 29,10 | 0,2964 | 0,2634 | 0,2546 | 0,8457 | 2,6193 | 22,7136 | 0,34% | 1,85% | 1,14% | 5,17% | 24,43% |
| 2,3-DIMETHYLTHIOPHENE | 637 | 40,50 | 0,2709 | 0,2582 | 0,5841 | 0,8643 | 1,4061 | 25,5060 | 0,70% | 1,63% | | 5,68% | 17,93% |
| 2,3-DIMETHYLUNDECANE | 671,4 | 17,61 | 0,5590 | 0,2482 | 0,5947 | 0,8390 | 2,0290 | 67,1396 | 0,78% | 1,52% | | 2,64% | 25,73% |
| 2,3-PENTADIENE | 497 | 38,00 | 0,2184 | 0,2578 | 0,8813 | 0,8705 | 0,8800 | 24,4516 | 1,07% | 0,66% | 1,68% | 5,77% | 14,59% |
| 2,3-XYLENOL | 722,95 | 49,00 | 0,5157 | 0,2930 | 0,4143 | 0,8463 | 2,6093 | -12,4132 | 1,87% | 1,61% | 2,25% | 0,87% | 17,03% |
| 2,4,4-TRIMETHYL-1-PENTENE | 550 | 26,80 | 0,3011 | 0,2656 | 0,2589 | 0,8462 | 2,6117 | 24,2554 | 1,89% | 1,99% | 1,84% | 3,61% | 24,89% |
| 2,4,4-TRIMETHYL-2-PENTENE | 555 | 26,80 | 0,2971 | 0,2632 | 1,2985 | 1,0000 | 0,6902 | 28,1206 | 1,01% | 1,25% | 1,06% | 4,42% | 25,19% |
| 2,4,4-TRIMETHYLHEXANE | 581 | 24,60 | 0,3522 | 0,2659 | 0,4531 | 0,8489 | 1,9377 | 25,5129 | 1,64% | 1,95% | 2,95% | 2,89% | 23,10% |
| 2,4,6-TRIMETHYLPYRIDINE | 653 | 33,30 | 0,3749 | 0,2499 | 0,6387 | 0,8373 | 1,4820 | 36,9048 | 0,39% | 0,72% | | 5,97% | 21,48% |
| 2,4-DIAMINOTOLUENE | 804 | 43,80 | 0,5794 | 0,2466 | 1,2381 | 0,9955 | 1,0733 | 33,6148 | 0,48% | 0,32% | | 3,09% | 26,36% |
| 2,4-DICHLOROBENZOTRIFLUORIDE | 646 | 28,10 | 0,4344 | | 0,5531 | 0,8363 | 1,8307 | | 0,69% | 1,14% | | | |
| 2,4-DICHLOROTOLUENE | 705 | 35,90 | 0,3590 | 0,2547 | 0,7387 | 0,8746 | 1,3232 | 34,2230 | 0,49% | 0,49% | | 4,11% | 26,25% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2,4-DIMETHYL-1,3-DIOXOLANE-2-METHANOL | 621,3 | 35,40 | 0,5507 | | 0,4359 | 0,8241 | 2,5048 | | 0,57% | 1,57% | | | |
| 2,4-DIMETHYL-3-ETHYLPENTANE | 591 | 25,30 | 0,3530 | 0,2659 | 0,4931 | 0,8547 | 1,8418 | 25,4065 | 1,07% | 1,60% | | 2,71% | 21,48% |
| 2,4-DIMETHYLHEXANE | 553,5 | 25,60 | 0,3436 | 0,2657 | 0,2654 | 0,8392 | 2,7070 | 24,1314 | 0,42% | 0,77% | 0,69% | 2,81% | 21,84% |
| 2,4-DIMETHYLOCTANE | 600 | 21,70 | 0,4345 | 0,2636 | 0,7614 | 0,8530 | 1,4076 | 32,3049 | 0,82% | 1,02% | 1,57% | 1,66% | 27,65% |
| 2,4-DIMETHYLPENTANE | 519,8 | 27,40 | 0,3022 | 0,2642 | 0,3311 | 0,8352 | 2,1718 | 23,1212 | 0,52% | 1,18% | 0,80% | 4,68% | 20,25% |
| 2,4-DINITROPHENOL | 766,9 | 38,88 | 0,8160 | 0,2444 | 0,4579 | 0,8186 | 3,1415 | 31,1987 | 0,77% | 1,67% | | 1,96% | 30,83% |
| 2,4-DIPHENYL-4-METHYLPENTENE-1 | 835 | 20,00 | 0,5467 | 0,2417 | 0,3433 | 0,8273 | 2,9580 | 89,2339 | 0,91% | 1,17% | | 3,55% | 27,28% |
| 2,4-TOLUENE DIISOCYANATE | 725 | 30,40 | 0,6582 | 0,2476 | 0,6436 | 0,8722 | 2,2276 | 41,6302 | 2,35% | | | 1,39% | 17,97% |
| 2,4-XYLENOL | 707,65 | 44,00 | 0,5136 | 0,2682 | 0,3681 | 0,8368 | 2,7744 | 9,4468 | 1,69% | 2,33% | 2,72% | 2,56% | 11,87% |
| 2,5-DIHYDROFURAN | 542 | 55,00 | 0,2197 | 0,2607 | 0,9324 | 0,9185 | 0,8473 | 16,0636 | 1,09% | 2,78% | 0,71% | 5,90% | 24,78% |
| 2,5-DIMETHYL-1,5-HEXADIENE | 567 | 27,40 | 0,3238 | 0,2588 | 0,3769 | 0,8173 | 1,9811 | 32,5756 | 0,44% | 1,98% | 0,25% | 4,12% | 21,56% |
| 2,5-DIMETHYL-2,4-HEXADIENE | 597 | 27,40 | 0,3218 | 0,2444 | 1,3351 | 1,0000 | 0,7101 | 49,3856 | 1,57% | 2,74% | 0,96% | 6,19% | 30,46% |
| 2,5-DIMETHYLHEXANE | 550 | 24,90 | 0,3576 | 0,2615 | 0,2726 | 0,8394 | 2,7275 | 28,9342 | 0,60% | 0,99% | 0,71% | 3,61% | 21,00% |
| 2,5-DIMETHYLOCTANE | 603 | 21,70 | 0,4403 | 0,2581 | 0,6507 | 0,8419 | 1,6129 | 38,5295 | 1,93% | 1,86% | 2,11% | 2,94% | 27,24% |
| 2,5-DIMETHYLTHIOPHENE | 629,9 | 44,62 | 0,3085 | | 0,4182 | 0,8822 | 2,0836 | | 0,63% | | | | |
| 2,5-XYLENOL | 707,05 | 49,00 | 0,5638 | 0,2877 | 0,6548 | 0,8906 | 2,0044 | -9,6644 | 1,61% | 1,94% | | 1,02% | 17,02% |
| 2,6,8-TRIMETHYL-4-NONANONE | 658 | 19,70 | 0,6490 | 0,2531 | 0,5878 | 0,8334 | 2,2495 | 42,4552 | 0,82% | 1,73% | | 2,06% | 29,89% |
| 2,6-DIETHYLNAPHTHALENE | 807 | 25,80 | 0,5118 | | 0,5362 | 0,8265 | 2,0377 | | 0,31% | 1,80% | 1,48% | | |
| 2,6-DIMETHYL-4-HEPTANOL | 603 | 25,50 | 0,8022 | 0,2684 | 0,6527 | 0,8524 | 2,4525 | 6,2303 | 1,08% | 2,62% | | 1,86% | 20,66% |
| 2,6-DIMETHYLHEPTANE | 579 | 23,00 | 0,3927 | 0,2582 | 0,5505 | 0,8206 | 1,6828 | 36,2337 | 0,43% | 0,34% | 1,27% | 3,87% | 27,20% |
| 2,6-DIMETHYLNAPHTHALENE | 777 | 31,70 | 0,4177 | 0,2612 | 0,5785 | 0,8492 | 1,7492 | 34,0779 | 0,30% | 0,99% | 0,63% | 1,45% | 24,08% |
| 2,6-DIMETHYLOCTANE | 606 | 21,70 | 0,4386 | 0,2616 | 0,5640 | 0,8339 | 1,8010 | 34,9740 | 0,51% | 1,16% | 1,86% | 1,84% | 28,52% |
| 2,6-DIMETHYLPYRIDINE | 623,75 | 37,50 | 0,3453 | 0,2562 | 0,4439 | 0,8262 | 1,8649 | 27,1481 | 0,71% | 0,47% | 0,66% | 4,64% | 16,31% |
| 2,6-DINITROPHENOL | 770,1 | 39,05 | 0,8220 | | 0,4880 | 0,7959 | 2,8653 | | 0,65% | 1,73% | | | |
| 2,6-NAPHTHALENEDICARBOXYLIC ACID | 904 | 30,50 | 1,1601 | | 0,6868 | 0,8258 | 2,9883 | | 1,53% | 1,50% | | | |
| 2,6-TOLUENE DIISOCYANATE | 749 | 29,00 | 0,4338 | 0,2366 | 1,7063 | 1,0000 | 0,6202 | 70,0151 | 0,75% | 1,09% | | 5,51% | 23,01% |
| 2,6-XYLENOL | 701,05 | 43,00 | 0,4554 | 0,2880 | 0,3753 | 0,8471 | 2,5960 | -7,0139 | 1,91% | 2,25% | 2,05% | 1,01% | 17,66% |
| 2,7-DIMETHYLBENZOTHIOPHENE | 772,4 | 34,64 | 0,4220 | | 0,3520 | 0,8387 | 2,5534 | | 0,61% | 1,64% | | | |
| 2,7-DIMETHYLNAPHTHALENE | 775 | 32,30 | 0,4477 | 0,2674 | 0,5166 | 0,8477 | 2,0001 | 26,1193 | 0,38% | 1,90% | 0,86% | 1,25% | 6,48% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2,7-DIMETHYLOCTANE | 604 | 21,30 | 0,4420 | 0,2559 | 0,4075 | 0,8270 | 2,2920 | 42,0723 | 0,32% | 0,51% | 1,66% | 3,24% | 29,36% |
| 2-ACETOACETOXY ETHYL METHACRYLATE | 724,2 | 22,57 | 0,8156 | 0,2399 | 0,5973 | 0,8280 | 2,5843 | 57,8068 | 0,30% | | | 2,03% | 33,89% |
| 2-AMINO-2-METHYL-1-PROPANOL | 619,8 | 38,62 | 0,6466 | 0,2362 | 0,3919 | 0,7646 | 2,6155 | 37,2967 | 0,61% | 1,66% | | 3,85% | 29,36% |
| 2-AMINOETHOXYETHANOL | 735 | 59,00 | 0,5598 | 0,2927 | 0,4129 | 0,7920 | 2,4385 | -7,9579 | 2,06% | 1,40% | 7,83% | 2,02% | 4,13% |
| 2-BROMOBUTANE | 567 | 46,30 | 0,2684 | 0,2868 | 0,7077 | 0,8647 | 1,1696 | -0,7211 | 0,92% | 1,91% | 0,89% | 3,54% | 6,29% |
| 2-BROMOPROPANE | 532 | 55,10 | 0,2432 | 0,3291 | 0,2626 | 0,8611 | 2,3803 | -19,4389 | 3,21% | 2,99% | 4,46% | 6,53% | 7,91% |
| 2-BUTANOL | 535,9 | 41,88 | 0,5808 | 0,2522 | 2,0395 | 1,0000 | 0,6054 | 18,6985 | 1,01% | 1,60% | | 4,13% | 24,41% |
| 2-BUTOXIME | 608,5 | 42,04 | 0,6071 | 0,2426 | 0,7972 | 0,8177 | 1,6133 | 27,6011 | 1,06% | 1,63% | 2,81% | 4,71% | 23,28% |
| 2-BUTOXYETHANOL | 633,9 | 32,70 | 0,5143 | 0,2535 | 0,2676 | 0,8167 | 3,1856 | 29,1796 | 1,35% | 2,51% | 3,23% | 3,30% | 19,95% |
| 2-BUTYL-1-DECANOL | 707,6 | 17,13 | 1,1142 | | 0,6288 | 0,8202 | 3,1055 | | 1,36% | 1,51% | | | |
| 2-BUTYL-2-ETHYL-1,3-PROPANEDIOL | 732 | 25,97 | 0,6907 | 0,2429 | 0,2134 | 0,7899 | 3,9089 | 53,4329 | 1,46% | | | 3,06% | 27,90% |
| 2-BUTYLBENZOTHIOPHENE | 818,7 | 28,41 | 0,5280 | | 0,3181 | 0,8246 | 3,0131 | | 0,59% | 1,54% | | | |
| 2-BUTYL-NONAN-1-OL | 681,5 | 18,26 | 1,0762 | 0,2508 | 0,6039 | 0,8196 | 3,1202 | 37,0371 | 1,20% | 1,44% | | 1,79% | 28,19% |
| 2-BUTYL-OCTAN-1-OL | 667,3 | 19,41 | 0,9889 | | 0,6329 | 0,8319 | 2,8660 | | 0,79% | | | | |
| 2-CHLORO-1,1,1,2-TETRAFLUOROETHANE | 395,65 | 36,60 | 0,2877 | 0,2697 | 0,2647 | 0,8495 | 2,5580 | 10,6723 | 0,53% | 1,87% | 4,42% | 3,03% | 18,50% |
| 2-CHLORO-1,1,1-TRIFLUOROETHANE | 430 | 38,40 | 0,2465 | 0,2551 | 0,2673 | 0,8586 | 2,4166 | 21,6080 | 0,79% | 2,12% | | 4,82% | 21,32% |
| 2-CHLORO-1,1-DIFLUOROETHYLENE | 400,55 | 44,58 | 0,2116 | 0,2657 | 0,4372 | 0,8729 | 1,6529 | 12,3731 | 2,50% | 2,43% | 0,17% | 4,20% | 20,11% |
| 2-CHLOROETHANOL | 585 | 59,20 | 0,6578 | 0,2393 | 0,6545 | 0,8752 | 2,1891 | 17,8875 | 2,66% | | | 5,58% | 20,75% |
| 2-CHLOROPROPENE | 478 | 47,10 | 0,1515 | 0,2792 | 0,7543 | 0,9399 | 0,9262 | 9,3936 | 0,72% | 1,37% | 1,92% | 1,44% | 16,18% |
| 2-CYCLOHEXENE-1-ONE | 684,2 | 45,35 | 0,3063 | | 0,5749 | 0,8656 | 1,5214 | | 0,73% | 1,57% | | | |
| 2-CYCLOHEXENYL CYCLOHEXANONE | 792,8 | 29,33 | 0,4284 | 0,2586 | 0,5569 | 0,8286 | 1,7850 | 37,4379 | 0,60% | 1,70% | | 3,08% | 22,50% |
| 2-ETHOXYETHYL ACETATE | 607,3 | 31,66 | 0,5522 | 0,2641 | 0,4109 | 0,8401 | 2,7151 | 18,6107 | 2,32% | 2,58% | | 1,27% | 13,25% |
| 2-ETHYL BUTYRIC ACID | 655 | 34,10 | 0,6326 | 0,2548 | 0,5504 | 0,8231 | 2,2910 | 25,5064 | 0,75% | 0,91% | | 1,43% | 30,29% |
| 2-ETHYL HEXANOIC ACID | 674,6 | 27,78 | 0,8013 | 0,2482 | 0,7095 | 0,8158 | 2,1624 | 32,6914 | 1,12% | 2,07% | | 2,04% | 21,27% |
| 2-ETHYL-1-BUTANOL | 591,2 | 35,35 | 0,6330 | 0,2634 | 0,4048 | 0,7165 | 2,3092 | 13,8655 | 0,67% | | | 1,90% | 22,85% |
| 2-ETHYL-1-BUTENE | 511 | 33,00 | 0,2523 | 0,2677 | 0,6431 | 0,8544 | 1,2310 | 18,9035 | 0,81% | 1,77% | 1,11% | 3,72% | 19,61% |
| 2-ETHYL-1-HEXANOL | 640,4 | 27,56 | 0,5498 | 0,2548 | 0,2174 | 0,7328 | 2,8341 | 33,6798 | 0,94% | | | 3,24% | 24,05% |
| 2-ETHYL-1-HEXENE | 569 | 26,70 | 0,3577 | 0,2603 | 1,0253 | 1,0000 | 1,0027 | 30,1055 | 0,47% | 0,50% | | 3,39% | 23,73% |
| 2-ETHYL-1-PENTENE | 543 | 29,50 | 0,3073 | 0,2644 | 0,4017 | 0,8781 | 2,1526 | 23,0709 | 2,07% | 4,77% | 1,33% | 2,75% | 22,38% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2-ETHYL-2-HEXENAL | 636 | 26,40 | 0,4535 | 0,2300 | 0,2925 | 0,8297 | 2,9095 | 70,6258 | 1,06% | 2,82% | 1,99% | 5,87% | 29,51% |
| 2-ETHYLBENZOTHIOPHENE | 774 | 35,26 | 0,4283 | 0,2626 | 0,5741 | 0,8339 | 1,7503 | 25,3868 | 0,77% | 1,54% | 0,46% | 2,74% | 25,64% |
| 2-ETHYLHEXANAL | 619,2 | 26,79 | 0,4539 | 0,2596 | 0,7435 | 0,8552 | 1,4835 | 32,1387 | 0,80% | 1,26% | | 1,69% | 25,97% |
| 2-ETHYLHEXYL ACRYLATE | 655 | 20,70 | 0,6730 | 0,2527 | 0,6729 | 0,8763 | 2,1753 | 42,0175 | 0,60% | | | 1,64% | 25,74% |
| 2-ETHYLHEXYL BENZOATE | 755,6 | 18,68 | 0,6858 | 0,2451 | 0,6441 | 0,8356 | 2,1659 | 70,9550 | 0,78% | 1,65% | | 1,94% | 27,44% |
| 2-ETHYL-m-XYLENE | 671 | 30,20 | 0,4066 | 0,2598 | 0,3104 | 0,8401 | 2,7148 | 30,7693 | 0,71% | 0,87% | 2,01% | 2,56% | 21,37% |
| 2-ETHYLNAPHTHALENE | 771 | 31,70 | 0,4213 | 0,2520 | 0,3527 | 0,8475 | 2,5890 | 41,3517 | 2,05% | 2,20% | 2,82% | 4,30% | 21,68% |
| 2-ETHYL-p-XYLENE | 663 | 28,80 | 0,4114 | 0,2554 | 0,4257 | 0,8242 | 2,1111 | 37,2489 | 0,30% | 3,12% | 1,36% | 3,30% | 24,64% |
| 2-ETHYL-TETRAHYDROTHIOPHENE | 657,8 | 38,10 | 0,2515 | 0,2643 | 1,3497 | 1,0000 | 0,6145 | 24,4561 | 0,63% | 1,96% | | 4,61% | 19,80% |
| 2-ETHYLTHIOPHENE | 626,6 | 44,09 | 0,2931 | | 0,5441 | 0,8691 | 1,5674 | | 0,57% | 1,19% | | | |
| 2-FORMYL BENZOIC ACID | 772 | 38,30 | 0,8188 | 0,2222 | 1,0020 | 0,9071 | 1,6917 | 57,1062 | 0,33% | 0,18% | | 3,61% | 34,82% |
| 2-HEPTANOL | 608,3 | 30,00 | 0,5677 | 0,2556 | 3,8841 | 0,9969 | 0,2963 | 27,5254 | 0,39% | | | 4,31% | 19,56% |
| 2-HEPTANONE | 611,4 | 29,40 | 0,4190 | 0,2550 | 0,3172 | 0,8391 | 2,7330 | 33,8367 | 1,04% | 1,77% | 1,20% | 2,81% | 25,00% |
| 2-HEXANOL | 585,3 | 33,11 | 0,5530 | 0,2554 | 2,5568 | 1,0000 | 0,4560 | 24,1433 | 3,02% | 3,96% | | 4,23% | 20,98% |
| 2-HEXANONE | 587,61 | 32,87 | 0,3846 | 0,2544 | 0,3796 | 0,8317 | 2,2389 | 30,2045 | 0,91% | 2,04% | 0,59% | 3,93% | 23,08% |
| 2-HEXYNE | 549 | 35,30 | 0,2214 | 0,2628 | 0,4669 | 0,7636 | 1,3159 | 26,0084 | 0,29% | 0,74% | | 3,76% | 22,36% |
| 2-HYDROXYPROPYL METHACRYLATE | 663 | 31,40 | 0,7544 | 0,2541 | 0,8398 | 0,8426 | 1,8226 | 24,7756 | 1,46% | 0,87% | 3,04% | 1,66% | 25,65% |
| 2-MERCAPTOBENZOTHIAZOLE | 749 | 40,00 | 0,3321 | | 0,2409 | 0,8364 | 2,7815 | | 0,50% | 1,96% | | | |
| 2-METHOXY PROPANOL-1 | 588,4 | 39,40 | 0,4727 | 0,2453 | 0,4800 | 0,8534 | 2,2431 | 30,5686 | 0,72% | 1,64% | | 3,63% | 25,68% |
| 2-METHOXYETHANOL | 597,6 | 52,85 | 0,4543 | 0,2512 | 0,4183 | 0,8539 | 2,4536 | 18,4270 | 0,84% | 2,05% | | 4,74% | 12,15% |
| 2-METHYL BENZOTHIOPHENE | 768,7 | 35,00 | 0,3302 | 0,2465 | 0,2561 | 0,8399 | 2,7152 | 49,3481 | 1,32% | 2,80% | 1,73% | 4,90% | 24,30% |
| 2-METHYL OCTANAL | 638,3 | 25,00 | 0,5483 | | 0,5314 | 0,8175 | 2,1220 | | 0,62% | 1,39% | | | |
| 2-METHYL THIAINDAN | 788,6 | 37,09 | 0,3023 | 0,2571 | 0,6309 | 0,8749 | 1,4038 | 36,2396 | 0,59% | 1,17% | | 4,32% | 21,54% |
| 2-METHYL-1,3-PROPANEDIOL | 697 | 53,50 | 0,7144 | 0,2663 | 0,9441 | 0,8634 | 1,5838 | 8,6451 | 1,39% | 0,98% | 2,42% | 2,79% | 20,69% |
| 2-METHYL-1-BUTANOL | 575,4 | 39,40 | 0,5877 | 0,2547 | 1,8378 | 0,9998 | 0,6860 | 17,4482 | 1,46% | 1,46% | | 4,91% | 17,72% |
| 2-METHYL-1-BUTENE | 465 | 34,47 | 0,2341 | 0,2617 | 0,7217 | 0,8765 | 1,0912 | 21,1707 | 0,23% | 0,98% | 0,30% | 5,25% | 20,79% |
| 2-METHYL-1-BUTENE-3-YNE | 492 | 43,80 | 0,1370 | 0,2752 | 0,2117 | 0,8543 | 2,1636 | 11,7979 | 0,67% | 0,77% | 0,01% | 3,69% | 20,77% |
| 2-METHYL-1-HEPTANOL | 608,5 | 28,57 | 0,7623 | 0,2708 | 0,5114 | 0,8248 | 2,7835 | 3,6262 | 0,77% | 1,26% | | 1,48% | 22,22% |
| 2-METHYL-1-HEPTENE | 567 | 26,00 | 0,3551 | 0,2584 | 0,5187 | 0,8548 | 1,7655 | 33,2549 | 0,56% | 1,56% | 2,63% | 3,46% | 26,08% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2-METHYL-1-HEXANOL | 595 | 30,30 | 0,7733 | 0,2561 | 0,5921 | 0,8190 | 2,4656 | 18,1690 | 0,76% | 1,04% | 10,14% | 1,72% | 21,77% |
| 2-METHYL-1-HEXENE | 538 | 28,70 | 0,3094 | 0,2612 | 0,3011 | 0,8245 | 2,2646 | 27,1290 | 0,21% | 1,76% | 0,19% | 4,03% | 23,72% |
| 2-METHYL-1-NONENE | 616 | 21,90 | 0,4527 | 0,2533 | 0,5584 | 0,8300 | 1,8437 | 46,2270 | 0,82% | 1,25% | 0,18% | 3,04% | 32,61% |
| 2-METHYL-1-OCTENE | 593 | 23,80 | 0,4051 | 0,2528 | 0,4771 | 0,8394 | 1,9835 | 42,2242 | 0,35% | 1,89% | 0,03% | 4,32% | 27,62% |
| 2-METHYL-1-PENTANOL | 604,4 | 34,50 | 0,5100 | 0,2544 | 0,1263 | 0,7624 | 3,4403 | 25,0648 | 0,35% | | | 5,01% | 21,17% |
| 2-METHYL-1-PENTENE | 505 | 31,90 | 0,2611 | 0,2641 | 0,3388 | 0,8269 | 1,9486 | 21,6635 | 0,46% | 0,87% | 0,15% | 4,52% | 21,60% |
| 2-METHYL-1-PROPANOL | 547,8 | 42,95 | 0,5857 | 0,2492 | 1,8067 | 1,0000 | 0,6968 | 19,0437 | 2,39% | 2,31% | 8,09% | 5,77% | 22,06% |
| 2-METHYL-1-TRIDECANOL | 707,7 | 17,13 | 1,1154 | | 0,6349 | 0,8211 | 3,0872 | | 1,55% | 1,53% | | | |
| 2-METHYL-1-UNDECANOL | 665,9 | 19,56 | 1,0345 | | 0,5871 | 0,8204 | 3,1019 | | 1,14% | 1,41% | | | |
| 2-METHYL-2-AMINOBUTANE | 526 | 36,60 | 0,3202 | 0,2819 | 0,6882 | 0,8748 | 1,3328 | 5,7344 | 0,72% | 1,24% | | 1,27% | 6,97% |
| 2-METHYL-2-BUTANOL | 543,7 | 37,10 | 0,4820 | 0,2592 | 2,7232 | 0,8476 | 0,4352 | 18,5767 | 2,37% | 2,05% | 6,07% | 4,10% | 19,62% |
| 2-METHYL-2-BUTENE | 470 | 34,20 | 0,2870 | 0,2538 | 0,3107 | 0,8582 | 2,3481 | 24,5650 | 1,45% | 1,79% | 1,95% | 6,46% | 22,02% |
| 2-METHYL-2-PENTENAL | 605 | 32,60 | 0,3494 | 0,2395 | 0,2329 | 0,8320 | 2,8650 | 47,7572 | 0,43% | 2,31% | 1,08% | 5,97% | 31,43% |
| 2-METHYL-2-PENTENE | 514 | 31,60 | 0,2445 | 0,2608 | 1,2005 | 1,0000 | 0,6927 | 26,5056 | 1,02% | 1,18% | 2,12% | 4,97% | 16,89% |
| 2-METHYL-2-PROPANOL | 506,2 | 39,72 | 0,6152 | 0,2557 | 2,4686 | 1,0000 | 0,5035 | 16,6563 | 0,96% | 3,42% | 4,02% | 3,00% | 22,38% |
| 2-METHYL-3-ETHYLPENTANE | 567,1 | 27,00 | 0,3297 | 0,2603 | 0,6959 | 0,8522 | 1,2996 | 28,4192 | 1,40% | 1,43% | 1,51% | 5,59% | 25,27% |
| 2-METHYLBENZOFURAN | 697 | 36,40 | 0,3752 | 0,2541 | 0,3342 | 0,8506 | 2,5404 | 32,9728 | 1,30% | 2,11% | | 3,63% | 22,29% |
| 2-METHYLBUTYRALDEHYDE | 543,2 | 38,29 | 0,3779 | 0,2634 | 0,2692 | 0,8362 | 2,7865 | 16,9905 | 1,73% | 4,34% | 0,94% | 3,03% | 20,96% |
| 2-METHYLBUTYRIC ACID | 643 | 38,90 | 0,5894 | 0,2524 | 0,6996 | 0,8439 | 1,8305 | 24,4843 | 0,82% | 0,92% | | 2,06% | 24,96% |
| 2-METHYLDECANE | 631,8 | 19,82 | 0,5230 | 0,2530 | 0,6991 | 0,8426 | 1,6919 | 49,5848 | 0,45% | 0,89% | | 2,79% | 24,46% |
| 2-METHYL-DODECAN-1-OL | 682,5 | 18,26 | 1,0722 | 0,2500 | 0,5985 | 0,8190 | 3,1339 | 38,7872 | 1,07% | 1,44% | | 1,75% | 28,49% |
| 2-METHYLDODECANE | 668 | 17,17 | 0,6188 | 0,2474 | 0,4800 | 0,8364 | 2,5880 | 66,4390 | 0,69% | 1,55% | | 2,25% | 26,48% |
| 2-METHYLHEPTANAL | 605,7 | 26,82 | 0,4869 | 0,2567 | 0,7938 | 0,7871 | 1,3818 | 32,0548 | 0,76% | 1,21% | | 3,24% | 23,21% |
| 2-METHYLHEPTANE | 559,7 | 25,00 | 0,3795 | 0,2585 | 0,4217 | 0,8348 | 2,0782 | 32,0569 | 0,60% | 0,82% | 2,23% | 4,03% | 20,58% |
| 2-METHYLHEXANAL | 592 | 28,50 | 0,4609 | 0,2539 | 0,3591 | 0,8175 | 2,5061 | 33,1767 | 0,47% | 1,84% | 0,94% | 3,25% | 23,58% |
| 2-METHYLHEXANE | 530,4 | 27,40 | 0,3280 | 0,2626 | 0,3388 | 0,8380 | 2,2560 | 25,0218 | 0,70% | 2,19% | 1,85% | 3,99% | 21,49% |
| 2-METHYLHEXANOIC ACID | 666 | 31,10 | 0,6957 | | 0,6784 | 0,8313 | 2,0733 | | 0,77% | 1,98% | | | |
| 2-METHYLINDENE | 711 | 34,60 | 0,3508 | 0,2538 | 0,3430 | 0,8267 | 2,2516 | 37,0059 | 0,41% | 0,88% | 0,97% | 4,18% | 22,13% |
| 2-METHYLNAPHTHALENE | 761 | 35,00 | 0,3781 | 0,2551 | 0,3434 | 0,8531 | 2,5005 | 35,9448 | 4,71% | 1,11% | 0,72% | 3,77% | 21,86% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 2-METHYLNONANE | 610 | 21,20 | 0,4723 | 0,2547 | 0,4177 | 0,8245 | 2,3360 | 43,7662 | 1,12% | 2,05% | 1,40% | 2,78% | 29,28% |
| 2-METHYLOCTANE | 582,87 | 23,10 | 0,4602 | 0,2587 | 0,5285 | 0,8413 | 1,9820 | 33,0678 | 0,66% | 1,40% | 3,47% | 2,66% | 23,15% |
| 2-METHYLOCTANOIC ACID | 694 | 25,40 | 0,7913 | 0,2514 | 0,5420 | 0,8249 | 2,7301 | 34,2838 | 0,76% | 1,69% | | 1,47% | 26,39% |
| 2-METHYLPENTANE | 497,7 | 30,40 | 0,2791 | 0,2685 | 0,3279 | 0,8404 | 2,1294 | 17,7302 | 0,65% | 1,86% | 1,42% | 3,46% | 18,48% |
| 2-METHYLPROPANAL | 507 | 41,00 | 0,3622 | 0,2570 | 0,2988 | 0,8395 | 2,6076 | 19,6035 | 0,73% | 1,66% | | 3,60% | 22,86% |
| 2-METHYLPYRIDINE | 621 | 46,00 | 0,2990 | 0,2676 | 0,4666 | 0,8273 | 1,6544 | 16,1333 | 1,50% | 1,60% | 0,83% | 3,19% | 6,87% |
| 2-METHYLTETRAHYDROFURAN | 537 | 37,58 | 0,2816 | 0,2481 | 0,6992 | 0,9002 | 1,2610 | 30,2594 | 0,73% | 1,56% | | 7,28% | 37,00% |
| 2-METHYLTHIACYCLOPENTANE | 628,4 | 41,83 | 0,2489 | 0,2622 | 1,0635 | 1,0000 | 0,7993 | 23,0267 | 0,74% | 1,85% | | 4,59% | 19,92% |
| 2-METHYLTHIOPHENE | 609 | 49,10 | 0,2389 | 0,2780 | 0,3198 | 0,8336 | 1,9603 | 8,6871 | 1,32% | 2,04% | 1,25% | 1,97% | 21,84% |
| 2-METHYLTRIDECANE | 684,1 | 16,04 | 0,6649 | 0,2445 | 0,4841 | 0,8367 | 2,7057 | 76,8449 | 0,60% | 1,59% | | 2,08% | 27,47% |
| 2-METHYLUNDECANE | 650,7 | 18,42 | 0,5718 | 0,2502 | 0,5370 | 0,8322 | 2,2209 | 57,5253 | 0,74% | 1,48% | | 2,46% | 25,38% |
| 2-NITROPROPANE | 594 | 44,50 | 0,3836 | 0,2525 | 0,3695 | 0,8598 | 2,3994 | 24,4996 | 5,38% | 4,89% | 7,87% | 3,82% | 19,95% |
| 2-NONANOL | 649,5 | 25,41 | 0,6092 | 0,2613 | 0,5528 | 0,7506 | 1,9950 | 27,2788 | 1,00% | | | 1,46% | 18,06% |
| 2-NONANONE | 652,5 | 24,10 | 0,4979 | 0,2491 | 0,5328 | 0,8109 | 1,9601 | 49,5785 | 1,19% | 1,80% | 0,66% | 3,45% | 25,14% |
| 2-NORBORNENE | 583 | 39,30 | 0,1590 | | 0,2534 | 0,8445 | 1,9944 | | 0,66% | 2,59% | 0,08% | | |
| 2-n-PROPYLTHIOPHENE | 649,2 | 38,97 | 0,3407 | | 0,5666 | 0,8718 | 1,6453 | | 0,73% | 1,16% | | | |
| 2-OCTANOL | 629,8 | 27,49 | 0,5881 | 0,2523 | 0,3144 | 0,7063 | 2,4233 | 32,4086 | 0,27% | | | 4,66% | 17,68% |
| 2-OCTANONE | 632,7 | 26,40 | 0,4549 | 0,2528 | 0,4779 | 0,8149 | 2,0245 | 41,3742 | 0,68% | 1,49% | 0,31% | 2,93% | 25,32% |
| 2-OXAZOLIDONE | 930,5 | 54,88 | 0,3944 | | 0,4714 | 0,8422 | 1,9934 | | 0,75% | 2,41% | | | |
| 2-PENTANETHIOL | 584,3 | 35,36 | 0,2685 | 0,2709 | 1,1450 | 1,0000 | 0,7612 | 17,3940 | 0,61% | 1,05% | | 2,79% | 14,43% |
| 2-PENTANOL | 561 | 37,00 | 0,5550 | 0,2526 | 2,1821 | 0,2948 | 0,8134 | 22,7135 | 0,63% | | | 5,82% | 21,93% |
| 2-PENTANONE | 561,08 | 36,94 | 0,3433 | 0,2546 | 0,3621 | 0,8304 | 2,1650 | 26,4859 | 0,19% | 3,67% | 2,03% | 4,22% | 31,05% |
| 2-PENTOXYETHANOL | 641,2 | 30,36 | 0,6228 | 0,2606 | 0,3370 | 0,8173 | 3,1720 | 20,2119 | 0,60% | 2,90% | 4,80% | 1,46% | 23,39% |
| 2-PENTYNE | 519 | 40,30 | 0,1752 | 0,2631 | 1,1208 | 1,0000 | 0,6558 | 22,1577 | 1,07% | 4,09% | 0,53% | 4,18% | 21,29% |
| 2-PHENYL-2-PROPANOL | 660 | 34,90 | 0,6924 | 0,2641 | 0,7009 | 0,8798 | 2,1316 | 11,6537 | 2,17% | 2,79% | | 1,30% | 16,47% |
| 2-PHENYLBUTENE-1 | 666 | 30,10 | 0,3536 | 0,2562 | 1,1994 | 1,0000 | 0,8293 | 36,9174 | 0,54% | 0,67% | | 4,04% | 26,94% |
| 2-PHENYLETHANOL | 684 | 39,20 | 0,7429 | 0,2509 | 0,7628 | 0,8856 | 2,0617 | 20,2176 | 5,61% | 6,34% | | 2,80% | 19,74% |
| 2-PROPYLBENZOTHIOPHENE | 807,5 | 31,56 | 0,4782 | | 0,3343 | 0,8263 | 2,7559 | | 0,62% | 1,38% | | | |
| 2-PYRROLIDONE | 802 | 61,70 | 0,4324 | 0,2478 | 0,3796 | 0,8239 | 2,3600 | 26,6962 | 1,60% | 3,93% | 13,12% | 3,33% | 26,34% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 3-(METHYLMERCAPTO)PROPANAL | 650 | 40,20 | 0,4168 | 0,2418 | 0,7134 | 0,8546 | 1,4597 | 37,0887 | 0,61% | 1,37% | 3,12% | 5,55% | 30,90% |
| 3-(N,N-DIMETHYLAMINO) PROPYLAMINE | 593,3 | 35,86 | 0,4544 | 0,2679 | 0,5120 | 0,8596 | 2,0949 | 12,8708 | 0,60% | 1,30% | | 1,67% | 20,78% |
| 3,3,3-TRIFLUOROPROPENE | 378,59 | 36,09 | 0,2653 | | 0,5350 | 0,9264 | 1,6452 | | 1,40% | | | | |
| 3,3,5-TRIMETHYLHEPTANE | 609,5 | 23,20 | 0,3847 | 0,2643 | 0,3784 | 0,8263 | 2,2065 | 29,8969 | 1,79% | 1,84% | 2,17% | 2,80% | 21,01% |
| 3,3-DIETHYLPENTANE | 610,05 | 26,75 | 0,3381 | 0,2644 | 0,3005 | 0,8494 | 2,5596 | 25,4373 | 1,37% | 2,45% | 2,41% | 3,75% | 28,25% |
| 3,3-DIMETHYL-1-BUTENE | 480 | 32,90 | 0,2285 | 0,2814 | 0,2198 | 0,8510 | 2,5334 | 6,5981 | 2,77% | 2,94% | 5,44% | 2,51% | 19,44% |
| 3,3-DIMETHYL-1-BUTYNE | 488,5 | 36,75 | 0,1615 | 0,2889 | 0,3519 | 0,8513 | 1,6521 | 1,5820 | 0,62% | 1,52% | | 2,92% | 14,99% |
| 3,3-DIMETHYL-2-BUTANONE | 564 | 33,20 | 0,3273 | 0,2604 | 0,2814 | 0,8460 | 2,6147 | 24,3730 | 0,99% | 1,50% | | 3,75% | 21,32% |
| 3,3-DIMETHYLHEXANE | 562 | 26,50 | 0,3202 | 0,2581 | 0,3153 | 0,8394 | 2,3403 | 30,1689 | 0,60% | 1,16% | 0,47% | 6,36% | 25,87% |
| 3,3-DIMETHYLPENTANE | 536,4 | 29,50 | 0,2679 | 0,2744 | 0,2865 | 0,8510 | 2,3527 | 14,8760 | 0,47% | 1,29% | 0,78% | 1,84% | 18,13% |
| 3,4-DICHLORO-1-BUTENE | 589 | 38,50 | 0,2959 | 0,2589 | 0,3315 | 0,7700 | 1,8522 | 25,0839 | 1,51% | | | 4,70% | 20,88% |
| 3,4-DICHLOROANILINE | 800 | 41,10 | 0,4678 | 0,2461 | 0,3170 | 0,8321 | 2,8624 | 39,2208 | 0,74% | 1,54% | | 3,71% | 22,31% |
| 3,4-DICHLOROPHENYL ISOCYANATE | 730,3 | 34,09 | 0,5050 | 0,2460 | 0,7934 | 0,7734 | 1,4020 | 42,4559 | 0,67% | 1,50% | | 4,31% | 25,00% |
| 3,4-DIMETHYLHEXANE | 568,8 | 26,90 | 0,3381 | 0,2626 | 0,2642 | 0,8408 | 2,7034 | 26,5213 | 0,33% | 1,16% | 0,67% | 4,16% | 20,07% |
| 3,4-DIMETHYLTHIOPHENE | 642,8 | 41,89 | 0,2786 | 0,2660 | 0,6410 | 0,8729 | 1,3243 | 19,0100 | 0,59% | 1,45% | | 3,74% | 19,14% |
| 3,4-XYLENOL | 729,95 | 50,00 | 0,5763 | 0,2826 | 0,4213 | 0,8393 | 2,7297 | -6,0129 | 2,20% | 1,90% | 3,02% | 1,41% | 17,32% |
| 3,5-DIISOPROPYL TOLUENE | 681,4 | 22,39 | 0,4887 | 0,2563 | 0,6101 | 0,8428 | 1,8300 | 42,4158 | 0,77% | 1,39% | | 2,70% | 24,38% |
| 3,5-DIMETHYLBENZOFURAN | 713,7 | 32,16 | 0,4222 | 0,2509 | 0,3738 | 0,8513 | 2,5285 | 40,2684 | 0,59% | | | 3,50% | 24,14% |
| 3,5-DIMETHYLBENZOTHIOPHENE | 784,8 | 34,64 | 0,4247 | 0,2573 | 0,5166 | 0,8831 | 2,0918 | 32,4743 | 1,97% | | | 2,61% | 22,77% |
| 3,5-XYLENOL | 715,65 | 36,00 | 0,4852 | 0,2375 | 1,6053 | 1,0000 | 0,7108 | 47,6203 | 1,77% | 2,30% | 1,64% | 6,32% | 4,86% |
| 3-AMINO-1-PROPANOL | 649 | 55,00 | 0,8273 | 0,2499 | 0,5068 | 0,8181 | 2,9343 | 15,4070 | 0,72% | 0,89% | | 1,29% | 27,19% |
| 3-CHLORO-o-XYLENE | 685,1 | 33,88 | 0,3424 | | 0,4301 | 0,8301 | 1,9232 | | 0,57% | 1,96% | | | |
| 3-CHLOROPROPENE | 514,15 | 47,10 | 0,1478 | 0,2604 | 1,0410 | 0,9802 | 0,6648 | 20,6251 | 1,09% | | 0,58% | 5,90% | 20,48% |
| 3-CHLOROPROPYLTRIMETHOXYSILANE | 647,3 | 21,34 | 0,5349 | 0,2415 | 0,7358 | 0,7786 | 1,5426 | 66,9437 | 3,97% | | 1,53% | 4,10% | 26,63% |
| 3-ETHYL HEPTANAL | 623,8 | 23,64 | 0,5671 | | 0,5808 | 0,8731 | 2,2162 | | 0,73% | | | | |
| 3-ETHYL-1-HEPTANOL | 636,7 | 25,46 | 0,8657 | 0,2582 | 1,3052 | 0,9646 | 1,3304 | 20,0182 | 2,22% | 2,46% | 6,22% | 1,54% | 25,34% |
| 3-ETHYL-1-HEXENE | 553,9 | 26,04 | 0,3600 | 0,2602 | 0,2466 | 0,8334 | 2,8374 | 29,4091 | 0,65% | 3,72% | 2,79% | 3,81% | 23,65% |
| 3-ETHYL-1-PENTENE | 530 | 30,30 | 0,3019 | 0,2736 | 0,2250 | 0,8302 | 2,6772 | 13,4418 | 0,62% | 3,89% | 1,69% | 2,50% | 18,43% |
| 3-ETHYL-2,5-DIMETHYLTHIOPHENE | 669 | 32,60 | 0,3794 | | 0,5242 | 0,8488 | 1,8058 | | 0,77% | 2,53% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 3-ETHYLBENZOTHIOPHENE | 776,5 | 35,26 | 0,4292 | 0,2607 | 0,5497 | 0,8581 | 1,8949 | 27,4712 | 0,75% | 1,41% | | 2,56% | 22,19% |
| 3-ETHYLDODECANE | 691,4 | 16,22 | 0,5995 | | 0,5051 | 0,8284 | 2,3905 | | 0,73% | 1,50% | | | |
| 3-ETHYLHEPTANE | 590 | 23,90 | 0,4080 | 0,2581 | 0,5238 | 0,8488 | 1,8839 | 34,4107 | 0,97% | 1,61% | | 3,54% | 23,06% |
| 3-ETHYLHEXANE | 565,5 | 26,10 | 0,3605 | 0,2575 | 0,2771 | 0,8381 | 2,7020 | 31,2263 | 0,43% | 1,05% | 1,17% | 5,10% | 25,11% |
| 3-ETHYL-o-XYLENE | 680 | 28,80 | 0,3621 | 0,2517 | 0,8824 | 0,8642 | 1,1136 | 46,3548 | 0,38% | 0,61% | 0,12% | 4,24% | 19,93% |
| 3-ETHYLPENTANE | 540,6 | 28,90 | 0,3091 | 0,2667 | 0,3337 | 0,8413 | 2,2268 | 21,4862 | 0,34% | 1,95% | 0,55% | 2,94% | 19,46% |
| 3-HEPTANOL | 605,4 | 30,73 | 0,5511 | 0,2624 | 0,4706 | 0,7792 | 2,1928 | 19,3633 | 2,83% | | | 1,79% | 21,34% |
| 3-HEPTANONE | 606,6 | 29,20 | 0,4076 | 0,2505 | 0,5360 | 0,8150 | 1,7538 | 38,3605 | 0,78% | 1,48% | 0,29% | 4,60% | 24,11% |
| 3-HEXANONE | 582,82 | 33,20 | 0,3801 | 0,2556 | 0,4023 | 0,8297 | 2,1211 | 28,5921 | 1,94% | 1,90% | 0,99% | 4,03% | 21,15% |
| 3-HEXYNE | 544 | 35,30 | 0,2183 | 0,2606 | 0,8168 | 0,6491 | 0,8351 | 26,8204 | 1,34% | | | 5,95% | 20,93% |
| 3-HYDROXY-2-METHYL PROPIONALDEHYDE | 615 | 45,90 | 0,7928 | | 1,0682 | 0,8781 | 1,5140 | | 2,33% | 1,66% | 3,46% | | |
| 3-HYDROXYBUTYROLACTONE | 830,6 | 53,97 | 0,6127 | 0,2324 | 0,4037 | 0,8307 | 2,8895 | 39,1294 | 0,51% | | | 3,81% | 30,44% |
| 3-MERCAPTOPROPIONIC ACID | 729 | 50,20 | 0,5885 | 0,2639 | 0,9094 | 0,8369 | 1,4174 | 17,2791 | 2,76% | | 0,52% | 3,19% | 37,08% |
| 3-METHOXYISOPROPYLAMINE | 548 | 40,90 | 0,4227 | 0,2772 | 0,2749 | 0,8300 | 2,9037 | 6,2989 | 0,49% | 1,31% | | 0,88% | 9,62% |
| 3-METHOXYPROPIONITRILE | 638 | 36,30 | 0,4597 | 0,2163 | 0,7689 | 0,9079 | 1,5201 | 62,6606 | 0,60% | 0,94% | | 9,02% | 31,00% |
| 3-METHYL SULFOLANE | 817 | 42,40 | 0,4191 | 0,2426 | 0,6179 | 0,8477 | 1,6577 | 43,4943 | 0,77% | 1,18% | | 4,91% | 38,96% |
| 3-METHYL-1,2-BUTADIENE | 490 | 38,30 | 0,1874 | 0,2650 | 1,3721 | 1,0000 | 0,5332 | 20,4367 | 1,14% | 0,98% | 0,48% | 4,35% | 14,82% |
| 3-METHYL-1,4-PENTADIENE | 497 | 34,90 | 0,2468 | 0,2730 | 0,5461 | 0,8784 | 1,4605 | 12,5450 | 0,75% | 1,68% | 0,80% | 3,22% | 18,31% |
| 3-METHYL-1-BUTANOL | 577,2 | 39,30 | 0,5900 | 0,2551 | 1,9115 | 1,0000 | 0,6561 | 17,2566 | 1,46% | 2,57% | | 5,06% | 18,48% |
| 3-METHYL-1-BUTENE | 452,7 | 35,30 | 0,2097 | 0,2748 | 0,4160 | 0,8757 | 1,7062 | 11,2509 | 0,70% | 2,76% | 0,49% | 3,19% | 12,84% |
| 3-METHYL-1-BUTYNE | 463,2 | 42,00 | 0,3081 | 0,2927 | 0,2784 | 0,8529 | 2,5030 | -2,0603 | 6,53% | 6,59% | 4,55% | 1,13% | 11,90% |
| 3-METHYL-1-HEXENE | 528 | 29,50 | 0,3057 | 0,2687 | 0,2882 | 0,8259 | 2,3211 | 17,9350 | 0,53% | 1,24% | 0,13% | 3,60% | 20,13% |
| 3-METHYL-1-PENTANOL | 588 | 34,00 | 0,7230 | 0,2505 | 0,2820 | 0,7977 | 3,6706 | 20,4114 | 3,58% | 3,80% | | 3,93% | 20,76% |
| 3-METHYL-1-PENTENE | 495 | 32,90 | 0,2640 | 0,2741 | 0,2714 | 0,8568 | 2,4435 | 11,7783 | 1,83% | 1,90% | 2,68% | 2,97% | 18,03% |
| 3-METHYL-2-BUTANOL | 556,1 | 38,70 | 0,5016 | 0,2611 | 2,7074 | 1,0000 | 0,4070 | 16,0614 | 2,27% | 3,33% | | 4,12% | 16,88% |
| 3-METHYL-2-PENTANONE | 573 | 33,20 | 0,3886 | 0,2586 | 0,2633 | 0,8276 | 2,7861 | 25,2292 | 0,72% | 6,98% | 2,07% | 3,42% | 22,79% |
| 3-METHYL-3-ETHYLPENTANE | 576,5 | 28,10 | 0,3050 | 0,2676 | 0,2788 | 0,8499 | 2,5505 | 21,5086 | 0,56% | 0,85% | 2,15% | 3,47% | 20,24% |
| 3-METHYL-3-PENTANOL | 575,6 | 35,20 | 0,4318 | 0,2662 | 0,2736 | 0,8272 | 2,9600 | 14,9319 | 2,72% | | | 2,58% | 15,33% |
| 3-METHYLBUTYRALDEHYDE | 543,2 | 38,29 | 0,3820 | 0,2651 | 0,5622 | 0,8569 | 1,7274 | 15,5249 | 0,65% | 1,34% | | 2,69% | 19,51% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 3-METHYL-cis-2-PENTENE | 515 | 32,90 | 0,2585 | 0,2644 | 0,4749 | 0,8232 | 1,5210 | 21,5102 | 0,52% | 1,28% | 0,79% | 4,53% | 20,20% |
| 3-METHYLCYCLOPENTENE | 526 | 41,30 | 0,2296 | 0,2774 | 0,8583 | 0,8991 | 0,9245 | 8,2834 | 1,23% | 2,03% | 1,52% | 4,02% | 13,76% |
| 3-METHYLDECANE | 634,1 | 19,89 | 0,5204 | 0,2520 | 0,6019 | 0,8703 | 2,0128 | 50,6968 | 0,63% | | | 2,33% | 24,68% |
| 3-METHYLDODECANE | 669 | 17,19 | 0,6156 | 0,2465 | 0,5019 | 0,8495 | 2,5567 | 68,4292 | 0,72% | | | 2,05% | 26,59% |
| 3-METHYLHEPTANE | 563,6 | 25,50 | 0,3723 | 0,2569 | 0,4299 | 0,8334 | 2,0181 | 32,6414 | 0,81% | 0,96% | 2,59% | 4,94% | 24,98% |
| 3-METHYLHEXANAL | 595 | 28,50 | 0,4570 | 0,2488 | 0,4606 | 0,8339 | 2,1692 | 38,2952 | 0,54% | | 1,30% | 4,11% | 28,34% |
| 3-METHYLHEXANE | 535,2 | 28,10 | 0,3204 | 0,2592 | 0,3606 | 0,8342 | 2,1138 | 26,9222 | 0,60% | 1,25% | 0,99% | 5,66% | 23,99% |
| 3-METHYLNONANE | 613 | 21,60 | 0,4649 | 0,2535 | 0,4054 | 0,8284 | 2,3843 | 44,2732 | 0,24% | 0,91% | 1,61% | 3,48% | 27,32% |
| 3-METHYLOCTANE | 590,15 | 23,40 | 0,4123 | 0,2578 | 0,4410 | 0,8330 | 2,1054 | 36,2761 | 1,51% | 1,86% | 1,91% | 3,13% | 25,27% |
| 3-METHYLPENTANE | 504,6 | 31,20 | 0,2702 | 0,2666 | 0,3141 | 0,8389 | 2,1441 | 19,0017 | 1,03% | 1,49% | 0,94% | 4,49% | 16,64% |
| 3-METHYLPYRIDINE | 645 | 46,60 | 0,2978 | 0,2613 | 0,2987 | 0,8458 | 2,3739 | 20,5163 | 0,83% | 1,59% | 1,14% | 3,93% | 13,47% |
| 3-METHYLTHIOPHENE | 613 | 49,10 | 0,2397 | 0,2741 | 0,4009 | 0,8244 | 1,6510 | 11,0408 | 1,19% | 1,56% | 0,75% | 3,11% | 21,37% |
| 3-METHYL-trans-2-PENTENE | 517 | 31,90 | 0,2627 | 0,2568 | 1,3531 | 1,0000 | 0,6196 | 28,8502 | 0,59% | 1,76% | 4,00% | 6,21% | 22,54% |
| 3-METHYLTRIDECANE | 684,7 | 16,06 | 0,6668 | 0,2438 | 0,5055 | 0,8356 | 2,6120 | 78,5840 | 0,75% | 1,60% | | 2,11% | 27,66% |
| 3-METHYLUNDECANE | 652,3 | 18,47 | 0,5690 | 0,2492 | 0,4700 | 0,8495 | 2,5566 | 58,9904 | 0,55% | | | 2,23% | 25,66% |
| 3-NITROBENZOTRIFLUORIDE | 667 | 28,00 | 0,5364 | 0,2322 | 0,4015 | 0,8402 | 2,7134 | 63,4949 | 1,89% | 2,73% | | 4,50% | 29,72% |
| 3-NONANONE | 648,1 | 24,53 | 0,4629 | 0,2519 | 0,8835 | 0,8217 | 1,2517 | 46,0991 | 0,65% | 0,91% | | 3,70% | 22,43% |
| 3-OCTANONE | 627,7 | 27,04 | 0,4406 | 0,2511 | 0,4537 | 0,8281 | 2,1296 | 40,2507 | 0,70% | 1,07% | | 4,23% | 21,36% |
| 3-PENTANOL | 559,6 | 37,14 | 0,5143 | 0,2530 | 0,1765 | 0,0003 | 1,0308 | 23,9211 | 2,03% | | | 5,94% | 21,13% |
| 3-PENTANONE | 560,95 | 37,40 | 0,3448 | 0,2578 | 0,3648 | 0,8284 | 2,1410 | 24,6477 | 0,67% | 6,07% | 0,54% | 3,44% | 16,38% |
| 4-((2-HYDROXYETHOXY)CARBONYL) BENZOIC ACID | 871,4 | 29,60 | 0,9669 | | 0,5285 | 0,8167 | 3,1841 | | 1,02% | 1,45% | | | |
| 4-(2-METHOXYETHYL)MORPHOLINE | 669,8 | 31,33 | 0,4696 | | 0,7280 | 0,8147 | 1,4867 | | 0,65% | 1,42% | | | |
| 4,4'-DIISOPROPYLBIPHENYL | 813,6 | 18,41 | 0,6164 | | 0,4412 | 0,8243 | 2,6789 | | 0,56% | 1,63% | | | |
| 4,4'-DINITRODIPHENYLAMINE | 926 | 26,20 | 1,0247 | | 0,5568 | 0,8165 | 3,1903 | | 1,38% | 1,01% | | | |
| 4,4'-DINITROTRIPHENYLAMINE | 946 | 20,00 | 1,0900 | | 0,5886 | 0,8161 | 3,1984 | | 1,38% | 0,99% | | | |
| 4,6-DIMETHYLDIBENZOTHIOPHENE | 939,4 | 29,81 | 0,4902 | | 0,3578 | 0,8269 | 2,6863 | | 0,67% | 1,78% | | | |
| 4,6-DINITRO-o-sec-BUTYLPHENOL | 793,9 | 27,50 | 1,0079 | | 0,6928 | 0,8402 | 2,7145 | | 1,32% | | | | |
| 4-[(TETRAHYDRO-2-FURANYL)OXY]-1-BUTANOL | 694,3 | 30,90 | 0,9319 | | 0,5489 | 0,8231 | 3,0434 | | 0,95% | 1,30% | | | |
| 4-[2-(2-AMINOETHOXY)ETHYL]MORPHOLINE | 706,9 | 28,50 | 0,6933 | | 0,7336 | 0,8357 | 1,9372 | | 1,30% | 1,25% | 1,65% | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 4-CARBOXYBENZALDEHYDE | 966 | 38,20 | 0,8174 | | 0,4438 | 0,8162 | 3,1971 | | 0,78% | 1,66% | | | |
| 4-CHLORO-3-NITROBENZOTRIFLUORIDE | 686 | 27,40 | 0,6038 | 0,2410 | 0,6260 | 0,8771 | 2,1651 | 52,0513 | 1,77% | | | 2,82% | 30,99% |
| 4-CHLORO-o-XYLENE | 689,1 | 33,22 | 0,3471 | | 0,5286 | 0,8394 | 1,6788 | | 0,57% | 1,75% | | | |
| 4-ETHYL-m-XYLENE | 665 | 28,80 | 0,4140 | 0,2555 | 0,3496 | 0,8365 | 2,5110 | 36,9301 | 0,50% | 2,99% | 2,06% | 2,99% | 25,11% |
| 4-ETHYL-o-XYLENE | 667 | 28,80 | 0,4114 | 0,2543 | 0,3407 | 0,8355 | 2,5381 | 38,2418 | 0,26% | 0,57% | 1,91% | 3,44% | 23,19% |
| 4-HEPTANONE | 602 | 29,20 | 0,4120 | 0,2553 | 0,3130 | 0,8398 | 2,7217 | 33,5318 | 0,37% | 1,10% | 2,67% | 2,92% | 23,93% |
| 4-HYDROXYACETOPHENONE | 860 | 44,50 | 0,6409 | 0,2480 | 0,6476 | 0,8762 | 2,1769 | 31,4660 | 5,25% | | | 2,09% | 27,96% |
| 4-HYDROXYBUTYRALDEHYDE | 599 | 44,80 | 0,8404 | 0,2382 | 0,5602 | 0,7959 | 2,6350 | 26,1409 | 2,00% | | 1,19% | 2,02% | 29,97% |
| 4-HYDROXYSTYRENE | 736 | 45,20 | 0,5090 | | 0,5754 | 0,8267 | 1,9220 | | 0,85% | 1,19% | 3,31% | | |
| 4-ISOBUTYLSTYRENE | 735 | 23,80 | 0,4631 | 0,2417 | 0,4806 | 0,8272 | 2,0926 | 70,3550 | 0,68% | 1,48% | 1,45% | 4,46% | 26,50% |
| 4-METHOXYPHENYLACETIC ACID | 768 | 39,00 | 0,8984 | | 0,5986 | 0,8342 | 2,8079 | | 0,53% | 0,70% | | | |
| 4-METHYL DIBENZOTHIOPHENE | 904,1 | 33,78 | 0,4414 | | 0,3281 | 0,8221 | 2,6182 | | 0,44% | | | | |
| 4-METHYL-1-HEPTENE | 557,3 | 26,04 | 0,3591 | 0,2591 | 0,6594 | 0,8744 | 1,4772 | 30,8149 | 0,62% | 1,39% | | 3,87% | 24,13% |
| 4-METHYL-1-HEXENE | 534 | 30,40 | 0,3024 | 0,2715 | 0,4581 | 0,8245 | 1,6921 | 15,2381 | 0,62% | 2,79% | 1,22% | 3,07% | 18,49% |
| 4-METHYL-1-OCTANOL | 631,7 | 24,84 | 0,8697 | 0,2564 | 0,6730 | 0,8505 | 2,5416 | 21,5880 | 2,08% | | | 1,51% | 26,99% |
| 4-METHYL-1-PENTENE | 496 | 32,20 | 0,2389 | 0,2716 | 1,1615 | 1,0000 | 0,7026 | 15,6413 | 1,21% | 1,84% | 1,37% | 3,88% | 19,21% |
| 4-METHYL-2-PENTANOL | 574,4 | 34,70 | 0,5730 | 0,2665 | 1,3602 | 1,0000 | 0,9518 | 11,0909 | 0,46% | 0,78% | | 1,90% | 17,81% |
| 4-METHYL-cis-2-PENTENE | 499 | 32,20 | 0,2442 | 0,2699 | 1,1357 | 1,0000 | 0,7310 | 17,0947 | 0,75% | 2,54% | 2,25% | 3,96% | 19,19% |
| 4-METHYL-CYCLOHEXANE-METHANOL | 647,6 | 32,43 | 0,6295 | 0,2792 | 0,9661 | 0,8147 | 1,3907 | 4,5193 | 0,74% | 0,89% | | 4,04% | 31,32% |
| 4-METHYLCYCLOPENTENE | 527 | 41,30 | 0,2357 | 0,2811 | 1,0428 | 0,9528 | 0,7773 | 6,7888 | 1,59% | 2,84% | 1,35% | 1,97% | 14,47% |
| 4-METHYLHEPTANE | 561,7 | 25,40 | 0,3707 | 0,2579 | 0,4038 | 0,8312 | 2,0993 | 32,1943 | 0,70% | 0,83% | 2,55% | 4,53% | 21,99% |
| 4-METHYLNONANE | 610 | 21,60 | 0,4651 | 0,2578 | 0,5457 | 0,8214 | 1,8863 | 39,4453 | 1,52% | 2,44% | 2,21% | 2,18% | 27,49% |
| 4-METHYLOCTANE | 587,65 | 23,40 | 0,4129 | 0,2575 | 0,4669 | 0,8302 | 2,0014 | 36,2157 | 1,66% | 1,96% | 2,51% | 3,42% | 26,15% |
| 4-METHYLPHENANTHRENE | 895,3 | 27,21 | 0,4401 | 0,2343 | 1,2057 | 1,0000 | 0,9356 | 89,8813 | 0,55% | 1,02% | | 5,72% | 28,24% |
| 4-METHYLPYRIDINE | 646,15 | 46,60 | 0,3010 | 0,2628 | 0,2800 | 0,8487 | 2,5147 | 19,6123 | 0,77% | 1,32% | 1,18% | 3,40% | 11,86% |
| 4-METHYL-trans-2-PENTENE | 501 | 32,20 | 0,2552 | 0,2696 | 1,1705 | 1,0000 | 0,7201 | 17,0527 | 0,94% | 2,24% | 0,86% | 3,89% | 19,70% |
| 4-NONANONE | 643,7 | 24,53 | 0,4988 | 0,2575 | 0,5927 | 0,8235 | 1,8482 | 38,0465 | 0,76% | 0,95% | | 1,58% | 22,98% |
| 4-OCTANONE | 623,8 | 27,04 | 0,4204 | 0,2562 | 1,5766 | 1,0000 | 0,6681 | 36,6834 | 0,65% | 0,78% | | 3,68% | 21,28% |
| 5-ETHYLIDENE-2-NORBORNENE | 629 | 34,00 | 0,3141 | 0,2657 | 0,4294 | 0,8391 | 1,8645 | 22,2808 | 0,33% | 0,82% | | 3,08% | 20,18% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| 5-ETHYL-m-XYLENE | 655 | 27,50 | 0,4169 | 0,2510 | 0,3203 | 0,8407 | 2,7052 | 43,1580 | 0,44% | 1,06% | 2,27% | 3,68% | 28,00% |
| 5-HEXEN-2-ONE | 586,8 | 34,13 | 0,4174 | 0,2489 | 0,4107 | 0,8604 | 2,3906 | 31,7495 | 0,50% | | | 4,43% | 30,04% |
| 5-METHYL-1-HEXANOL | 605 | 30,30 | 0,7807 | 0,2700 | 0,5602 | 0,8139 | 2,5748 | 8,3731 | 0,75% | 0,73% | | 3,17% | 26,16% |
| 5-METHYL-1-HEXENE | 528 | 28,70 | 0,3105 | 0,2643 | 0,4422 | 0,8596 | 1,9076 | 22,4187 | 1,17% | 1,78% | 0,79% | 3,62% | 22,48% |
| 5-METHYL-2-HEXANONE | 601 | 29,70 | 0,4344 | 0,2568 | 0,3201 | 0,8380 | 2,7524 | 29,7072 | 0,99% | 1,34% | | 2,95% | 26,16% |
| 5-METHYLINDAN | 711,2 | 35,22 | 0,3262 | 0,2622 | 0,3919 | 0,8731 | 2,2163 | 27,0639 | 0,60% | | | 3,16% | 21,04% |
| 5-METHYLNONANE | 610 | 21,60 | 0,4562 | 0,2557 | 0,4342 | 0,8251 | 2,2237 | 41,9288 | 2,50% | 3,26% | 2,67% | 2,96% | 27,06% |
| 5-NONANONE | 640 | 23,20 | 0,5137 | 0,2423 | 0,3515 | 0,8328 | 2,8491 | 57,4406 | 1,21% | 2,12% | 1,05% | 4,31% | 26,27% |
| 5-o-TOLYL-2-PENTENE | 702,6 | 25,16 | 0,4794 | 0,2523 | 0,5286 | 0,8342 | 2,0136 | 46,2279 | 0,61% | 1,48% | | 3,12% | 27,00% |
| 6-AMINOHEXANAMIDE | 807,8 | 34,56 | 0,6975 | 0,2480 | 0,8020 | 0,8447 | 1,8067 | 37,1409 | 1,36% | 1,33% | 0,84% | 2,05% | 26,69% |
| 6-AMINOHEXANOL | 665 | 34,40 | 0,9689 | | 0,4734 | 0,7989 | 3,3208 | | 0,81% | 0,83% | | | |
| 6-METHYL-1-HEPTENE | 558 | 26,00 | 0,3555 | 0,2592 | 0,3814 | 0,8487 | 2,2468 | 30,2121 | 0,97% | 1,84% | 0,16% | 3,88% | 24,63% |
| 6-METHYL-1-OCTANOL | 633,4 | 24,84 | 0,8745 | 0,2555 | 0,6723 | 0,8501 | 2,5482 | 23,5589 | 1,68% | | | 1,56% | 26,98% |
| 7-METHYL-1-OCTENE | 579 | 23,80 | 0,4045 | | 0,4657 | 0,8387 | 2,0269 | | 0,82% | 1,37% | 0,13% | | |
| 8-HYDROXYQUINOLINE | 788 | 43,60 | 0,5223 | 0,2651 | 0,4935 | 0,8249 | 2,2050 | 18,0060 | 0,75% | 1,05% | | 1,12% | 16,64% |
| 8-METHYL-1-NONANOL | 676,7 | 23,93 | 0,6107 | 0,2551 | 0,1633 | 0,6649 | 2,7406 | 38,9499 | 0,67% | | | 3,25% | 24,54% |
| 8-METHYL-1-NONENE | 619 | 21,90 | 0,4523 | | 0,6370 | 0,8382 | 1,6684 | | 0,77% | 1,17% | 0,17% | | |
| 8-METHYLQUINOLINE | 787 | 43,00 | 0,3582 | 0,2736 | 0,4098 | 0,8422 | 2,0761 | 11,6091 | 2,60% | 2,93% | 2,70% | 2,21% | 12,88% |
| ACENAPHTHALENE | 792 | 32,00 | 0,3987 | | 0,8703 | 0,8556 | 1,1837 | | 0,80% | 1,48% | 2,48% | | |
| ACENAPHTHENE | 803,15 | 31,00 | 0,3811 | 0,2302 | 1,1835 | 1,0000 | 0,8801 | 77,4423 | 1,08% | 4,23% | 0,96% | 7,25% | 15,84% |
| ACETAL | 539,7 | 32,20 | 0,4869 | 0,2842 | 0,4702 | 0,8635 | 2,3463 | -3,1778 | 3,30% | 3,30% | 3,44% | 1,47% | 16,34% |
| ACETALDOL | 620 | 45,90 | 0,7966 | 0,2149 | 0,7252 | 0,8697 | 2,2613 | 37,4761 | 0,55% | | | 8,85% | 21,18% |
| ACETALDOXIME | 568 | 60,40 | 0,6384 | 0,2506 | 0,5091 | 0,8480 | 2,5817 | 15,9804 | 0,93% | 1,48% | | 1,14% | 14,86% |
| ACETAMIDE | 761 | 66,00 | 0,4210 | 0,2156 | 0,6860 | 0,8091 | 1,4557 | 42,6861 | 0,74% | 1,82% | 0,78% | 8,69% | 28,78% |
| ACETAMINOPHEN | 736 | 42,60 | 0,7997 | | 0,4701 | 0,8049 | 2,9329 | | 1,09% | 1,28% | 2,93% | | |
| ACETANILIDE | 825 | 37,30 | 0,5646 | 0,2364 | 0,7474 | 0,8681 | 1,7162 | 52,9305 | 0,44% | 0,75% | | 4,03% | 30,25% |
| ACETIC ANHYDRIDE | 606 | 40,00 | 0,4553 | 0,2446 | 0,3544 | 0,8340 | 2,6197 | 32,8202 | 0,66% | 2,89% | 2,95% | 3,50% | 27,32% |
| ACETOACETANILIDE | 879 | 30,30 | 0,7946 | 0,2337 | 0,4906 | 0,8217 | 2,9445 | 64,9966 | 0,76% | 1,10% | | 2,43% | 31,03% |
| ACETOACETIC ACID | 678,5 | 46,97 | 0,7073 | | 0,4316 | 0,8119 | 2,9102 | | 0,73% | 1,43% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| ACETOIN | 607,4 | 44,63 | 0,5263 | 0,2469 | 0,3487 | 0,8158 | 2,7729 | 25,6665 | 0,66% | 1,69% | | 3,30% | 25,99% |
| ACETONE | 508,2 | 47,01 | 0,3065 | 0,2433 | 0,3262 | 0,8554 | 2,3401 | 26,1497 | 0,21% | 1,72% | 3,22% | 6,03% | 30,84% |
| ACETONE CYANOHYDRIN | 620 | 42,50 | 0,7673 | 0,2440 | 0,6013 | 0,8250 | 2,4470 | 25,0133 | 0,70% | 0,77% | | 1,79% | 28,14% |
| ACETONITRILE | 545,5 | 48,50 | 0,3419 | 0,1963 | 0,5871 | 0,9211 | 1,6928 | 53,2912 | 2,80% | 4,98% | | 13,33% | 33,90% |
| ACETOPHENONE | 709,6 | 40,10 | 0,3830 | 0,2572 | 0,3213 | 0,8459 | 2,6164 | 27,5582 | 0,64% | 1,13% | | 3,11% | 19,92% |
| ACETOVANILLONE | 786 | 36,50 | 0,7856 | | 0,4265 | 0,8163 | 3,1940 | | 0,60% | 0,87% | | | |
| ACETOXYACETIC ACID | 764 | 43,20 | 0,7104 | | 0,4242 | 0,8230 | 3,0462 | | 0,80% | 2,11% | | | |
| ACETYL CHLORIDE | 508 | 57,40 | 0,3340 | 0,2643 | 0,3929 | 0,8751 | 2,1908 | 9,8426 | 5,11% | 6,28% | | 4,39% | 20,12% |
| ACETYLENE | 308,3 | 61,38 | 0,1912 | 0,2708 | 0,3171 | 0,8842 | 2,0788 | 5,6077 | 0,45% | 2,34% | | 2,84% | 19,28% |
| ACETYLSALICYLIC ACID | 765 | 32,70 | 0,8327 | 0,2411 | 0,6540 | 0,8212 | 2,4009 | 42,0633 | 0,99% | 1,19% | 2,67% | 1,91% | 29,28% |
| ACRIDINE | 905 | 36,40 | 0,4400 | 0,2536 | 0,3367 | 0,8412 | 2,6960 | 39,3017 | 1,37% | 2,25% | 0,85% | 3,92% | 19,66% |
| ACROLEIN | 506 | 50,00 | 0,3198 | 0,2333 | 1,1458 | 1,0000 | 0,7943 | 29,1775 | 6,62% | 7,11% | 3,76% | 9,51% | 27,56% |
| ACROLEIN CYANOHYDRIN | 639 | 45,10 | 0,8435 | 0,2357 | 0,7375 | 0,8661 | 2,3102 | 29,2745 | 0,65% | | | 1,78% | 30,72% |
| ACRYLIC ACID | 615 | 56,60 | 0,5383 | 0,2447 | 1,3654 | 0,9999 | 0,9050 | 21,8008 | 2,76% | | 0,59% | 3,66% | 34,30% |
| ACRYLONITRILE | 540 | 46,60 | 0,3107 | 0,2256 | 0,3355 | 0,8621 | 2,3662 | 39,6531 | 1,04% | | | 7,84% | 30,33% |
| ACRYLOXY PROPIONIC ACID | 729,5 | 34,41 | 0,8018 | 0,2366 | 0,6675 | 0,8579 | 2,4276 | 43,7958 | 1,45% | | | 1,85% | 30,40% |
| ADAMANTANE | 703 | 29,20 | 0,1853 | | 0,2134 | 0,8570 | 2,4402 | | 0,47% | | 0,40% | | |
| ADIPIC ACID | 841 | 37,00 | 0,7778 | 0,2343 | 0,2658 | 0,7906 | 3,8854 | 51,9736 | 1,57% | 1,36% | | 2,77% | 32,26% |
| ADIPONITRILE | 781 | 28,30 | 0,6588 | 0,1925 | 0,6419 | 0,8720 | 2,2301 | 120,3553 | 0,26% | | | 11,06% | 58,74% |
| AIR | 132,45 | 37,74 | 0,0000 | 0,2943 | 0,1592 | 0,8955 | 1,9493 | 1,1017 | 1,35% | 5,17% | 3,70% | 3,25% | 5,13% |
| ALLYL ACETATE | 559 | 36,80 | 0,3879 | 0,2566 | 0,5197 | 0,8922 | 1,9861 | 23,5024 | 0,49% | 0,96% | | 2,88% | 23,06% |
| ALLYL ACRYLATE | 575,5 | 33,96 | 0,4264 | | 1,0631 | 0,8901 | 1,0289 | | 0,80% | 1,15% | | | |
| ALLYL ALCOHOL | 545,1 | 56,20 | 0,5697 | 0,2482 | 0,6706 | 0,8421 | 1,8559 | 15,7122 | 0,90% | 1,31% | | 4,23% | 21,68% |
| ALLYL ETHER | 550,6 | 31,99 | 0,2762 | 0,2555 | 1,2535 | 1,0000 | 0,6965 | 32,2124 | 0,61% | 1,45% | | 5,19% | 21,53% |
| ALLYL GLYCIDYL ETHER | 629 | 36,80 | 0,4087 | 0,2580 | 0,4173 | 0,8375 | 2,2135 | 24,6489 | 0,81% | 1,73% | | 3,12% | 22,69% |
| ALLYL METHACRYLATE | 600 | 30,20 | 0,3881 | 0,2542 | 0,2802 | 0,8146 | 2,6184 | 34,0517 | 1,28% | 3,01% | | 3,83% | 24,48% |
| ALLYLAMINE | 505 | 51,70 | 0,3265 | 0,2547 | 0,5545 | 0,8502 | 1,5863 | 15,9444 | 0,72% | 1,35% | | 6,56% | 3,15% |
| ALLYLIDENE DIACETATE | 639,1 | 28,64 | 0,5702 | 0,2526 | 0,6463 | 0,8172 | 1,8582 | 33,6162 | 0,68% | 1,35% | | 2,56% | 24,70% |
| ALLYL-TERT-BUTYLPEROXIDE | 563 | 28,80 | 0,4020 | 0,2747 | 0,3063 | 0,8393 | 2,7298 | 9,0901 | 1,11% | 2,02% | | 1,81% | 19,17% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| alpha-EPICHLOROHYDRIN | 615 | 49,00 | 0,2523 | 0,2409 | 0,1860 | 0,8373 | 2,7656 | 33,4555 | 2,54% | 2,71% | | 7,41% | 34,93% |
| alpha-HYDROXYISOBUTYRAMIDE | 771,7 | 53,42 | 0,6453 | | 0,4252 | 0,8308 | 2,8876 | | 0,68% | 1,37% | | | |
| alpha-HYDROXYISOBUTYRIC ACID | 664 | 49,20 | 0,9833 | | 0,5064 | 0,8119 | 3,2961 | | 1,35% | 0,93% | | | |
| alpha-METHYLBENZYL ALCOHOL | 699 | 37,70 | 0,4382 | 0,2522 | 1,6060 | 0,9968 | 0,6705 | 32,2115 | 0,78% | 1,32% | | 4,29% | 23,18% |
| alpha-METHYLBENZYL ALCOHOL FORMATE | 690 | 32,30 | 0,4377 | 0,2556 | 0,5050 | 0,8343 | 1,9690 | 32,3382 | 0,29% | 0,42% | | 3,40% | 24,66% |
| alpha-METHYLSTYRENE | 654 | 33,60 | 0,3230 | 0,2581 | 0,5287 | 0,8296 | 1,5837 | 32,4918 | 0,45% | 1,74% | 0,62% | 3,34% | 27,06% |
| alpha-PHELLANDRENE | 649 | 28,20 | 0,3807 | 0,2680 | 0,8440 | 0,8508 | 1,1802 | 24,5708 | 0,49% | 2,65% | 0,35% | 1,57% | 25,41% |
| alpha-PINENE | 644 | 27,60 | 0,2209 | 0,2528 | 0,0952 | 0,7921 | 2,7026 | 48,7669 | 0,27% | | | 7,43% | 31,70% |
| alpha-TERPINENE | 649 | 28,00 | 0,3721 | 0,2562 | 0,3592 | 0,8299 | 2,2765 | 35,4751 | 0,38% | 0,91% | 1,12% | 4,82% | 24,11% |
| alpha-TERPINEOL | 675 | 29,50 | 0,6992 | | 0,5969 | 0,8572 | 2,4373 | | 0,66% | | | | |
| alpha-TOCOPHEROL | 964,3 | 10,80 | 1,0314 | 0,2316 | 0,6695 | 0,8341 | 2,8240 | 187,1195 | 0,99% | | | 1,96% | 32,99% |
| AMINOACETONITRILE | 638 | 54,40 | 0,4657 | | 1,3040 | 1,0000 | 0,8759 | | 1,61% | 2,09% | 3,11% | | |
| AMINOCAPRONITRILE | 697 | 30,50 | 0,6532 | | 0,4091 | 0,8271 | 2,9608 | | 0,33% | 0,81% | 1,21% | | |
| AMMONIA | 405,65 | 112,80 | 0,2526 | 0,2460 | 0,2988 | 0,8652 | 2,3219 | 8,6398 | 0,09% | 2,79% | 9,86% | 5,25% | 25,61% |
| AMMONIUM SULFIDE | 479 | 31,54 | 0,1657 | 0,1904 | 0,4632 | 0,9338 | 1,5801 | 83,5138 | 0,70% | | | 12,47% | 40,58% |
| ANETHOLE | 723 | 29,00 | 0,4846 | 0,2428 | 0,4721 | 0,8298 | 2,1976 | 53,3405 | 0,74% | 1,29% | | 4,20% | 32,29% |
| ANILINE | 699 | 53,10 | 0,3775 | 0,2593 | 0,3454 | 0,8219 | 2,3066 | 17,9623 | 0,48% | 3,25% | 0,81% | 4,01% | 28,47% |
| ANISOLE | 645,6 | 42,50 | 0,3502 | 0,2639 | 0,3299 | 0,8431 | 2,4133 | 18,4118 | 0,10% | 0,72% | | 3,11% | 19,46% |
| ANTHRACENE | 873 | 29,00 | 0,4857 | 0,2289 | 0,3634 | 0,8403 | 2,7122 | 85,6306 | 4,25% | 6,22% | 3,11% | 5,01% | 35,14% |
| ANTHRAQUINONE | 900 | 31,50 | 0,6807 | 0,2390 | 0,6837 | 0,8811 | 2,1158 | 62,5716 | 3,63% | 5,99% | | 3,69% | 25,74% |
| ANTIMONY TRICHLORIDE | 794 | 48,20 | 0,1706 | 0,2188 | 0,2015 | 0,8570 | 2,4405 | 66,0097 | 1,24% | | | 10,69% | 44,64% |
| ARGON | 150,86 | 48,98 | 0,0000 | 0,2941 | 0,2020 | 0,9085 | 1,8138 | 0,8738 | 0,45% | 2,54% | 5,88% | 2,74% | 13,27% |
| ARSENIC (III) CHLORIDE | 629 | 52,60 | 0,3020 | 0,2599 | 0,2743 | 0,8480 | 2,5460 | 18,3791 | 0,54% | 2,30% | 3,14% | 3,84% | 21,33% |
| ARSENIC TRIOXIDE | 1200 | 40,00 | 0,0611 | | 0,1786 | 0,8784 | 2,1485 | | 0,44% | 2,19% | | | |
| ARSINE | 373 | 65,50 | 0,0105 | 0,2779 | 0,2375 | 0,8807 | 1,5191 | 6,4884 | 0,68% | 3,51% | 0,37% | 4,74% | 54,74% |
| AZELAIC ACID | 844 | 27,20 | 0,8923 | 0,2331 | 0,4695 | 0,7265 | 2,7213 | 65,2914 | 0,79% | | | 3,69% | 38,45% |
| BENZALDEHYDE | 695 | 46,50 | 0,3127 | 0,2597 | 0,4359 | 0,8387 | 1,8335 | 23,1728 | 0,48% | 0,58% | 1,40% | 3,88% | 20,70% |
| BENZAMIDE | 824 | 50,50 | 0,5585 | 0,2549 | 0,3744 | 0,8227 | 2,8030 | 22,4851 | 0,67% | 1,50% | | 2,41% | 24,20% |
| BENZANTHRACENE | 979 | 23,90 | 0,5692 | | 0,6727 | 0,8313 | 1,8249 | | 0,87% | 1,56% | 0,35% | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| BENZENE | 562,05 | 48,95 | 0,2103 | 0,2698 | 0,1919 | 0,8469 | 2,5997 | 13,4541 | 0,52% | 1,75% | 1,47% | 3,59% | 19,05% |
| BENZENE-1,2,4-TRICARBOXYLIC ACID TRIMETHYL ESTER | 821,7 | 23,34 | 0,8845 | 0,2400 | 0,6746 | 0,8480 | 2,5814 | 62,3067 | 3,97% | | | 1,70% | 29,93% |
| BENZIDINE | 929 | 33,00 | 0,7347 | | 0,4697 | 0,8204 | 2,8657 | | 0,75% | 0,96% | | | |
| BENZOIC ACID | 751 | 44,70 | 0,6028 | 0,2481 | 2,0345 | 1,0000 | 0,6177 | 29,5477 | 2,17% | 4,15% | 2,33% | 3,43% | 26,77% |
| BENZONITRILE | 702,3 | 42,15 | 0,3432 | 0,2467 | 0,5039 | 0,8501 | 1,7603 | 37,0711 | 0,27% | 1,76% | | 4,88% | 35,60% |
| BENZOPHENONE | 830 | 33,52 | 0,5019 | 0,2632 | 0,3663 | 0,8382 | 2,7503 | 25,4462 | 2,51% | 1,93% | | 1,69% | 16,40% |
| BENZOTHIOPHENE | 764 | 47,60 | 0,3071 | 0,2840 | 0,3136 | 0,8582 | 2,4230 | 7,0833 | 2,18% | 3,20% | | 2,08% | 15,50% |
| BENZOTRICHLORIDE | 737 | 33,40 | 0,2599 | 0,2539 | 0,5051 | 0,8551 | 1,5394 | 43,6533 | 0,68% | 1,50% | | 5,08% | 27,05% |
| BENZOTRIFLUORIDE | 559,9 | 32,10 | 0,2998 | 0,2522 | 0,4891 | 0,8191 | 1,5963 | 33,4748 | 0,92% | 2,53% | 0,58% | 5,49% | 26,39% |
| BENZOYL CHLORIDE | 697 | 40,60 | 0,4159 | 0,2610 | 0,8356 | 0,9602 | 1,3648 | 22,3078 | 0,37% | 0,39% | | 2,09% | 23,57% |
| BENZYL ACETATE | 699 | 31,80 | 0,4733 | 0,2593 | 0,4480 | 0,8340 | 2,2745 | 30,1669 | 0,91% | 1,83% | | 1,52% | 28,96% |
| BENZYL ALCOHOL | 720,15 | 43,74 | 0,3631 | 0,2450 | 0,0725 | 0,7243 | 2,7828 | 37,5766 | 0,58% | | | 7,62% | 9,61% |
| BENZYL CHLORIDE | 686 | 39,10 | 0,3136 | 0,2537 | 0,3743 | 0,7959 | 1,8648 | 33,2898 | 0,59% | 3,03% | 5,70% | 4,97% | 25,82% |
| BENZYL DICHLORIDE | 731 | 36,50 | 0,3264 | 0,2570 | 0,5731 | 0,9137 | 1,6991 | 33,9398 | 0,46% | 1,19% | | 2,66% | 28,99% |
| BENZYL ETHYL ETHER | 662 | 31,10 | 0,4332 | 0,2501 | 0,8554 | 0,9173 | 1,3169 | 36,9214 | 0,48% | 2,07% | | 4,95% | 25,12% |
| BENZYL FORMATE | 698 | 35,90 | 0,4203 | 0,2553 | 0,6056 | 0,8395 | 1,6671 | 31,7559 | 0,75% | 1,14% | 3,13% | 2,87% | 27,73% |
| BENZYL MERCAPTAN | 718 | 40,60 | 0,3126 | 0,2624 | 0,3777 | 0,8241 | 1,9725 | 25,9317 | 1,18% | 2,44% | 1,09% | 2,58% | 26,48% |
| BENZYLAMINE | 684 | 43,20 | 0,4011 | 0,2620 | 0,2932 | 0,8371 | 2,7698 | 20,1612 | 0,72% | 1,12% | | 2,63% | 12,24% |
| beta-PHELLANDRENE | 648 | 28,20 | 0,3766 | 0,2659 | 0,5628 | 0,8177 | 1,6123 | 26,0269 | 0,55% | 1,85% | 0,22% | 1,91% | 25,43% |
| beta-PINENE | 643 | 27,60 | 0,3249 | 0,2549 | 0,2863 | 0,8478 | 2,5848 | 41,3826 | 2,00% | 3,15% | | 4,20% | 22,33% |
| beta-TERPINEOL | 665,2 | 30,12 | 0,6872 | 0,2738 | 0,4333 | 0,8186 | 2,8876 | 1,8988 | 0,62% | 1,09% | | 1,03% | 21,31% |
| BICYCLO[2.2.1]HEPTANE | 594 | 36,96 | 0,1636 | | 0,1781 | 0,8525 | 2,5090 | | 0,50% | 2,60% | | | |
| BICYCLO[2.2.2]OCTANE | 625 | 34,20 | 0,2054 | 0,2417 | 0,2826 | 0,8701 | 2,2557 | 45,2152 | 0,81% | | 3,45% | 4,82% | 13,89% |
| BICYCLOHEXYL | 727 | 25,60 | 0,4276 | 0,2549 | 0,3985 | 0,8563 | 2,4510 | 43,7668 | 1,70% | 2,62% | | 3,43% | 24,30% |
| BIPHENYL | 773 | 33,80 | 0,4029 | 0,2551 | 0,2858 | 0,8350 | 2,8089 | 35,9357 | 0,97% | 1,73% | 0,18% | 3,94% | 20,30% |
| BIS-(2-AMINOETHYL)ETHER | 655,8 | 44,21 | 0,6152 | | 1,7655 | 0,9998 | 0,7358 | | 0,77% | 0,82% | | | |
| BIS(alpha-METHYLBENZYL) ETHER | 770,6 | 19,92 | 0,4834 | 0,2419 | 0,3834 | 0,7456 | 2,1264 | 87,6077 | 0,71% | | | 4,99% | 26,55% |
| BIS(CHLOROMETHYL)ETHER | 579 | 45,80 | 0,3239 | 0,2541 | 0,3782 | 0,8348 | 2,0658 | 23,1531 | 0,69% | 1,50% | | 4,32% | 26,83% |
| BIS(CYANOETHYL)ETHER | 783 | 28,30 | 0,7775 | 0,1978 | 0,6674 | 0,8609 | 2,3842 | 108,0962 | 1,26% | | | 8,58% | 74,72% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| BIS(DIFLUOROMETHYL)ETHER | 420,25 | 42,28 | 0,3676 | 0,2636 | 0,6322 | 0,8542 | 1,5173 | 11,6303 | 0,79% | 1,18% | | 3,62% | 18,32% |
| BIS(TRIFLUOROMETHYL)SULFIDE | 376,75 | 30,58 | 0,2638 | 0,2806 | 0,3955 | 0,8877 | 2,0369 | 4,5624 | 0,61% | | | 2,30% | 17,38% |
| BIS[3-(TRIMETHOXYSILYL)PROPYL]DISULFIDE | 736,2 | 13,09 | 1,1551 | 0,2452 | 0,6856 | 0,8253 | 2,9981 | 63,2543 | 1,88% | | | 2,00% | 34,73% |
| BORON TRIBROMIDE | 573,15 | 48,70 | 0,2599 | 0,2766 | 0,5306 | 0,9263 | 1,6462 | 7,4442 | 1,74% | | | 2,58% | 17,61% |
| BORON TRICHLORIDE | 451,95 | 38,71 | 0,1505 | 0,2436 | 0,1193 | 0,8403 | 2,7122 | 29,5090 | 0,70% | 1,87% | | 9,30% | 98,32% |
| BORON TRIFLUORIDE | 260,9 | 49,90 | 0,4337 | 0,2565 | 0,3048 | 0,8356 | 2,7965 | 6,7109 | 2,80% | 5,17% | 2,22% | 4,30% | 11,80% |
| BROMINE | 584,15 | 103,00 | 0,1290 | 0,3008 | 0,1923 | 0,8672 | 2,2947 | -2,3953 | 1,88% | 2,30% | 1,26% | 1,26% | 18,20% |
| BROMOBENZENE | 670,15 | 45,19 | 0,2506 | 0,2629 | 0,3384 | 0,8414 | 1,9750 | 21,7146 | 1,95% | 2,79% | 0,67% | 4,52% | 20,15% |
| BROMOCHLORODIFLUOROMETHANE | 426,15 | 42,54 | 0,1871 | 0,2749 | 1,2278 | 1,0000 | 0,5857 | 9,8878 | 2,68% | 4,80% | 1,63% | 4,44% | 8,84% |
| BROMOCHLOROMETHANE | 557 | 64,70 | 0,2064 | 0,2727 | 0,9884 | 1,0000 | 0,8004 | 9,3472 | 0,67% | 1,27% | | 3,04% | 12,38% |
| BROMODIFLUOROMETHANE | 411,98 | 51,32 | 0,2050 | 0,2665 | 0,1860 | 0,8411 | 2,5531 | 10,1415 | 0,49% | 5,63% | | 5,85% | 27,15% |
| BROMOETHANE | 503,8 | 55,65 | 0,2053 | 0,2750 | 0,2729 | 0,8691 | 2,2694 | 8,1641 | 2,13% | 3,04% | | 2,72% | 18,99% |
| BROMOMETHANE | 464 | 69,29 | 0,1534 | 0,2717 | 0,2977 | 0,8562 | 1,8182 | 8,0807 | 1,35% | 2,89% | 1,34% | 4,25% | 16,78% |
| BROMOTRICHLOROMETHANE | 606 | 49,70 | 0,1920 | 0,2800 | 0,2097 | 0,8551 | 2,4693 | 7,1944 | 0,46% | 2,06% | 1,21% | 3,22% | 16,46% |
| BROMOTRIFLUOROETHYLENE | 432 | 44,80 | 0,1754 | 0,2815 | 0,9747 | 1,0000 | 0,7586 | 7,2186 | 0,76% | 2,07% | 0,74% | 1,38% | 8,80% |
| BROMOTRIFLUOROMETHANE | 340,15 | 39,70 | 0,1704 | 0,2762 | 0,8466 | 1,0000 | 0,8890 | 7,5443 | 0,56% | 1,63% | | 3,76% | 14,96% |
| BUTANAL | 537,2 | 44,10 | 0,2826 | 0,2588 | 0,5336 | 0,8785 | 1,5897 | 19,6031 | 0,70% | 1,65% | | 4,52% | 23,26% |
| BUTYL VINYL ETHER | 536 | 31,20 | 0,3802 | 0,2620 | 0,4320 | 0,8367 | 2,0599 | 21,7616 | 0,88% | 1,60% | | 3,05% | 24,82% |
| BUTYRONITRILE | 585,4 | 38,80 | 0,3601 | 0,2303 | 0,4198 | 0,8735 | 2,2114 | 45,9701 | 1,86% | 2,91% | | 7,12% | 27,90% |
| CAMPHENE | 638 | 27,50 | 0,2957 | 0,2520 | 0,2782 | 0,8342 | 2,3910 | 45,2875 | 0,35% | 1,04% | | 4,92% | 19,78% |
| CAMPHOR | 709 | 29,90 | 0,3190 | 0,2560 | 0,3027 | 0,8525 | 2,5101 | 40,6994 | 0,92% | 2,71% | | 2,95% | 22,08% |
| CARBAMYL CHLORIDE | 517 | 73,80 | 0,4446 | | 0,3989 | 0,8197 | 2,2980 | | 0,69% | 1,39% | | | |
| CARBON DIOXIDE | 304,21 | 73,83 | 0,2236 | 0,2728 | 0,2806 | 0,8684 | 2,2782 | 4,1585 | 0,30% | 1,20% | 8,47% | 2,07% | 17,06% |
| CARBON DISULFIDE | 552 | 79,00 | 0,1107 | 0,2891 | 0,2771 | 0,8872 | 1,8956 | 2,1296 | 0,72% | 1,17% | 13,18% | 1,92% | 19,70% |
| CARBON MONOXIDE | 132,92 | 34,99 | 0,0482 | 0,2903 | 0,1623 | 0,8778 | 2,1566 | 1,4078 | 0,27% | 1,55% | 11,37% | 3,00% | 10,04% |
| CARBON TETRACHLORIDE | 556,35 | 45,60 | 0,1926 | 0,2721 | 0,2022 | 0,8525 | 2,4909 | 12,9812 | 0,58% | 1,69% | 4,18% | 3,77% | 17,81% |
| CARBON TETRAFLUORIDE | 227,51 | 37,45 | 0,1790 | 0,2811 | 0,4352 | 0,8494 | 1,4376 | 3,5302 | 1,18% | 1,99% | 0,86% | 3,37% | 15,27% |
| CARBONYL FLUORIDE | 297 | 57,60 | 0,2829 | 0,3291 | 0,1335 | 0,8201 | 3,1083 | -14,1169 | 1,86% | 3,85% | 0,93% | 0,84% | 11,36% |
| CARBONYL SULFIDE | 378,8 | 63,49 | 0,0970 | 0,2744 | 0,1931 | 0,8735 | 2,2104 | 6,4994 | 0,43% | 1,87% | 12,08% | 5,65% | 17,58% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| CELLOBIOSE | 1235 | 39,21 | 0,8442 | | 0,5243 | 0,8273 | 2,9563 | | 0,78% | 1,02% | | | |
| CHLORINE | 417,15 | 77,10 | 0,0688 | 0,2777 | 0,4057 | 0,8530 | 1,1810 | 5,7845 | 0,58% | 2,06% | 0,49% | 4,41% | 16,26% |
| CHLORINE TRIFLUORIDE | 433,7 | 45,78 | 0,3371 | 0,2040 | 0,7776 | 0,8631 | 1,2293 | 42,4463 | 2,73% | 1,20% | 1,46% | 10,67% | 36,71% |
| CHLOROACETALDEHYDE | 555 | 53,70 | 0,3297 | 0,2355 | 0,2273 | 0,8336 | 2,8335 | 29,5368 | 0,63% | 2,52% | | 5,29% | 27,81% |
| CHLOROACETIC ACID | 686 | 57,80 | 0,5461 | 0,2304 | 0,3184 | 0,8223 | 3,0601 | 32,0100 | 0,81% | 1,74% | | 4,93% | 34,35% |
| CHLOROACETYL CHLORIDE | 581 | 51,10 | 0,3540 | 0,2568 | 0,3242 | 0,8175 | 2,2919 | 18,5229 | 0,53% | | | 3,87% | 21,06% |
| CHLOROCYCLOHEXANE | 638 | 38,27 | 0,2611 | 0,2631 | 0,2576 | 0,8531 | 2,5000 | 23,9624 | 0,76% | 2,32% | | 4,02% | 20,02% |
| CHLORODIFLUOROMETHANE | 369,3 | 49,71 | 0,2192 | 0,2678 | 0,4493 | 0,8383 | 1,4998 | 9,5406 | 0,99% | 2,15% | 1,73% | 4,31% | 18,29% |
| CHLOROFLUOROMETHANE | 427 | 56,20 | 0,2108 | 0,2486 | 0,7881 | 0,8852 | 0,9284 | 18,9856 | 4,28% | 6,06% | 1,08% | 6,24% | 24,41% |
| CHLOROFORM | 536,4 | 54,72 | 0,2219 | 0,2765 | 0,6193 | 0,8434 | 1,1567 | 8,0991 | 2,57% | 3,17% | 0,08% | 3,35% | 10,28% |
| CHLOROMETHYL METHYL ETHER | 521 | 50,30 | 0,2698 | 0,2653 | 0,7419 | 0,8932 | 1,1568 | 15,3448 | 0,75% | 1,18% | | 1,52% | 26,97% |
| CHLOROPENTAFLUOROETHANE | 353,15 | 31,57 | 0,2514 | 0,2757 | 0,3593 | 0,8398 | 1,8949 | 8,0816 | 0,82% | 1,95% | 1,56% | 2,96% | 19,82% |
| CHLOROPRENE | 525 | 42,60 | 0,1974 | 0,2611 | 0,2432 | 0,8605 | 2,3300 | 21,2436 | 0,03% | 1,35% | | 5,51% | 17,33% |
| CHLOROTRIFLUOROETHYLENE | 379,15 | 40,53 | 0,2442 | 0,2735 | 0,3009 | 0,8617 | 2,2631 | 8,8788 | 0,84% | 2,03% | | 1,76% | 18,11% |
| CHLOROTRIFLUOROMETHANE | 302 | 38,70 | 0,1717 | 0,2775 | 0,2067 | 0,8587 | 2,4157 | 6,2746 | 0,31% | 1,83% | 2,22% | 3,52% | 16,49% |
| CHRYSENE | 979 | 23,90 | 0,6030 | | 0,3294 | 0,8180 | 3,1550 | | 0,61% | 1,70% | 0,39% | | |
| CINNAMIC ACID | 797 | 35,40 | 0,7121 | 0,2339 | 0,3486 | 0,7908 | 3,1789 | 50,2526 | 1,50% | | | 4,12% | 33,11% |
| cis,trans-2,4-HEXADIENE | 538 | 33,50 | 0,2754 | 0,2534 | 0,2982 | 0,8264 | 2,1647 | 31,4787 | 0,56% | 2,36% | 0,14% | 5,34% | 24,96% |
| cis-1,2-DICHLOROETHYLENE | 544 | 51,90 | 0,1349 | 0,2598 | 1,6854 | 0,9456 | 0,3872 | 21,1029 | 0,38% | 0,98% | | 5,80% | 20,27% |
| cis-1,2-DIMETHYLCYCLOHEXANE | 606,15 | 29,38 | 0,2324 | 0,2544 | 1,2535 | 0,9848 | 0,6421 | 41,9757 | 0,40% | 0,78% | 0,50% | 5,89% | 15,16% |
| cis-1,2-DIMETHYLCYCLOPENTANE | 565,15 | 34,45 | 0,2662 | 0,2698 | 0,2869 | 0,8464 | 2,3023 | 17,0339 | 0,89% | 1,57% | 2,49% | 3,41% | 18,27% |
| cis-1,3-DICHLOROPROPENE | 594,4 | 47,04 | 0,2278 | 0,2617 | 0,7269 | 0,8740 | 1,0744 | 20,2801 | 0,70% | 1,68% | | 4,74% | 19,97% |
| cis-1,3-DIMETHYLCYCLOHEXANE | 591,15 | 29,38 | 0,2366 | 0,2639 | 1,2468 | 1,0000 | 0,6506 | 30,1653 | 0,31% | 0,73% | 0,42% | 4,47% | 17,20% |
| cis-1,3-DIMETHYLCYCLOPENTANE | 551 | 34,45 | 0,2743 | 0,2812 | 0,4003 | 0,8496 | 1,8654 | 6,4743 | 0,37% | 1,48% | 3,57% | 1,51% | 21,33% |
| cis-1,3-PENTADIENE | 499 | 37,40 | 0,1470 | 0,2559 | 1,3828 | 1,0000 | 0,4963 | 28,3087 | 2,87% | 2,67% | 0,54% | 6,99% | 23,72% |
| cis-1,4-DIMETHYLCYCLOHEXANE | 598,15 | 29,38 | 0,2311 | 0,2598 | 1,3142 | 1,0000 | 0,6076 | 35,7892 | 0,43% | 0,31% | 0,35% | 5,06% | 14,86% |
| cis-1,8-TERPIN | 694,8 | 29,49 | 1,0801 | | 0,5694 | 0,8140 | 3,2468 | | 0,86% | 1,01% | | | |
| cis-1-PROPENYLBENZENE | 671 | 33,60 | 0,3411 | 0,2573 | 0,8442 | 0,8877 | 1,1339 | 34,3929 | 0,81% | 1,93% | 1,76% | 2,78% | 27,54% |
| cis-2-BUTENE | 435,5 | 42,10 | 0,2019 | 0,2702 | 0,3984 | 0,8355 | 1,5731 | 12,0599 | 0,95% | 1,36% | 1,22% | 4,50% | 17,36% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| cis-2-DECENE | 621 | 21,80 | 0,4752 | 0,2513 | 0,3510 | 0,8152 | 2,5778 | 48,5755 | 0,64% | 2,12% | 2,96% | 3,51% | 25,58% |
| cis-2-DODECENE | 663 | 18,90 | 0,5692 | | 0,4154 | 0,8105 | 2,5628 | | 0,67% | 1,73% | 4,23% | | |
| cis-2-HEPTENE | 543,7 | 28,40 | 0,3363 | 0,2568 | 0,3017 | 0,8497 | 2,5540 | 30,8333 | 0,69% | 3,89% | 1,66% | 4,20% | 24,32% |
| cis-2-HEXENE | 511,4 | 31,60 | 0,2874 | 0,2600 | 0,4515 | 0,8442 | 1,7295 | 24,9747 | 0,56% | 2,23% | 1,79% | 4,57% | 22,77% |
| cis-2-METHYLCYCLOHEXANOL | 614 | 37,90 | 0,6805 | 0,2658 | 0,3917 | 0,8213 | 3,0828 | 8,1511 | 6,14% | 1,75% | 2,59% | 1,61% | 17,87% |
| cis-2-NONENE | 598,1 | 23,70 | 0,4304 | | 0,8035 | 0,9084 | 1,3948 | | 0,35% | 1,03% | | | |
| cis-2-OCTENE | 572 | 25,90 | 0,3889 | 0,2549 | 0,3620 | 0,8547 | 2,4751 | 35,9436 | 0,86% | 1,09% | 4,85% | 3,67% | 24,70% |
| cis-2-PENTENE | 475 | 36,40 | 0,2454 | 0,2716 | 0,3552 | 0,8379 | 1,8820 | 13,9712 | 0,62% | 3,32% | 2,53% | 2,24% | 19,07% |
| cis-2-PHENYLBUTENE-2 | 685 | 30,10 | 0,3564 | 0,2482 | 0,4058 | 0,8292 | 2,0451 | 47,8355 | 0,82% | 1,58% | | 4,74% | 24,02% |
| cis-3-HEPTENE | 545 | 28,40 | 0,2949 | 0,2588 | 0,3325 | 0,8227 | 2,0722 | 31,3088 | 0,28% | 0,64% | 0,28% | 4,51% | 18,89% |
| cis-3-HEXENE | 509 | 31,70 | 0,2787 | 0,2634 | 0,3913 | 0,8329 | 1,8491 | 22,4145 | 0,31% | 1,11% | 1,47% | 4,06% | 20,40% |
| cis-3-METHYLCYCLOHEXANOL | 625 | 37,90 | 0,6943 | 0,2682 | 0,5673 | 0,8012 | 2,2935 | 6,2069 | 0,45% | 1,81% | 0,96% | 1,37% | 20,54% |
| cis-3-OCTENE | 569 | 25,90 | 0,3800 | 0,2551 | 0,2813 | 0,8385 | 2,7449 | 35,6803 | 1,37% | 4,21% | 1,75% | 4,26% | 24,34% |
| cis-4-METHYLCYCLOHEXANOL | 622 | 37,90 | 0,6880 | 0,2699 | 0,4008 | 0,8218 | 3,0716 | 5,2415 | 1,10% | 1,73% | 2,74% | 1,12% | 20,21% |
| cis-4-OCTENE | 568 | 25,90 | 0,3854 | 0,2551 | 0,2829 | 0,8379 | 2,7542 | 35,3419 | 1,34% | 6,40% | 1,76% | 4,27% | 24,18% |
| cis-CROTONALDEHYDE | 554 | 45,90 | 0,3241 | | 1,0413 | 0,9387 | 0,9113 | | 1,18% | 2,04% | 2,88% | | |
| cis-CROTONIC ACID | 647 | 47,00 | 0,5723 | 0,2403 | 0,6166 | 0,8373 | 1,9932 | 29,5208 | 0,83% | | | 3,84% | 30,37% |
| cis-CROTONITRILE | 568 | 38,80 | 0,3787 | 0,2225 | 0,6093 | 0,8499 | 1,5305 | 50,5913 | 4,94% | 3,17% | 1,67% | 8,94% | 34,01% |
| cis-DECAHYDRONAPHTHALENE | 703,6 | 32,00 | 0,2791 | 0,2640 | 0,5419 | 0,8179 | 1,4026 | 30,4714 | 1,72% | 1,67% | 1,85% | 4,26% | 20,61% |
| cis-DICYANO-1-BUTENE | 796 | 29,50 | 0,6639 | | 0,5679 | 0,8292 | 2,3308 | | 0,24% | 0,83% | | | |
| cis-STILBENE | 784 | 27,40 | 0,4758 | 0,2506 | 0,3634 | 0,8406 | 2,7064 | 49,8288 | 1,50% | 1,69% | | 3,10% | 24,69% |
| CITRACONIC ACID | 829 | 42,40 | 0,9269 | | 0,5194 | 0,8187 | 3,1394 | | 0,79% | 1,12% | | | |
| CROTYL GLYCOL ETHER | 643,9 | 33,87 | 0,5532 | 0,2518 | 0,5591 | 0,7997 | 1,9940 | 30,3867 | 0,76% | | | 2,54% | 25,38% |
| CUMENE | 631 | 32,09 | 0,3274 | 0,2626 | 1,2646 | 0,9977 | 0,7415 | 27,4205 | 1,97% | 1,91% | 1,53% | 3,66% | 19,25% |
| CYANOGEN | 400,15 | 59,24 | 0,2756 | 0,2615 | 0,9049 | 0,9995 | 1,0129 | 9,5918 | 0,10% | 1,95% | | 3,61% | 17,62% |
| CYANOGEN CHLORIDE | 449 | 59,90 | 0,3221 | 0,2363 | 0,7362 | 0,9604 | 1,3632 | 20,4664 | 0,55% | 1,09% | | 5,12% | 14,89% |
| CYCLOBUTANE | 459,93 | 49,80 | 0,1847 | 0,2701 | 0,2545 | 0,8692 | 2,2675 | 9,6317 | 0,48% | 1,95% | 1,79% | 5,74% | 17,30% |
| CYCLOHEPTANE | 604,2 | 38,20 | 0,2408 | 0,2725 | 0,2653 | 0,8585 | 2,4188 | 14,9107 | 0,64% | 1,69% | 0,58% | 2,91% | 19,96% |
| CYCLOHEPTENE | 598 | 40,10 | 0,2517 | 0,2786 | 1,2066 | 1,0000 | 0,6865 | 10,0273 | 0,73% | 2,42% | 2,66% | 1,91% | 20,02% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| CYCLOHEXANE | 553,8 | 40,80 | 0,2081 | 0,2730 | 0,3133 | 0,8336 | 1,8785 | 13,3342 | 0,49% | 1,22% | 0,48% | 3,47% | 17,81% |
| CYCLOHEXANECARBOXALDEHYDE | 639,4 | 35,79 | 0,3827 | 0,2552 | 0,3146 | 0,8450 | 2,6316 | 29,5007 | 1,20% | | 0,78% | 3,53% | 22,86% |
| CYCLOHEXANOL | 650,1 | 42,60 | 0,3690 | 0,2575 | 3,0023 | 1,0000 | 0,3143 | 23,7782 | 2,46% | 4,00% | 9,28% | 4,68% | 23,96% |
| CYCLOHEXANONE | 653 | 40,00 | 0,2990 | 0,2454 | 0,2767 | 0,8503 | 2,5448 | 37,6232 | 0,44% | 1,22% | | 5,86% | 33,38% |
| CYCLOHEXANONE OXIME | 715 | 46,90 | 0,4620 | | 0,2868 | 0,8270 | 2,9632 | | 0,57% | 1,30% | | | |
| CYCLOHEXENE | 560,4 | 43,50 | 0,2123 | 0,2723 | 0,5878 | 0,8470 | 1,2020 | 13,5910 | 1,70% | 2,28% | 1,30% | 3,91% | 18,02% |
| CYCLOHEXYL ACETATE | 648 | 31,20 | 0,4209 | 0,2622 | 0,4867 | 0,8173 | 1,9184 | 24,5894 | 0,44% | 2,42% | 0,85% | 2,71% | 26,38% |
| CYCLOHEXYL FORMATE | 645 | 35,20 | 0,3679 | 0,2629 | 0,2771 | 0,8392 | 2,7313 | 23,1350 | 1,40% | 1,46% | 1,60% | 2,61% | 26,23% |
| CYCLOHEXYL HYDROPEROXIDE | 685 | 42,10 | 0,7571 | 0,2632 | 0,6471 | 0,8267 | 2,2811 | 10,3128 | 0,83% | 0,78% | | 1,40% | 23,77% |
| CYCLOHEXYL ISOCYANATE | 633 | 34,70 | 0,5247 | 0,2514 | 0,7056 | 0,8472 | 1,6887 | 32,6760 | 0,95% | 0,88% | | 1,69% | 15,91% |
| CYCLOHEXYL MERCAPTAN | 664 | 39,70 | 0,2641 | 0,2695 | 0,2265 | 0,8458 | 2,6186 | 18,0993 | 1,19% | 2,46% | 0,24% | 3,07% | 25,48% |
| CYCLOHEXYLAMINE | 615 | 42,00 | 0,3604 | 0,2767 | 0,3005 | 0,8482 | 2,5783 | 7,6224 | 3,52% | 3,47% | 3,90% | 1,91% | 10,61% |
| CYCLOHEXYLBENZENE | 744 | 28,80 | 0,3783 | 0,2644 | 1,5193 | 1,0000 | 0,6569 | 33,0709 | 0,72% | 1,11% | | 1,83% | 29,09% |
| CYCLOOCTANE | 647,2 | 35,60 | 0,2524 | 0,2709 | 0,1928 | 0,8392 | 2,7320 | 19,1910 | 0,39% | 1,29% | 1,15% | 3,05% | 18,21% |
| CYCLOOCTENE | 632 | 36,80 | 0,2804 | 0,2711 | 1,0469 | 1,0000 | 0,8613 | 16,1682 | 0,78% | 0,72% | | 3,31% | 18,81% |
| CYCLOPENTADIENE | 507 | 51,50 | 0,2020 | 0,2741 | 0,5239 | 0,9428 | 1,5039 | 8,7905 | 1,82% | 3,78% | | 3,73% | 17,36% |
| CYCLOPENTANE | 511,7 | 45,10 | 0,1949 | 0,2691 | 0,3229 | 0,8496 | 1,8673 | 12,6704 | 0,33% | 2,63% | 1,99% | 5,85% | 16,07% |
| CYCLOPENTANONE | 624,5 | 46,00 | 0,2876 | 0,2469 | 0,5742 | 0,8508 | 1,4326 | 30,5607 | 1,18% | 1,72% | 2,87% | 6,30% | 33,99% |
| CYCLOPENTENE | 507 | 48,00 | 0,1961 | 0,2763 | 0,5187 | 0,8593 | 1,3153 | 8,9979 | 1,24% | 2,76% | 1,20% | 3,47% | 15,81% |
| CYCLOPENTYLACETIC ACID | 708 | 36,20 | 0,6144 | 0,2521 | 0,9197 | 0,8419 | 1,4623 | 28,7743 | 1,67% | | | 2,47% | 25,19% |
| CYCLOPENTYLAMINE | 584 | 46,40 | 0,3294 | 0,2702 | 1,0433 | 1,0000 | 0,9397 | 10,6340 | 0,66% | 0,94% | | 3,73% | 9,80% |
| CYCLOPROPANE | 398 | 55,40 | 0,1278 | 0,2776 | 0,2344 | 0,8713 | 2,1266 | 6,3601 | 0,76% | 1,36% | 2,90% | 3,83% | 18,98% |
| CYCLOPROPANE CARBOXYLIC ACID | 671 | 59,95 | 0,6048 | 0,2644 | 1,1685 | 0,9838 | 1,1796 | 8,9419 | 1,95% | | 1,47% | 1,39% | 21,48% |
| CYCLOPROPANECARBOXAMIDE | 779,1 | 57,39 | 0,5726 | | 0,3910 | 0,8208 | 2,7541 | | 0,53% | 2,12% | | | |
| CYCLOPROPYL CYANIDE | 621,9 | 44,62 | 0,3415 | 0,2202 | 0,7029 | 0,9056 | 1,3828 | 49,9114 | 2,16% | | 0,72% | 9,04% | 38,42% |
| CYCLOPROPYLAMINE | 508,6 | 57,48 | 0,3038 | 0,2649 | 0,4136 | 0,8833 | 2,0888 | 10,3942 | 0,61% | | | 3,45% | 23,60% |
| DECAFLUOROBUTANE | 386,35 | 23,23 | 0,3664 | 0,2710 | 0,3392 | 0,8339 | 2,3797 | 12,6324 | 0,81% | 1,48% | | 2,45% | 18,60% |
| DECAMETHYLCYCLOPENTASILOXANE | 617,4 | 10,35 | 0,6223 | 0,2485 | 1,4470 | 1,0000 | 0,9334 | 100,1402 | 0,73% | 0,65% | | 2,75% | 26,27% |
| DECAMETHYLTETRASILOXANE | 599,4 | 11,90 | 0,6596 | 0,2627 | 0,8760 | 0,8824 | 1,6465 | 39,8932 | 0,36% | 0,54% | | 1,45% | 23,28% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| DECAN-1,10-DIOL | 747 | 21,10 | 0,9194 | 0,2184 | 0,5893 | 0,8155 | 2,7946 | 95,1973 | 1,60% | | | 4,93% | 45,48% |
| DECANAL | 674 | 26,00 | 0,5201 | 0,2696 | 1,3294 | 1,0000 | 0,9208 | 15,1008 | 0,97% | 0,26% | | 2,02% | 22,32% |
| DEHYDROABIETIC ACID | 828 | 17,50 | 0,9154 | | 0,4999 | 0,8166 | 3,1862 | | 1,07% | 0,97% | | | |
| DEHYDROABIETYLAMINE | 863 | 17,00 | 0,7415 | | 0,5466 | 0,8236 | 2,5783 | | 0,65% | 1,17% | | | |
| DEUTERIUM OXIDE | 643,89 | 216,71 | 0,3658 | 0,2253 | 0,3817 | 0,8616 | 2,3397 | 9,2306 | 0,41% | 2,25% | 1,84% | 10,61% | 29,87% |
| DI-(2-CHLOROETHOXY)METHANE | 696,2 | 30,66 | 0,5230 | 0,2465 | 0,5206 | 0,8473 | 2,2096 | 43,1492 | 0,75% | 1,48% | | 3,09% | 26,06% |
| DI(2-CHLOROETHYL)ETHER | 666 | 35,90 | 0,3940 | 0,2470 | 0,5600 | 0,7820 | 1,5759 | 39,0941 | 2,06% | | 0,16% | 5,18% | 30,51% |
| DI-2-ETHYLHEXYLAMINE | 702 | 14,70 | 0,9179 | 0,2485 | 0,5470 | 0,8193 | 2,9825 | 61,3790 | 0,38% | 1,44% | | 1,32% | 28,14% |
| DIACETYL | 546,9 | 43,84 | 0,3641 | 0,2536 | 0,4756 | 0,7969 | 1,7420 | 22,4789 | 0,69% | 1,93% | | 4,02% | 22,91% |
| DIALLYL MALEATE | 693 | 23,30 | 0,7886 | 0,2450 | 0,6328 | 0,8281 | 2,4012 | 48,5172 | 0,76% | 1,02% | | 1,64% | 28,02% |
| DIALLYL PHTHALATE | 790,2 | 20,96 | 0,7345 | | 0,6942 | 0,8294 | 2,1077 | | 0,93% | 1,68% | | | |
| DIALLYL SULFIDE | 653,53 | 33,59 | 0,0824 | 0,2492 | 0,8597 | 0,0000 | 0,5464 | 51,5157 | 1,75% | | | 10,38% | 26,68% |
| DIALLYLAMINE | 556 | 33,20 | 0,4483 | 0,2768 | 0,6652 | 0,8506 | 1,6210 | 10,8892 | 0,81% | 0,92% | | 3,24% | 15,62% |
| DIAMANTANE | 791 | 22,60 | 0,1633 | | 0,2512 | 0,8727 | 2,2217 | | 0,47% | 3,46% | | | |
| DIAMYL KETONE | 678,5 | 20,52 | 0,5928 | 0,2479 | 0,5398 | 0,8087 | 2,1713 | 58,4583 | 0,75% | | | 2,65% | 23,98% |
| DIAMYLAMINE | 639 | 21,20 | 0,6767 | 0,2521 | 0,4218 | 0,8266 | 2,9720 | 39,2313 | 0,83% | 1,44% | | 1,98% | 26,57% |
| DIBENZOFURAN | 824 | 36,40 | 0,3988 | 0,2632 | 0,3227 | 0,8448 | 2,6343 | 29,2953 | 2,73% | 3,32% | 1,96% | 1,63% | 20,83% |
| DIBENZOPYRROLE | 899 | 32,60 | 0,4938 | | 0,4834 | 0,8635 | 2,3470 | | 2,33% | 4,84% | 0,60% | | |
| DIBENZOTHIOPHENE | 897 | 38,60 | 0,3983 | | 0,3598 | 0,8524 | 2,5113 | | 0,52% | 1,62% | | | |
| DIBORANE | 289,8 | 40,53 | 0,1311 | 0,2845 | 0,5261 | 0,8614 | 1,1240 | 3,9371 | 1,33% | 2,22% | 0,79% | 3,16% | 12,21% |
| DIBROMODIFLUOROMETHANE | 478 | 40,70 | 0,1085 | 0,2496 | 0,1498 | 0,8296 | 2,1614 | 27,4955 | 0,73% | | | 11,35% | 19,68% |
| DIBROMOMETHANE | 611 | 71,70 | 0,2095 | 0,2869 | 0,3604 | 0,8346 | 1,6913 | 2,5050 | 2,15% | 2,29% | 2,85% | 1,70% | 4,78% |
| DIBUTYL MALEATE | 716 | 19,00 | 0,8994 | 0,2450 | 0,5395 | 0,8206 | 2,9859 | 55,2378 | 0,67% | 1,06% | | 2,12% | 37,58% |
| DIBUTYL SEBACATE | 768 | 13,20 | 1,1245 | 0,2375 | 0,6695 | 0,8262 | 2,9791 | 93,1325 | 0,36% | 1,81% | 6,37% | 1,91% | 44,70% |
| DIBUTYL TEREPHTHALATE | 787,2 | 16,94 | 0,9642 | 0,2358 | 0,6735 | 0,8409 | 2,7020 | 84,6367 | 1,44% | | | 1,70% | 37,36% |
| DICHLOROACETALDEHYDE | 555 | 49,50 | 0,3437 | 0,2561 | 0,2767 | 0,8421 | 2,6800 | 18,7086 | 0,85% | 1,94% | | 3,84% | 22,19% |
| DICHLOROACETIC ACID | 686 | 51,70 | 0,5550 | 0,2531 | 0,4730 | 0,8227 | 2,3611 | 21,2056 | 0,79% | 1,11% | | 1,41% | 30,77% |
| DICHLOROACETYL CHLORIDE | 585 | 46,10 | 0,3089 | 0,2686 | 0,5460 | 0,8498 | 1,5578 | 12,9711 | 0,70% | 1,32% | | 3,22% | 19,69% |
| DICHLORODIETHYLSILANE | 595,75 | 30,60 | 0,3189 | 0,2733 | 1,4200 | 1,0000 | 0,6502 | 15,7454 | 0,79% | 1,40% | | 2,40% | 14,97% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| DICHLORODIFLUOROMETHANE | 384,95 | 41,25 | 0,1797 | 0,2765 | 0,2133 | 0,8588 | 2,4139 | 7,9500 | 0,40% | 1,41% | 6,10% | 3,53% | 15,52% |
| DICHLOROFLUOROMETHANE | 451,58 | 51,84 | 0,2048 | 0,2712 | 0,2039 | 0,8506 | 2,5401 | 9,4991 | 0,40% | 1,38% | 2,11% | 3,93% | 18,33% |
| DICHLOROMETHANE | 510 | 60,80 | 0,1986 | 0,2633 | 0,6974 | 0,8397 | 1,0008 | 13,8040 | 2,43% | 1,39% | 1,03% | 4,83% | 18,20% |
| DICHLOROSILANE | 451,5 | 45,99 | 0,1630 | 0,2781 | 0,1835 | 0,8416 | 2,3573 | 8,4924 | 0,50% | | | 3,09% | 11,22% |
| DICYANDIAMIDE | 834 | 53,40 | 0,6924 | | 0,3769 | 0,8170 | 3,1787 | | 0,62% | 1,13% | | | |
| DICYCLOHEXYL SULFIDE | 802 | 26,50 | 0,3955 | 0,2676 | 0,4602 | 0,8475 | 2,0595 | 30,5250 | 0,86% | 1,91% | 4,56% | 1,46% | 14,32% |
| DICYCLOPENTADIENE | 660 | 30,60 | 0,2880 | 0,2645 | 0,1777 | 0,8300 | 2,9026 | 36,3411 | 0,54% | 1,88% | 0,46% | 1,21% | 26,16% |
| DIETHANOLAMINE | 736,6 | 42,70 | 0,9529 | 0,2170 | 0,6949 | 0,8459 | 2,6157 | 44,7989 | 1,95% | 1,52% | | 6,10% | 24,15% |
| DIETHYL CARBONATE | 576 | 33,90 | 0,4857 | 0,2567 | 0,4199 | 0,8520 | 2,5175 | 22,6412 | 6,76% | 6,79% | | 2,79% | 25,92% |
| DIETHYL DISULFIDE | 642 | 38,70 | 0,3469 | 0,2695 | 0,3555 | 0,8610 | 2,3813 | 14,6396 | 2,87% | 2,74% | 2,90% | 2,12% | 24,34% |
| DIETHYL ETHER | 466,7 | 36,40 | 0,2811 | 0,2641 | 0,6670 | 0,8231 | 1,2031 | 17,3234 | 1,88% | 2,17% | 4,71% | 4,58% | 20,72% |
| DIETHYL MALEATE | 680 | 26,10 | 0,6658 | 0,2614 | 0,6397 | 0,8705 | 2,2508 | 21,7207 | 1,09% | | | 1,46% | 37,86% |
| DIETHYL MALONATE | 653 | 27,80 | 0,6155 | 0,2519 | 1,2153 | 0,9886 | 1,1394 | 35,3118 | 0,38% | | | 1,76% | 31,28% |
| DIETHYL PHTHALATE | 776 | 22,60 | 0,6249 | 0,2410 | 0,3618 | 0,8211 | 3,0866 | 70,6470 | 1,61% | 2,68% | | 2,92% | 28,05% |
| DIETHYL SUCCINATE | 663 | 25,30 | 0,6995 | 0,2525 | 0,4271 | 0,8261 | 2,9815 | 37,0306 | 5,60% | 3,60% | 4,63% | 1,32% | 21,47% |
| DIETHYL SULFATE | 749 | 64,80 | 0,3865 | 0,3829 | 1,1724 | 1,0000 | 0,8888 | -66,5830 | 1,26% | | 1,23% | 9,82% | 2,78% |
| DIETHYL SULFIDE | 557,15 | 39,60 | 0,2900 | 0,2665 | 0,4631 | 0,8343 | 1,6547 | 16,7189 | 0,84% | 2,59% | 1,49% | 4,01% | 17,36% |
| DIETHYLALUMINUM CHLORIDE | 723,15 | 30,00 | 0,3177 | | 1,4195 | 1,0000 | 0,6508 | | 0,86% | 1,49% | | | |
| DIETHYLAMINE | 496,6 | 37,10 | 0,3039 | 0,2611 | 0,5112 | 0,8212 | 1,5510 | 19,6684 | 0,46% | 2,55% | 1,02% | 4,22% | 16,71% |
| DIETHYLENE GLYCOL | 744,6 | 46,00 | 0,6221 | 0,2291 | 0,5980 | 0,8411 | 2,2033 | 39,6026 | 2,81% | | | 6,68% | 31,09% |
| DIETHYLENE GLYCOL DIETHYL ETHER | 624 | 23,70 | 0,6807 | 0,2550 | 0,5158 | 0,8439 | 2,6504 | 31,1923 | 0,97% | 1,76% | | 1,40% | 25,18% |
| DIETHYLENE GLYCOL DIMETHYL ETHER | 608 | 28,60 | 0,5775 | 0,2553 | 0,3995 | 0,8345 | 2,8181 | 29,2730 | 0,90% | 0,76% | | 1,46% | 32,68% |
| DIETHYLENE GLYCOL DI-n-BUTYL ETHER | 680 | 17,60 | 0,8455 | 0,2499 | 0,6662 | 0,8495 | 2,5566 | 48,1100 | 4,99% | | | 1,82% | 27,36% |
| DIETHYLENE GLYCOL ETHYL ETHER ACETATE | 660 | 24,20 | 0,7145 | 0,2490 | 0,7478 | 0,8858 | 2,0595 | 40,5756 | 2,66% | 4,38% | | 1,52% | 26,60% |
| DIETHYLENE GLYCOL MONOBUTYL ETHER ACETATE | 679 | 20,60 | 0,8420 | 0,2487 | 0,4892 | 0,8218 | 3,0709 | 44,7616 | 1,10% | | 2,16% | 1,46% | 27,38% |
| DIETHYLENE GLYCOL MONOPROPYL ETHER | 679,8 | 30,02 | 0,6114 | 0,2609 | 0,3516 | 0,8216 | 3,0753 | 23,2658 | 1,70% | 2,27% | 7,41% | 1,43% | 23,59% |
| DIETHYLSULFITE | 624 | 37,70 | 0,5065 | 0,2758 | 0,5240 | 0,8714 | 2,2385 | 4,4868 | 1,02% | 3,52% | | 1,40% | 21,78% |
| DIFLUOROMETHANE | 351,255 | 57,84 | 0,2771 | 0,2440 | 0,3318 | 0,8589 | 2,2045 | 15,0288 | 0,95% | 2,12% | 0,76% | 5,93% | 24,62% |
| DIFLUOROMETHYL TRIFLUOROMETHYL ETHER | 354,49 | 33,76 | 0,3253 | 0,2642 | 0,3510 | 0,8412 | 2,2196 | 11,1244 | 0,67% | 1,66% | 3,57% | 5,00% | 32,02% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| DIGLYCOLIC ACID | 820 | 44,20 | 1,0807 | | 0,5794 | 0,8155 | 3,2113 | | 1,20% | 1,14% | | | |
| DIHEXYL ADIPATE | 767 | 13,20 | 1,0935 | 0,2422 | 0,6494 | 0,8168 | 2,9658 | 84,0208 | 2,12% | 1,65% | 5,28% | 2,57% | 45,37% |
| DIIODOMETHANE | 747 | 54,70 | 0,1405 | 0,2379 | 0,0875 | 0,8347 | 2,8133 | 42,4285 | 1,14% | 2,59% | 4,66% | 10,04% | 23,55% |
| DIISOBUTYL ETHER | 562 | 25,30 | 0,4243 | 0,2703 | 0,2884 | 0,8327 | 2,8509 | 15,5705 | 0,39% | 4,62% | 1,12% | 1,87% | 23,22% |
| DIISOBUTYL KETONE | 615 | 24,80 | 0,5116 | 0,2581 | 0,3889 | 0,8411 | 2,6972 | 29,2046 | 3,31% | 3,12% | | 2,77% | 26,07% |
| DIISOBUTYL PHTHALATE | 762 | 17,80 | 0,9158 | 0,2503 | 0,5777 | 0,8248 | 2,8873 | 50,6067 | 1,06% | 1,73% | | 2,03% | 27,48% |
| DIISOBUTYLAMINE | 580 | 25,70 | 0,4854 | 0,2689 | 0,9813 | 0,9628 | 1,2452 | 15,2826 | 0,48% | | | 1,76% | 16,45% |
| DIISONONYL PHTHALATE | 835 | 10,80 | 1,0312 | | 0,6012 | 0,8227 | 3,0519 | | 1,44% | 1,35% | 1,80% | | |
| DIISOOCTYL PHTHALATE | 851 | 11,80 | 1,0880 | 0,2367 | 0,7181 | 0,8215 | 2,7183 | 127,4306 | 1,72% | 1,89% | 1,31% | 2,40% | 31,78% |
| DIISOPENTYLSULFIDE | 664,4 | 21,81 | 0,5971 | 0,2580 | 0,7533 | 0,8916 | 1,8199 | 33,6089 | 0,84% | | | 1,65% | 25,49% |
| DIISOPROPYL ETHER | 500,05 | 28,80 | 0,3387 | 0,2699 | 1,2124 | 1,0000 | 0,7901 | 15,9634 | 0,74% | 3,87% | 0,79% | 3,13% | 20,53% |
| DIISOPROPYL KETONE | 576 | 30,20 | 0,4044 | 0,2630 | 1,0361 | 0,9966 | 1,0609 | 21,6134 | 1,04% | 1,02% | | 3,12% | 21,87% |
| DIISOPROPYL SULFIDE | 585,2 | 32,25 | 0,3144 | 0,2782 | 0,2709 | 0,8464 | 2,6083 | 8,5188 | 1,16% | 2,42% | 1,30% | 1,68% | 19,13% |
| DIKETENE | 616 | 59,60 | 0,3821 | | 0,6875 | 0,8136 | 1,3647 | | 1,50% | | 1,33% | | |
| DILACTIC ACID | 660 | 34,80 | 0,9068 | | 0,5392 | 0,8240 | 3,0261 | | 0,70% | 0,73% | 2,85% | | |
| DIMERCAPTOETHYL ETHER | 720 | 36,90 | 0,4193 | 0,2454 | 0,5847 | 0,8460 | 1,7357 | 41,6618 | 1,01% | 1,46% | | 4,31% | 32,04% |
| DIMETHYL CARBONATE | 548 | 45,00 | 0,3846 | 0,2490 | 0,4117 | 0,8666 | 2,3035 | 23,3811 | 1,05% | 2,39% | | 4,18% | 25,15% |
| DIMETHYL DISULFIDE | 615 | 53,60 | 0,2059 | 0,2756 | 0,4394 | 0,8261 | 1,4532 | 10,1319 | 1,00% | 1,33% | 1,28% | 3,10% | 22,17% |
| DIMETHYL ETHER | 400,1 | 53,70 | 0,2002 | 0,2736 | 0,5121 | 0,8494 | 1,3199 | 7,5304 | 1,89% | 3,30% | 1,06% | 3,71% | 17,04% |
| DIMETHYL MALEATE | 675 | 32,20 | 0,5624 | 0,2391 | 0,3770 | 0,8276 | 2,8346 | 46,4885 | 0,61% | 1,80% | 2,51% | 3,94% | 32,63% |
| DIMETHYL PHTHALATE | 766 | 27,80 | 0,6568 | 0,2443 | 1,1014 | 0,9645 | 1,3317 | 50,7668 | 0,45% | | | 2,06% | 34,51% |
| DIMETHYL SILANE | 402 | 35,60 | 0,1300 | 0,2704 | 0,2257 | 0,8728 | 2,2196 | 14,9326 | 2,97% | 1,83% | | 4,50% | 15,51% |
| DIMETHYL SUCCINATE | 657 | 32,80 | 0,6223 | 0,2505 | 0,6347 | 0,8760 | 2,1794 | 30,1366 | 3,95% | | | 2,19% | 23,82% |
| DIMETHYL SULFIDE | 503,04 | 55,30 | 0,1943 | 0,2662 | 0,2737 | 0,8496 | 2,0632 | 12,2665 | 1,35% | 2,40% | 1,67% | 5,42% | 19,32% |
| DIMETHYL SULFOXIDE | 729 | 56,50 | 0,2806 | 0,2353 | 1,3601 | 1,0000 | 0,6427 | 38,7376 | 2,12% | 2,15% | 1,51% | 6,74% | 40,47% |
| DIMETHYL TEREPHTHALATE | 777,4 | 27,60 | 0,5807 | 0,2358 | 0,6187 | 0,8792 | 2,1388 | 64,8937 | 0,89% | | | 3,91% | 35,30% |
| DIMETHYL-1,4-CYCLOHEXANEDICARBOXYLATE | 736 | 24,90 | 0,6412 | 0,2420 | 0,3620 | 0,8198 | 3,1143 | 55,6848 | 1,61% | 1,73% | 6,87% | 3,54% | 34,19% |
| DIMETHYL-2,6-NAPHTHALENEDICARBOXYLATE | 883 | 24,85 | 0,6853 | | 0,4158 | 0,8247 | 3,0108 | | 0,45% | 1,21% | | | |
| DIMETHYLACETYLENE | 473,2 | 48,70 | 0,2385 | 0,2648 | 0,3213 | 0,8397 | 1,9946 | 13,5117 | 0,22% | 1,30% | 0,58% | 3,85% | 15,74% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| DIMETHYLALUMINUM CHLORIDE | 619 | 36,20 | 0,1834 | 0,2253 | 0,7407 | 0,3061 | 0,7176 | 64,9174 | 1,23% | | | 10,93% | 27,81% |
| DIMETHYLAMINE | 437,2 | 53,40 | 0,2999 | 0,2611 | 1,2686 | 0,8804 | 0,7039 | 11,4630 | 2,91% | 3,48% | 1,67% | 5,78% | 19,69% |
| DIMETHYLCHLOROSILANE | 472 | 36,20 | 0,2526 | 0,2677 | 0,5495 | 0,9315 | 1,5996 | 14,1320 | 0,79% | 2,37% | | 4,33% | 16,13% |
| DIMETHYLDICHLOROSILANE | 520,35 | 34,90 | 0,2675 | 0,2756 | 1,2377 | 1,0000 | 0,6883 | 12,3105 | 0,66% | 1,13% | 3,39% | 2,37% | 11,99% |
| DIMETHYLDIMETHOXYSILANE | 524 | 26,60 | 0,2629 | 0,2495 | 2,5091 | 0,3687 | 0,4909 | 44,1929 | 0,90% | | | 7,93% | 13,78% |
| DIMETHYLETHANOLAMINE | 571,82 | 41,40 | 0,7110 | 0,2612 | 0,4717 | 0,8213 | 2,7986 | 11,0371 | 1,03% | 1,24% | | 1,31% | 23,92% |
| DIMETHYLKETENE | 470,2 | 42,35 | 0,3112 | | 0,5765 | 0,9242 | 1,6644 | | 1,02% | | 8,01% | | |
| DI-n-BUTYL ETHER | 584,1 | 24,60 | 0,4476 | 0,2586 | 0,4532 | 0,8290 | 2,1510 | 31,2464 | 0,61% | 1,45% | 1,47% | 2,78% | 28,71% |
| DI-n-BUTYL PHTHALATE | 781 | 17,50 | 0,9569 | 0,2466 | 0,6769 | 0,8410 | 2,7005 | 59,0742 | 2,95% | | | 2,50% | 39,22% |
| DI-n-BUTYL SULFATE | 814 | 60,00 | 0,3651 | 0,4635 | 0,3097 | 0,8140 | 2,3694 | -151,9301 | 0,56% | | 3,98% | 16,84% | 13,31% |
| DI-n-BUTYL SULFIDE | 652 | 25,79 | 0,4665 | 0,2560 | 0,3620 | 0,8419 | 2,6842 | 34,7705 | 0,60% | | | 3,29% | 28,55% |
| DI-n-BUTYL SULFONE | 767 | 25,40 | 0,6877 | 0,2416 | 0,4822 | 0,8218 | 2,6881 | 57,6829 | 0,71% | 1,04% | | 2,53% | 36,94% |
| DI-n-BUTYLAMINE | 602,3 | 25,70 | 0,5296 | 0,2618 | 0,3499 | 0,8319 | 2,8661 | 23,6400 | 4,15% | 2,15% | 2,58% | 2,07% | 22,24% |
| DI-n-DECYL PHTHALATE | 905 | 9,95 | 0,8906 | 0,2194 | 0,5538 | 0,8273 | 2,9577 | 237,0580 | 1,82% | 2,60% | | 5,02% | 54,31% |
| DI-n-HEXYL ETHER | 658 | 18,16 | 0,7105 | 0,2486 | 0,5296 | 0,8147 | 2,5192 | 52,8256 | 0,67% | 1,30% | 2,44% | 1,97% | 36,30% |
| DI-n-HEXYL PHTHALATE | 793 | 14,00 | 1,1245 | 0,2377 | 0,8582 | 0,8333 | 2,3823 | 86,8567 | 0,97% | 0,92% | 1,74% | 1,89% | 39,90% |
| DI-n-NONYL PHTHALATE | 866 | 10,70 | 0,9961 | 0,2434 | 2,5826 | 1,0000 | 0,6880 | 128,8476 | 5,84% | | 2,58% | 3,90% | 54,32% |
| DI-n-OCTYL ETHER | 707 | 14,40 | 0,9336 | 0,2423 | 0,5266 | 0,8166 | 3,1048 | 74,0253 | 0,80% | 1,28% | 1,84% | 1,55% | 41,39% |
| DI-n-OCTYL TEREPHTHALATE | 855 | 11,60 | 1,0895 | 0,2342 | 0,6565 | 0,8154 | 2,9303 | 139,9874 | 1,49% | 1,77% | 1,24% | 1,65% | 32,14% |
| DI-n-OCTYLAMINE | 734 | 12,60 | 0,8187 | 0,2256 | 0,5988 | 0,8395 | 2,6470 | 153,7267 | 0,31% | | | 2,92% | 33,70% |
| DINONYL ETHER | 736 | 13,00 | 1,0021 | 0,2426 | 0,6434 | 0,8326 | 2,8536 | 84,3969 | 0,77% | | | 1,76% | 45,56% |
| DINONYLPHENOL | 902 | 12,40 | 1,1246 | | 0,6356 | 0,8204 | 3,1018 | | 1,54% | 1,33% | | | |
| DI-n-PENTYL ETHER | 622 | 20,90 | 0,6012 | 0,2534 | 0,3865 | 0,8292 | 2,9190 | 40,1165 | 1,76% | 7,03% | 2,48% | 2,03% | 32,33% |
| DI-n-PROPYL DISULFIDE | 675 | 30,30 | 0,4370 | 0,2649 | 0,4514 | 0,8396 | 2,1489 | 22,9727 | 0,87% | 2,08% | 2,92% | 1,72% | 28,39% |
| DI-n-PROPYL ETHER | 530,6 | 30,28 | 0,3688 | 0,2652 | 0,3257 | 0,8497 | 2,5547 | 18,0463 | 1,31% | 2,61% | 3,35% | 3,29% | 22,41% |
| DI-n-PROPYL SULFIDE | 608 | 30,80 | 0,3740 | 0,2600 | 0,3140 | 0,8459 | 2,6169 | 26,5464 | 1,22% | 2,63% | 1,50% | 3,39% | 26,35% |
| DI-n-PROPYL SULFONE | 763 | 31,10 | 0,5821 | 0,2415 | 0,6579 | 0,8343 | 1,8917 | 51,1393 | 0,26% | 0,16% | | 3,41% | 35,81% |
| DI-n-PROPYLAMINE | 550 | 31,40 | 0,4497 | 0,2689 | 0,3371 | 0,8397 | 2,7230 | 12,8536 | 2,04% | 1,36% | 2,10% | 2,00% | 17,56% |
| DIPHENYL DISULFIDE | 829,8 | 35,69 | 0,5697 | | 0,1953 | 0,7410 | 3,0566 | | 0,46% | | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| DIPHENYL ETHER | 766,8 | 30,80 | 0,4389 | 0,2557 | 0,5177 | 0,8818 | 2,1066 | 38,2131 | 1,60% | 2,17% | | 2,29% | 29,58% |
| DIPHENYLACETYLENE | 832 | 29,00 | 0,3836 | | 0,4407 | 0,8342 | 2,0279 | | 0,69% | 1,31% | | | |
| DIPHENYLAMINE | 817 | 31,80 | 0,5297 | 0,2493 | 0,4465 | 0,8506 | 2,5400 | 44,8019 | 0,94% | 1,37% | | 2,68% | 23,79% |
| DIPHENYLDICHLOROSILANE | 814 | 23,30 | 0,4283 | 0,2423 | 1,5414 | 0,9077 | 0,7030 | 78,9489 | 2,08% | | 1,43% | 6,43% | 31,94% |
| DIPHENYLMETHANE | 760 | 27,10 | 0,4816 | 0,2424 | 0,3373 | 0,8349 | 2,8093 | 60,6971 | 1,01% | 0,90% | | 4,39% | 27,27% |
| DIPROPYL MALEATE | 691 | 22,00 | 0,7815 | 0,2468 | 0,4602 | 0,8224 | 3,0598 | 47,3724 | 1,06% | 1,56% | | 1,49% | 34,06% |
| DIPROPYLENE GLYCOL n-BUTYL ETHER | 647,1 | 20,96 | 1,0022 | 0,2563 | 0,6887 | 0,8371 | 2,7688 | 22,6580 | 4,88% | | | 2,79% | 26,02% |
| DIPROPYLENE GLYCOL t-BUTYL ETHER | 667 | 22,30 | 0,9966 | | 0,5451 | 0,8169 | 3,1784 | | 1,14% | 1,68% | 2,71% | | |
| DI-sec-BUTYL ETHER | 559 | 25,30 | 0,4319 | 0,2687 | 0,3501 | 0,8446 | 2,6378 | 17,0032 | 2,11% | 2,50% | 2,51% | 1,77% | 20,52% |
| DISILANE | 432 | 51,30 | 0,0939 | 0,3179 | 0,2010 | 0,8765 | 2,1727 | -13,1838 | 1,00% | 2,51% | | 1,60% | 10,57% |
| DI-t-BUTYL PEROXIDE | 547 | 24,80 | 0,4031 | 0,2794 | 0,2874 | 0,8353 | 2,8026 | 4,0898 | 0,90% | 1,72% | | 1,68% | 19,53% |
| DI-tert-BUTYL DISULFIDE | 689,7 | 31,59 | 0,4020 | | 0,4985 | 0,8838 | 2,0832 | | 0,72% | | | | |
| DI-tert-BUTYL ETHER | 550 | 23,23 | 0,2985 | 0,2555 | 1,3931 | 1,0000 | 0,6436 | 41,8556 | 0,84% | 1,08% | | 5,57% | 26,14% |
| DI-tert-BUTYL SULFIDE | 623,2 | 25,91 | 0,3008 | | 0,3200 | 0,8223 | 2,1513 | | 0,65% | 1,60% | | | |
| DIVINYL ETHER | 463 | 42,50 | 0,2911 | | 0,2846 | 0,8535 | 2,4948 | | 1,22% | 2,20% | | | |
| DODECAMETHYLCYCLOHEXASILOXANE | 645,8 | 9,01 | 0,7095 | 0,2488 | 1,0301 | 0,8643 | 1,4485 | 110,4236 | 0,32% | 0,72% | | 2,16% | 26,83% |
| DODECAMETHYLPENTASILOXANE | 628,4 | 9,45 | 0,7202 | 0,2560 | 0,6975 | 0,8104 | 2,0201 | 79,9501 | 0,90% | 1,35% | | 1,84% | 25,93% |
| DODECANAL | 705,1 | 23,20 | 0,6808 | | 0,8094 | 0,8681 | 1,8060 | | 0,77% | 1,83% | | | |
| DODECANEDIOIC ACID | 847 | 21,50 | 1,0418 | | 0,6052 | 0,8228 | 3,0495 | | 1,58% | | | | |
| EICOSAMETHYLNONASILOXANE | 707,2 | 5,75 | 1,0500 | 0,2430 | 0,7591 | 0,8065 | 2,4719 | 179,4168 | 1,18% | 1,70% | | 2,21% | 32,35% |
| epsilon-CAPROLACTAM | 818,2 | 46,21 | 0,3850 | 0,2504 | 1,6483 | 0,9995 | 0,6061 | 35,6519 | 0,73% | 1,30% | 0,78% | 4,33% | 20,39% |
| ERUCIC ACID | 809,9 | 10,21 | 1,2417 | 0,2247 | 0,6893 | 0,8194 | 3,1246 | 190,0232 | 1,70% | | | 2,03% | 29,58% |
| ETHANE | 305,32 | 48,72 | 0,0995 | 0,2817 | 0,2968 | 0,8812 | 1,7252 | 4,6079 | 0,50% | 1,39% | 8,04% | 3,76% | 16,20% |
| ETHANESULFONYL CHLORIDE | 682 | 47,40 | 0,3688 | 0,2541 | 0,4383 | 0,8747 | 2,1869 | 24,7931 | 1,40% | | | 3,46% | 23,02% |
| ETHANOL | 514 | 61,37 | 0,6436 | 0,2377 | 0,8136 | 0,9028 | 1,7934 | 16,0242 | 1,65% | 1,06% | 1,93% | 6,02% | 28,63% |
| ETHYL ACETATE | 523,3 | 38,80 | 0,3664 | 0,2549 | 0,6536 | 0,8532 | 1,4653 | 22,6752 | 1,17% | 1,79% | 1,12% | 4,40% | 22,77% |
| ETHYL ACETOACETATE | 642,9 | 32,70 | 0,5552 | 0,2461 | 0,4691 | 0,8514 | 2,5275 | 35,5185 | 0,68% | | | 3,44% | 24,24% |
| ETHYL ACRYLATE | 553 | 36,80 | 0,3718 | 0,2549 | 1,1131 | 1,0000 | 0,9302 | 24,4371 | 0,59% | 0,75% | | 4,90% | 21,37% |
| ETHYL ALUMINUM DICHLORIDE | 646,05 | 18,60 | 0,5338 | 0,1451 | 0,3625 | 0,8248 | 2,7992 | 225,0709 | 0,57% | 3,23% | | 28,15% | 141,04% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| ETHYL BENZOATE | 698 | 31,80 | 0,4771 | 0,2573 | 0,8664 | 0,9534 | 1,4182 | 31,6033 | 0,86% | 0,73% | | 1,70% | 17,94% |
| ETHYL CAPRATE | 688,1 | 17,88 | 0,6253 | 0,2427 | 1,6725 | 0,9877 | 0,7943 | 77,4723 | 0,76% | 0,82% | | 3,60% | 27,46% |
| ETHYL CAPRYLATE | 649 | 21,18 | 0,6114 | 0,2503 | 0,5073 | 0,8288 | 2,4170 | 47,7863 | 0,74% | 1,58% | | 2,10% | 25,62% |
| ETHYL CHLORIDE | 460,35 | 52,70 | 0,1886 | 0,2662 | 0,3426 | 0,8448 | 1,7499 | 12,3886 | 0,49% | 2,60% | 1,85% | 4,85% | 19,64% |
| ETHYL CHLOROFORMATE | 508,15 | 45,00 | 0,8350 | 0,2806 | 0,5734 | 0,8216 | 2,6938 | -4,4726 | 0,73% | 0,95% | | 2,42% | 15,85% |
| ETHYL CYANOACETATE | 679 | 33,40 | 0,5584 | 0,2184 | 0,3577 | 0,8186 | 2,8474 | 66,1056 | 0,26% | | | 7,78% | 38,92% |
| ETHYL ERUCATE | 808,2 | 8,82 | 1,1236 | | 0,6726 | 0,8262 | 2,9790 | | 1,43% | | | | |
| ETHYL FLUORIDE | 375,31 | 50,28 | 0,2179 | 0,2607 | 0,4145 | 0,8792 | 1,7490 | 12,2235 | 0,36% | 1,90% | 2,39% | 4,93% | 22,42% |
| ETHYL FORMATE | 508,4 | 47,40 | 0,2847 | 0,2579 | 0,5466 | 0,8182 | 1,4108 | 18,1861 | 1,27% | 1,84% | 0,90% | 5,03% | 21,87% |
| ETHYL HYDROGEN SULFATE | 857 | 89,80 | 0,4939 | | 0,7837 | 0,8624 | 1,4950 | | 0,93% | 0,83% | | | |
| ETHYL HYDROPEROXIDE | 560 | 65,81 | 0,4656 | | 1,5339 | 1,0000 | 0,7311 | | 0,83% | 0,74% | | | |
| ETHYL IODIDE | 554 | 47,11 | 0,1674 | 0,2501 | 0,9763 | 1,0000 | 0,7594 | 27,9397 | 1,49% | 1,02% | | 7,35% | 21,13% |
| ETHYL ISOAMYL KETONE | 617 | 27,27 | 0,4242 | 0,2568 | 0,1888 | 0,7624 | 2,7748 | 34,7008 | 0,55% | | | 4,00% | 22,64% |
| ETHYL ISOBUTYL ETHER | 519,2 | 30,41 | 0,3552 | 0,2719 | 0,7294 | 0,8757 | 1,3345 | 12,6010 | 0,74% | 1,08% | | 2,45% | 19,32% |
| ETHYL ISOBUTYRATE | 553,15 | 30,40 | 0,4264 | 0,2634 | 0,3169 | 0,8387 | 2,7407 | 21,1905 | 0,53% | 3,61% | 1,20% | 1,85% | 17,83% |
| ETHYL ISOPROPYL ETHER | 489 | 34,10 | 0,3056 | 0,2793 | 1,1881 | 1,0000 | 0,7695 | 7,1710 | 1,57% | 2,23% | 0,84% | 1,57% | 18,62% |
| ETHYL ISOPROPYL KETONE | 567 | 33,20 | 0,3891 | 0,2659 | 1,0498 | 0,9755 | 1,0126 | 19,9235 | 0,74% | 0,55% | | 1,44% | 22,87% |
| ETHYL ISOVALERATE | 587,95 | 28,40 | 0,4000 | 0,2636 | 1,3800 | 1,0000 | 0,7514 | 24,7323 | 1,86% | 4,22% | 1,15% | 2,65% | 24,22% |
| ETHYL LACTATE | 606,95 | 37,40 | 0,6032 | 0,2601 | 0,5641 | 0,8640 | 2,3399 | 16,5068 | 0,84% | | | 1,31% | 22,39% |
| ETHYL LAURATE | 716,3 | 15,29 | 0,6992 | 0,2358 | 0,1754 | 0,7798 | 4,0577 | 107,4928 | 0,40% | | | 4,00% | 29,58% |
| ETHYL LEVULINATE | 666,1 | 29,24 | 0,6071 | 0,2463 | 0,5296 | 0,8563 | 2,4518 | 40,4865 | 0,65% | | | 2,24% | 26,52% |
| ETHYL LINOLEATE | 777,8 | 11,27 | 0,9443 | 0,2300 | 0,6442 | 0,8381 | 2,7508 | 165,4015 | 0,85% | | | 2,08% | 25,71% |
| ETHYL LINOLENATE | 779,8 | 11,50 | 0,9334 | 0,2313 | 0,5493 | 0,8223 | 3,0377 | 161,0002 | 0,72% | 1,93% | | 1,80% | 23,62% |
| ETHYL MERCAPTAN | 499,15 | 54,90 | 0,1878 | 0,2699 | 0,5467 | 0,8428 | 1,2095 | 11,1175 | 1,05% | 2,16% | 1,66% | 4,92% | 16,36% |
| ETHYL METHACRYLATE | 577 | 32,50 | 0,3432 | 0,2505 | 0,3779 | 0,8292 | 2,0962 | 33,1934 | 0,36% | 1,50% | | 6,10% | 22,36% |
| ETHYL METHYL DISULFIDE | 628,9 | 46,15 | 0,3010 | | 0,4550 | 0,8945 | 1,9606 | | 0,65% | | | | |
| ETHYL MYRISTATE | 738,7 | 13,23 | 0,7642 | 0,2296 | 0,7552 | 0,7702 | 1,8880 | 141,7435 | 0,85% | 1,39% | | 3,86% | 31,38% |
| ETHYL n-BUTYRATE | 571 | 29,50 | 0,4011 | 0,2503 | 0,3385 | 0,8470 | 2,5977 | 35,8632 | 0,64% | 2,86% | | 4,35% | 24,21% |
| ETHYL n-HEXYL ETHER | 583 | 24,60 | 0,4944 | 0,2576 | 0,3718 | 0,8192 | 2,5720 | 30,5864 | 0,72% | 2,25% | 1,14% | 2,64% | 28,59% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| ETHYL n-OCTYL SULFIDE | 700 | 24,00 | 0,5346 | 0,2725 | 0,3594 | 0,8323 | 2,8589 | 15,8104 | 2,46% | 1,54% | | 1,46% | 13,08% |
| ETHYL n-PENTYL SULFIDE | 633,2 | 27,97 | 0,4349 | | 0,5699 | 0,8420 | 1,8035 | | 0,74% | 1,40% | | | |
| ETHYL OLEATE | 772,1 | 10,98 | 0,9426 | 0,2245 | 0,6599 | 0,8402 | 2,7139 | 179,5312 | 1,54% | | | 1,97% | 35,06% |
| ETHYL PHENYL ACETATE | 702,1 | 28,53 | 0,5251 | 0,2525 | 0,5184 | 0,8388 | 2,1869 | 38,4626 | 0,61% | 1,48% | | 2,57% | 24,48% |
| ETHYL PROPIONATE | 546 | 33,62 | 0,3944 | 0,2539 | 0,4348 | 0,8193 | 2,0090 | 27,6032 | 0,95% | 2,15% | 0,44% | 4,15% | 22,46% |
| ETHYL PROPYL DISULFIDE | 660 | 36,12 | 0,3910 | 0,2746 | 0,4228 | 0,8679 | 2,2847 | 8,8783 | 0,63% | | | 1,54% | 19,31% |
| ETHYL PROPYL SULFIDE | 583,9 | 34,46 | 0,3331 | 0,2655 | 0,3403 | 0,8586 | 2,4171 | 19,2283 | 1,29% | 2,36% | | 2,80% | 20,42% |
| ETHYL STEARATE | 777,9 | 10,19 | 0,8985 | 0,2179 | 0,5452 | 0,7841 | 2,7562 | 228,6961 | 0,82% | 1,17% | | 3,72% | 36,74% |
| ETHYL t-BUTYL SULFIDE | 588 | 31,30 | 0,2861 | 0,2689 | 0,2157 | 0,8385 | 2,7448 | 19,1103 | 0,33% | 1,53% | 0,46% | 3,72% | 21,73% |
| ETHYL TERT-BUTYL DISULFIDE | 659,9 | 30,76 | 0,3471 | 0,2695 | 0,5339 | 0,8720 | 1,7557 | 18,8632 | 0,71% | 1,36% | | 2,48% | 19,69% |
| ETHYL tert-PENTYL ETHER | 546 | 27,40 | 0,3382 | 0,2654 | 1,1595 | 1,0000 | 0,8371 | 23,4701 | 0,56% | 1,22% | 4,87% | 3,49% | 16,99% |
| ETHYL THIOLACETATE | 590,55 | 40,75 | 0,3098 | 0,2641 | 0,7345 | 0,8852 | 1,2430 | 18,7490 | 0,61% | 0,82% | | 3,59% | 20,03% |
| ETHYL VANILLIN | 748 | 32,70 | 1,0728 | | 0,5791 | 0,8161 | 3,1979 | | 1,00% | 0,83% | | | |
| ETHYL VINYL ETHER | 475,15 | 40,70 | 0,2665 | 0,2698 | 0,3531 | 0,8500 | 2,0352 | 12,8814 | 0,83% | 1,45% | | 2,50% | 18,13% |
| ETHYL-3-ETHOXYPROPIONATE | 621 | 26,60 | 0,4975 | 0,2564 | 0,4119 | 0,8156 | 2,3893 | 34,7678 | 0,66% | 1,65% | 0,98% | 1,53% | 33,68% |
| ETHYLACETYLENE | 440 | 46,00 | 0,2470 | 0,2703 | 0,9863 | 0,8963 | 0,8246 | 10,3506 | 1,84% | 2,68% | 0,11% | 4,05% | 22,47% |
| ETHYLAL | 524 | 32,80 | 0,4297 | 0,2661 | 0,2693 | 0,8293 | 2,9169 | 14,5378 | 3,30% | 6,28% | 1,04% | 2,90% | 22,70% |
| ETHYLAMINE | 456,15 | 56,20 | 0,2848 | 0,2664 | 0,3191 | 0,8048 | 1,9962 | 10,5836 | 0,23% | 1,19% | 2,29% | 3,34% | 3,56% |
| ETHYLBENZENE | 617,15 | 36,09 | 0,3035 | 0,2620 | 0,3935 | 0,8355 | 1,9278 | 24,3802 | 0,98% | 1,12% | 1,43% | 3,93% | 20,20% |
| ETHYLBENZENE HYDROPEROXIDE | 737 | 37,90 | 0,8130 | 0,2573 | 0,7255 | 0,8319 | 2,1823 | 17,7454 | 1,73% | 1,14% | 3,25% | 1,44% | 25,29% |
| ETHYLCHLOROACETATE | 618 | 37,90 | 0,3932 | 0,2480 | 1,2119 | 1,0000 | 0,8693 | 33,0229 | 0,65% | 0,73% | | 4,83% | 28,10% |
| ETHYLCYCLOHEXANE | 609,15 | 30,40 | 0,2455 | 0,2590 | 1,2720 | 1,0000 | 0,6471 | 34,2425 | 0,32% | 0,61% | 1,08% | 5,73% | 21,19% |
| ETHYLCYCLOPENTANE | 569,5 | 34,00 | 0,2701 | 0,2668 | 0,6607 | 0,8475 | 1,2158 | 20,2346 | 1,69% | 1,71% | 2,00% | 4,43% | 18,40% |
| ETHYLENE | 282,34 | 50,41 | 0,0862 | 0,2825 | 0,2296 | 0,8729 | 1,9291 | 4,1267 | 0,41% | 1,29% | 3,74% | 3,67% | 15,34% |
| ETHYLENE CARBONATE | 806 | 67,70 | 0,4423 | 0,2235 | 0,5731 | 0,8971 | 1,9321 | 36,1102 | 5,47% | 5,00% | | 8,61% | 52,25% |
| ETHYLENE GLYCOL | 720 | 82,00 | 0,5068 | 0,2383 | 1,5219 | 1,0000 | 0,7758 | 19,2899 | 1,42% | 1,25% | 3,52% | 7,66% | 17,31% |
| ETHYLENE GLYCOL DIACETATE | 653 | 30,90 | 0,5595 | 0,2456 | 0,3837 | 0,8321 | 2,8627 | 39,6699 | 5,39% | 1,93% | | 2,85% | 31,25% |
| ETHYLENE GLYCOL DIACRYLATE | 689 | 27,00 | 0,6618 | 0,2441 | 0,7257 | 0,8889 | 2,0228 | 46,6285 | 0,37% | | | 2,01% | 27,53% |
| ETHYLENE GLYCOL DINITRATE | 654 | 40,40 | 0,7904 | 0,2500 | 0,6199 | 0,8420 | 2,5069 | 23,2174 | 0,59% | 0,73% | | 1,37% | 17,52% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| ETHYLENE OXIDE | 469,15 | 71,90 | 0,1974 | 0,2565 | 0,4891 | 0,8541 | 1,3817 | 12,6224 | 0,46% | 1,78% | 0,89% | 6,34% | 19,90% |
| ETHYLENEDIAMINE | 593 | 62,90 | 0,4724 | 0,2546 | 0,3064 | 0,8308 | 2,8879 | 14,0060 | 3,45% | 4,36% | 2,22% | 4,02% | 6,33% |
| ETHYLENEIMINE | 537 | 68,50 | 0,2007 | 0,2385 | 2,5343 | 0,9789 | 0,2871 | 22,9186 | 0,90% | 1,74% | | 10,21% | 12,34% |
| ETHYLIDENE DIACETATE | 627 | 31,40 | 0,5263 | 0,2537 | 0,7343 | 0,8389 | 1,6137 | 29,3146 | 1,18% | 1,00% | 3,00% | 3,29% | 25,98% |
| ETHYLNORBORNENE | 625 | 30,60 | 0,2605 | 0,2571 | 0,4507 | 0,8550 | 1,6912 | 36,4640 | 0,90% | 1,92% | | 4,79% | 21,19% |
| ETHYLTRICHLOROSILANE | 559,95 | 33,30 | 0,2698 | 0,2800 | 0,8549 | 0,8850 | 1,0012 | 10,5355 | 0,92% | 0,98% | | 1,34% | 13,03% |
| ETHYNYLBENZENE | 650 | 42,80 | 0,2264 | 0,2720 | 0,3044 | 0,8260 | 1,9466 | 16,8711 | 0,48% | 2,04% | 2,74% | 2,33% | 21,70% |
| FLUORANTHENE | 905 | 26,10 | 0,5875 | | 0,7008 | 0,9003 | 1,8975 | | 6,80% | 5,25% | | | |
| FLUORENE | 826 | 30,00 | 0,4042 | | 0,4581 | 0,8231 | 1,9817 | | 0,31% | 0,89% | 0,17% | | |
| FLUORINE | 144,12 | 51,72 | 0,0530 | 0,2876 | 0,3314 | 0,8864 | 1,3930 | 1,4127 | 0,65% | 1,82% | 0,90% | 3,91% | 13,92% |
| FLUOROBENZENE | 560,09 | 45,51 | 0,2472 | 0,2654 | 0,3451 | 0,8505 | 1,9983 | 15,9871 | 0,68% | 1,87% | | 4,18% | 20,87% |
| FORMALDEHYDE | 420 | 65,90 | 0,1679 | 0,2068 | 0,9139 | 0,9234 | 0,7804 | 28,2758 | 0,63% | 1,05% | | 17,50% | 74,33% |
| FORMAMIDE | 771 | 78,00 | 0,4124 | 0,1913 | 0,5298 | 0,8484 | 1,8763 | 47,9904 | 0,62% | 2,74% | | 15,31% | 38,62% |
| FORMANILIDE | 787 | 41,10 | 0,5449 | | 0,4837 | 0,8259 | 2,3090 | | 0,75% | 1,18% | | | |
| FORMIC ACID | 588 | 58,10 | 0,3125 | 0,1673 | 0,4404 | 0,8326 | 1,7631 | 61,1205 | 3,68% | | 0,67% | 21,45% | 75,49% |
| FUMARIC ACID | 771 | 49,80 | 0,9885 | | 0,4358 | 0,7997 | 3,6147 | | 1,41% | 2,08% | 0,79% | | |
| FUMARONITRILE | 657 | 37,30 | 0,5566 | 0,1984 | 0,3106 | 0,8199 | 3,1140 | 77,0069 | 0,56% | 2,18% | 3,96% | 7,58% | 43,26% |
| FURAN | 490,15 | 55,00 | 0,2015 | 0,2698 | 0,5040 | 0,8173 | 1,2938 | 10,9429 | 0,14% | 1,08% | 0,59% | 4,32% | 8,28% |
| FURAN 2,5-DICARBOXYLIC ACID | 894,5 | 44,66 | 1,0134 | | 0,6694 | 0,8356 | 2,7960 | | 1,14% | | | | |
| FURFURAL | 670,15 | 56,60 | 0,3678 | 0,2633 | 0,5278 | 0,8434 | 1,7304 | 14,7276 | 0,66% | 1,23% | 0,82% | 2,85% | 24,37% |
| FURFURYL ALCOHOL | 632 | 53,50 | 0,7341 | 0,2581 | 0,5129 | 0,8372 | 2,7678 | 8,9212 | 1,02% | | 1,42% | 2,40% | 21,09% |
| GALLIUM TRICHLORIDE | 694 | 38,20 | 0,4577 | 0,1996 | 0,5946 | 0,8969 | 1,9347 | 78,3260 | 3,42% | | | 9,55% | 61,67% |
| gamma-BUTYROLACTONE | 731 | 51,30 | 0,3603 | | 0,5332 | 0,8596 | 1,7506 | | 1,01% | | 0,68% | | |
| gamma-TERPINENE | 661 | 28,00 | 0,3762 | 0,2621 | 0,4781 | 0,8203 | 1,8341 | 31,9904 | 0,66% | 1,88% | 0,56% | 2,11% | 27,25% |
| gamma-VALEROLACTONE | 727 | 48,40 | 0,4030 | 0,2547 | 0,5087 | 0,8873 | 2,0417 | 25,0254 | 2,14% | 2,40% | | 2,03% | 40,24% |
| GERMANIUM TETRACHLORIDE | 550 | 38,50 | 0,2411 | 0,2760 | 0,2915 | 0,8454 | 2,1771 | 11,0894 | 2,35% | 4,11% | 1,15% | 2,45% | 19,50% |
| GERMANIUM TETRAFLUORIDE | 352 | 46,04 | 0,2231 | 0,2627 | 0,2912 | 0,8536 | 2,1271 | 11,9082 | 0,50% | 2,66% | | 2,60% | 19,75% |
| GERMANIUM TETRAHYDRIDE | 308 | 55,50 | 0,1506 | 0,3025 | 0,4647 | 0,9474 | 1,4667 | -3,7176 | 5,46% | | | 1,94% | 12,52% |
| GLUTARALDEHYDE | 660 | 35,90 | 0,5373 | 0,2267 | 0,5074 | 0,8136 | 2,1499 | 54,7872 | 0,68% | 2,28% | 1,68% | 5,89% | 31,05% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| GLUTARIC ACID | 840 | 42,70 | 0,7526 | 0,2273 | 1,1620 | 0,8366 | 1,3225 | 51,2918 | 1,26% | 1,65% | 2,07% | 4,93% | 29,64% |
| GLUTARIC ANHYDRIDE | 838 | 58,00 | 0,5372 | 0,2556 | 0,6013 | 0,8840 | 2,0809 | 20,0540 | 2,96% | 3,07% | | 1,48% | 38,32% |
| GLUTARONITRILE | 782 | 31,50 | 0,6033 | 0,1852 | 0,5716 | 0,8674 | 2,2925 | 118,5400 | 5,47% | 7,65% | 3,70% | 14,44% | 61,79% |
| GLYCERYL TRIACETATE | 701,4 | 23,33 | 0,8758 | 0,2460 | 0,5031 | 0,8206 | 3,0976 | 42,5390 | 1,01% | 1,45% | | 1,46% | 26,71% |
| GLYCINE | 1021 | 67,40 | 0,6860 | | 0,3879 | 0,8194 | 3,1233 | | 0,62% | 1,58% | | | |
| GLYCOL ALDEHYDE | 609,3 | 66,44 | 0,7684 | | 0,3840 | 0,8106 | 3,3277 | | 0,66% | 2,40% | | | |
| GLYCOLIC ACID | 616 | 73,10 | 1,0592 | | 0,5783 | 0,8171 | 3,1754 | | 1,13% | 0,61% | | | |
| HALOTHANE | 496 | 39,20 | 0,2750 | 0,2751 | 0,2272 | 0,8451 | 2,6304 | 9,9673 | 4,21% | 2,33% | 0,75% | 2,47% | 15,10% |
| HEPTAFLUOROPROPYL METHYL ETHER | 437,7 | 24,81 | 0,4035 | 0,2584 | 0,5222 | 0,8469 | 1,8707 | 25,2658 | 0,71% | 1,40% | | 3,15% | 22,67% |
| HEPTANAL | 620 | 31,60 | 0,4058 | 0,2607 | 0,4353 | 0,8681 | 2,2821 | 25,9433 | 0,67% | 2,31% | | 2,25% | 19,31% |
| HEXACHLOROBENZENE | 825 | 28,50 | 0,4971 | | 2,7373 | 0,0000 | 1,0227 | | 1,30% | | | | |
| HEXACHLOROCYCLOPENTADIENE | 746 | 30,10 | 0,3834 | 0,2540 | 0,4729 | 0,8464 | 1,9664 | 42,6343 | 0,63% | 1,35% | | 3,74% | 22,48% |
| HEXACHLOROETHANE | 695 | 33,40 | 0,2386 | | 0,1509 | 0,8118 | 2,6475 | | 0,41% | 2,40% | | | |
| HEXACOSAMETHYLDODECASILOXANE | 751,3 | 4,70 | 1,3096 | 0,2464 | 0,6645 | 0,8101 | 3,3417 | 164,9102 | 1,55% | | | 3,85% | 30,44% |
| HEXADECAMETHYLCYCLOOCTASILOXANE | 689,2 | 6,92 | 0,8826 | 0,2445 | 0,5027 | 0,8199 | 3,1121 | 153,4554 | 0,87% | 1,43% | | 1,32% | 31,66% |
| HEXADECAMETHYLHEPTASILOXANE | 671,8 | 6,77 | 0,8864 | 0,2407 | 1,5412 | 0,9934 | 1,0951 | 178,4883 | 0,74% | 1,08% | | 1,93% | 29,26% |
| HEXAETHYLBENZENE | 746 | 17,30 | 0,7534 | 0,2526 | 0,8840 | 0,9067 | 1,8321 | 55,6578 | 0,86% | 2,36% | 1,23% | 1,30% | 23,45% |
| HEXAFLUORO-1,3-BUTADIENE | 409,9 | 31,31 | 0,3510 | 0,2645 | 1,3822 | 1,0000 | 0,7037 | 15,7336 | 0,87% | 0,98% | | 3,56% | 21,36% |
| HEXAFLUOROACETONE | 357,14 | 28,37 | 0,3636 | 0,2652 | 0,1626 | 0,8154 | 3,2139 | 13,9712 | 1,16% | 4,63% | 1,55% | 4,16% | 1,80% |
| HEXAFLUOROBENZENE | 516,73 | 32,73 | 0,3953 | 0,2546 | 0,2699 | 0,8331 | 2,8434 | 25,7732 | 0,65% | 3,05% | 0,68% | 3,56% | 22,93% |
| HEXAFLUOROETHANE | 293,03 | 30,43 | 0,2549 | 0,2778 | 0,2585 | 0,8511 | 2,4486 | 5,5686 | 0,33% | 1,86% | 1,76% | 2,49% | 16,66% |
| HEXAMETHYLBENZENE | 758 | 27,70 | 0,4956 | 0,2475 | 1,1033 | 0,9909 | 1,1186 | 48,8150 | 0,95% | 2,32% | 0,61% | 3,90% | 19,66% |
| HEXAMETHYLCYCLOTRISILOXANE | 554,2 | 17,80 | 0,4962 | 0,2673 | 1,6326 | 1,0000 | 0,7020 | 25,0756 | 0,92% | 0,95% | | 2,53% | 21,07% |
| HEXAMETHYLDISILAZANE | 544 | 19,20 | 0,5101 | 0,2598 | 0,5430 | 0,8743 | 2,2005 | 32,7137 | 1,70% | 2,43% | | 2,13% | 22,76% |
| HEXAMETHYLDISILOXANE | 519 | 19,20 | 0,4142 | 0,2672 | 0,2707 | 0,8247 | 2,8308 | 24,6152 | 0,87% | 3,48% | 0,56% | 2,52% | 18,58% |
| HEXAMETHYLENEIMINE | 624 | 42,70 | 0,3454 | 0,2757 | 0,2971 | 0,8477 | 2,5862 | 8,7360 | 2,13% | 3,68% | | 1,83% | 9,77% |
| HEXAMETHYLENETETRAMINE | 837 | 36,80 | 0,2994 | | 0,2558 | 0,8456 | 2,6218 | | 0,48% | 2,20% | | | |
| HEXANAL | 594 | 34,60 | 0,3618 | 0,2606 | 0,5013 | 0,8605 | 1,8624 | 24,1709 | 0,70% | 1,16% | | 2,94% | 19,48% |
| HEXANENITRILE | 633,8 | 33,00 | 0,4343 | 0,2447 | 0,4727 | 0,8713 | 2,2402 | 40,9552 | 1,33% | 5,91% | | 3,91% | 25,66% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| HMX | 1030 | 25,00 | 1,1318 | | 0,7010 | 0,8305 | 2,8939 | | 1,30% | | | | |
| HYDRAZOBENZENE | 939 | 30,90 | 0,6718 | 0,2311 | 0,4406 | 0,8218 | 2,8294 | 78,7974 | 0,70% | 1,16% | | 3,26% | 27,45% |
| HYDROGEN BROMIDE | 363,15 | 85,52 | 0,0734 | 0,2832 | 0,5191 | 0,8943 | 1,0456 | 2,9690 | 0,98% | 1,32% | 0,25% | 3,64% | 14,72% |
| HYDROGEN CHLORIDE | 324,65 | 83,10 | 0,1315 | 0,2677 | 0,2288 | 0,8767 | 2,1698 | 5,9877 | 1,55% | 2,07% | 1,35% | 3,65% | 26,28% |
| HYDROGEN CYANIDE | 457 | 54,00 | 0,4043 | 0,1917 | 0,5825 | 0,9063 | 1,8359 | 42,0086 | 4,55% | | | 9,12% | 42,62% |
| HYDROGEN IODIDE | 423,85 | 83,10 | 0,0381 | 0,2883 | 0,3946 | 0,8631 | 1,1132 | 2,5624 | 0,30% | 1,68% | 0,60% | 3,55% | 13,86% |
| HYDROGEN PEROXIDE | 730,15 | 217,00 | 0,3582 | 0,2685 | 0,4272 | 0,8756 | 2,1837 | 3,3570 | 0,42% | 1,21% | | 1,62% | 15,70% |
| HYDROGEN SELENIDE | 411,15 | 89,20 | 0,0542 | 0,2876 | 0,1117 | 0,8601 | 2,3944 | 2,3908 | 1,27% | 3,84% | | 3,48% | 4,46% |
| HYDROGEN SULFIDE | 373,53 | 89,63 | 0,0942 | 0,2825 | 0,1748 | 0,8686 | 2,2761 | 3,0181 | 0,25% | 1,55% | 10,76% | 3,18% | 14,20% |
| HYDROXYACETONITRILE | 664 | 59,30 | 0,8007 | 0,2097 | 0,7845 | 0,8400 | 2,0271 | 39,2313 | 0,65% | 0,91% | | 5,64% | 39,02% |
| HYDROXYCAPROIC ACID | 683 | 36,40 | 1,1375 | | 0,6083 | 0,8156 | 3,2107 | | 1,41% | 0,82% | | | |
| IBUPROFEN | 765 | 29,80 | 1,0101 | 0,3028 | 0,6953 | 0,8394 | 2,7278 | -42,0001 | 1,62% | | | 4,73% | 12,79% |
| IMIDAZOLE | 844,8 | 105,50 | 0,4138 | 0,2862 | 0,5664 | 0,7998 | 1,6572 | -1,8061 | 0,57% | 1,24% | | 1,54% | 17,14% |
| INDENE | 687 | 38,20 | 0,3338 | 0,2555 | 0,3053 | 0,8520 | 2,5181 | 32,2215 | 2,99% | 3,76% | 1,64% | 3,22% | 26,69% |
| INDOLE | 790 | 43,00 | 0,3763 | 0,2371 | 0,5783 | 0,8348 | 1,6221 | 48,7143 | 0,65% | 1,32% | 0,04% | 6,60% | 6,84% |
| IODINE | 819,15 | 116,54 | 0,1115 | 0,2988 | 0,2140 | 0,8759 | 2,1803 | -2,8926 | 1,57% | 3,71% | | 2,46% | 27,55% |
| IODOBENZENE | 721,15 | 45,19 | 0,2466 | 0,2652 | 0,3489 | 0,8406 | 1,9273 | 21,7784 | 0,40% | 1,04% | 0,65% | 3,94% | 19,80% |
| IRON PENTACARBONYL | 559,65 | 31,53 | 0,2938 | 0,2669 | 1,5510 | 1,0000 | 0,5710 | 21,2688 | 2,09% | | 0,16% | 3,56% | 17,78% |
| ISOAGATHOLAL | 790 | 16,70 | 1,0832 | | 0,6068 | 0,8194 | 3,1236 | | 1,21% | 1,44% | | | |
| ISOBUTANE | 407,8 | 36,40 | 0,1835 | 0,2741 | 0,6853 | 0,8842 | 1,0305 | 10,8558 | 1,38% | 1,81% | 3,04% | 4,61% | 15,69% |
| ISOBUTENE | 417,9 | 40,00 | 0,1948 | 0,2723 | 0,3292 | 0,8528 | 1,8473 | 10,9236 | 1,04% | 1,21% | 2,74% | 4,14% | 16,58% |
| ISOBUTYL ACETATE | 560,8 | 30,10 | 0,4340 | 0,2542 | 1,4335 | 1,0000 | 0,7520 | 29,4842 | 1,12% | 4,08% | 2,58% | 4,74% | 25,16% |
| ISOBUTYL ACRYLATE | 587 | 29,50 | 0,4551 | 0,2617 | 0,5366 | 0,8512 | 1,9805 | 22,8949 | 0,74% | 1,00% | | 2,36% | 22,07% |
| ISOBUTYL CHLORIDE | 528 | 39,00 | 0,2416 | 0,2622 | 0,3629 | 0,8173 | 1,7413 | 19,6714 | 1,57% | 1,95% | 0,99% | 6,37% | 18,51% |
| ISOBUTYL FORMATE | 551,35 | 38,81 | 0,3896 | 0,2779 | 0,4312 | 0,8274 | 2,0295 | 5,2696 | 0,73% | 2,17% | | 1,57% | 10,36% |
| ISOBUTYL ISOBUTYRATE | 601,89 | 26,10 | 0,4006 | 0,2680 | 1,4498 | 0,9994 | 0,7140 | 22,8353 | 0,74% | 2,18% | | 1,82% | 22,77% |
| ISOBUTYL MERCAPTAN | 559 | 40,60 | 0,2528 | 0,2723 | 0,3279 | 0,8427 | 2,0303 | 13,0112 | 1,91% | 2,10% | 2,07% | 2,97% | 20,06% |
| ISOBUTYL METHACRYLATE | 612 | 26,70 | 0,4205 | 0,2589 | 0,3001 | 0,8341 | 2,7801 | 31,5206 | 0,28% | 1,18% | 1,32% | 2,99% | 22,46% |
| ISOBUTYLAMINE | 513,73 | 42,15 | 0,3627 | 0,2701 | 0,2429 | 0,8330 | 2,8461 | 9,6512 | 2,19% | 4,04% | 0,68% | 3,58% | 4,97% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| ISOBUTYLBENZENE | 650 | 30,50 | 0,3817 | 0,2735 | 0,3189 | 0,8386 | 2,5508 | 14,5466 | 0,35% | 2,48% | 1,80% | 1,29% | 20,52% |
| iso-BUTYLCYCLOHEXANE | 642,1 | 25,85 | 0,3536 | 0,2669 | 0,8107 | 0,8864 | 1,2129 | 27,6013 | 0,65% | 1,05% | | 1,81% | 27,33% |
| ISOBUTYLENE GLYCOL | 626,3 | 50,33 | 0,8765 | 0,2681 | 0,6347 | 0,8432 | 2,6614 | 3,5849 | 0,82% | | | 2,82% | 19,33% |
| ISOBUTYL-tert-BUTYL ETHER | 558,3 | 25,61 | 0,3494 | 0,2781 | 1,1330 | 0,9712 | 0,8731 | 11,0518 | 0,81% | 1,04% | 0,39% | 1,36% | 21,79% |
| ISOBUTYRIC ACID | 605 | 37,00 | 0,6140 | 0,2213 | 0,3807 | 0,8257 | 2,9894 | 47,8441 | 1,76% | | | 7,21% | 38,81% |
| ISOBUTYRIC ANHYDRIDE | 631,5 | 27,19 | 0,5926 | 0,2712 | 0,6253 | 0,8786 | 2,1464 | 12,0287 | 2,25% | | | 2,62% | 29,97% |
| ISOBUTYRONITRILE | 565 | 37,60 | 0,3384 | 0,2333 | 0,5134 | 0,8484 | 1,7210 | 44,2194 | 0,75% | 1,52% | | 6,75% | 33,90% |
| ISOPENTANE | 460,4 | 33,80 | 0,2279 | 0,2710 | 0,2507 | 0,8548 | 2,3951 | 13,8762 | 0,37% | 1,66% | 1,65% | 3,93% | 18,83% |
| ISOPENTYL ISOVALERATE | 637 | 22,00 | 0,5785 | 0,2504 | 0,3577 | 0,8266 | 2,9723 | 40,9398 | 2,79% | 1,63% | 2,95% | 4,28% | 26,92% |
| ISOPHORONE | 707,6 | 30,90 | 0,4165 | 0,2543 | 0,5817 | 0,9014 | 1,8869 | 37,3403 | 0,93% | | | 3,05% | 23,41% |
| ISOPHORONE DIISOCYANATE | 765 | 25,20 | 0,6660 | | 0,5732 | 0,8345 | 2,3445 | | 0,88% | 1,69% | | | |
| ISOPHTHALIC ACID | 1007 | 39,50 | 1,0613 | | 0,6009 | 0,8204 | 3,1024 | | 1,05% | 1,36% | | | |
| ISOPHTHALOYL CHLORIDE | 768 | 33,30 | 0,6455 | 0,2501 | 0,6226 | 0,8300 | 2,1162 | 35,3237 | 0,38% | 0,29% | | 2,17% | 28,21% |
| ISOPRENE | 484 | 38,50 | 0,1583 | 0,2649 | 1,3072 | 1,0000 | 0,5301 | 20,0617 | 1,15% | 1,00% | 0,18% | 5,76% | 18,97% |
| ISOPROPANOL | 508,3 | 47,65 | 0,6630 | 0,2454 | 1,3702 | 0,9976 | 1,0478 | 17,0320 | 2,73% | 3,19% | 6,70% | 4,46% | 25,50% |
| ISOPROPYL ACETATE | 532 | 32,90 | 0,3678 | 0,2554 | 1,2055 | 1,0000 | 0,8408 | 26,9180 | 1,02% | 1,18% | | 4,34% | 25,37% |
| ISOPROPYL ACRYLATE | 560 | 33,10 | 0,4051 | 0,2660 | 0,4436 | 0,8707 | 2,2473 | 16,5036 | 0,81% | | 2,86% | 2,13% | 20,32% |
| ISOPROPYL BUTYL ETHER | 549 | 27,40 | 0,4032 | 0,2702 | 0,3231 | 0,8179 | 2,4729 | 15,9595 | 0,56% | 5,00% | 0,15% | 1,64% | 23,99% |
| ISOPROPYL CHLORIDE | 489 | 45,40 | 0,1986 | 0,2736 | 0,7891 | 0,8876 | 0,9431 | 10,2319 | 0,47% | 1,81% | 0,73% | 4,51% | 16,71% |
| ISOPROPYL IODIDE | 578 | 51,20 | 0,2380 | 0,2987 | 0,3390 | 0,8808 | 2,1185 | -5,5053 | 2,61% | 3,04% | | 1,42% | 9,79% |
| ISOPROPYL ISOBUTYL ETHER | 537 | 27,90 | 0,3785 | 0,2786 | 0,3503 | 0,8188 | 2,2710 | 7,2316 | 0,66% | 4,72% | 1,03% | 1,29% | 20,97% |
| ISOPROPYL MERCAPTAN | 517 | 47,50 | 0,2138 | 0,2830 | 0,2315 | 0,8559 | 2,4428 | 4,4474 | 2,05% | 2,19% | 2,61% | 2,10% | 17,01% |
| ISOPROPYL PALMITATE | 766,2 | 10,90 | 0,8688 | 0,2223 | 0,6116 | 0,7886 | 2,4885 | 195,7746 | 0,85% | 1,60% | | 3,56% | 34,80% |
| ISOPROPYLAMINE | 471,85 | 45,40 | 0,2759 | 0,2677 | 0,5504 | 0,7664 | 1,3049 | 11,9086 | 0,62% | 0,92% | 2,42% | 4,27% | 24,95% |
| ISOPROPYLCYCLOHEXANE | 627 | 28,50 | 0,3295 | 0,2628 | 0,2909 | 0,8482 | 2,5789 | 28,6385 | 0,63% | 1,07% | | 3,22% | 25,23% |
| ISOPROPYLCYCLOPENTANE | 593 | 30,40 | 0,3030 | 0,2631 | 0,4834 | 0,8524 | 1,7058 | 25,4780 | 1,25% | 1,84% | 3,61% | 4,33% | 22,65% |
| ISOQUINOLINE | 803,15 | 51,00 | 0,3035 | 0,2827 | 0,2937 | 0,8474 | 2,4392 | 4,4735 | 0,60% | 1,46% | 1,98% | 1,18% | 15,50% |
| ISOVALERIC ACID | 629,09 | 36,88 | 0,6818 | 0,2406 | 0,5767 | 0,8173 | 2,2987 | 31,1181 | 0,65% | | | 4,15% | 41,73% |
| ISOXAZOLE | 590 | 61,00 | 0,2568 | 0,2472 | 0,2868 | 0,8609 | 2,3839 | 22,1560 | 1,75% | 1,28% | | 6,20% | 28,79% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ITACONIC ACID | 821 | 42,40 | 0,9247 | | 0,4965 | 0,8152 | 3,2186 | | 0,82% | 1,18% | | | |
| KETENE | 370 | 58,10 | 0,1257 | 0,2720 | 1,1884 | 1,0000 | 0,5467 | 7,9815 | 1,18% | 2,66% | | 5,11% | 17,02% |
| KRYPTON | 209,35 | 55,02 | 0,0000 | 0,2906 | 0,1943 | 0,9046 | 1,8528 | 1,7957 | 0,35% | 1,70% | | 3,07% | 13,66% |
| LACTONITRILE | 643 | 50,30 | 0,7886 | 0,2195 | 0,8637 | 0,8679 | 1,8735 | 35,2870 | 0,34% | 0,34% | | 6,79% | 31,28% |
| LEVULINIC ACID | 738 | 40,20 | 0,7557 | 0,2172 | 0,4444 | 0,8224 | 3,0599 | 51,7062 | 0,71% | 0,96% | | 7,65% | 33,26% |
| LINOLEIC ACID | 775 | 14,10 | 1,1801 | 0,2288 | 0,6791 | 0,8229 | 3,0473 | 103,6769 | 1,37% | 1,35% | | 1,87% | 43,40% |
| LINOLENIC ACID | 780 | 14,40 | 1,1870 | 0,2373 | 0,6719 | 0,8210 | 3,0885 | 88,9636 | 1,72% | 1,73% | | 2,23% | 31,99% |
| L-MENTHOL | 658 | 27,10 | 0,7796 | 0,2567 | 0,7215 | 0,8714 | 2,2384 | 18,8540 | 3,50% | 4,27% | | 2,24% | 22,72% |
| L-PHENYLALANINE | 854 | 34,70 | 0,8516 | | 0,4173 | 0,8088 | 3,3736 | | 1,35% | 1,62% | 1,76% | | |
| LYSINE | 821 | 35,30 | 1,0127 | | 0,5630 | 0,8170 | 3,1345 | | 1,01% | 0,92% | | | |
| MALEIC ACID | 773 | 49,90 | 0,9976 | | 0,5343 | 0,8151 | 3,2204 | | 0,97% | 0,99% | | | |
| MALEONITRILE | 704 | 37,30 | 0,5575 | | 1,5094 | 0,9997 | 0,8236 | | 3,70% | 5,20% | 2,11% | | |
| MALONIC ACID | 834 | 61,00 | 0,7383 | | 0,4746 | 0,7826 | 2,6350 | | 0,78% | | | | |
| MALONONITRILE | 715 | 40,40 | 0,5016 | 0,1742 | 0,3383 | 0,8321 | 2,8634 | 96,6377 | 0,44% | 1,83% | | 17,06% | 58,81% |
| m-CHLOROANILINE | 751 | 45,90 | 0,4198 | 0,2661 | 0,4129 | 0,8440 | 2,2916 | 19,5504 | 0,50% | 6,87% | | 1,59% | 19,21% |
| m-CHLOROBENZOYL CHLORIDE | 724 | 36,80 | 0,4542 | | 1,0334 | 0,9887 | 1,1386 | | 0,38% | 0,31% | | | |
| m-CHLORONITROBENZENE | 742 | 39,80 | 0,4919 | 0,2458 | 0,3895 | 0,8448 | 2,6346 | 37,0384 | 2,06% | 4,55% | 3,39% | 3,95% | 11,03% |
| m-CHLOROPHENOL | 729 | 53,20 | 0,4856 | 0,2800 | 0,6473 | 0,9052 | 1,8473 | 2,6727 | 3,75% | 4,53% | | 1,51% | 17,84% |
| m-CRESOL | 705,85 | 45,60 | 0,4480 | 0,2513 | 0,5258 | 0,7714 | 1,7537 | 25,2046 | 1,62% | 2,27% | 2,28% | 5,38% | 29,42% |
| m-CYMENE | 649 | 28,10 | 0,3780 | 0,2552 | 0,6333 | 0,8554 | 1,5366 | 38,4404 | 0,18% | 1,12% | 2,62% | 4,03% | 21,79% |
| m-DIBROMOBENZENE | 761 | 46,60 | 0,2932 | 0,2742 | 0,3452 | 0,8591 | 2,2027 | 11,7097 | 1,25% | 2,08% | 1,66% | 2,69% | 18,52% |
| m-DICHLOROBENZENE | 683,95 | 40,70 | 0,2790 | 0,2624 | 0,3711 | 0,8434 | 1,9744 | 25,2754 | 0,55% | 1,44% | 0,49% | 3,04% | 25,49% |
| m-DIETHYLBENZENE | 663 | 28,80 | 0,3540 | 0,2582 | 0,6855 | 0,8497 | 1,3763 | 36,2849 | 0,83% | 1,32% | | 3,41% | 23,31% |
| m-DIISOPROPYLBENZENE | 684 | 24,50 | 0,3587 | 0,2813 | 1,4884 | 1,0000 | 0,6535 | 16,5110 | 1,93% | 2,95% | | 4,63% | 26,21% |
| m-DIVINYLBENZENE | 692 | 31,20 | 0,3734 | 0,2497 | 0,7712 | 0,8926 | 1,3154 | 44,2880 | 0,35% | 0,31% | | 4,24% | 29,64% |
| MELAMINE | 1008 | 58,58 | 0,6973 | | 0,6260 | 0,8633 | 2,3491 | | 1,05% | | | | |
| MERCURY | 1735 | 1608,03 | -0,1645 | 0,3906 | 0,1420 | 0,9748 | 1,2517 | -6,2081 | 2,37% | 8,53% | 1,15% | 2,43% | 14,49% |
| MERCURY DICHLORIDE | 972 | 115,21 | 0,2563 | 0,2548 | 0,2694 | 0,8566 | 2,4465 | 15,6954 | 0,38% | 2,04% | | 4,18% | 24,95% |
| MESITYL OXIDE | 600 | 34,10 | 0,3254 | 0,2464 | 0,5281 | 0,8148 | 1,5616 | 39,5820 | 0,66% | 1,33% | 0,24% | 5,81% | 26,22% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| MESITYLENE | 637,3 | 31,27 | 0,3985 | 0,2550 | 0,4151 | 0,8496 | 2,2393 | 32,6536 | 0,20% | 0,84% | 1,43% | 3,76% | 22,91% |
| METHACROLEIN | 530 | 42,50 | 0,2456 | 0,2459 | 0,4467 | 0,8529 | 1,6501 | 30,6287 | 0,71% | 1,78% | | 6,13% | 23,53% |
| METHACRYLONITRILE | 554 | 38,80 | 0,3013 | 0,2306 | 0,2312 | 0,8423 | 2,6767 | 45,7926 | 4,63% | 7,70% | 1,13% | 7,14% | 32,05% |
| METHANE | 190,564 | 45,99 | 0,0115 | 0,2894 | 0,2170 | 0,9082 | 1,8172 | 2,0509 | 0,33% | 2,04% | 8,33% | 3,60% | 14,39% |
| METHANOL | 512,5 | 80,84 | 0,5658 | 0,2263 | 0,7619 | 0,9142 | 1,7582 | 16,9781 | 1,40% | 5,36% | 10,13% | 7,69% | 35,66% |
| METHOXYACETONE | 584,1 | 42,13 | 0,3805 | 0,2493 | 0,5790 | 0,8925 | 1,7710 | 27,5149 | 0,18% | | | 3,97% | 24,30% |
| METHOXYDIHYDROPYRAN | 599 | 39,30 | 0,3669 | 0,2659 | 0,3307 | 0,8327 | 2,4104 | 15,6252 | 0,66% | 1,39% | | 3,18% | 22,90% |
| METHYL ACETATE | 506,55 | 47,50 | 0,3313 | 0,2564 | 0,5648 | 0,8254 | 1,4988 | 17,9514 | 2,39% | 3,45% | 0,45% | 4,83% | 21,76% |
| METHYL ACRYLATE | 536 | 42,50 | 0,3423 | 0,2495 | 0,3704 | 0,8576 | 2,2812 | 24,1483 | 0,24% | 0,34% | | 6,01% | 20,51% |
| METHYL alpha-HYDROXYISOBUTYRATE | 585,1 | 34,88 | 0,5444 | 0,2533 | 0,4532 | 0,8494 | 2,5582 | 24,8003 | 0,55% | 1,54% | | 2,28% | 24,68% |
| METHYL alpha-METHOXYISOBUTYRATE | 589,3 | 29,35 | 0,4212 | | 0,4836 | 0,8373 | 2,0094 | | 0,59% | 1,67% | | | |
| METHYL BENZOATE | 693 | 35,90 | 0,4205 | 0,2567 | 0,3074 | 0,8379 | 2,7554 | 31,0545 | 3,27% | 3,70% | 2,25% | 2,43% | 15,58% |
| METHYL CAPRYLATE | 650,7 | 23,84 | 0,4947 | 0,2558 | 1,4544 | 1,0000 | 0,8036 | 41,1642 | 1,36% | 1,16% | | 2,50% | 25,27% |
| METHYL CHLORIDE | 416,25 | 66,80 | 0,1510 | 0,2686 | 0,3041 | 0,8591 | 1,8107 | 8,6823 | 0,65% | 2,10% | 0,94% | 4,26% | 16,32% |
| METHYL CHLOROACETATE | 600 | 45,00 | 0,4340 | 0,2524 | 0,5009 | 0,8297 | 1,9569 | 23,7940 | 1,56% | 2,04% | 0,89% | 2,85% | 28,05% |
| METHYL CHLOROFORMATE | 525 | 53,60 | 0,3921 | 0,2680 | 0,5851 | 0,8449 | 1,6645 | 8,6214 | 0,77% | 1,11% | | 2,78% | 18,93% |
| METHYL CYANOACETATE | 687 | 38,10 | 0,5413 | 0,2266 | 0,3598 | 0,8311 | 2,8823 | 56,0311 | 0,55% | 1,27% | | 2,96% | 45,48% |
| METHYL DECANOATE | 686,9 | 19,42 | 0,5491 | 0,2429 | 1,5955 | 1,0000 | 0,7711 | 74,4822 | 0,72% | 0,78% | | 4,12% | 26,86% |
| METHYL DICHLOROSILANE | 483 | 39,50 | 0,2758 | 0,2658 | 0,2474 | 0,8507 | 2,5375 | 12,9355 | 3,95% | 5,41% | 7,69% | 6,17% | 12,79% |
| METHYL DIETHANOLAMINE | 741,9 | 41,60 | 0,6286 | 0,2489 | 0,5923 | 0,8248 | 2,1561 | 27,3364 | 0,83% | 1,42% | | 3,20% | 23,20% |
| METHYL DODECANOATE | 712 | 16,50 | 0,6644 | 0,2370 | 0,6689 | 0,7983 | 1,9509 | 97,2350 | 0,65% | 1,03% | | 3,54% | 29,26% |
| METHYL EICOSANOATE | 797,9 | 9,59 | 0,9021 | | 0,6505 | 0,7620 | 2,3480 | | 0,87% | 1,58% | | | |
| METHYL ERUCATE | 806,2 | 9,38 | 1,0984 | 0,2199 | 0,6030 | 0,8176 | 3,1634 | 234,4497 | 1,12% | 1,97% | | 1,78% | 32,65% |
| METHYL ETHYL ETHER | 437,8 | 44,00 | 0,2314 | 0,2678 | 1,0577 | 1,0000 | 0,7788 | 11,7313 | 1,73% | 2,05% | | 4,85% | 19,47% |
| METHYL ETHYL KETONE | 535,5 | 41,50 | 0,3234 | 0,2531 | 0,3273 | 0,8480 | 2,3524 | 24,8282 | 0,33% | 1,56% | 2,32% | 3,84% | 24,64% |
| METHYL ETHYL SULFIDE | 533 | 42,60 | 0,2091 | 0,2552 | 0,5103 | 0,8223 | 1,3173 | 24,8983 | 0,48% | 1,07% | 0,03% | 6,30% | 26,72% |
| METHYL FLUORIDE | 317,42 | 58,75 | 0,1947 | 0,2474 | 0,2956 | 0,8771 | 2,1653 | 13,1601 | 0,59% | 2,37% | 4,20% | 6,33% | 20,86% |
| METHYL FORMATE | 487,2 | 60,00 | 0,2556 | 0,2570 | 0,4365 | 0,8345 | 1,6414 | 14,4770 | 0,51% | 1,22% | 2,15% | 5,32% | 22,42% |
| METHYL HYDROPEROXIDE | 566,1 | 92,44 | 0,4827 | | 0,5379 | 0,8512 | 2,0537 | | 0,64% | 1,20% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| METHYL IODIDE | 528,2 | 66,00 | 0,1567 | 0,2669 | 0,2671 | 0,8490 | 1,8554 | 12,0805 | 3,46% | 4,97% | 1,80% | 4,97% | 19,84% |
| METHYL ISOBUTYL ETHER | 497 | 34,10 | 0,3078 | 0,2706 | 0,2287 | 0,8378 | 2,7563 | 12,5550 | 0,56% | 4,53% | 0,21% | 3,54% | 18,96% |
| METHYL ISOBUTYL KETONE | 574,6 | 32,70 | 0,3557 | 0,2575 | 0,2690 | 0,8388 | 2,7393 | 27,2253 | 2,59% | 1,45% | | 3,86% | 24,60% |
| METHYL ISOBUTYRATE | 540,7 | 34,32 | 0,3637 | 0,2579 | 0,3194 | 0,8204 | 2,3659 | 24,0659 | 0,85% | 2,04% | 0,45% | 3,97% | 21,70% |
| METHYL ISOCYANATE | 488 | 54,80 | 0,3007 | 0,2484 | 0,2358 | 0,8403 | 2,7114 | 21,1000 | 0,51% | 1,90% | | 3,21% | 11,73% |
| METHYL ISOPROPENYL KETONE | 566 | 38,90 | 0,2862 | 0,2509 | 0,6148 | 0,8631 | 1,3769 | 30,4672 | 0,66% | 1,41% | | 5,11% | 23,44% |
| METHYL ISOPROPYL ETHER | 464,48 | 37,62 | 0,2656 | 0,2705 | 0,5634 | 0,8500 | 1,4004 | 12,6099 | 0,81% | 2,04% | 0,94% | 3,35% | 19,41% |
| METHYL ISOPROPYL KETONE | 553,4 | 38,00 | 0,3208 | 0,2596 | 0,4211 | 0,7898 | 1,7253 | 22,0602 | 0,97% | 8,22% | 1,20% | 4,75% | 23,08% |
| METHYL ISOPROPYL SULFIDE | 553,1 | 40,21 | 0,2461 | 0,2711 | 0,5766 | 0,8673 | 1,3613 | 13,8095 | 0,55% | 2,12% | | 3,87% | 12,02% |
| METHYL LACTATE | 607,3 | 42,35 | 0,5297 | 0,2476 | 0,5116 | 0,8492 | 2,2702 | 25,0807 | 0,62% | 1,56% | | 3,78% | 23,30% |
| METHYL MERCAPTAN | 469,95 | 72,30 | 0,1582 | 0,2722 | 0,4040 | 0,8485 | 1,4266 | 7,4581 | 3,24% | 3,82% | 1,46% | 4,95% | 19,09% |
| METHYL METHACRYLATE | 566 | 36,80 | 0,2802 | 0,2552 | 0,2964 | 0,7670 | 1,8910 | 29,7037 | 0,55% | 1,60% | | 4,66% | 22,77% |
| METHYL MYRISTATE | 741,2 | 14,21 | 0,6979 | 0,2335 | 1,7272 | 1,0000 | 0,8137 | 129,6612 | 1,47% | 1,40% | | 3,41% | 32,52% |
| METHYL n-BUTYL ETHER | 512,74 | 33,71 | 0,3130 | 0,2624 | 0,2263 | 0,8364 | 2,7818 | 19,8463 | 0,57% | 3,80% | 0,22% | 4,63% | 22,10% |
| METHYL n-BUTYL SULFIDE | 593 | 34,70 | 0,3229 | 0,2610 | 0,3006 | 0,8378 | 2,4107 | 24,0500 | 0,73% | 1,31% | 1,12% | 3,96% | 24,88% |
| METHYL n-BUTYRATE | 554,5 | 34,73 | 0,3775 | 0,2533 | 0,5903 | 0,8214 | 1,5557 | 27,5227 | 1,69% | 2,54% | 3,74% | 5,14% | 22,05% |
| METHYL NONAFLUORO-N-BUTYL ETHER | 468,45 | 22,30 | 0,4322 | 0,2597 | 0,6243 | 0,8138 | 1,5918 | 28,0641 | 4,21% | | 0,82% | 3,07% | 22,06% |
| METHYL n-PENTYL ETHER | 546,49 | 30,42 | 0,3442 | 0,2633 | 0,2689 | 0,8286 | 2,5981 | 22,8107 | 0,41% | 2,85% | 0,13% | 3,17% | 25,02% |
| METHYL n-PROPYL ETHER | 476,25 | 38,01 | 0,2770 | 0,2692 | 0,2299 | 0,8441 | 2,6472 | 13,8340 | 2,39% | 2,86% | 0,78% | 2,72% | 20,80% |
| METHYL n-PROPYL SULFIDE | 565 | 39,70 | 0,2737 | 0,2671 | 0,2589 | 0,8417 | 2,4551 | 17,2486 | 0,37% | 1,62% | 0,84% | 3,10% | 22,86% |
| METHYL OLEATE | 764 | 12,80 | 1,0494 | 0,2397 | 0,5856 | 0,8187 | 3,1392 | 96,2078 | 1,15% | 0,62% | | 1,90% | 46,98% |
| METHYL PALMITATE | 762,2 | 12,35 | 0,7765 | 0,2264 | 1,7388 | 1,0000 | 0,8657 | 169,7665 | 1,69% | 1,50% | | 3,87% | 33,97% |
| METHYL PALMITOLEATE | 744,4 | 14,15 | 0,9974 | 0,2404 | 0,5832 | 0,8229 | 3,0484 | 86,7827 | 1,08% | 1,64% | | 1,52% | 43,43% |
| METHYL para-TOLUATE | 718,4 | 31,78 | 0,3662 | | 0,1635 | 0,7164 | 2,3544 | | 0,54% | | | | |
| METHYL PENTYL SULFIDE | 611,9 | 30,81 | 0,3653 | 0,2594 | 0,5021 | 0,8144 | 1,7340 | 28,6298 | 0,92% | 1,52% | 0,48% | 3,74% | 22,49% |
| METHYL PHENYL SULFIDE | 712,8 | 42,06 | 0,3080 | 0,2666 | 0,2366 | 0,8176 | 2,5336 | 20,9173 | 0,40% | | | 2,78% | 14,48% |
| METHYL PROPIONATE | 530,6 | 40,04 | 0,3466 | 0,2558 | 0,3543 | 0,8227 | 2,1714 | 22,0582 | 1,00% | 1,98% | 0,57% | 4,53% | 22,41% |
| METHYL sec-BUTYL ETHER | 498 | 34,10 | 0,3062 | 0,2670 | 0,5265 | 0,8340 | 1,5544 | 15,4418 | 0,76% | 4,13% | 0,60% | 4,39% | 18,33% |
| METHYL SILANE | 352,5 | 47,00 | 0,1314 | 0,3066 | 0,5461 | 0,9561 | 1,2684 | -5,8411 | 0,21% | | | 1,02% | 4,24% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| METHYL SILICATE | 562,8 | 28,73 | 0,4442 | 0,2674 | 0,3486 | 0,8424 | 2,6749 | 17,1956 | 0,48% | 1,65% | 2,31% | 1,84% | 18,14% |
| METHYL STEARATE | 781,1 | 10,84 | 0,8595 | 0,2181 | 1,7228 | 1,0000 | 0,9353 | 219,6386 | 1,98% | 1,81% | | 4,79% | 35,68% |
| METHYL t-BUTYL SULFIDE | 570 | 35,40 | 0,2334 | 0,2722 | 0,3069 | 0,8176 | 1,9202 | 15,7966 | 0,42% | 1,19% | 0,22% | 3,73% | 19,57% |
| METHYL tert-BUTYL ETHER | 497,1 | 32,86 | 0,2465 | 0,2642 | 1,2240 | 1,0000 | 0,6801 | 21,3400 | 0,63% | 1,16% | | 4,72% | 20,95% |
| METHYL tert-PENTYL ETHER | 534 | 30,40 | 0,2981 | 0,2606 | 0,2691 | 0,8482 | 2,5786 | 25,3206 | 0,94% | 1,42% | 3,58% | 4,50% | 19,56% |
| METHYL t-PENTYL SULFIDE | 632 | 31,30 | 0,2836 | 0,2592 | 0,2276 | 0,8416 | 2,6892 | 32,7553 | 0,65% | 2,95% | 1,70% | 4,39% | 21,12% |
| METHYL TRICHLOROSILANE | 517 | 35,30 | 0,2634 | 0,2705 | 1,3824 | 1,0000 | 0,5956 | 15,7316 | 3,64% | | 0,96% | 3,88% | 14,76% |
| METHYL VINYL DICHLOROSILANE | 544,1 | 29,40 | 0,2928 | 0,2505 | 0,5305 | 0,8442 | 1,5406 | 37,7583 | 0,70% | 1,81% | | 6,31% | 16,17% |
| METHYL VINYL ETHER | 437 | 46,70 | 0,2416 | 0,2603 | 1,0514 | 1,0000 | 0,7990 | 14,8256 | 0,88% | 1,16% | | 5,83% | 16,44% |
| METHYL-3-MERCAPTOPROPIONATE | 644 | 39,26 | 0,3990 | | 0,7489 | 0,8634 | 1,3759 | | 0,78% | 1,38% | | | |
| METHYL-4-FORMYLBENZOATE | 759,5 | 31,69 | 0,6107 | 0,2282 | 0,6332 | 0,8775 | 2,1603 | 60,8410 | 2,44% | | | 6,15% | 23,64% |
| METHYLACETYLENE | 402,4 | 56,30 | 0,2115 | 0,2706 | 0,3018 | 0,8332 | 1,9338 | 8,0617 | 0,62% | 1,78% | 0,74% | 3,84% | 15,87% |
| METHYLAL | 480,6 | 39,50 | 0,2856 | 0,2463 | 0,1353 | 0,8212 | 3,0858 | 27,2097 | 0,96% | 3,53% | 0,66% | 7,45% | 45,54% |
| METHYLAMINE | 430,05 | 74,60 | 0,2814 | 0,2593 | 0,8236 | 0,8644 | 1,0432 | 9,5867 | 0,33% | 0,65% | 0,68% | 4,81% | 2,48% |
| METHYLCYCLOHEXANE | 572,1 | 34,80 | 0,2361 | 0,2715 | 0,6317 | 0,8468 | 1,1886 | 17,2539 | 1,64% | 2,10% | 0,87% | 3,60% | 18,80% |
| METHYLCYCLOPENTADIENE | 541 | 44,30 | 0,2376 | 0,2743 | 0,5352 | 0,8557 | 1,4055 | 10,2020 | 0,70% | 1,10% | | 3,40% | 17,65% |
| METHYLCYCLOPENTADIENE DIMER | 675 | 26,40 | 0,4229 | | 0,5876 | 0,8451 | 1,7354 | | 0,75% | 1,34% | | | |
| METHYLCYCLOPENTANE | 532,7 | 37,90 | 0,2288 | 0,2712 | 0,5735 | 0,8458 | 1,2793 | 14,7516 | 0,47% | 1,54% | 2,10% | 4,02% | 17,49% |
| METHYLETHANOLAMINE | 630 | 52,20 | 0,5855 | 0,2523 | 0,3940 | 0,8242 | 2,8050 | 17,8829 | 0,77% | 1,27% | | 2,33% | 25,14% |
| METHYLGERMANIUM TRICHLORIDE | 595,4 | 39,51 | 0,2243 | 0,2684 | 1,1934 | 1,0000 | 0,6747 | 18,3992 | 0,92% | 1,36% | 1,38% | 4,25% | 18,82% |
| METHYLGLUTARONITRILE | 742 | 28,80 | 0,6381 | 0,2143 | 0,5941 | 0,8323 | 2,1986 | 91,8061 | 0,82% | 1,34% | | 4,34% | 54,02% |
| METHYLNORBORNENE | 600 | 34,40 | 0,2108 | 0,2601 | 0,9559 | 0,9900 | 0,8362 | 30,3063 | 0,72% | 1,70% | | 5,15% | 20,18% |
| m-ETHYLSTYRENE | 670,7 | 29,36 | 0,3955 | 0,2531 | 0,7343 | 0,8664 | 1,3984 | 40,7857 | 0,80% | 1,69% | | 3,23% | 28,21% |
| m-ETHYLTOLUENE | 637,15 | 31,50 | 0,3649 | 0,2585 | 0,7506 | 0,8768 | 1,3137 | 30,8897 | 0,31% | 1,49% | 3,37% | 3,39% | 24,05% |
| m-METHYLSTYRENE | 657 | 32,90 | 0,3487 | 0,2504 | 0,7415 | 0,8796 | 1,3059 | 39,6140 | 0,76% | 1,22% | | 4,79% | 26,25% |
| m-NITROANILINE | 815 | 44,20 | 0,7297 | | 0,4018 | 0,8182 | 3,1518 | | 2,05% | 0,52% | | | |
| MONOBUTYL SULFATE | 889,2 | 76,10 | 0,4390 | | 1,0171 | 0,9134 | 1,1008 | | 0,93% | 2,02% | | | |
| MONOCHLOROBENZENE | 632,35 | 45,19 | 0,2499 | 0,2641 | 0,3383 | 0,8423 | 1,9860 | 19,3208 | 0,55% | 2,08% | 2,72% | 4,46% | 19,64% |
| MONOCHLOROSILANE | 399,2 | 53,01 | 0,1327 | | 0,4393 | 0,8578 | 1,3352 | | 0,92% | 1,69% | 1,16% | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| MONOMETHYL TEREPHTHALATE | 797,8 | 31,08 | 0,8770 | | 0,4604 | 0,8135 | 3,2584 | | 0,62% | | | | |
| MONOMETHYL UREA | 836,5 | 63,53 | 0,5690 | | 0,1657 | 0,7299 | 3,0986 | | 0,60% | | | | |
| MONOOLEIN | 856,9 | 12,01 | 1,0985 | 0,2316 | 0,6780 | 0,8294 | 2,9161 | 144,9219 | 1,35% | | | 1,69% | 33,76% |
| MONO-TERT-BUTYLHYDROQUINONE | 805,5 | 37,65 | 0,7321 | | 0,6591 | 0,8653 | 2,3216 | | 2,22% | | | | |
| MORPHOLINE | 618 | 53,40 | 0,3579 | 0,2693 | 0,3073 | 0,8473 | 2,5925 | 10,1223 | 1,67% | 2,98% | | 2,59% | 19,93% |
| m-PHENYLENEDIAMINE | 824 | 51,80 | 0,5464 | 0,2486 | 0,7144 | 0,9067 | 1,8321 | 28,9353 | 0,59% | 1,99% | | 2,43% | 9,27% |
| m-TERPHENYL | 883 | 24,80 | 0,6509 | 0,2451 | 0,5021 | 0,8449 | 2,6321 | 61,2293 | 0,65% | 1,12% | | 2,77% | 27,84% |
| m-TOLUALCOHOL | 681 | 39,10 | 0,7508 | 0,2736 | 0,4429 | 0,8227 | 3,0523 | -0,8895 | 0,83% | 0,57% | 4,66% | 1,35% | 24,96% |
| m-TOLUALDEHYDE | 691 | 36,70 | 0,4332 | 0,2458 | 0,8609 | 0,8847 | 1,2810 | 38,9209 | 0,63% | 0,83% | | 4,80% | 28,43% |
| m-TOLUIC ACID | 754 | 39,01 | 0,6809 | | 0,3859 | 0,7615 | 2,7119 | | 0,75% | 1,77% | | | |
| m-TOLUIDINE | 707 | 42,80 | 0,4348 | 0,2536 | 1,3279 | 0,8997 | 0,8153 | 27,6161 | 4,91% | 3,17% | 0,16% | 4,32% | 29,19% |
| m-XYLENE | 617 | 35,41 | 0,3265 | 0,2581 | 0,3602 | 0,8466 | 2,2015 | 27,1365 | 0,56% | 1,10% | 1,33% | 4,31% | 21,54% |
| N-(2-HYDROXYETHYL)PIPERAZINE | 780 | 49,37 | 0,4203 | 0,2863 | 1,3428 | 1,0000 | 0,8024 | -2,6911 | 1,75% | 2,15% | | 1,37% | 19,39% |
| N,N'-BIS(2-HYDROXYETHYL)ETHYLENEDIAMINE | 781,8 | 38,04 | 1,1400 | 0,2584 | 0,7159 | 0,8315 | 2,8749 | 10,1620 | 1,25% | | | 1,59% | 26,57% |
| N,N'-DI(2-HYDROXYETHYL)PIPERAZINE | 825,3 | 38,80 | 0,6303 | | 0,5862 | 0,7999 | 2,0955 | | 0,68% | 1,28% | 3,90% | | |
| N,N-DIETHYLANILINE | 702 | 28,50 | 0,4262 | 0,2523 | 1,5041 | 1,0000 | 0,7081 | 43,8756 | 1,50% | 2,15% | 0,15% | 4,48% | 14,89% |
| N,N-DIETHYLHYDROXYLAMINE | 567 | 41,30 | 0,7154 | 0,2712 | 1,2451 | 0,9776 | 1,2300 | 5,6539 | 1,33% | 1,68% | | 1,54% | 13,24% |
| N,N-DIETHYLMETHYLAMINE | 506,1 | 33,43 | 0,3051 | 0,2725 | 0,3846 | 0,8521 | 2,0562 | 11,9810 | 0,62% | | | 2,59% | 18,83% |
| N,N-DIMETHYLACETAMIDE | 658 | 40,30 | 0,3635 | 0,2310 | 1,1552 | 1,0000 | 0,8802 | 49,1998 | 0,88% | 0,31% | | 7,42% | 25,64% |
| N,N-DIMETHYLANILINE | 687,15 | 36,30 | 0,4022 | 0,2540 | 1,0607 | 0,9989 | 1,0293 | 31,5900 | 1,17% | 2,61% | | 4,36% | 6,03% |
| N,N-DIMETHYLFORMAMIDE | 649,6 | 44,20 | 0,3177 | 0,2200 | 0,3945 | 0,8419 | 2,0230 | 53,5364 | 0,67% | 2,23% | 0,85% | 10,07% | 35,04% |
| N,N-DIMETHYL-n-BUTYLAMINE | 538 | 29,30 | 0,3403 | 0,2666 | 0,4286 | 0,8357 | 1,9414 | 20,4475 | 0,73% | 1,38% | | 2,83% | 16,85% |
| N,N'-DI-tert-BUTYLETHYLENEDIAMINE | 625 | 21,60 | 0,6278 | | 0,7338 | 0,8869 | 1,9229 | | 0,88% | 1,27% | 8,14% | | |
| N-AMINOETHYL ETHANOLAMINE | 698 | 44,60 | 1,0473 | 0,2524 | 0,6010 | 0,8216 | 3,0765 | 14,5460 | 0,93% | 1,20% | | 2,13% | 27,80% |
| N-AMINOETHYL PIPERAZINE | 710,7 | 37,87 | 0,5271 | 0,2618 | 0,4410 | 0,8496 | 2,5554 | 18,0693 | 0,68% | | | 2,18% | 20,98% |
| NAPHTHACENE | 987 | 23,90 | 0,5653 | | 0,3021 | 0,8172 | 3,1740 | | 0,55% | 2,54% | | | |
| NAPHTHALENE | 748,4 | 40,50 | 0,3020 | 0,2603 | 0,3757 | 0,8201 | 1,9035 | 28,3468 | 2,05% | 5,27% | 2,76% | 4,19% | 18,87% |
| n-BUTANE | 425,12 | 37,96 | 0,2002 | 0,2732 | 0,3515 | 0,8609 | 1,8323 | 11,0274 | 0,50% | 1,24% | 3,23% | 3,66% | 17,39% |
| n-BUTYL ACETATE | 575,4 | 30,90 | 0,4394 | 0,2574 | 0,2927 | 0,8317 | 2,8701 | 26,4717 | 1,24% | 1,17% | 1,43% | 2,97% | 25,86% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| n-BUTYL ACRYLATE | 598 | 29,10 | 0,4817 | 0,2620 | 0,3423 | 0,8361 | 2,7882 | 24,7392 | 2,49% | 1,92% | | 1,36% | 27,29% |
| n-BUTYL BENZOATE | 724 | 25,90 | 0,5767 | 0,2518 | 0,5908 | 0,8610 | 2,1552 | 42,4754 | 0,22% | | | 1,83% | 31,94% |
| n-BUTYL CHLORIDE | 539,2 | 37,21 | 0,2472 | 0,2561 | 0,3613 | 0,8338 | 1,8648 | 26,9281 | 1,25% | 2,20% | | 5,42% | 22,44% |
| n-BUTYL FORMATE | 559 | 35,10 | 0,3878 | 0,2559 | 0,3014 | 0,8260 | 2,5688 | 24,8192 | 0,55% | 2,45% | 1,04% | 4,33% | 23,98% |
| n-BUTYL ISOCYANATE | 568 | 34,40 | 0,4145 | 0,2438 | 0,7391 | 0,8668 | 1,4269 | 34,7451 | 0,81% | 0,90% | | 6,81% | 17,46% |
| n-BUTYL MERCAPTAN | 570,1 | 39,70 | 0,2714 | 0,2628 | 0,3027 | 0,8489 | 2,2641 | 19,9285 | 1,90% | 1,88% | 2,15% | 4,54% | 23,15% |
| n-BUTYL METHACRYLATE | 619 | 26,30 | 0,4467 | 0,2519 | 1,2974 | 1,0000 | 0,8623 | 40,1531 | 0,95% | 0,79% | | 4,24% | 27,26% |
| n-BUTYL n-BUTYRATE | 616 | 25,40 | 0,4815 | 0,2535 | 0,3401 | 0,8354 | 2,8001 | 36,8875 | 0,54% | 1,60% | 2,23% | 3,22% | 28,59% |
| n-BUTYL PROPIONATE | 594,6 | 28,00 | 0,4644 | 0,2558 | 0,6875 | 0,8371 | 1,5814 | 30,9078 | 0,51% | 1,12% | 0,54% | 3,41% | 26,16% |
| n-BUTYL STEARATE | 764 | 11,10 | 1,0246 | 0,2496 | 0,5354 | 0,8126 | 3,2806 | 84,5226 | 1,52% | 2,57% | 7,69% | 3,37% | 48,22% |
| n-BUTYL VALERATE | 629 | 23,30 | 0,5955 | 0,2539 | 0,4779 | 0,8195 | 2,4324 | 36,5345 | 0,41% | | 0,12% | 1,97% | 30,10% |
| n-BUTYLAMINE | 531,9 | 42,00 | 0,3292 | 0,2650 | 0,2128 | 0,8307 | 2,8897 | 14,5190 | 0,67% | 2,31% | 3,03% | 4,16% | 8,54% |
| n-BUTYLBENZENE | 660,5 | 28,90 | 0,3941 | 0,2606 | 0,4570 | 0,8342 | 1,9927 | 31,7276 | 1,09% | 1,33% | 2,07% | 2,37% | 21,06% |
| n-BUTYLBENZENE HYDROPEROXIDE | 762,5 | 29,44 | 0,9570 | | 0,5658 | 0,8236 | 3,0336 | | 0,92% | 1,61% | | | |
| n-BUTYLCYCLOHEXANE | 667 | 25,70 | 0,2743 | 0,2579 | 1,4616 | 1,0000 | 0,5900 | 45,1019 | 2,37% | 2,28% | 4,01% | 4,85% | 26,25% |
| n-BUTYLCYCLOPENTANE | 621 | 27,20 | 0,3719 | 0,2592 | 0,4222 | 0,8300 | 2,0284 | 32,6715 | 1,67% | 3,42% | 1,55% | 3,63% | 24,24% |
| n-BUTYLHYDROPEROXIDE | 565 | 52,10 | 0,8658 | 0,3040 | 0,5256 | 0,8212 | 2,9662 | -18,8557 | 0,44% | 1,13% | | 4,03% | 8,64% |
| n-BUTYRIC ACID | 615,7 | 40,60 | 0,6750 | 0,2297 | 0,6326 | 0,8677 | 2,2883 | 36,0001 | 1,05% | | | 5,36% | 31,16% |
| n-CROTYL ACETATE | 585,4 | 33,14 | 0,4383 | 0,2578 | 0,6109 | 0,8456 | 1,7156 | 24,9299 | 0,76% | 1,28% | | 2,98% | 22,60% |
| n-DECANE | 617,7 | 21,10 | 0,4923 | 0,2517 | 0,3786 | 0,8255 | 2,5740 | 48,7183 | 0,63% | 1,25% | 1,08% | 3,09% | 23,60% |
| n-DECYL FORMATE | 672 | 19,90 | 0,7118 | 0,2481 | 0,4023 | 0,8196 | 3,1201 | 52,3236 | 0,80% | | 1,63% | 1,68% | 26,77% |
| n-DECYL MERCAPTAN | 696 | 21,30 | 0,5874 | 0,2417 | 0,4265 | 0,8384 | 2,7461 | 61,7352 | 2,68% | 2,51% | 2,80% | 4,48% | 35,24% |
| n-DECYLAMINE | 663 | 21,80 | 0,6664 | 0,2477 | 0,3931 | 0,8228 | 3,0498 | 46,8876 | 3,23% | 4,41% | 3,05% | 2,90% | 26,55% |
| n-DECYLBENZENE | 753 | 17,70 | 0,6797 | 0,2468 | 0,4354 | 0,8284 | 2,9359 | 70,6521 | 3,60% | 3,19% | 1,85% | 1,58% | 36,33% |
| n-DECYLCYCLOHEXANE | 751,25 | 16,50 | 0,6627 | 0,2471 | 0,6254 | 0,8239 | 2,1736 | 75,4421 | 2,50% | 3,38% | 0,56% | 1,71% | 38,28% |
| n-DODECANE | 658 | 18,20 | 0,5764 | 0,2466 | 0,4299 | 0,8171 | 2,5617 | 65,9614 | 0,80% | 1,22% | 2,82% | 2,95% | 23,98% |
| n-DODECANOIC ACID | 743 | 19,30 | 0,8983 | 0,2406 | 1,7644 | 1,0000 | 0,9472 | 68,5455 | 1,33% | 1,24% | 5,67% | 2,13% | 30,17% |
| n-DODECYLAMINE | 696 | 18,80 | 0,7638 | 0,2440 | 0,4622 | 0,8242 | 3,0208 | 58,4215 | 6,04% | 7,16% | 4,36% | 2,58% | 31,65% |
| n-DODECYLBENZENE | 780 | 15,60 | 0,7333 | 0,2446 | 0,5563 | 0,8180 | 2,4936 | 88,1905 | 0,97% | 2,40% | 0,60% | 1,62% | 40,58% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| n-EICOSANE | 768 | 11,60 | 0,9069 | 0,2335 | 0,5596 | 0,8140 | 2,8872 | 140,6330 | 1,09% | 2,24% | 0,73% | 1,80% | 26,44% |
| NEOABIETIC ACID | 812 | 16,70 | 0,8598 | | 0,4693 | 0,8166 | 3,1878 | | 0,88% | 1,02% | | | |
| NEOHEXANOIC ACID | 653 | 34,10 | 0,5671 | 0,2396 | 0,5961 | 0,8143 | 1,9649 | 38,2979 | 0,43% | 1,41% | 2,98% | 6,24% | 26,59% |
| NEOPENTANE | 433,8 | 31,96 | 0,1957 | 0,2756 | 0,1821 | 0,8476 | 2,5887 | 11,6811 | 0,64% | 1,99% | 1,13% | 2,89% | 18,73% |
| N-ETHYL-2-METHYLALLYLAMINE | 556 | 31,80 | 0,3550 | 0,2673 | 0,3511 | 0,8232 | 2,2132 | 19,1731 | 0,60% | 1,73% | 3,62% | 2,28% | 14,91% |
| N-ETHYLANILINE | 698,55 | 35,80 | 0,4149 | 0,2522 | 0,2587 | 0,8115 | 2,7998 | 34,8546 | 0,39% | 1,10% | | 4,13% | 18,76% |
| N-ETHYLMORPHOLINE | 617 | 36,83 | 0,3327 | | 0,4968 | 0,8459 | 1,7451 | | 0,80% | 1,44% | | | |
| n-HENEICOSANE | 778 | 11,10 | 0,9420 | 0,2315 | 0,5191 | 0,8173 | 3,1709 | 153,5489 | 2,02% | 2,28% | 1,42% | 1,71% | 26,88% |
| n-HEPTACOSANE | 826 | 8,83 | 1,2136 | 0,2265 | 0,6766 | 0,8193 | 3,1268 | 205,7583 | 2,33% | | 1,02% | 1,58% | 28,32% |
| n-HEPTADECANE | 736 | 13,40 | 0,7697 | 0,2364 | 0,5331 | 0,8075 | 2,6166 | 117,2450 | 0,25% | 0,55% | 0,17% | 2,57% | 26,58% |
| n-HEPTADECYLBENZENE | 826 | 12,10 | 0,9195 | 0,2374 | 0,6550 | 0,8237 | 2,5996 | 130,0828 | 1,55% | 1,17% | 1,02% | 1,82% | 46,82% |
| n-HEPTANE | 540,2 | 27,40 | 0,3495 | 0,2602 | 0,3529 | 0,8368 | 2,2644 | 27,8526 | 0,48% | 1,61% | 3,16% | 3,73% | 21,16% |
| n-HEPTANOIC ACID | 677,3 | 30,43 | 0,7599 | 0,2495 | 0,6874 | 0,8105 | 2,1088 | 32,0655 | 0,92% | 2,27% | | 1,68% | 25,49% |
| n-HEPTYL ACETATE | 637 | 23,30 | 0,5943 | 0,2552 | 0,3880 | 0,8301 | 2,9014 | 36,4577 | 0,43% | 2,67% | 2,45% | 1,48% | 31,85% |
| n-HEPTYL FORMATE | 628 | 25,40 | 0,5337 | 0,2525 | 0,3250 | 0,8261 | 2,9812 | 38,2995 | 2,49% | 1,59% | 1,69% | 2,52% | 30,96% |
| n-HEPTYL MERCAPTAN | 645 | 27,70 | 0,4226 | 0,2534 | 0,3490 | 0,8401 | 2,5698 | 37,8125 | 2,19% | 1,98% | 2,51% | 3,76% | 30,65% |
| n-HEPTYLAMINE | 607 | 28,50 | 0,5077 | 0,2553 | 0,2948 | 0,8238 | 3,0303 | 29,8627 | 2,80% | 3,67% | 2,03% | 3,33% | 18,98% |
| n-HEPTYLBENZENE | 714 | 21,80 | 0,5272 | 0,2504 | 0,3771 | 0,8364 | 2,7813 | 55,0342 | 4,36% | 4,32% | 2,01% | 2,22% | 31,59% |
| n-HEXACOSANE | 819 | 9,10 | 1,1544 | 0,2267 | 0,6098 | 0,8135 | 3,2596 | 201,1113 | 2,51% | | 1,30% | 1,53% | 28,83% |
| n-HEXADECANE | 723 | 14,00 | 0,7174 | 0,2366 | 0,5435 | 0,8042 | 2,4387 | 113,3416 | 0,26% | 0,69% | 0,27% | 3,00% | 26,72% |
| n-HEXADECANOIC ACID | 785 | 14,90 | 0,9919 | 0,2348 | 2,0172 | 1,0000 | 0,8844 | 104,2859 | 5,22% | | 7,88% | 2,19% | 33,58% |
| n-HEXADECYLBENZENE | 818 | 12,70 | 0,8996 | 0,2414 | 0,6736 | 0,8252 | 2,4908 | 113,2628 | 0,34% | 0,81% | 1,10% | 2,00% | 46,65% |
| n-HEXANE | 507,6 | 30,25 | 0,3013 | 0,2633 | 0,2982 | 0,8491 | 2,4179 | 22,0561 | 0,98% | 1,66% | 2,69% | 3,97% | 19,41% |
| n-HEXANOIC ACID | 660,2 | 33,08 | 0,7330 | 0,2397 | 1,5794 | 1,0000 | 0,9374 | 37,4155 | 0,24% | | | 4,50% | 26,40% |
| n-HEXYL ACETATE | 618 | 25,40 | 0,5396 | 0,2550 | 0,3604 | 0,8317 | 2,8706 | 33,8382 | 1,06% | 3,28% | 2,40% | 1,95% | 29,65% |
| n-HEXYL FORMATE | 607 | 28,00 | 0,4830 | 0,2504 | 0,2721 | 0,8201 | 3,0652 | 35,9236 | 0,51% | 2,92% | 0,90% | 4,40% | 27,80% |
| n-HEXYL MERCAPTAN | 623 | 30,80 | 0,3681 | 0,2559 | 0,3799 | 0,8402 | 2,2280 | 32,1096 | 1,61% | 1,92% | 2,36% | 4,21% | 28,27% |
| n-HEXYLAMINE | 584 | 31,80 | 0,4577 | 0,2570 | 0,2618 | 0,8234 | 3,0378 | 25,0393 | 2,13% | 4,32% | 1,73% | 3,88% | 15,77% |
| n-HEXYLBENZENE | 698 | 23,80 | 0,4790 | 0,2518 | 0,4098 | 0,8372 | 2,4671 | 48,5841 | 2,13% | 2,83% | 1,90% | 2,94% | 28,87% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| NIACIN | 760 | 46,40 | 0,5958 | | 0,3570 | 0,8241 | 3,0232 | | 0,56% | 1,57% | | | |
| NICKEL CARBONYL | 452,55 | 30,40 | 0,4631 | 0,2738 | 0,3660 | 0,8439 | 2,6501 | 5,9689 | 4,43% | | 0,38% | 1,95% | 16,18% |
| NICOTINONITRILE | 703 | 41,20 | 0,4215 | 0,2272 | 0,4329 | 0,8499 | 2,2645 | 51,6450 | 1,32% | 1,96% | 2,73% | 6,82% | 22,46% |
| NITROETHANE | 593 | 51,60 | 0,3803 | 0,2412 | 0,3738 | 0,8610 | 2,3821 | 28,2597 | 5,83% | 5,21% | 3,82% | 5,28% | 22,98% |
| NITROGEN | 126,2 | 34,00 | 0,0377 | 0,2908 | 0,1901 | 0,8900 | 2,0107 | 1,3475 | 0,31% | 1,66% | 3,91% | 2,98% | 13,80% |
| NITROGEN TRIFLUORIDE | 234 | 44,61 | 0,1200 | 0,2779 | 0,4284 | 0,8671 | 1,3232 | 4,7535 | 0,32% | 0,68% | | 4,21% | 18,43% |
| NITROGEN TRIOXIDE | 425 | 69,90 | 0,4312 | | 0,2776 | 0,8290 | 2,9133 | | 0,51% | | | | |
| NITROMETHANE | 588,15 | 63,10 | 0,3480 | 0,2310 | 0,3693 | 0,8659 | 2,3124 | 28,5796 | 3,93% | 5,11% | 2,73% | 6,32% | 32,80% |
| NITROSYL CHLORIDE | 440,65 | 91,20 | 0,3005 | 0,3061 | 0,5561 | 0,9242 | 1,6649 | -5,9067 | 2,04% | 2,12% | | 0,89% | 0,59% |
| NITROUS OXIDE | 309,57 | 72,45 | 0,1409 | 0,2753 | 0,3111 | 0,8132 | 1,5587 | 4,3989 | 1,04% | 1,87% | 0,07% | 3,23% | 17,07% |
| N-METHYL-2-PYRROLIDONE | 721,6 | 45,20 | 0,3732 | 0,2407 | 0,3526 | 0,8543 | 2,4813 | 38,2720 | 1,28% | 4,27% | | 5,86% | 30,38% |
| N-METHYLACETAMIDE | 718 | 49,80 | 0,4351 | 0,2239 | 0,2870 | 0,8304 | 2,8965 | 46,2710 | 0,83% | 1,90% | | 7,33% | 32,33% |
| N-METHYLANILINE | 701,55 | 52,00 | 0,4750 | 0,2883 | 0,5273 | 0,8784 | 2,1485 | -4,6745 | 2,81% | 2,39% | | 1,58% | 1,50% |
| N-METHYLCYCLOHEXYLAMINE | 622 | 34,90 | 0,3855 | 0,2654 | 0,3115 | 0,8355 | 2,5990 | 18,7598 | 0,75% | 1,58% | | 2,74% | 20,91% |
| N-METHYLFORMAMIDE | 721 | 56,20 | 0,4100 | 0,2062 | 0,5979 | 0,8466 | 1,6832 | 53,3193 | 0,75% | 1,63% | | 11,34% | 40,58% |
| N-METHYLPYRROLE | 610 | 47,70 | 0,2128 | 0,2710 | 1,4269 | 0,9775 | 0,5391 | 17,3192 | 0,80% | 1,04% | 1,01% | 1,34% | 19,12% |
| N-METHYLPYRROLIDINE | 550 | 42,00 | 0,2258 | 0,2755 | 0,6097 | 0,8778 | 1,2619 | 10,3670 | 0,74% | 1,29% | | 3,41% | 17,52% |
| N-METHYLTHIOPYRROLIDONE | 869 | 43,20 | 0,2381 | | 0,4797 | 0,8633 | 1,5593 | | 0,30% | 1,45% | | | |
| N-NITROSODIETHANOLAMINE | 887,1 | 48,36 | 0,9833 | 0,2424 | 0,6459 | 0,8345 | 2,8170 | 28,4563 | 0,93% | | | 1,84% | 29,71% |
| N-NITROSODIMETHYLAMINE | 661 | 48,90 | 0,2738 | 0,2284 | 0,6320 | 0,8340 | 1,2792 | 45,4824 | 0,83% | 2,02% | 0,29% | 8,49% | 28,07% |
| n-NONADECANE | 758 | 12,10 | 0,8522 | 0,2334 | 0,5824 | 0,8026 | 2,6145 | 137,9881 | 0,95% | 1,22% | 0,36% | 2,32% | 26,84% |
| n-NONANE | 594,6 | 22,90 | 0,4435 | 0,2544 | 0,4046 | 0,8255 | 2,3023 | 41,4328 | 0,29% | 0,93% | 0,94% | 3,28% | 23,08% |
| n-NONANOIC ACID | 710,7 | 25,14 | 0,7787 | 0,2507 | 1,6788 | 0,9835 | 0,9097 | 40,7316 | 0,58% | 0,49% | | 1,51% | 27,18% |
| n-NONYL ACETATE | 661 | 19,90 | 0,7036 | 0,2553 | 0,4616 | 0,8194 | 2,8040 | 40,4816 | 0,38% | 0,71% | 2,02% | 1,55% | 34,78% |
| n-NONYL FORMATE | 656 | 21,40 | 0,6504 | 0,2507 | 0,3697 | 0,8204 | 3,1030 | 45,5670 | 0,86% | | 1,39% | 1,87% | 25,82% |
| n-NONYL MERCAPTAN | 681 | 23,10 | 0,5260 | 0,2491 | 0,3985 | 0,8250 | 2,5968 | 49,8716 | 4,13% | 4,38% | 2,71% | 3,24% | 34,36% |
| n-NONYL n-UNDECYL PHTHALATE | 914,6 | 9,95 | 0,9080 | | 0,6203 | 0,8378 | 2,7576 | | 0,69% | | | | |
| n-NONYLAMINE | 648 | 23,60 | 0,6171 | 0,2530 | 0,3691 | 0,8241 | 3,0237 | 38,5157 | 3,02% | 5,29% | 2,95% | 2,06% | 25,21% |
| n-OCTACOSANE | 832 | 8,50 | 1,2375 | 0,2256 | 0,6633 | 0,8149 | 3,2252 | 217,2250 | 3,45% | 3,01% | 1,47% | 1,60% | 29,30% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| n-OCTADECANE | 747 | 12,70 | 0,8114 | 0,2347 | 0,5664 | 0,8054 | 2,5832 | 128,1272 | 0,57% | 0,84% | 0,15% | 2,47% | 26,22% |
| n-OCTADECYLBENZENE | 834 | 11,60 | 0,9505 | 0,2346 | 0,5587 | 0,8230 | 3,0461 | 142,6682 | 1,44% | 1,38% | 1,75% | 1,66% | 47,99% |
| n-OCTANE | 568,7 | 24,90 | 0,3996 | 0,2569 | 0,3597 | 0,8321 | 2,3840 | 34,8744 | 0,58% | 1,14% | 1,00% | 3,38% | 23,07% |
| n-OCTANOIC ACID | 694,26 | 27,79 | 0,7734 | 0,2466 | 0,6388 | 0,7999 | 2,2377 | 37,8278 | 0,96% | 1,73% | | 2,58% | 25,15% |
| n-OCTYL ACETATE | 652 | 21,50 | 0,6558 | 0,2525 | 0,5209 | 0,8071 | 2,3879 | 41,9332 | 1,82% | | 0,80% | 1,67% | 33,09% |
| n-OCTYL FORMATE | 645 | 23,30 | 0,5871 | 0,2520 | 0,3435 | 0,8217 | 3,0740 | 41,2146 | 6,13% | | 0,96% | 1,90% | 32,72% |
| n-OCTYL MERCAPTAN | 667,3 | 25,20 | 0,4497 | 0,2509 | 0,3790 | 0,8329 | 2,4751 | 45,5545 | 1,39% | 1,54% | 2,45% | 3,77% | 32,88% |
| n-OCTYLAMINE | 627 | 25,80 | 0,5694 | 0,2552 | 0,3411 | 0,8245 | 3,0149 | 32,7358 | 2,41% | 4,61% | 2,58% | 2,34% | 22,29% |
| n-OCTYLBENZENE | 729 | 20,20 | 0,5670 | 0,2482 | 0,3804 | 0,8317 | 2,8713 | 62,5268 | 3,08% | 3,25% | 1,94% | 2,19% | 33,38% |
| NONANAL | 658,5 | 26,80 | 0,4733 | 0,2627 | 1,2157 | 0,9901 | 0,9669 | 27,0745 | 0,86% | 2,10% | | 2,32% | 20,42% |
| NONYLPHENOL | 770 | 20,70 | 0,8795 | 0,2446 | 0,4051 | 0,8042 | 3,4926 | 52,8635 | 2,06% | 1,31% | | 1,94% | 29,20% |
| n-PENTADECANE | 708 | 14,80 | 0,6863 | 0,2384 | 0,5292 | 0,8044 | 2,4124 | 102,3182 | 0,27% | 2,05% | 0,27% | 3,06% | 26,26% |
| n-PENTADECANOIC ACID | 774 | 15,70 | 0,9639 | 0,2345 | 1,9167 | 1,0000 | 0,9191 | 99,2306 | 5,65% | | 7,17% | 2,18% | 33,10% |
| n-PENTADECYLBENZENE | 809 | 13,30 | 0,8567 | 0,2421 | 0,6086 | 0,8242 | 2,6216 | 107,3728 | 0,65% | 1,29% | 1,27% | 1,86% | 44,81% |
| n-PENTANE | 469,7 | 33,70 | 0,2515 | 0,2679 | 0,2950 | 0,8513 | 2,2388 | 16,2371 | 0,56% | 1,19% | 1,43% | 3,97% | 18,22% |
| n-PENTANOIC ACID | 639,16 | 36,30 | 0,7066 | 0,2357 | 0,4970 | 0,8100 | 2,6105 | 36,6779 | 0,32% | | | 4,72% | 28,95% |
| n-PENTYL ACETATE | 599,9 | 27,70 | 0,4478 | 0,2540 | 0,2855 | 0,8289 | 2,9261 | 34,1645 | 1,79% | 2,09% | 1,23% | 3,39% | 28,07% |
| n-PENTYL MERCAPTAN | 598 | 34,70 | 0,3207 | 0,2624 | 0,4116 | 0,8330 | 1,9107 | 23,7713 | 1,87% | 1,86% | 1,87% | 3,37% | 26,42% |
| n-PENTYLAMINE | 555 | 35,80 | 0,4070 | 0,2607 | 0,2328 | 0,8243 | 3,0189 | 19,7656 | 1,81% | 4,47% | 0,98% | 3,85% | 12,30% |
| n-PENTYLBENZENE | 679,9 | 26,04 | 0,4378 | 0,2534 | 0,5579 | 0,8264 | 1,7886 | 43,0288 | 3,81% | | 1,03% | 3,82% | 23,74% |
| n-PENTYLCYCLOHEXANE | 669,2 | 23,85 | 0,4612 | 0,2586 | 0,4880 | 0,8600 | 2,2062 | 36,6263 | 0,70% | 1,71% | | 2,30% | 22,89% |
| n-PROPYL ACETATE | 549,73 | 33,60 | 0,3889 | 0,2531 | 0,5310 | 0,8167 | 1,7088 | 28,7630 | 1,11% | 1,31% | 0,71% | 4,52% | 23,09% |
| n-PROPYL ACRYLATE | 569 | 32,50 | 0,4315 | 0,2597 | 0,5746 | 0,8362 | 1,7657 | 23,0542 | 0,80% | 1,16% | | 2,93% | 22,92% |
| n-PROPYL FORMATE | 538 | 40,20 | 0,3088 | 0,2567 | 0,5920 | 0,7951 | 1,3482 | 22,9857 | 1,38% | 1,73% | 0,71% | 5,18% | 22,08% |
| n-PROPYL IODIDE | 586,3 | 41,52 | 0,2230 | 0,2521 | 0,8939 | 0,9835 | 0,9230 | 29,8883 | 0,44% | 1,42% | | 6,60% | 20,09% |
| n-PROPYL ISOBUTYRATE | 579,4 | 28,40 | 0,4838 | 0,2650 | 0,3326 | 0,8150 | 2,6916 | 19,1935 | 0,57% | 2,42% | 1,96% | 1,73% | 23,58% |
| n-PROPYL MERCAPTAN | 536,6 | 46,30 | 0,2318 | 0,2689 | 0,2976 | 0,8448 | 2,0908 | 13,6297 | 1,99% | 2,07% | 1,97% | 3,76% | 21,09% |
| n-PROPYL METHACRYLATE | 599 | 29,10 | 0,3966 | 0,2582 | 0,2547 | 0,8298 | 2,9065 | 31,0089 | 1,69% | 2,11% | | 2,67% | 26,05% |
| n-PROPYL n-BUTYRATE | 593,7 | 27,20 | 0,4335 | 0,2535 | 0,4659 | 0,8062 | 1,9682 | 36,3085 | 0,46% | 3,99% | 0,30% | 3,71% | 28,65% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| n-PROPYL PROPIONATE | 568,6 | 30,60 | 0,4487 | 0,2564 | 0,2961 | 0,8313 | 2,8791 | 26,9616 | 0,33% | 3,33% | 6,04% | 3,13% | 25,46% |
| n-PROPYLAMINE | 496,95 | 47,40 | 0,2798 | 0,2636 | 1,0718 | 0,8312 | 0,8052 | 14,7560 | 1,14% | 4,15% | 1,22% | 4,89% | 6,08% |
| n-PROPYLBENZENE | 638,35 | 32,00 | 0,3444 | 0,2634 | 0,4751 | 0,8364 | 1,7970 | 26,6533 | 0,81% | 1,09% | 1,70% | 2,38% | 19,59% |
| n-PROPYLBENZENE HYDROPEROXIDE | 746,8 | 32,90 | 0,9058 | | 0,5550 | 0,8242 | 2,9589 | | 0,69% | 1,52% | | | |
| n-PROPYLCYCLOHEXANE | 639,15 | 28,07 | 0,2595 | 0,2608 | 1,3190 | 1,0000 | 0,6410 | 36,5436 | 1,35% | 1,42% | 0,72% | 4,62% | 24,64% |
| n-PROPYLCYCLOPENTANE | 596 | 30,20 | 0,3266 | 0,2623 | 0,5412 | 0,8376 | 1,5753 | 26,3840 | 1,38% | 1,57% | 1,68% | 4,15% | 21,63% |
| n-TETRACOSANE | 804 | 9,80 | 1,0710 | 0,2284 | 0,5559 | 0,8124 | 3,2859 | 183,0294 | 1,34% | 2,48% | 0,97% | 1,54% | 28,26% |
| n-TETRADECANE | 693 | 15,70 | 0,6430 | 0,2401 | 0,5090 | 0,8079 | 2,3926 | 92,7429 | 0,32% | 1,05% | 0,33% | 3,18% | 26,04% |
| n-TETRADECANOIC ACID | 763 | 16,40 | 0,9535 | 0,2334 | 1,9271 | 1,0000 | 0,9059 | 96,4996 | 5,25% | | 6,47% | 2,63% | 34,03% |
| n-TETRADECYLAMINE | 722 | 16,60 | 0,8609 | 0,2415 | 1,0027 | 0,8104 | 1,7296 | 70,1646 | 8,82% | | 1,04% | 2,15% | 35,15% |
| n-TETRADECYLBENZENE | 800 | 14,00 | 0,8130 | 0,2428 | 0,6255 | 0,8234 | 2,4628 | 101,1496 | 1,01% | 1,41% | 1,18% | 1,75% | 43,94% |
| n-TRICOSANE | 796 | 10,20 | 1,0262 | 0,2293 | 0,5437 | 0,8142 | 3,2430 | 173,8344 | 1,11% | 2,40% | 1,50% | 1,58% | 27,50% |
| n-TRIDECANE | 675 | 16,80 | 0,6174 | 0,2433 | 0,4659 | 0,8143 | 2,5169 | 78,4645 | 0,41% | 0,91% | 0,25% | 2,97% | 25,31% |
| n-TRIDECANOIC ACID | 754 | 17,90 | 0,9134 | 0,2380 | 1,8236 | 1,0000 | 0,9275 | 79,8725 | 3,41% | 3,03% | 5,99% | 2,16% | 31,35% |
| n-TRIDECYLBENZENE | 790 | 14,80 | 0,7799 | 0,2440 | 0,5467 | 0,8203 | 2,6617 | 92,5333 | 1,63% | 2,02% | 1,20% | 1,66% | 41,80% |
| n-UNDECANE | 639 | 19,50 | 0,5303 | 0,2488 | 0,4782 | 0,8122 | 2,2228 | 58,4006 | 1,07% | 1,33% | 0,55% | 3,21% | 24,06% |
| n-UNDECANOIC ACID | 732 | 20,90 | 0,8531 | 0,2426 | 1,7694 | 1,0000 | 0,9104 | 60,6117 | 0,94% | 1,01% | 4,72% | 2,15% | 29,09% |
| n-UNDECYLBENZENE | 764 | 16,72 | 0,7287 | 0,2469 | 0,4628 | 0,8275 | 2,9531 | 73,1556 | 4,82% | 3,60% | 2,27% | 1,55% | 37,47% |
| o-ANISIDINE | 736 | 42,40 | 0,4447 | 0,2547 | 0,2920 | 0,8302 | 2,8990 | 27,2180 | 2,14% | 3,15% | | 3,18% | 23,33% |
| o-CHLOROANILINE | 722 | 45,90 | 0,4213 | 0,2578 | 0,3928 | 0,8566 | 2,4470 | 22,5683 | 3,23% | 3,59% | | 3,14% | 13,57% |
| o-CHLOROBENZOIC ACID | 792 | 40,30 | 0,6637 | | 0,4736 | 0,8200 | 2,6482 | | 0,76% | | | | |
| o-CHLORONITROBENZENE | 757 | 39,80 | 0,4864 | 0,2497 | 1,2560 | 0,9711 | 0,9344 | 36,5292 | 5,40% | | 0,26% | 3,14% | 13,57% |
| o-CHLOROPHENOL | 675 | 50,00 | 0,4372 | 0,2744 | 0,5211 | 0,8883 | 2,0307 | 6,7952 | 5,79% | 6,68% | | 1,54% | 13,03% |
| o-CHLOROTOLUENE | 656 | 39,10 | 0,3044 | 0,2587 | 0,3394 | 0,8439 | 2,2003 | 26,1343 | 0,49% | 0,82% | | 4,51% | 23,97% |
| o-CRESOL | 697,55 | 50,10 | 0,4339 | 0,2688 | 0,2428 | 0,8226 | 3,0544 | 9,7797 | 1,55% | 1,67% | 1,87% | 2,95% | 33,37% |
| OCTADECAMETHYLOCTASILOXANE | 688,9 | 6,24 | 0,9837 | 0,2533 | 1,0056 | 0,8652 | 1,8757 | 129,3124 | 0,21% | 0,52% | | 4,30% | 18,80% |
| OCTAFLUORO-2-BUTENE | 392 | 23,30 | 0,2922 | 0,2417 | 0,2936 | 0,8551 | 2,4703 | 39,4919 | 1,11% | 1,66% | 1,84% | 8,74% | 22,99% |
| OCTAFLUOROCYCLOBUTANE | 388,37 | 27,77 | 0,3558 | 0,2719 | 0,2295 | 0,8303 | 2,8936 | 10,6143 | 0,22% | 1,50% | 0,29% | 2,33% | 16,04% |
| OCTAFLUOROPROPANE | 345,05 | 26,80 | 0,3280 | 0,2780 | 0,9392 | 0,9965 | 1,0573 | 5,5754 | 0,30% | | | 2,06% | 17,48% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| OCTAHYDRO-PENTALENE-1-CARBOXYLIC ACID | 799,5 | 33,37 | 0,6928 | | 0,6214 | 0,8629 | 2,3548 | | 1,01% | | | | |
| OCTAMETHYLCYCLOTETRASILOXANE | 586,5 | 13,17 | 0,5837 | 0,2572 | 0,5695 | 0,7600 | 1,9232 | 56,5328 | 0,59% | 1,32% | | 2,53% | 19,66% |
| OCTAMETHYLTRISILOXANE | 564,4 | 14,60 | 0,5377 | 0,2667 | 0,3551 | 0,8304 | 2,8956 | 30,1784 | 1,25% | 2,13% | | 1,30% | 19,95% |
| OCTANAL | 638,9 | 29,60 | 0,4420 | 0,2667 | 1,0413 | 0,9547 | 1,0996 | 20,2245 | 0,85% | 1,08% | | 1,97% | 18,44% |
| o-CYMENE | 657 | 29,00 | 0,3662 | 0,2566 | 1,1259 | 1,0000 | 0,9065 | 36,8862 | 0,76% | 1,00% | | 3,88% | 20,61% |
| o-DICHLOROBENZENE | 705 | 40,70 | 0,2192 | 0,2553 | 1,6310 | 1,0000 | 0,4680 | 35,3958 | 0,76% | 1,05% | | 5,56% | 26,69% |
| o-DIETHYLBENZENE | 668 | 28,80 | 0,3395 | 0,2534 | 1,3037 | 1,0000 | 0,7383 | 43,2293 | 0,74% | 1,54% | 0,26% | 4,70% | 19,44% |
| o-ETHYLANILINE | 704 | 37,40 | 0,4620 | 0,2594 | 0,9829 | 0,9157 | 1,1804 | 26,2592 | 0,64% | 0,56% | | 1,79% | 16,30% |
| o-ETHYLPHENOL | 703 | 42,90 | 0,4763 | 0,2770 | 0,2749 | 0,8237 | 3,0322 | 5,6046 | 3,30% | 3,71% | 3,40% | 1,36% | 27,79% |
| o-ETHYLSTYRENE | 666,7 | 29,36 | 0,3962 | 0,2497 | 0,7102 | 0,8673 | 1,4457 | 44,0385 | 0,79% | 0,94% | | 4,28% | 26,69% |
| o-ETHYLTOLUENE | 650 | 32,90 | 0,3353 | 0,2605 | 0,4465 | 0,8317 | 1,8487 | 29,1441 | 0,37% | 0,78% | | 3,33% | 21,41% |
| OLEIC ACID | 781 | 13,90 | 1,1822 | 0,2349 | 0,7477 | 0,8258 | 2,7966 | 93,8205 | 0,40% | 0,39% | | 1,75% | 46,34% |
| o-METHYLSTYRENE | 659 | 34,70 | 0,3412 | 0,2594 | 0,5903 | 0,8303 | 1,4954 | 29,1521 | 0,27% | 0,48% | | 3,56% | 22,16% |
| o-NITROANISOLE | 782 | 37,60 | 0,5613 | 0,2444 | 0,5667 | 0,8308 | 2,0922 | 41,2944 | 0,79% | 1,07% | | 3,08% | 26,80% |
| o-NITRODIPHENYLAMINE | 835 | 28,70 | 0,7669 | | 0,7238 | 0,8734 | 2,2127 | | 0,82% | | | | |
| o-NITROTOLUENE | 720 | 38,00 | 0,4878 | 0,2536 | 0,5159 | 0,8732 | 2,2151 | 32,1651 | 3,53% | 3,33% | | 1,71% | 11,78% |
| o-PHENYLENEDIAMINE | 781 | 51,80 | 0,5389 | 0,2509 | 0,5077 | 0,8329 | 2,2341 | 24,6568 | 0,56% | 1,05% | | 2,82% | 24,83% |
| o-TERPHENYL | 857 | 29,90 | 0,5513 | 0,2889 | 0,3325 | 0,8252 | 2,9995 | -11,1374 | 4,53% | 4,37% | | 2,03% | 10,19% |
| o-TOLUALDEHYDE | 694 | 36,70 | 0,4346 | 0,2453 | 0,4295 | 0,8615 | 2,3689 | 39,8726 | 0,36% | | | 3,89% | 25,44% |
| o-TOLUIC ACID | 751 | 38,60 | 0,6572 | 0,2468 | 0,3710 | 0,8195 | 3,1210 | 32,9003 | 0,69% | 1,18% | | 2,41% | 27,54% |
| o-TOLUIDINE | 716,5 | 47,00 | 0,3842 | 0,2691 | 0,2958 | 0,8319 | 2,6207 | 14,3423 | 2,37% | 1,53% | 2,81% | 1,74% | 17,42% |
| OXAZOLE | 554 | 63,20 | 0,2310 | | 0,4956 | 0,8821 | 1,5521 | | 1,78% | 3,21% | | | |
| OXYGEN | 154,58 | 50,43 | 0,0222 | 0,2899 | 0,2128 | 0,9011 | 1,8652 | 1,3486 | 0,35% | 1,45% | 4,95% | 3,74% | 13,90% |
| o-XYLENE | 630,3 | 37,32 | 0,3101 | 0,2611 | 0,3355 | 0,8551 | 2,3172 | 23,8703 | 0,41% | 1,61% | 0,74% | 3,96% | 20,06% |
| OZONE | 261 | 55,70 | 0,2119 | 0,2505 | 0,2147 | 0,8538 | 2,4890 | 9,9921 | 2,05% | 5,31% | 11,39% | 8,08% | 34,69% |
| p,alpha-DIMETHYLBENZYL ALCOHOL | 695,9 | 34,92 | 0,5945 | 0,2614 | 0,5568 | 0,8338 | 2,2182 | 18,9779 | 0,79% | 1,87% | | 1,51% | 23,17% |
| p-AMINOAZOBENZENE | 877 | 29,00 | 0,6345 | | 0,4065 | 0,8212 | 2,8739 | | 0,67% | 1,05% | | | |
| p-AMINODIPHENYL | 867 | 32,90 | 0,5419 | | 0,8779 | 0,9315 | 1,4925 | | 0,27% | | | | |
| p-AMINODIPHENYLAMINE | 867 | 31,90 | 0,6940 | | 0,5451 | 0,8226 | 2,4603 | | 0,72% | 0,90% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| PARALDEHYDE | 579 | 35,00 | 0,4368 | 0,2792 | 0,1774 | 0,8096 | 3,3533 | 3,5612 | 2,10% | 3,35% | 2,43% | 1,57% | 24,64% |
| p-BROMOTOLUENE | 699 | 43,70 | 0,3179 | 0,2813 | 0,9981 | 1,0000 | 0,9677 | 5,7178 | 0,98% | 1,70% | | 1,23% | 15,46% |
| p-CHLOROANILINE | 754 | 45,90 | 0,4210 | 0,2561 | 0,3627 | 0,8371 | 2,4850 | 26,4629 | 0,60% | 1,36% | | 2,58% | 17,80% |
| p-CHLOROBENZOTRIFLUORIDE | 601 | 30,10 | 0,3715 | 0,2495 | 0,6284 | 0,8539 | 1,5344 | 38,5583 | 0,70% | 1,18% | | 5,04% | 29,03% |
| p-CHLORONITROBENZENE | 751 | 39,80 | 0,4874 | 0,2407 | 0,8033 | 0,8596 | 1,4424 | 41,3233 | 1,15% | 1,68% | 0,76% | 5,52% | 11,49% |
| p-CHLOROPHENOL | 738 | 53,20 | 0,4849 | 0,2743 | 0,6450 | 0,9043 | 1,8567 | 6,9338 | 3,34% | 3,61% | | 1,10% | 16,16% |
| p-CHLOROTOLUENE | 660 | 39,10 | 0,3123 | 0,2610 | 0,2615 | 0,8446 | 2,6378 | 24,0891 | 0,63% | 1,44% | | 3,85% | 23,26% |
| p-CRESOL | 704,65 | 51,50 | 0,5072 | 0,2697 | 0,3122 | 0,8268 | 2,9665 | 5,4840 | 5,22% | 5,10% | 3,46% | 2,72% | 34,92% |
| p-CUMYLPHENOL | 834 | 28,60 | 0,6888 | 0,2679 | 0,3672 | 0,8159 | 3,2041 | 16,8588 | 1,23% | 1,92% | 1,73% | 1,24% | 12,56% |
| p-CYMENE | 652 | 28,00 | 0,3738 | 0,2559 | 0,4670 | 0,8424 | 1,9392 | 38,0849 | 1,00% | 2,69% | 2,11% | 3,62% | 22,19% |
| p-DICHLOROBENZENE | 684,75 | 40,70 | 0,2846 | 0,2607 | 0,3370 | 0,8276 | 2,0419 | 26,4825 | 0,44% | 1,27% | 3,90% | 3,46% | 25,30% |
| p-DIETHYLBENZENE | 657,9 | 28,03 | 0,4028 | 0,2550 | 0,6567 | 0,8413 | 1,5127 | 39,2059 | 1,73% | 2,51% | 2,03% | 3,53% | 23,00% |
| p-DIISOPROPYLBENZENE | 689 | 24,50 | 0,3900 | 0,2577 | 1,5491 | 1,0000 | 0,6522 | 43,1548 | 0,65% | 1,03% | | 4,00% | 23,12% |
| p-DIISOPROPYLBENZENE HYDROPEROXIDE | 810 | 24,90 | 0,9279 | 0,2472 | 0,6868 | 0,8234 | 2,5041 | 43,9800 | 1,36% | 1,01% | 2,62% | 1,56% | 28,19% |
| p-DIMETHYLAMINOBENZALDEHYDE | 832 | 30,70 | 0,5272 | 0,2258 | 0,6664 | 0,8999 | 1,9018 | 81,9692 | 1,86% | 3,92% | | 5,15% | 42,07% |
| p-DIVINYLBENZENE | 691,5 | 30,77 | 0,3830 | 0,2473 | 0,3714 | 0,8412 | 2,3373 | 47,0444 | 0,65% | 1,84% | | 4,22% | 24,63% |
| PENTACHLOROETHANE | 665 | 36,80 | 0,2455 | 0,2523 | 0,4624 | 0,8764 | 1,6835 | 36,6930 | 1,17% | | | 5,68% | 25,78% |
| PENTACHLOROFLUOROETHANE | 624 | 33,40 | 0,2450 | 0,2522 | 0,1744 | 0,8356 | 2,7974 | 38,5768 | 0,73% | 2,68% | | 4,23% | 25,45% |
| PENTAETHYLENE GLYCOL DIMETHYL ETHER | 769,8 | 16,67 | 1,1388 | 0,2420 | 0,6904 | 0,8281 | 2,9421 | 68,3967 | 1,19% | | | 3,45% | 47,56% |
| PENTAFLUORO(TRIFLUOROMETHYL)SULFUR | 381,3 | 33,71 | 0,2796 | 0,2973 | 0,5850 | 0,9024 | 1,4993 | -6,7520 | 0,15% | 0,84% | | 0,99% | 10,43% |
| PENTAFLUOROETHANE | 339,165 | 36,20 | 0,3053 | 0,2669 | 0,2829 | 0,8505 | 2,5417 | 10,3482 | 0,60% | 1,33% | 6,02% | 3,16% | 18,00% |
| PENTAFLUOROETHYL METHYL ETHER | 406,83 | 28,87 | 0,3535 | 0,2568 | 0,4880 | 0,8500 | 1,8446 | 22,7122 | 0,59% | 1,58% | | 3,79% | 22,33% |
| PENTAFLUOROETHYL TRIFLUOROVINYL ETHER | 401 | 28,00 | 0,4493 | | 0,6253 | 0,8464 | 1,7071 | | 0,75% | 1,34% | | | |
| PENTAFLUOROPHENOL | 609 | 40,00 | 0,5030 | 0,2630 | 0,3647 | 0,8370 | 2,7719 | 15,9482 | 2,41% | 4,15% | | 1,77% | 19,06% |
| PENTAMETHYLBENZENE | 719,15 | 28,70 | 0,4637 | 0,2561 | 0,6634 | 0,8834 | 1,7308 | 38,0079 | 0,51% | 0,88% | 1,38% | 2,21% | 22,02% |
| PENTANAL | 566,1 | 38,45 | 0,3132 | 0,2567 | 1,0194 | 1,0000 | 0,9608 | 23,8430 | 4,02% | 1,11% | | 4,96% | 22,75% |
| PERCHLORIC ACID | 631 | 38,60 | 0,0498 | 0,1701 | 0,0793 | 0,8503 | 2,4935 | 108,8243 | 0,63% | | | 35,18% | 104,90% |
| PERCHLORYL FLUORIDE | 368,4 | 53,70 | 0,1726 | 0,2822 | 0,2817 | 0,8573 | 1,9839 | 3,9437 | 0,48% | 1,56% | 8,01% | 2,50% | 15,64% |
| PERFLUOROBUTANOIC ACID | 530 | 26,50 | 0,7925 | 0,2413 | 0,3134 | 0,7975 | 3,6765 | 37,0176 | 0,52% | | | 2,35% | 29,00% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| PERFLUOROMETHYLCYCLOPENTANE | 451,437 | 21,72 | 0,4111 | 0,2667 | 0,2486 | 0,8261 | 2,9823 | 19,5525 | 0,57% | 1,63% | | 2,58% | 20,73% |
| PERFLUORO-n-DODECANE | 570,5 | 9,72 | 0,6209 | | 0,5459 | 0,8418 | 2,3520 | | 0,69% | | | | |
| PERFLUORO-n-HEPTANE | 475,65 | 16,10 | 0,5429 | 0,2557 | 0,7311 | 0,8404 | 1,6564 | 40,6971 | 0,52% | 0,79% | | 2,77% | 18,30% |
| PERFLUORO-n-HEXADECANE | 620,8 | 6,35 | 0,6461 | 0,1964 | 0,6668 | 0,8700 | 2,1053 | 424,5324 | 0,54% | | | 5,77% | 42,70% |
| PERFLUORO-n-HEXANE | 449,55 | 18,02 | 0,4965 | 0,2628 | 0,5341 | 0,8207 | 1,9880 | 27,1619 | 0,13% | 1,63% | | 1,86% | 17,98% |
| PERFLUORO-n-NONANE | 523,9 | 12,96 | 0,5253 | 0,2448 | 0,4612 | 0,8315 | 2,3620 | 80,7851 | 0,67% | | | 3,35% | 26,31% |
| PERFLUORO-n-OCTANE | 502,2 | 14,78 | 0,5084 | 0,2536 | 0,2302 | 0,8094 | 3,3591 | 52,0713 | 1,69% | 2,72% | | 2,99% | 23,83% |
| PERFLUORO-n-PENTANE | 423,1 | 20,47 | 0,4016 | 0,2663 | 1,3752 | 1,0000 | 0,7602 | 20,7250 | 0,50% | 0,71% | | 2,92% | 19,79% |
| p-ETHYLPHENOL | 716,45 | 42,90 | 0,5154 | 0,2691 | 1,0907 | 0,8283 | 1,0927 | 11,1672 | 0,74% | 3,01% | 1,30% | 2,25% | 20,77% |
| p-ETHYLSTYRENE | 674 | 29,36 | 0,3965 | 0,2529 | 0,6573 | 0,8627 | 1,5467 | 41,4631 | 0,70% | 0,93% | | 3,06% | 29,86% |
| p-ETHYLTOLUENE | 640,2 | 32,30 | 0,3666 | 0,2670 | 0,6714 | 0,8535 | 1,4165 | 22,5535 | 2,93% | 2,96% | 2,86% | 1,64% | 23,36% |
| PHENANTHRENE | 869 | 29,00 | 0,4707 | 0,2221 | 0,4169 | 0,8531 | 2,5003 | 93,0340 | 1,59% | 2,01% | 1,15% | 8,04% | 33,11% |
| PHENETOLE | 647,15 | 34,20 | 0,4179 | 0,2546 | 0,3259 | 0,8413 | 2,6939 | 30,4892 | 1,42% | 2,44% | | 3,24% | 26,65% |
| PHENOL | 694,25 | 61,30 | 0,4435 | 0,2754 | 0,2584 | 0,8250 | 3,0049 | 3,1734 | 4,19% | 4,13% | 4,74% | 2,12% | 35,68% |
| PHENOTHIAZINE | 923 | 40,01 | 0,5796 | | 0,3428 | 0,8231 | 3,0443 | | 0,61% | 1,18% | | | |
| PHENYL ISOCYANATE | 653 | 40,60 | 0,4123 | 0,2615 | 0,5305 | 0,8910 | 1,9999 | 21,9463 | 2,47% | 3,03% | | 1,49% | 14,54% |
| PHENYL MERCAPTAN | 689 | 47,40 | 0,2628 | 0,2675 | 0,3018 | 0,8238 | 2,1087 | 17,9853 | 1,95% | 2,17% | 0,89% | 2,94% | 22,18% |
| PHENYLACETONITRILE | 732 | 34,60 | 0,4715 | 0,2273 | 1,0278 | 0,9847 | 1,1729 | 62,5777 | 1,34% | 1,13% | | 7,07% | 33,95% |
| PHENYLHYDRAZINE | 761 | 49,10 | 0,5351 | 0,2583 | 0,6200 | 0,8889 | 2,0229 | 21,8698 | 6,95% | | | 1,29% | 2,47% |
| PHENYLMETHYLDICHLOROSILANE | 689 | 28,70 | 0,4022 | 0,2664 | 0,4236 | 0,8389 | 2,1651 | 26,8889 | 0,39% | 0,64% | | 1,42% | 25,68% |
| PHENYLTRICHLOROSILANE | 688 | 29,60 | 0,3956 | 0,2637 | 0,4595 | 0,8498 | 2,0611 | 27,5332 | 0,46% | 0,96% | | 1,98% | 23,58% |
| PHOSGENE | 455 | 56,74 | 0,2013 | 0,2788 | 0,3192 | 0,8413 | 1,8410 | 5,2701 | 1,45% | 1,78% | 1,79% | 3,61% | 14,19% |
| PHOSPHINE | 324,75 | 65,40 | 0,0452 | 0,3001 | 0,2627 | 0,9126 | 1,7734 | -0,5545 | 1,40% | 2,97% | | 0,90% | 22,28% |
| PHOSPHORUS (RED) | 993,75 | 83,29 | 0,0051 | | 0,3172 | 0,9523 | 1,4272 | | 0,14% | | | | |
| PHOSPHORUS OXYCHLORIDE | 602,15 | 34,40 | 0,0832 | 0,2108 | 1,6849 | 1,0000 | 0,3562 | 78,3635 | 4,16% | | 0,17% | 14,05% | 102,37% |
| PHOSPHORUS TRICHLORIDE | 563,15 | 56,70 | 0,2344 | 0,2971 | 0,2742 | 0,8671 | 2,2959 | -3,1339 | 4,54% | 3,99% | 2,54% | 1,27% | 7,08% |
| PHOSPHORUS TRIFLUORIDE | 271,1 | 43,27 | 0,2121 | 0,2804 | 0,1923 | 0,8479 | 2,5827 | 3,5862 | 2,47% | 4,86% | 2,53% | 2,84% | 14,53% |
| PHTHALAN | 700 | 42,85 | 0,3715 | 0,2598 | 0,3051 | 0,8441 | 2,6463 | 23,1845 | 0,66% | 3,43% | | 3,07% | 20,60% |
| PHTHALIC ACID | 800 | 39,50 | 1,0585 | | 0,5641 | 0,8149 | 3,2253 | | 1,07% | 0,95% | | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| PHTHALIDE | 830,9 | 50,95 | 0,5360 | 0,2665 | 0,6221 | 0,8889 | 2,0234 | 13,6863 | 5,21% | | | 1,14% | 16,88% |
| p-HYDROQUINONE | 838,8 | 58,91 | 0,4858 | 0,2455 | 0,2808 | 0,6941 | 2,2085 | 29,6744 | 0,48% | | | 4,30% | 25,41% |
| p-HYDROXYBENZALDEHYDE | 844 | 49,90 | 0,6172 | 0,2395 | 0,8814 | 0,9293 | 1,6194 | 34,2043 | 0,56% | 0,90% | | 4,37% | 20,38% |
| PIMELIC ACID | 842 | 32,80 | 0,8114 | 0,2459 | 0,3600 | 0,7423 | 3,0235 | 47,2873 | 0,73% | | | 1,56% | 37,23% |
| PIPERAZINE | 638 | 55,30 | 0,4138 | | 0,2654 | 0,8291 | 2,9133 | | 0,56% | 1,69% | | | |
| PIPERIDINE | 594,05 | 46,51 | 0,2428 | 0,2730 | 1,1014 | 0,9997 | 0,7590 | 12,1064 | 0,61% | 0,95% | 3,01% | 3,30% | 11,00% |
| p-ISOPROPENYL PHENOL | 742,7 | 39,36 | 0,5236 | | 0,3783 | 0,7954 | 2,4973 | | 0,70% | 1,51% | | | |
| p-MENTHANE HYDROPEROXIDE | 711 | 29,50 | 0,9007 | 0,2794 | 0,5222 | 0,8203 | 3,0681 | -12,1537 | 0,81% | 1,03% | | 1,95% | 22,99% |
| p-METHYLSTYRENE | 665 | 33,60 | 0,3175 | 0,2664 | 0,8853 | 0,8760 | 1,0385 | 28,5418 | 0,54% | 0,95% | 0,56% | 1,41% | 20,64% |
| p-NITROANILINE | 851 | 44,20 | 0,7824 | | 0,4301 | 0,8172 | 3,1722 | | 1,11% | 0,74% | | | |
| p-NITROTOLUENE | 743 | 32,07 | 0,4252 | 0,2205 | 0,5541 | 0,8916 | 1,9929 | 78,2707 | 3,03% | | | 7,33% | 27,85% |
| p-PHENETIDINE | 754 | 35,70 | 0,5351 | 0,2573 | 0,3947 | 0,8279 | 2,6563 | 30,9185 | 0,32% | 1,90% | | 1,42% | 24,31% |
| p-PHENYLENEDIAMINE | 796 | 51,80 | 0,5386 | 0,2480 | 0,3218 | 0,8240 | 3,0242 | 27,6844 | 0,56% | 1,37% | | 3,00% | 25,62% |
| PROPADIENE | 394 | 52,50 | 0,1041 | 0,2682 | 1,4143 | 0,9998 | 0,4285 | 11,8114 | 0,78% | 1,02% | | 5,29% | 18,90% |
| PROPANAL | 503,6 | 50,38 | 0,2813 | 0,2549 | 0,9590 | 1,0000 | 0,9530 | 18,7753 | 0,89% | 4,02% | | 4,58% | 26,60% |
| PROPANE | 369,83 | 42,48 | 0,1523 | 0,2774 | 0,5427 | 0,8811 | 1,1904 | 7,7000 | 0,85% | 1,37% | 5,41% | 3,67% | 16,79% |
| PROPARGYL ALCOHOL | 588,8 | 61,90 | 0,4567 | 0,2405 | 0,5666 | 0,8893 | 2,0186 | 22,2074 | 0,71% | | | 4,08% | 27,06% |
| PROPARGYL CHLORIDE | 541 | 53,00 | 0,1500 | 0,2444 | 0,2420 | 0,8583 | 2,1059 | 26,0827 | 0,72% | 2,31% | | 9,88% | 21,71% |
| PROPENYL CYCLOHEXENE | 636 | 31,20 | 0,3420 | 0,2612 | 0,6703 | 0,8486 | 1,3729 | 28,0940 | 0,67% | 1,30% | 3,55% | 3,97% | 22,85% |
| PROPIONIC ACID | 600,81 | 46,68 | 0,5796 | 0,2254 | 1,0828 | 0,9748 | 1,2519 | 36,3457 | 0,36% | | | 6,52% | 36,33% |
| PROPIONIC ANHYDRIDE | 623 | 32,70 | 0,5599 | 0,2586 | 0,4038 | 0,8379 | 2,7551 | 23,7050 | 1,93% | 2,98% | 1,12% | 1,34% | 27,35% |
| PROPIONITRILE | 561,3 | 42,60 | 0,3501 | 0,2165 | 0,4293 | 0,8788 | 2,1439 | 49,5840 | 3,14% | 3,99% | | 9,97% | 30,41% |
| PROPYL CHLORIDE | 503,15 | 44,25 | 0,2150 | 0,2621 | 0,3025 | 0,8335 | 1,9476 | 17,8884 | 1,24% | 2,57% | 1,35% | 5,38% | 22,32% |
| PROPYLENE | 364,85 | 46,00 | 0,1376 | 0,2782 | 0,3855 | 0,8535 | 1,4709 | 6,8923 | 0,68% | 1,76% | 2,43% | 3,65% | 15,10% |
| PROPYLENE GLYCOL 1-tert-BUTYL ETHER | 600,7 | 27,20 | 0,4863 | 0,2553 | 0,5706 | 0,8389 | 1,9212 | 32,4660 | 0,68% | 1,36% | | 2,81% | 23,58% |
| PROPYLENE GLYCOL 2-tert-BUTYL ETHER | 600,6 | 27,20 | 0,4867 | 0,2554 | 0,4159 | 0,8275 | 2,4114 | 32,3290 | 0,56% | 1,53% | | 2,81% | 23,59% |
| PROPYLENE GLYCOL MONOALLYL ETHER | 616,6 | 33,76 | 0,4797 | 0,2571 | 1,2961 | 0,9210 | 0,9006 | 25,7932 | 0,69% | 1,15% | | 3,16% | 23,18% |
| PROPYLENE GLYCOL MONOMETHYL ETHER | 579,8 | 41,13 | 0,4427 | 0,2520 | 1,1931 | 1,0000 | 0,9513 | 23,5337 | 1,50% | 0,98% | | 4,31% | 29,28% |
| PROPYLENE GLYCOL MONOMETHYL ETHER ACETATE | 597,9 | 30,09 | 0,4807 | 0,2548 | 1,3276 | 1,0000 | 0,8756 | 30,5148 | 0,84% | 0,82% | 1,82% | 3,20% | 23,56% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| PROPYLENE GLYCOL n-BUTYL ETHER | 624,9 | 27,39 | 0,5008 | 0,2485 | 1,0305 | 0,8889 | 1,1701 | 40,7484 | 0,85% | 1,04% | | 4,19% | 29,44% |
| PROPYLENEIMINE | 539,9 | 54,79 | 0,2295 | 0,2572 | 0,1097 | 0,7781 | 2,5286 | 18,6964 | 0,54% | | | 5,76% | 20,57% |
| p-TERPHENYL | 908 | 29,90 | 0,6426 | 0,2753 | 0,3599 | 0,8193 | 3,1253 | 5,6268 | 1,14% | 1,56% | 1,05% | 0,82% | 14,68% |
| p-tert-AMYLPHENOL | 752 | 29,80 | 0,5635 | | 0,3507 | 0,8266 | 2,9709 | | 0,42% | 0,55% | | | |
| p-tert-BUTYL ETHYLBENZENE | 684 | 23,80 | 0,4347 | 0,2533 | 0,4441 | 0,8231 | 2,1159 | 48,2823 | 0,39% | 0,73% | 1,03% | 3,51% | 23,67% |
| p-tert-BUTYLCATECHOL | 776 | 37,70 | 0,7344 | 0,2829 | 0,4605 | 0,8218 | 2,9191 | -7,2329 | 1,05% | 0,97% | | 1,99% | 13,05% |
| p-tert-BUTYLPHENOL | 734 | 33,40 | 0,5094 | 0,2652 | 0,2581 | 0,8151 | 3,2216 | 18,9553 | 2,02% | 3,73% | | 2,17% | 19,70% |
| p-tert-BUTYLSTYRENE | 709 | 24,80 | 0,4216 | 0,2499 | 0,3170 | 0,8394 | 2,7285 | 53,8921 | 1,87% | 2,30% | 1,84% | 3,79% | 24,32% |
| p-tert-OCTYLPHENOL | 765 | 22,80 | 0,6326 | | 0,3667 | 0,8216 | 3,0763 | | 0,55% | 0,57% | | | |
| p-TOLUALDEHYDE | 715,8 | 39,22 | 0,3827 | 0,2540 | 0,3427 | 0,8505 | 2,5421 | 31,2211 | 0,78% | 2,04% | | 3,58% | 23,27% |
| p-TOLUIC ACID | 775 | 38,00 | 0,6291 | | 0,2669 | 0,8025 | 3,4710 | | 0,54% | 1,91% | | | |
| p-TOLUIDINE | 693,15 | 40,00 | 0,4722 | 0,2444 | 0,3603 | 0,8409 | 2,7021 | 35,0057 | 2,22% | 3,48% | 1,08% | 4,33% | 28,69% |
| p-XYLENE | 616,2 | 35,11 | 0,3218 | 0,2581 | 0,2957 | 0,8508 | 2,5362 | 27,6054 | 0,54% | 1,08% | 5,93% | 3,91% | 21,38% |
| PYRAZINE | 626 | 54,90 | 0,2030 | 0,2496 | 0,2115 | 0,8518 | 2,5201 | 26,7548 | 1,84% | 2,46% | | 5,05% | 5,57% |
| PYRAZOLE | 734 | 66,00 | 0,2868 | 0,2352 | 0,2437 | 0,8444 | 2,6412 | 32,4628 | 0,64% | 1,51% | | 6,75% | 17,34% |
| PYRENE | 936 | 26,10 | 0,5074 | | 0,4627 | 0,8575 | 2,4329 | | 2,65% | 3,44% | 1,65% | | |
| PYRIDAZINE | 774 | 54,90 | 0,2035 | 0,2242 | 0,4965 | 0,8413 | 1,3740 | 52,3062 | 1,17% | | 1,20% | 10,85% | 23,51% |
| PYRIDINE | 619,95 | 56,30 | 0,2386 | 0,2697 | 0,4121 | 0,8252 | 1,6262 | 13,3416 | 0,57% | 1,15% | 0,84% | 2,93% | 14,90% |
| PYRIMIDINE | 638 | 54,90 | 0,2105 | 0,2458 | 0,1643 | 0,8404 | 2,7107 | 29,1878 | 1,17% | | 1,03% | 6,76% | 6,89% |
| PYRROLE | 639,75 | 65,30 | 0,2976 | 0,2584 | 0,9157 | 0,8881 | 0,9811 | 15,8176 | 0,33% | 0,93% | 0,28% | 5,29% | 11,18% |
| PYRROLIDINE | 568,55 | 56,10 | 0,2668 | 0,2767 | 0,4650 | 0,8108 | 1,5397 | 6,5268 | 0,23% | 0,72% | | 3,35% | 10,18% |
| QUINALDINE | 769 | 33,50 | 0,3591 | 0,2426 | 1,3901 | 1,0000 | 0,7063 | 56,0628 | 1,81% | 2,06% | | 6,07% | 18,39% |
| QUINOLINE | 782,15 | 48,60 | 0,3465 | 0,2768 | 0,3365 | 0,8564 | 2,4492 | 8,1080 | 1,18% | 2,42% | 2,85% | 1,41% | 18,04% |
| QUINONE | 683 | 59,60 | 0,4945 | 0,2796 | 0,4328 | 0,8443 | 2,4362 | -0,0941 | 0,65% | 0,94% | 10,75% | 1,80% | 9,17% |
| RADON | 377,5 | 62,80 | 0,0000 | 0,2806 | 0,0000 | 0,6244 | 0,9530 | 7,6376 | 0,76% | | | 4,83% | 15,48% |
| RDX | 895,2 | 41,60 | 1,0118 | | 0,5487 | 0,8162 | 3,1956 | | 1,09% | 1,16% | 1,64% | | |
| SACCHARIN | 968 | 57,25 | 0,6157 | | 0,7433 | 0,8411 | 1,7725 | | 1,20% | 1,10% | 0,99% | | |
| SALICYLIC ACID | 739 | 51,80 | 0,8512 | 0,2752 | 0,4706 | 0,8173 | 3,1715 | -2,8598 | 1,61% | 1,43% | | 0,80% | 22,16% |
| SEBACIC ACID | 845 | 25,00 | 0,9608 | 0,2338 | 0,7014 | 0,7247 | 2,2249 | 66,5845 | 0,88% | | | 3,40% | 39,90% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| sec-BUTENYL ACETATE | 563,5 | 33,07 | 0,3922 | 0,2636 | 0,8632 | 0,8595 | 1,1882 | 19,9471 | 0,76% | 1,12% | | 3,14% | 20,94% |
| sec-BUTYL ACETATE | 561 | 31,70 | 0,3954 | 0,2675 | 1,2848 | 1,0000 | 0,8096 | 17,6614 | 0,63% | 3,37% | 0,36% | 2,09% | 21,55% |
| sec-BUTYL ACRYLATE | 580 | 29,70 | 0,4418 | 0,2636 | 1,2865 | 1,0000 | 0,8680 | 21,2229 | 0,51% | 1,02% | | 2,69% | 21,21% |
| sec-BUTYL CHLORIDE | 520,6 | 39,00 | 0,2907 | 0,2682 | 0,2893 | 0,8569 | 2,4431 | 14,3053 | 1,65% | 2,74% | 1,80% | 3,54% | 18,55% |
| sec-BUTYL FORMATE | 546 | 35,80 | 0,3489 | 0,2636 | 1,2910 | 1,0000 | 0,7510 | 18,9263 | 0,45% | 1,99% | 2,43% | 3,98% | 20,17% |
| sec-BUTYL MERCAPTAN | 554 | 40,60 | 0,2506 | 0,2743 | 0,3006 | 0,8496 | 2,1883 | 11,3185 | 1,82% | 2,09% | 2,08% | 2,69% | 19,50% |
| sec-BUTYLAMINE | 514,3 | 40,00 | 0,2815 | 0,2642 | 0,3655 | 0,8225 | 1,9033 | 16,7144 | 0,45% | 2,13% | 0,49% | 4,90% | 9,56% |
| sec-BUTYLBENZENE | 664,54 | 29,50 | 0,2791 | 0,2605 | 1,2340 | 1,0000 | 0,7186 | 35,4935 | 0,93% | 3,66% | 1,11% | 4,50% | 18,48% |
| sec-BUTYLCYCLOHEXANE | 654 | 25,85 | 0,3516 | 0,2589 | 0,8722 | 0,9005 | 1,1338 | 38,6935 | 0,78% | 1,10% | | 3,13% | 28,64% |
| sec-BUTYL-tert-BUTYL ETHER | 559,4 | 25,61 | 0,3489 | 0,2728 | 0,7489 | 0,8722 | 1,2820 | 16,2488 | 0,80% | 1,36% | 0,56% | 2,16% | 20,97% |
| SILANE | 269,7 | 48,40 | 0,0938 | 0,3138 | 0,4312 | 0,9557 | 1,4001 | -5,2683 | 4,01% | | | 3,10% | 20,35% |
| SITOSTEROL | 953 | 11,20 | 1,0543 | | 0,5853 | 0,8184 | 3,1474 | | 1,13% | 1,21% | | | |
| STIGMASTEROL | 953,6 | 11,38 | 1,0631 | | 0,5906 | 0,8183 | 3,1479 | | 1,29% | 1,65% | | | |
| STYRENE | 636 | 38,40 | 0,2971 | 0,2612 | 0,7900 | 0,8464 | 1,0848 | 25,6853 | 2,91% | 1,97% | 0,36% | 3,87% | 23,11% |
| STYRENE GLYCOL | 776,4 | 39,24 | 0,6159 | | 0,4092 | 0,8232 | 2,8213 | | 0,70% | 1,52% | | | |
| SUBERIC ACID | 843 | 29,70 | 0,8514 | 0,2317 | 0,6347 | 0,6705 | 2,0631 | 64,7206 | 0,78% | | | 4,12% | 36,47% |
| SUCCINIC ANHYDRIDE | 811 | 67,30 | 0,5322 | | 0,6439 | 0,8962 | 1,9417 | | 5,31% | 5,73% | | | |
| SUCCINIMIDE | 858 | 59,70 | 0,4834 | 0,2250 | 0,2841 | 0,8133 | 2,9358 | 43,9976 | 0,62% | | | 6,60% | 30,74% |
| SUCCINONITRILE | 770 | 35,40 | 0,5587 | 0,1781 | 0,3866 | 0,8251 | 2,7622 | 112,4766 | 0,75% | 1,94% | | 15,22% | 63,45% |
| SUCROSE | 1086 | 26,90 | 0,3653 | 0,2213 | 0,3771 | 0,8331 | 2,2035 | 128,9169 | 0,65% | 1,79% | | 13,94% | 30,09% |
| SULFOLANE | 853 | 50,30 | 0,3823 | 0,2355 | 0,3301 | 0,8483 | 2,5768 | 45,0809 | 0,54% | 1,40% | | 6,39% | 41,64% |
| SULFUR DIOXIDE | 430,75 | 78,84 | 0,2454 | 0,2671 | 0,3840 | 0,8366 | 1,7943 | 6,9935 | 1,58% | 1,17% | 4,27% | 3,35% | 18,38% |
| SULFUR HEXAFLUORIDE | 318,69 | 37,60 | 0,2151 | 0,2796 | 0,1845 | 0,8441 | 2,6181 | 5,3163 | 0,88% | 1,60% | | 2,00% | 15,65% |
| SULFUR TRIOXIDE | 490,85 | 82,10 | 0,4240 | 0,2726 | 0,8633 | 0,0001 | 0,9655 | 7,6107 | 3,55% | 4,93% | | 1,61% | 24,48% |
| SULFURYL CHLORIDE | 545 | 46,10 | 0,1764 | 0,2491 | 1,4547 | 0,8788 | 0,5008 | 28,9159 | 0,89% | 1,42% | | 7,18% | 27,66% |
| SYRINGOL | 752,2 | 37,85 | 0,6551 | 0,2570 | 0,4390 | 0,8322 | 2,8603 | 22,0306 | 0,70% | 1,40% | | 1,46% | 24,41% |
| t-BUTYL ACETOACETATE | 636,5 | 27,73 | 0,5832 | | 0,5033 | 0,8348 | 2,3840 | | 0,74% | 1,27% | | | |
| t-BUTYL HYDROPEROXIDE | 552 | 43,40 | 0,6623 | 0,2720 | 0,7009 | 0,8274 | 1,9365 | 3,0810 | 0,60% | 0,71% | | 1,13% | 20,49% |
| TEREPHTHALDEHYDE | 739 | 36,70 | 0,5832 | | 0,3369 | 0,8186 | 3,0484 | | 0,62% | 1,59% | 1,07% | | |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| TEREPHTHALIC ACID | 883,6 | 34,86 | 0,9469 | | 0,5977 | 0,8291 | 2,9221 | | 0,82% | | | | |
| TEREPHTHALOYL CHLORIDE | 755,4 | 38,20 | 0,6730 | 0,2701 | 0,4659 | 0,8352 | 2,8037 | 6,2814 | 0,73% | 1,32% | | 1,02% | 15,03% |
| TERPINOLENE | 667 | 28,20 | 0,3762 | 0,2572 | 0,6672 | 0,8267 | 1,4183 | 37,7590 | 0,51% | 1,39% | 0,13% | 3,49% | 25,31% |
| tert-BUTYL ACETATE | 545 | 31,70 | 0,3396 | 0,2667 | 1,2705 | 1,0000 | 0,7684 | 17,7058 | 1,35% | 2,06% | | 3,86% | 17,94% |
| tert-BUTYL CHLORIDE | 507 | 39,00 | 0,1914 | 0,2796 | 0,1949 | 0,8512 | 2,5305 | 8,7260 | 0,79% | 2,82% | 0,34% | 2,61% | 17,19% |
| tert-BUTYL ETHYL ETHER | 509,4 | 29,34 | 0,3162 | 0,2689 | 0,4965 | 0,8329 | 1,6610 | 17,7522 | 0,66% | 1,64% | | 2,89% | 17,62% |
| tert-BUTYL FORMATE | 537 | 35,80 | 0,2944 | 0,2748 | 0,2114 | 0,8361 | 2,7873 | 12,7926 | 0,58% | 1,97% | 4,10% | 1,28% | 20,64% |
| tert-BUTYL MERCAPTAN | 530 | 40,60 | 0,1914 | 0,2879 | 0,1585 | 0,8421 | 2,6809 | 2,9204 | 0,93% | 2,59% | 0,32% | 1,81% | 16,90% |
| tert-BUTYL METHACRYLATE | 588,3 | 27,27 | 0,3977 | 0,2672 | 0,9050 | 0,8523 | 1,1406 | 20,5504 | 0,63% | 1,13% | | 2,89% | 20,03% |
| tert-BUTYLAMINE | 483,9 | 38,40 | 0,2748 | 0,2689 | 0,3636 | 0,7536 | 1,6219 | 12,9977 | 1,06% | 3,03% | 2,02% | 5,00% | 14,76% |
| tert-BUTYLBENZENE | 660 | 29,70 | 0,2674 | 0,2663 | 1,4085 | 1,0000 | 0,6029 | 30,3092 | 1,00% | 1,70% | 0,13% | 2,93% | 19,02% |
| tert-BUTYLCYCLOHEXANE | 652 | 26,60 | 0,2991 | 0,2669 | 0,3785 | 0,8084 | 1,8615 | 30,1949 | 0,74% | 5,32% | | 2,39% | 27,28% |
| tert-BUTYLFORMAMIDE | 692 | 35,60 | 0,4491 | 0,2371 | 0,4170 | 0,8267 | 2,2839 | 49,6367 | 0,73% | 1,45% | | 4,92% | 27,70% |
| tert-DODECYL MERCAPTAN | 691 | 18,60 | 0,6098 | 0,2498 | 0,5965 | 0,8278 | 2,1052 | 59,5512 | 1,05% | 1,10% | 2,15% | 2,36% | 25,82% |
| tert-NONYL MERCAPTAN | 659 | 23,40 | 0,4514 | 0,2476 | 0,3943 | 0,8073 | 2,2707 | 55,7466 | 0,41% | 2,39% | 1,43% | 4,08% | 24,96% |
| tert-OCTYL MERCAPTAN | 627 | 25,90 | 0,3001 | 0,2629 | 0,3380 | 0,8315 | 2,1178 | 33,3545 | 0,59% | 1,93% | 0,71% | 3,85% | 20,52% |
| TETRACHLOROETHYLENE | 620 | 44,90 | 0,2138 | 0,2646 | 1,1517 | 1,0000 | 0,6842 | 18,9588 | 1,19% | 1,54% | 0,86% | 4,98% | 46,67% |
| TETRACHLOROSILANE | 507 | 35,90 | 0,2318 | 0,2710 | 0,3484 | 0,8160 | 1,7585 | 14,9931 | 0,50% | 1,40% | 1,76% | 3,91% | 15,46% |
| TETRADECAMETHYLHEXASILOXANE | 653,2 | 8,04 | 0,7769 | 0,2481 | 1,0812 | 0,8590 | 1,4679 | 121,7177 | 1,07% | 0,70% | | 1,76% | 26,86% |
| TETRAETHYL LEAD | 655 | 21,25 | 0,4812 | 0,2366 | 0,5133 | 0,8304 | 2,0485 | 71,1687 | 2,11% | 2,22% | 1,65% | 7,97% | 23,11% |
| TETRAETHYL SILANE | 606 | 24,00 | 0,4002 | 0,2673 | 0,4428 | 0,8426 | 2,0957 | 23,6192 | 0,33% | 1,55% | 6,37% | 2,44% | 15,19% |
| TETRAETHYLENE GLYCOL | 795 | 25,90 | 0,9174 | 0,2294 | 0,5309 | 0,8213 | 3,0834 | 65,6827 | 1,93% | 1,98% | | 3,28% | 39,19% |
| TETRAETHYLENE GLYCOL DIMETHYL ETHER | 705 | 19,40 | 0,9652 | 0,2508 | 0,6939 | 0,8437 | 2,6528 | 43,1054 | 1,22% | | | 3,39% | 43,03% |
| TETRAETHYLENE GLYCOL MONOETHYL ETHER | 732 | 23,60 | 0,9045 | 0,2630 | 0,5142 | 0,8199 | 3,1131 | 14,3703 | 0,80% | 1,33% | | 1,60% | 24,67% |
| TETRAETHYLENE GLYCOL MONOMETHYL ETHER | 720 | 26,01 | 0,9717 | 0,2660 | 0,5542 | 0,8205 | 3,1004 | 6,0368 | 0,93% | 1,28% | | 1,83% | 24,37% |
| TETRAFLUOROETHYLENE | 306,45 | 39,44 | 0,2265 | 0,2702 | 0,2901 | 0,8353 | 2,0567 | 8,6278 | 0,45% | 1,41% | 0,44% | 3,58% | 20,18% |
| TETRAFLUOROHYDRAZINE | 309,35 | 37,10 | 0,2233 | 0,2776 | 0,5294 | 0,9427 | 1,5054 | 5,8456 | 5,03% | 7,50% | | 3,00% | 5,75% |
| TETRAHYDROFURAN | 540,15 | 51,90 | 0,2254 | 0,2676 | 0,4609 | 0,8403 | 1,4945 | 12,8776 | 1,48% | 2,65% | 1,37% | 4,63% | 23,02% |
| TETRAHYDROPYRAN | 572,04 | 47,71 | 0,2162 | 0,2744 | 0,4302 | 0,8543 | 1,6076 | 9,5070 | 0,52% | 1,66% | | 4,22% | 22,87% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| TETRAHYDROTHIOPHENE | 631,95 | 51,60 | 0,1996 | 0,2596 | 0,4962 | 0,8347 | 1,3374 | 20,8478 | 0,63% | 1,39% | 0,60% | 6,73% | 27,94% |
| TETRAMANTANE | 867,7 | 15,51 | 0,2726 | | 0,2349 | 0,8448 | 2,6344 | | 0,59% | 2,91% | | | |
| TETRAMETHYLETHYLENEDIAMINE | 569 | 28,20 | 0,3915 | 0,2642 | 0,2927 | 0,8277 | 2,6545 | 22,6624 | 0,62% | 1,78% | 0,74% | 2,88% | 21,12% |
| TETRAMETHYLSILANE | 450,4 | 28,14 | 0,2240 | 0,2722 | 0,4753 | 0,8181 | 1,4119 | 16,4522 | 0,33% | 0,91% | 0,56% | 3,56% | 19,65% |
| TETRAPHENYLETHYLENE | 996 | 17,10 | 0,7285 | | 0,4105 | 0,8192 | 3,1295 | | 0,59% | 1,31% | | | |
| TETRAPHENYLMETHANE | 983 | 17,90 | 0,6794 | | 0,3912 | 0,8116 | 3,0177 | | 0,70% | 1,73% | 1,34% | | |
| THIACYCLOPROPANE | 547 | 67,80 | 0,1610 | 0,2599 | 0,2134 | 0,8625 | 2,3568 | 14,7340 | 0,48% | 1,52% | | 5,80% | 25,07% |
| THIAINDAN | 759,8 | 37,07 | 0,3327 | 0,2425 | 0,5440 | 0,8622 | 1,6588 | 50,5066 | 0,56% | 1,43% | | 5,56% | 25,31% |
| THIOGLYCOLIC ACID | 733 | 61,00 | 0,5598 | 0,2394 | 0,9534 | 0,9546 | 1,4090 | 27,0081 | 0,43% | | | 3,50% | 28,04% |
| THIONYL CHLORIDE | 567 | 44,30 | 0,0946 | 0,2221 | 1,1494 | 1,0000 | 0,5465 | 51,1264 | 3,80% | 1,89% | | 14,51% | 45,96% |
| THIOPHENE | 579,35 | 56,90 | 0,1970 | 0,2722 | 0,2632 | 0,8331 | 2,0214 | 10,9362 | 1,22% | 1,81% | 1,30% | 3,71% | 23,86% |
| THIOUREA | 854 | 82,30 | 0,3586 | | 0,2501 | 0,8342 | 2,8229 | | 0,53% | 1,53% | | | |
| THYMOL | 698,25 | 34,08 | 0,7226 | 0,2646 | 0,6559 | 0,8656 | 2,3169 | 6,2003 | 2,51% | | | 2,09% | 28,82% |
| TIN(IV) CHLORIDE | 591,85 | 37,44 | 0,2613 | 0,2668 | 0,3121 | 0,8201 | 2,0136 | 20,0819 | 0,63% | 1,48% | 1,49% | 3,56% | 19,11% |
| TOLUENE | 591,75 | 41,08 | 0,2640 | 0,2641 | 0,3312 | 0,8448 | 2,0808 | 19,6570 | 0,52% | 1,52% | 0,87% | 4,08% | 20,12% |
| trans,trans-2,4-HEXADIENE | 535 | 33,50 | 0,2821 | 0,2540 | 0,2226 | 0,8407 | 2,7045 | 29,8530 | 0,66% | 1,67% | 0,35% | 5,11% | 24,70% |
| trans-1,2-DICHLOROETHYLENE | 516,5 | 55,10 | 0,2234 | 0,2768 | 0,2439 | 0,8602 | 2,3929 | 7,6368 | 3,58% | 1,56% | 2,86% | 2,63% | 12,57% |
| trans-1,2-DIMETHYLCYCLOHEXANE | 596,15 | 29,38 | 0,2379 | 0,2590 | 0,9368 | 0,9057 | 0,8685 | 35,3102 | 0,35% | 0,84% | 0,34% | 5,60% | 14,56% |
| trans-1,2-DIMETHYLCYCLOPENTANE | 553,15 | 34,45 | 0,2698 | 0,2789 | 0,2677 | 0,8542 | 2,4840 | 8,5623 | 0,93% | 1,43% | | 1,63% | 21,23% |
| trans-1,3,3,3-TETRAFLUOROPROPENE | 382,51 | 36,62 | 0,3238 | 0,2662 | 0,2132 | 0,8313 | 2,8773 | 11,7210 | 1,12% | 2,68% | | 3,28% | 18,20% |
| trans-1,3-DICHLOROPROPENE | 606,5 | 47,04 | 0,2234 | 0,2596 | 0,4610 | 0,7851 | 1,3798 | 22,5491 | 0,65% | 1,91% | | 4,93% | 20,43% |
| trans-1,3-DIMETHYLCYCLOHEXANE | 598 | 29,38 | 0,2335 | 0,2598 | 1,3230 | 1,0000 | 0,6061 | 35,8366 | 0,43% | 0,36% | 0,49% | 4,98% | 14,82% |
| trans-1,3-DIMETHYLCYCLOPENTANE | 553 | 34,45 | 0,2699 | 0,2785 | 0,8718 | 0,8830 | 0,9636 | 9,3441 | 2,72% | 2,68% | 0,68% | 2,31% | 20,98% |
| trans-1,3-HEXADIENE | 521,1 | 33,54 | 0,2783 | 0,2595 | 0,2657 | 0,8511 | 2,5319 | 24,4498 | 0,56% | 2,00% | | 4,31% | 22,70% |
| trans-1,3-PENTADIENE | 500 | 37,40 | 0,1162 | 0,2595 | 1,5655 | 1,0000 | 0,4071 | 26,6664 | 3,45% | 3,05% | 1,42% | 6,18% | 24,58% |
| trans-1,4-DIETHYLCYCLOHEXANE | 649,9 | 28,17 | 0,3846 | 0,2731 | 0,8058 | 0,8849 | 1,2775 | 14,2374 | 0,73% | 1,00% | | 2,10% | 18,63% |
| trans-1,4-DIMETHYLCYCLOHEXANE | 587,7 | 29,40 | 0,2548 | 0,2647 | 0,4392 | 0,8295 | 1,6173 | 27,8555 | 0,50% | 1,05% | 0,65% | 4,01% | 16,92% |
| trans-1,8-TERPIN | 702,7 | 29,49 | 1,0818 | | 0,6105 | 0,8203 | 3,1050 | | 1,16% | 1,59% | | | |
| trans-1-PROPENYLBENZENE | 670 | 33,60 | 0,3393 | 0,2553 | 0,6992 | 0,8561 | 1,3256 | 35,7454 | 0,83% | 1,46% | 1,44% | 3,59% | 27,00% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| trans-2,2,4,6,6-PENTAMETHYL-3-HEPTENE | 637,8 | 19,64 | 0,3619 | | 0,5386 | 0,8470 | 1,7130 | | 0,58% | 1,64% | | | |
| trans-2,n-HEXYL-DECAHYDRONAPHTHALENE | 777,2 | 18,14 | 0,4668 | | 0,3544 | 0,8261 | 2,6099 | | 0,61% | 2,86% | 5,56% | | |
| trans-2-BUTENE | 428,6 | 41,00 | 0,2176 | 0,2720 | 0,3341 | 0,8594 | 1,9420 | 10,6691 | 1,36% | 1,32% | 1,09% | 3,68% | 17,25% |
| trans-2-DECENE | 619 | 21,80 | 0,4820 | 0,2509 | 0,4294 | 0,8139 | 2,2680 | 49,1146 | 0,70% | 1,61% | 2,24% | 3,44% | 25,06% |
| trans-2-DODECENE | 663 | 18,90 | 0,5693 | | 0,4723 | 0,8108 | 2,3437 | | 0,73% | 1,44% | 3,73% | | |
| trans-2-EICOSENE | 741,8 | 12,21 | 0,8784 | | 0,5033 | 0,8205 | 3,1008 | | 0,89% | 1,94% | 7,58% | | |
| trans-2-HEPTENE | 543,1 | 28,50 | 0,3366 | 0,2586 | 0,2742 | 0,8432 | 2,6619 | 28,7226 | 0,38% | 3,45% | 0,19% | 4,12% | 24,23% |
| trans-2-HEXENE | 509,8 | 31,68 | 0,2886 | 0,2623 | 0,4822 | 0,8473 | 1,6560 | 22,5498 | 0,54% | 1,79% | 0,88% | 4,35% | 22,74% |
| trans-2-METHYL-1,3-PENTADIENE | 530,3 | 33,80 | 0,2477 | 0,2574 | 0,4651 | 0,8263 | 1,5321 | 28,3422 | 0,56% | 1,90% | | 4,86% | 20,98% |
| trans-2-NONENE | 597,1 | 23,70 | 0,4304 | | 1,0416 | 0,9751 | 1,0876 | | 0,22% | 0,82% | | | |
| trans-2-OCTENE | 571,6 | 25,89 | 0,3840 | 0,2556 | 0,2907 | 0,8396 | 2,7247 | 35,2758 | 1,07% | 4,68% | 0,62% | 3,92% | 24,81% |
| trans-2-PENTADECENE | 701,6 | 15,67 | 0,6894 | | 0,4803 | 0,8284 | 2,7404 | | 0,57% | 1,81% | | | |
| trans-2-PENTENE | 474,2 | 36,60 | 0,2484 | 0,2709 | 0,4929 | 0,8493 | 1,5073 | 13,2990 | 1,04% | 1,36% | 1,14% | 3,68% | 18,01% |
| trans-2-PHENYLBUTENE-2 | 654 | 30,10 | 0,3610 | 0,2570 | 0,4315 | 0,8297 | 1,9733 | 34,6301 | 0,80% | 1,68% | | 3,78% | 22,32% |
| trans-3-HEPTENE | 540 | 28,50 | 0,3341 | 0,2604 | 0,3833 | 0,8434 | 2,1160 | 27,0702 | 1,06% | 2,36% | 2,80% | 3,78% | 22,67% |
| trans-3-HEXENE | 509 | 31,70 | 0,2854 | 0,2654 | 0,4091 | 0,8330 | 1,8137 | 20,8350 | 0,41% | 0,67% | 0,78% | 3,32% | 20,85% |
| trans-3-METHYLCYCLOHEXANOL | 627 | 37,90 | 0,6806 | 0,2605 | 0,4173 | 0,8159 | 2,9225 | 11,3017 | 0,81% | 1,27% | 2,24% | 2,86% | 19,57% |
| trans-3-OCTENE | 574 | 25,80 | 0,3438 | 0,2569 | 0,3216 | 0,8368 | 2,3885 | 36,2911 | 0,99% | 2,27% | 1,42% | 3,90% | 20,90% |
| trans-4-METHYLCYCLOHEXANOL | 622 | 37,90 | 0,6940 | 0,2679 | 0,4420 | 0,8117 | 2,8169 | 5,7441 | 0,94% | 1,22% | 1,97% | 1,43% | 20,08% |
| trans-4-OCTENE | 573 | 25,80 | 0,3393 | 0,2573 | 0,3383 | 0,8285 | 2,2398 | 36,0599 | 1,48% | 2,10% | 0,83% | 4,02% | 20,72% |
| trans-CROTONALDEHYDE | 565 | 38,70 | 0,3435 | | 0,3538 | 0,8606 | 2,3880 | | 3,19% | | 6,30% | | |
| trans-CROTONIC ACID | 666 | 47,00 | 0,5708 | 0,2514 | 0,2548 | 0,8079 | 3,3963 | 25,7060 | 0,83% | 1,76% | | 1,05% | 35,93% |
| trans-CROTONITRILE | 586 | 38,80 | 0,3977 | 0,2243 | 0,5285 | 0,8925 | 1,9820 | 50,0539 | 0,97% | 1,97% | | 6,76% | 30,68% |
| trans-DECAHYDRONAPHTHALENE | 687 | 32,00 | 0,2993 | 0,2713 | 0,2980 | 0,8507 | 2,4223 | 18,7884 | 0,89% | 2,22% | 2,43% | 2,83% | 20,04% |
| trans-STILBENE | 820 | 27,40 | 0,4874 | 0,2438 | 1,5884 | 1,0000 | 0,7170 | 64,6967 | 0,93% | 1,86% | | 4,34% | 25,98% |
| TRIALLYLAMINE | 592 | 24,60 | 0,4987 | 0,2605 | 0,4679 | 0,8276 | 2,2355 | 27,8055 | 1,51% | 1,79% | 4,46% | 2,17% | 22,68% |
| TRIAMANTANE | 834,5 | 18,39 | 0,1869 | | 0,2171 | 0,8511 | 2,3655 | | 0,50% | | | | |
| TRIAMYLAMINE | 660 | 15,00 | 0,8526 | 0,2488 | 0,6741 | 0,8282 | 2,4032 | 55,5523 | 0,60% | 0,58% | | 1,57% | 30,34% |
| TRIBROMOMETHANE | 696 | 60,90 | 0,1561 | 0,2856 | 0,2165 | 0,8073 | 1,9144 | 6,1166 | 0,92% | 1,98% | 2,65% | 1,67% | 8,61% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| TRICAPRIN | 876,6 | 4,55 | 1,3974 | 0,1719 | 0,6730 | 0,8036 | 3,5072 | 895,8996 | 2,25% | | | 7,63% | 57,74% |
| TRICAPRYLIN | 850,7 | 5,93 | 1,2174 | 0,1822 | 0,6683 | 0,8167 | 3,1844 | 622,9127 | 2,02% | | | 6,93% | 51,66% |
| TRICHLOROACETALDEHYDE | 565 | 44,10 | 0,3323 | 0,2668 | 0,5196 | 0,8426 | 1,6699 | 13,7013 | 0,71% | 1,31% | | 3,36% | 18,53% |
| TRICHLOROACETIC ACID | 688 | 48,10 | 0,5490 | 0,2630 | 1,0228 | 0,8992 | 1,2525 | 14,2093 | 0,85% | 0,79% | | 1,76% | 23,69% |
| TRICHLOROACETYL CHLORIDE | 604 | 43,20 | 0,2824 | 0,2821 | 0,3148 | 0,8632 | 2,3506 | 4,8280 | 1,77% | 2,70% | | 1,36% | 12,28% |
| TRICHLOROETHYLENE | 571 | 49,10 | 0,2166 | 0,2707 | 0,5869 | 0,8503 | 1,2294 | 13,1621 | 0,87% | 1,71% | 0,18% | 3,75% | 20,76% |
| TRICHLOROFLUOROMETHANE | 471,2 | 44,08 | 0,1894 | 0,2763 | 0,3348 | 0,8469 | 1,7755 | 9,1726 | 1,02% | 0,78% | 1,38% | 3,48% | 15,76% |
| TRICHLOROSILANE | 479 | 41,70 | 0,2031 | 0,2784 | 0,3187 | 0,8343 | 1,8430 | 7,5086 | 0,41% | 2,43% | | 3,79% | 15,99% |
| TRIDECAFLUOROHEPTANOIC ACID | 583 | 20,75 | 0,9562 | 0,2612 | 0,6820 | 0,7625 | 2,3681 | 15,6303 | 0,86% | | | 1,07% | 25,09% |
| TRIDECANAL | 720 | 22,38 | 0,7452 | 0,2631 | 0,6472 | 0,8611 | 2,3806 | 21,1761 | 1,32% | 1,43% | | 1,14% | 22,60% |
| TRIETHYL ALUMINUM | 678,15 | 89,30 | 0,8418 | 0,4531 | 0,9676 | 0,8710 | 1,7442 | -97,4719 | 1,05% | 1,14% | | 7,67% | 33,89% |
| TRIETHYL ESTER PHOSPHOROUS ACID | 664,4 | 53,77 | 0,3308 | 0,3805 | 0,9092 | 0,9365 | 1,0678 | -79,8897 | 0,91% | 1,35% | | 2,93% | 8,02% |
| TRIETHYL GALLIUM | 581,2 | 25,00 | 0,4957 | 0,2420 | 3,7237 | 1,0000 | 0,2896 | 52,7981 | 6,46% | | 8,06% | 5,64% | 26,39% |
| TRIETHYL ORTHOFORMATE | 585 | 26,76 | 0,5447 | 0,2714 | 0,5109 | 0,8502 | 2,3198 | 10,8147 | 0,73% | 1,29% | | 1,50% | 22,95% |
| TRIETHYL PHOSPHATE | 757 | 68,40 | 0,4145 | 0,4800 | 0,8814 | 0,9706 | 1,2844 | -135,1814 | 0,85% | | | 16,88% | 24,59% |
| TRIETHYLAMINE | 535,15 | 30,40 | 0,3162 | 0,2690 | 0,4919 | 0,8439 | 1,6971 | 17,0544 | 0,72% | 1,90% | 3,13% | 3,19% | 20,72% |
| TRIETHYLENE GLYCOL BIS(2-ETHYLHEXANOATE) | 820,7 | 10,94 | 1,0371 | 0,2277 | 0,6696 | 0,8336 | 2,8343 | 154,9897 | 1,16% | | | 2,38% | 47,90% |
| TRIETHYLENE GLYCOL DIMETHYL ETHER | 651 | 23,10 | 0,7915 | 0,2650 | 0,6233 | 0,8258 | 2,4300 | 22,2079 | 0,71% | 0,88% | | 4,92% | 38,47% |
| TRIETHYLENEDIAMINE | 655 | 39,10 | 0,4602 | | 0,3218 | 0,8346 | 2,8153 | | 0,55% | 1,23% | | | |
| TRIETHYLENETETRAMINE | 718 | 31,70 | 0,9735 | 0,2557 | 0,5452 | 0,8188 | 3,1365 | 18,3887 | 1,32% | 1,27% | | 1,62% | 26,42% |
| TRIFLUOROACETAMIDE | 648 | 50,59 | 0,4814 | | 0,1930 | 0,8066 | 3,4291 | | 1,55% | 3,94% | 5,86% | | |
| TRIFLUOROACETIC ACID | 491,25 | 32,58 | 0,5238 | 0,1972 | 0,2910 | 0,8203 | 3,1047 | 64,2599 | 2,26% | | 0,33% | 9,97% | 73,35% |
| TRIFLUOROIODOMETHANE | 396,44 | 39,53 | 0,1763 | 0,2762 | 0,2577 | 0,8710 | 2,2434 | 9,5913 | 0,43% | 1,62% | | 2,16% | 19,11% |
| TRIFLUOROMETHANE | 299,01 | 48,16 | 0,2641 | 0,2569 | 0,3539 | 0,8548 | 2,0388 | 10,8619 | 0,43% | 2,12% | 2,24% | 4,99% | 22,12% |
| TRIFLUOROMETHYL TRIFLUOROVINYL ETHER | 363 | 31,10 | 0,3497 | | 0,7064 | 0,8710 | 1,3576 | | 0,76% | 1,30% | | | |
| TRIISOBUTYL ALUMINUM | 690,1 | 17,59 | 0,4304 | 0,2519 | 0,5664 | 0,8944 | 1,9613 | 68,2945 | 0,75% | | | 3,15% | 23,97% |
| TRIMETHYL BORATE | 501,7 | 35,87 | 0,4161 | 0,2550 | 0,5237 | 0,8870 | 2,0455 | 16,8073 | 0,77% | | | 5,49% | 48,93% |
| TRIMETHYL SILANE | 432 | 31,90 | 0,1751 | 0,2738 | 0,6390 | 0,8996 | 1,1145 | 14,2981 | 0,72% | 1,42% | | 3,48% | 16,08% |
| TRIMETHYL SILANOL | 526,5 | 38,09 | 0,6341 | 0,2741 | 0,3150 | 0,6959 | 2,4839 | 4,0731 | 0,65% | | | 1,34% | 16,26% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| TRIMETHYLALUMINUM | 620 | 40,00 | 0,2179 | 0,2347 | 4,2700 | 0,4755 | 0,2782 | 47,5933 | 1,80% | 4,53% | | 9,62% | 40,95% |
| TRIMETHYLAMINE | 433,25 | 40,70 | 0,2062 | 0,2714 | 0,2484 | 0,8574 | 2,3157 | 11,6627 | 1,14% | 3,22% | 1,87% | 3,83% | 11,56% |
| TRIMETHYLCHLOROSILANE | 497,75 | 32,00 | 0,2701 | 0,2750 | 1,0471 | 0,9999 | 0,8396 | 13,6101 | 1,24% | 1,96% | 1,95% | 1,89% | 14,07% |
| TRIMETHYLENE SULFIDE | 602 | 58,60 | 0,1731 | 0,2533 | 0,4601 | 0,8383 | 1,3520 | 21,6281 | 0,48% | 1,41% | 0,03% | 8,01% | 20,68% |
| TRI-n-BUTYL BORATE | 743,15 | 19,89 | 0,1887 | 0,2929 | 0,9197 | 0,9843 | 0,8314 | 7,8205 | 0,70% | 1,02% | | 4,45% | 19,04% |
| TRI-n-BUTYLAMINE | 644 | 18,00 | 0,6943 | 0,2492 | 0,6107 | 0,8308 | 2,2700 | 50,4965 | 0,82% | 1,11% | | 2,45% | 28,04% |
| TRI-n-OCTYLAMINE | 782 | 10,10 | 0,9688 | 0,2432 | 0,6283 | 0,8333 | 2,8392 | 121,8625 | 2,02% | | | 3,17% | 47,73% |
| TRIOXANE | 604 | 58,20 | 0,3337 | 0,2594 | 0,2422 | 0,8363 | 2,7845 | 15,6212 | 0,66% | 2,24% | | 3,27% | 21,43% |
| TRIPHENYLENE | 990,8 | 28,70 | 0,6733 | 0,2402 | 0,5967 | 0,8606 | 2,3873 | 70,0054 | 0,76% | | | 2,56% | 28,71% |
| TRIPHENYLETHYLENE | 908 | 21,00 | 0,5998 | | 0,5444 | 0,8230 | 2,2268 | | 0,80% | 1,14% | 0,93% | | |
| TRIPHENYLMETHANE | 865 | 22,00 | 0,5735 | 0,2426 | 0,2847 | 0,8118 | 3,2496 | 78,6352 | 0,45% | 1,88% | 6,30% | 3,86% | 34,27% |
| TRIPHENYLPHOSPHINE | 1008 | 78,40 | 0,4517 | 0,5378 | 0,3507 | 0,8335 | 2,6304 | -227,0483 | 0,90% | | | 13,98% | 5,30% |
| TRIPROPYLENE GLYCOL MONOETHYL ETHER | 664 | 20,20 | 1,1610 | 0,2616 | 2,0560 | 1,0000 | 0,9881 | 8,1189 | 5,08% | | 10,22% | 2,01% | 28,25% |
| TRIPROPYLENE GLYCOL MONOMETHYL ETHER | 657 | 21,80 | 1,1254 | 0,2625 | 0,6379 | 0,8057 | 3,0637 | 7,8322 | 2,20% | | 1,58% | 2,79% | 26,91% |
| TRIS(2-METHOXYETHOXY)VINYLSILANE | 723,9 | 17,79 | 0,7150 | 0,2570 | 0,4494 | 0,8275 | 2,9533 | 42,0563 | 0,69% | | | 2,08% | 24,79% |
| UNDECANAL | 690 | 23,93 | 0,6352 | 0,2659 | 0,6607 | 0,8435 | 2,0302 | 18,0808 | 0,83% | 1,28% | | 1,29% | 22,81% |
| UNDECYL MERCAPTAN | 710 | 19,80 | 0,6388 | 0,2405 | 0,4020 | 0,8272 | 2,9594 | 67,6831 | 3,77% | 2,01% | 1,98% | 4,17% | 37,00% |
| UNDECYLAMINE | 682 | 20,20 | 0,7043 | 0,2437 | 0,7682 | 0,7939 | 1,8573 | 56,1769 | 8,68% | | 0,39% | 3,53% | 28,96% |
| VALERONITRILE | 610,3 | 35,80 | 0,4069 | 0,2381 | 0,4795 | 0,8777 | 2,1580 | 42,6780 | 2,93% | 3,49% | | 5,57% | 25,67% |
| VANADIUM OXYTRICHLORIDE | 636 | 37,40 | 0,1305 | 0,2388 | 0,1598 | 0,8373 | 2,2828 | 51,6363 | 0,19% | | | 10,46% | 44,71% |
| VANADIUM TETRACHLORIDE | 697 | 60,30 | 0,1858 | 0,3025 | 0,7309 | 0,9945 | 1,0838 | -9,8865 | 0,53% | | | 1,84% | 23,22% |
| VANILLIC ACID | 825,1 | 37,98 | 0,8503 | | 0,4596 | 0,8157 | 3,2080 | | 0,71% | 1,74% | | | |
| VANILLIN | 777 | 40,10 | 0,7573 | | 0,4430 | 0,8218 | 3,0716 | | 0,76% | 1,07% | | | |
| VINYL ACETATE | 519,13 | 39,58 | 0,3513 | 0,2487 | 0,9546 | 0,8335 | 0,9945 | 27,0609 | 1,86% | 3,73% | 3,55% | 6,11% | 24,61% |
| VINYL CHLORIDE | 432 | 56,70 | 0,1001 | 0,2745 | 0,0671 | 0,8372 | 2,7683 | 8,8600 | 0,68% | 1,55% | | 5,94% | 13,02% |
| VINYL FLUORIDE | 327,8 | 52,40 | 0,1429 | 0,2727 | 0,2155 | 0,8573 | 2,2705 | 6,3323 | 2,39% | | 2,04% | 5,55% | 16,00% |
| VINYL FORMATE | 498 | 50,20 | 0,2849 | 0,2614 | 1,4192 | 1,0000 | 0,6139 | 15,6212 | 0,94% | 1,65% | | 3,89% | 19,50% |
| VINYL PIVALATE | 556 | 29,50 | 0,3913 | 0,2698 | 0,5566 | 0,8428 | 1,7254 | 14,9524 | 0,66% | 1,12% | | 2,38% | 19,95% |
| VINYL PROPIONATE | 546 | 36,80 | 0,3802 | 0,2606 | 0,7591 | 0,8752 | 1,3328 | 20,3122 | 0,79% | 1,11% | | 3,23% | 21,02% |

| Name | $T_c$ / K | $P_c$ / bar | ω | $Z_{RA}$ | L | M | N | c ($cm^3 \cdot mol^{-1}$) | MAPE on: | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | $P^{sat}$ | $\Delta_{vap}H$ | $c^{sat}_{P,liq}$ | $v^{sat}_{liq}$ | $v_c$ |
| VINYLACETONITRILE | 584 | 38,80 | 0,3782 | 0,2183 | 1,0997 | 1,0000 | 0,9400 | 54,7210 | 3,09% | 4,10% | 1,26% | 9,86% | 39,93% |
| VINYLACETYLENE | 454 | 48,60 | 0,1069 | 0,2656 | 1,0000 | 1,0000 | 0,6724 | 15,3287 | 5,04% | 3,50% | 0,78% | 4,77% | 18,81% |
| VINYLCYCLOHEXANE | 599,4 | 32,70 | 0,2902 | 0,2671 | 0,3603 | 0,8224 | 1,9602 | 21,0929 | 0,67% | 2,51% | 1,48% | 3,54% | 19,64% |
| VINYLETHYLENE CARBONATE | 759,1 | 48,00 | 0,4733 | 0,2388 | 1,0706 | 0,9013 | 1,0880 | 35,7193 | 0,77% | 1,23% | 0,07% | 6,89% | 41,26% |
| VINYLNORBORNENE | 626 | 32,10 | 0,2487 | 0,2814 | 1,0106 | 1,0000 | 0,8480 | 15,8965 | 0,55% | 1,22% | | 4,35% | 22,85% |
| VINYLTRICHLOROSILANE | 543,15 | 30,60 | 0,2815 | 0,2535 | 0,6716 | 0,8850 | 1,2904 | 33,8882 | 0,68% | 1,25% | | 5,94% | 12,27% |
| VINYLTRIMETHOXYSILANE | 553,7 | 26,85 | 0,5514 | 0,2606 | 0,7692 | 0,8720 | 1,6472 | 21,1270 | 3,81% | | 0,68% | 1,98% | 25,38% |
| WATER | 647,096 | 220,64 | 0,3449 | 0,2289 | 0,4171 | 0,8758 | 2,1818 | 8,9670 | 0,56% | 1,99% | 3,49% | 9,53% | 29,26% |
| XENON | 289,74 | 58,40 | 0,0000 | 0,2880 | 0,3216 | 0,9451 | 1,4855 | 2,9153 | 0,38% | 1,87% | | 3,08% | 14,05% |
| XYLITOL | 941,8 | 59,37 | 0,9066 | | 0,5344 | 0,8157 | 3,0001 | | 0,71% | 1,41% | | | |
| DEUTERIUM | 38,35 | 16,62 | -0,1449 | 0,315 | 0,215 | 0,9921 | 1,1079 | -1,2543 | 1,87% | 5,84% | | 3,41% | 5,82% |
| HELIUM-4 | 5,2 | 2,27 | -0,3900 | 0,3355 | -0,0466 | 1,2473 | 0,5401 | -1,4608 | 3,02% | 7,68% | | 8,09% | 9,67% |
| HYDROGEN | 33,19 | 13,13 | -0,2160 | 0,3192 | 0,9444 | 3,0087 | 0,1762 | -1,3449 | 1,58% | 2,30% | | 5,21% | 8,70% |
| NEON | 44,4 | 26,53 | -0,0396 | 0,3004 | 0,3275 | 0,9699 | 1,2893 | -0,0712 | 0,26% | 2,62% | | 3,23% | 11,48% |

# Annexe B-1

# Banque de données des systèmes binaires
# Systèmes non associés

# How to read the charts

## Phase equilibrium and energetic properties diagrams

*T vs $x_1$, $y_1$ and P vs $x_1$, $y_1$ charts*

- Red: vapor phase data
  - Line (–): calculated
  - Symbol (∗): measured
- Blue: liquid phase data
  - Line (–): calculated
  - Symbol (+): measured
- Cyan: three phase line
  - Line (–): calculated
  - Symbol (▲): measured
- Purple: critical points data (either vapor-liquid or liquid-liquid)
  - Line (–): calculated critical point temperature for isobaric charts, calculated critical point pressure for isothermal charts
  - Symbol (●): measured
- Green: azeotropic data
  - Line (–): calculated azeotropic pressure for isothermal charts
  - Symbol (▲): measured
- Black square (□): calculated boiling temperature for isobaric charts, calculated saturation pressure for isothermal charts

*$h^M$ vs $z_1$ and $c_P{}^M$ vs $z_1$ charts*

- Line (–): calculated (one color for a given pressure)
- Symbol (x): measured (one color for each reference)

## Global Phase Equilibrium Diagrams (GPED)

*T vs P charts*

- Red: liquid-vapor critical point data
  - Line (–): calculated
  - Symbol (x): measured
- Purple line (–): calculated liquid-liquid critical line
- Blue line (–): calculated three phase line
- Green: azeotropic point data
  - Line (–): calculated
  - Symbol (x): measured
- Black line (–): saturation pressure curve

*T vs $x_1$, $y_1$*

- Red: liquid-vapor critical point data (either vapor-liquid or liquid-liquid)
  - Line (–): calculated
  - Symbol (∗): measured
- Purple line (–): calculated liquid-liquid critical line
- Green: azeotropic point data
  - Line (–): calculated
  - Symbol (∗): measured
- Blue (–), yellow (–) and cyan (–) lines: three phase lines

# NA-NA systems (AC = 1)

## METHANE (1) + PROPANE (2)

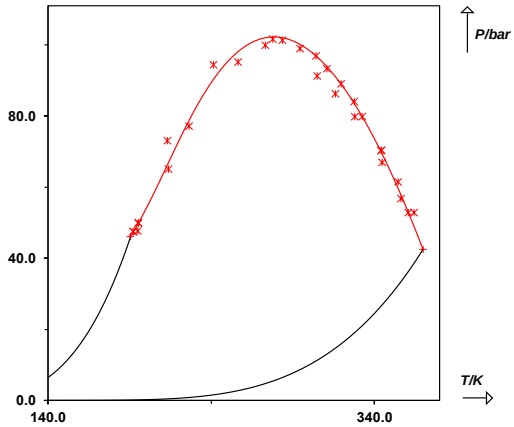
| | | |
|---|---|---|
| **CAS** | 74-82-8 | 74-98-6 |
| **InChiKey** | VNWKTOKETHGBQD-UHFFFAOYSA-N | ATUOYWHBWRKTHZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 190.56 | 369.83 |
| **$P_c$ / bar** | 45.99 | 42.48 |
| **ω** | 0.012 | 0.152 |

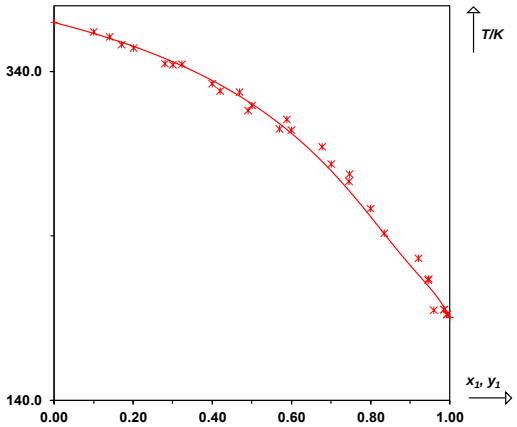
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 80.6
B/MPa = 75.7

*Deviations*
MAPE on x = 5.3 %
MAPE on y = 5.8 %
MAPE on $x_c$ = 9.4 %
MAPE on $P_c$ = 2.2 %
MAPE on $h^M$ = 29 %
MAPE on $c_P^M$ = 340 %



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**Isothermal phase equilibrium data**

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Poon, D. P. L. - Lu, B. C.-Y., Phase Equilibria for Systems Containing Nitrogen, Methane, and Propane, Advances in Cryogenic Engineering (1995) 292-299.

**T / K = 114.10**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4206 | 0.1812 | 0.9990 |
| 0.5930 | 0.2911 | 0.9995 |
| 0.7722 | 0.4102 | 0.9997 |
| 0.9653 | 0.6647 | 0.9998 |

Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-ethane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 9-12. doi:10.1021/je60052a022

**T / K = 130.37**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.862 | 0.3924 | 0.9999 |
| 2.344 | 0.5007 | 0.9999 |
| 2.896 | 0.6982 | 1.0000 |

Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-propane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 4-9. doi:10.1021/je60052a019

**T / K = 144.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.137 | 0.2109 | 0.9994 |
| 3.310 | 0.3005 | 0.9996 |
| 5.102 | 0.5258 | 0.9998 |
| 6.274 | 0.7200 | 0.9999 |
| 6.757 | 0.8306 | 0.9999 |
| 7.446 | 0.9287 | 1.0000 |

Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-propane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 4-9. doi:10.1021/je60052a019

**T / K = 158.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.724 | 0.0873 | 0.9958 |
| 3.551 | 0.1791 | 0.9979 |
| 6.895 | 0.3510 | 0.9989 |
| 9.549 | 0.5450 | 0.9992 |
| 12.14 | 0.8000 | 0.9996 |
| 12.89 | 0.8738 | 0.9997 |
| 13.38 | 0.9135 | 0.9997 |
| 13.89 | 0.9497 | 0.9998 |

Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-propane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 4-9. doi:10.1021/je60052a019

**T / K = 172.04**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.124 | 0.0692 | 0.9862 |
| 3.627 | 0.1196 | 0.9915 |
| 6.895 | 0.2270 | 0.9950 |
| 13.79 | 0.4909 | 0.9973 |
| 17.93 | 0.6907 | 0.9979 |
| 20.69 | 0.8423 | 0.9984 |
| 22.06 | 0.9032 | 0.9988 |
| 23.58 | 0.9650 | 0.9992 |

Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-propane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 4-9. doi:10.1021/je60052a019

**T / K = 187.43**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.827 | 0.0629 | 0.9656 |
| 6.895 | 0.1506 | 0.9839 |
| 13.79 | 0.3042 | 0.9907 |
| 20.69 | 0.4769 | 0.9929 |
| 27.58 | 0.6728 | 0.9937 |
| 33.78 | 0.8450 | 0.9947 |
| 37.23 | 0.9230 | 0.9958 |
| 38.96 | 0.9623 | 0.9968 |
| 40.40 | 0.9810 | 0.9980 |

Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-ethane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 9-12. doi:10.1021/je60052a022

**T / K = 192.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.068 | 0.0409 | 0.9355 |
| 3.447 | 0.0692 | 0.9601 |
| 5.171 | 0.1052 | 0.9718 |
| 6.895 | 0.1379 | 0.9783 |
| 13.79 | 0.2737 | 0.9874 |
| 20.68 | 0.4207 | 0.9899 |
| 27.58 | 0.5819 | 0.9913 |
| 34.47 | 0.7529 | 0.9919 |
| 39.65 | 0.8728 | 0.9924 |

| | | | |
|---|---|---|---|
| 44.06 | 0.9578 | 0.9941 | |
| 45.92 | 0.9782 | 0.9953 | |
| 46.47 | 0.9844 | 0.9957 | |
| 47.47 | 0.9926 | 0.9926 | CRIT |

Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-propane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 4-9. doi:10.1021/je60052a019

**T / K = 195.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.103 | 0.0377 | 0.9244 |
| 3.620 | 0.0667 | 0.9541 |
| 5.171 | 0.0958 | 0.9670 |
| 6.826 | 0.1263 | 0.9742 |
| 13.79 | 0.2545 | 0.9845 |
| 20.69 | 0.3969 | 0.9882 |
| 27.58 | 0.5392 | 0.9898 |
| 34.48 | 0.6947 | 0.9904 |
| 44.82 | 0.9061 | 0.9908 |
| 47.44 | 0.9546 | 0.9912 |
| 48.82 | 0.9719 | 0.9911 |
| 49.92 | 0.9856 | 0.9856 | CRIT |

Price, A. R. - Kobayashi, Riki, Low Temperature Vapor-Liquid Equilibrium in Light Hydrocarbon Mixtures: Methane-Ethane-Propane System., Journal of Chemical & Engineering Data 1 (1959) 40-52. doi:10.1021/je60001a007

**T / K = 199.82**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.1250 | 0.9591 |
| 7.929 | 0.1440 | 0.9700 |
| 13.79 | 0.2220 | 0.9792 |
| 14.82 | 0.2500 | 0.9810 |
| 41.37 | 0.7440 | 0.9852 |
| 42.40 | 0.7720 | 0.9842 |
| 51.71 | 0.9396 | 0.9851 |
| 52.75 | 0.9533 | 0.9854 |

Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-ethane-propane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 13-18. doi:10.1021/je60052a017

**T / K = 199.82**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.758 | 0.0427 | 0.9197 |
| 6.895 | 0.1149 | 0.9652 |
| 13.79 | 0.2335 | 0.9807 |
| 27.58 | 0.4937 | 0.9874 |
| 41.37 | 0.7472 | 0.9863 |
| 49.99 | 0.8979 | 0.9879 |

Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-ethane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 9-12. doi:10.1021/je60052a022

**T / K = 213.71**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.896 | 0.0205 | 0.7669 |
| 3.551 | 0.0443 | 0.8706 |
| 6.895 | 0.0899 | 0.9288 |
| 10.34 | 0.1358 | 0.9505 |
| 20.68 | 0.2709 | 0.9698 |
| 27.58 | 0.3656 | 0.9741 |
| 34.47 | 0.4580 | 0.9760 |
| 41.37 | 0.5563 | 0.9767 |
| 48.26 | 0.6555 | 0.9755 |
| 55.16 | 0.7573 | 0.9726 |
| 62.05 | 0.8600 | 0.9646 |
| 64.74 | 0.9053 | 0.9519 |

Webster, Leigh A. - Kidnay, Arthur J., Vapor–Liquid Equilibria for the Methane–Propane–Carbon Dioxide Systems at 230 K and 270 K, Journal of Chemical & Engineering Data 3 (2001) 759-764. doi:10.1021/je000307d

**T / K = 230.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.970 | 0.0657 | 0.8563 |
| 8.020 | 0.0759 | 0.8717 |
| 8.650 | 0.0855 | 0.8782 |
| 9.970 | 0.0994 | 0.8925 |
| 12.34 | 0.1244 | 0.9134 |
| 13.53 | 0.1372 | 0.9180 |
| 14.93 | 0.1524 | 0.9238 |
| 18.95 | 0.1972 | 0.9368 |
| 20.20 | 0.2128 | 0.9390 |
| 21.74 | 0.2269 | 0.9408 |
| 23.01 | 0.2436 | 0.9419 |
| 24.66 | 0.2550 | 0.9466 |
| 26.72 | 0.2758 | 0.9485 |
| 27.92 | 0.2864 | 0.9499 |
| 29.69 | 0.3178 | 0.9497 |
| 33.82 | 0.3526 | 0.9538 |
| 35.37 | 0.3738 | 0.9532 |
| 39.71 | 0.4126 | 0.9556 |
| 40.00 | 0.4179 | 0.9558 |

| | | |
|---|---|---|
| 41.74 | 0.4337 | 0.9515 |
| 43.99 | 0.4614 | 0.9546 |
| 45.75 | 0.4727 | 0.9531 |
| 50.57 | 0.5291 | 0.9537 |
| 55.13 | 0.5738 | 0.9524 |
| 60.50 | 0.6313 | 0.9495 |
| 65.66 | 0.6849 | 0.9448 |
| 69.46 | 0.7222 | 0.9407 |
| 70.00 | 0.7298 | 0.9415 |
| 71.25 | 0.7468 | 0.9369 |
| 72.70 | 0.7590 | 0.9334 |
| 74.22 | 0.7833 | 0.9279 |
| 76.21 | 0.8067 | 0.9214 |
| 77.20 | 0.8255 | 0.9175 |
| 77.67 | 0.8398 | 0.9155 |

Akers, W. W. - Burns, J. F. - Fairchild, W. R., Low-Temperature Phase Equilibria: Methane-Propane System, Industrial & Engineering Chemistry 12 (1954) 2531-2534. doi:10.1021/ie50540a038

**T / K = 241.48**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 6.895 | 0.0500 | 0.7650 | |
| 13.79 | 0.1120 | 0.8680 | |
| 20.68 | 0.1750 | 0.9020 | |
| 27.58 | 0.2370 | 0.9200 | |
| 34.47 | 0.3000 | 0.9300 | |
| 41.37 | 0.3610 | 0.9330 | |
| 48.26 | 0.4220 | 0.9360 | |
| 55.16 | 0.4850 | 0.9350 | |
| 62.05 | 0.5480 | 0.9330 | |
| 68.95 | 0.6090 | 0.9300 | |
| 75.84 | 0.6710 | 0.9190 | |
| 82.74 | 0.7340 | 0.9010 | |
| 89.63 | 0.7960 | 0.8720 | |
| 94.40 | 0.8350 | 0.8350 | CRIT |

Akers, W. W. - Burns, J. F. - Fairchild, W. R., Low-Temperature Phase Equilibria: Methane-Propane System, Industrial & Engineering Chemistry 12 (1954) 2531-2534. doi:10.1021/ie50540a038

**T / K = 256.48**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 6.895 | 0.0340 | 0.5600 | |
| 13.79 | 0.0890 | 0.7670 | |
| 20.68 | 0.1420 | 0.8320 | |
| 27.58 | 0.1970 | 0.8610 | |
| 34.47 | 0.2490 | 0.8800 | |
| 41.37 | 0.3030 | 0.8880 | |
| 48.26 | 0.3570 | 0.8900 | |
| 55.16 | 0.4100 | 0.8920 | |
| 62.05 | 0.4640 | 0.8910 | |
| 68.95 | 0.5180 | 0.8890 | |
| 75.84 | 0.5720 | 0.8820 | |
| 82.74 | 0.6360 | 0.8690 | |
| 89.63 | 0.7180 | 0.8450 | |
| 95.10 | 0.8000 | 0.8000 | CRIT |

Webster, Leigh A. - Kidnay, Arthur J., Vapor–Liquid Equilibria for the Methane–Propane–Carbon Dioxide Systems at 230 K and 270 K, Journal of Chemical & Engineering Data 3 (2001) 759-764. doi:10.1021/je000307d

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.540 | 0.0238 | 0.4184 |
| 8.120 | 0.0296 | 0.4536 |
| 9.040 | 0.0356 | 0.5003 |
| 9.310 | 0.0385 | 0.5119 |
| 10.73 | 0.0474 | 0.5752 |
| 11.89 | 0.0588 | 0.6089 |
| 13.31 | 0.0667 | 0.6526 |
| 14.34 | 0.0748 | 0.6670 |
| 15.35 | 0.0779 | 0.6874 |
| 15.44 | 0.0827 | 0.6881 |
| 16.94 | 0.0928 | 0.7160 |
| 18.25 | 0.1015 | 0.7269 |
| 19.17 | 0.1040 | 0.7416 |
| 19.56 | 0.1146 | 0.7418 |
| 21.70 | 0.1281 | 0.7608 |
| 23.44 | 0.1397 | 0.7713 |
| 25.63 | 0.1542 | 0.7859 |
| 26.63 | 0.1638 | 0.7919 |
| 27.98 | 0.1718 | 0.7969 |
| 28.57 | 0.1789 | 0.7998 |
| 30.31 | 0.1901 | 0.8073 |
| 30.53 | 0.1903 | 0.8083 |
| 34.07 | 0.2160 | 0.8211 |
| 38.73 | 0.2493 | 0.8345 |
| 47.02 | 0.3064 | 0.8468 |
| 55.02 | 0.3601 | 0.8543 |
| 53.80 | 0.3612 | 0.8467 |
| 58.27 | 0.3825 | 0.8520 |
| 58.38 | 0.3848 | 0.8518 |
| 65.46 | 0.4314 | 0.8553 |
| 66.87 | 0.4374 | 0.8546 |
| 70.34 | 0.4655 | 0.8539 |
| 75.49 | 0.5012 | 0.8494 |
| 80.00 | 0.5345 | 0.8426 |

| | | | |
|---|---|---|---|
| 84.13 | 0.5642 | 0.8356 | |
| 92.22 | 0.6429 | 0.8029 | |
| 92.92 | 0.6543 | 0.7937 | |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane-Propane System., Industrial & Engineering Chemistry 3 (1950) 534-539. doi:10.1021/ie50483a037

**T / K = 277.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 6.895 | 0.0099 | 0.2034 | |
| 10.34 | 0.0324 | 0.4432 | |
| 13.79 | 0.0549 | 0.5627 | |
| 17.24 | 0.0779 | 0.6382 | |
| 20.69 | 0.1008 | 0.6875 | |
| 24.13 | 0.1242 | 0.7235 | |
| 27.58 | 0.1471 | 0.7505 | |
| 31.03 | 0.1695 | 0.7677 | |
| 34.48 | 0.1923 | 0.7819 | |
| 37.92 | 0.2171 | 0.7966 | |
| 41.37 | 0.2378 | 0.8042 | |
| 44.82 | 0.2607 | 0.8099 | |
| 48.26 | 0.2834 | 0.8135 | |
| 51.71 | 0.3060 | 0.8159 | |
| 55.16 | 0.3289 | 0.8180 | |
| 58.61 | 0.3517 | 0.8188 | |
| 62.05 | 0.3769 | 0.8199 | |
| 65.50 | 0.3986 | 0.8205 | |
| 68.95 | 0.4226 | 0.8208 | |
| 72.40 | 0.4473 | 0.8211 | |
| 75.84 | 0.4719 | 0.8214 | |
| 79.29 | 0.4968 | 0.8217 | |
| 82.74 | 0.5225 | 0.8220 | |
| 93.08 | 0.6080 | 0.8217 | |
| 96.53 | 0.6434 | 0.8173 | |
| 99.97 | 0.6891 | 0.7924 | |
| 101.63 | 0.7459 | 0.7459 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane-Propane System., Industrial & Engineering Chemistry 3 (1950) 534-539. doi:10.1021/ie50483a037

**T / K = 294.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.34 | 0.0106 | 0.1513 |
| 13.79 | 0.0321 | 0.3435 |
| 17.24 | 0.0535 | 0.4750 |
| 20.69 | 0.0749 | 0.5338 |
| 24.13 | 0.0959 | 0.5853 |
| 27.58 | 0.1168 | 0.6231 |
| 31.03 | 0.1372 | 0.6501 |
| 34.48 | 0.1580 | 0.6721 |
| 37.92 | 0.1782 | 0.6908 |
| 41.37 | 0.1987 | 0.7038 |
| 44.82 | 0.2196 | 0.7141 |
| 48.26 | 0.2407 | 0.7228 |
| 51.71 | 0.2616 | 0.7300 |
| 55.16 | 0.2828 | 0.7357 |
| 58.61 | 0.3042 | 0.7403 |
| 62.05 | 0.3261 | 0.7442 |
| 65.50 | 0.3481 | 0.7471 |
| 68.95 | 0.3707 | 0.7497 |
| 72.40 | 0.3938 | 0.7520 |
| 75.84 | 0.4179 | 0.7539 |
| 79.29 | 0.4425 | 0.7553 |
| 82.74 | 0.4679 | 0.7567 |
| 86.19 | 0.4954 | 0.7570 |
| 89.63 | 0.5244 | 0.7561 |
| 93.08 | 0.5670 | 0.7503 |
| 96.53 | 0.6046 | 0.7309 |
| 98.87 | 0.6772 | 0.6772 CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane-Propane System., Industrial & Engineering Chemistry 3 (1950) 534-539. doi:10.1021/ie50483a037

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.79 | 0.0049 | 0.0521 |
| 17.24 | 0.0257 | 0.2184 |
| 20.69 | 0.0460 | 0.3255 |
| 24.13 | 0.0652 | 0.3949 |
| 27.58 | 0.0845 | 0.4472 |
| 31.03 | 0.1040 | 0.4884 |
| 34.48 | 0.1235 | 0.5209 |
| 37.92 | 0.1432 | 0.5481 |
| 41.37 | 0.1630 | 0.5714 |
| 44.82 | 0.1821 | 0.5911 |
| 48.26 | 0.2019 | 0.6073 |
| 51.71 | 0.2216 | 0.6210 |
| 55.16 | 0.2418 | 0.6321 |
| 58.61 | 0.2611 | 0.6420 |
| 62.05 | 0.2836 | 0.6503 |
| 65.50 | 0.3051 | 0.6572 |
| 68.95 | 0.3271 | 0.6635 |
| 72.40 | 0.3498 | 0.6691 |

| | | | |
|---|---|---|---|
| 75.84 | 0.3731 | 0.6738 | |
| 79.29 | 0.3969 | 0.6767 | |
| 82.74 | 0.4226 | 0.6779 | |
| 86.19 | 0.4511 | 0.6766 | |
| 89.63 | 0.4889 | 0.6643 | |
| 93.08 | 0.5610 | 0.6087 | |
| 93.29 | 0.5882 | 0.5882 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane-Propane System., Industrial & Engineering Chemistry 3 (1950) 534-539. doi:10.1021/ie50483a037

**T / K = 327.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 20.69 | 0.0104 | 0.0699 | |
| 24.13 | 0.0289 | 0.1663 | |
| 27.58 | 0.0480 | 0.2414 | |
| 31.03 | 0.0664 | 0.2964 | |
| 34.48 | 0.0852 | 0.3418 | |
| 37.92 | 0.1040 | 0.3797 | |
| 41.37 | 0.1227 | 0.4109 | |
| 44.82 | 0.1419 | 0.4361 | |
| 48.26 | 0.1612 | 0.4582 | |
| 51.71 | 0.1810 | 0.4768 | |
| 55.16 | 0.2008 | 0.4938 | |
| 58.61 | 0.2213 | 0.5086 | |
| 62.05 | 0.2430 | 0.5224 | |
| 65.50 | 0.2652 | 0.5351 | |
| 68.95 | 0.2885 | 0.5459 | |
| 72.40 | 0.3118 | 0.5532 | |
| 75.84 | 0.3361 | 0.5546 | |
| 79.29 | 0.3654 | 0.5473 | |
| 82.74 | 0.4101 | 0.5130 | |
| 83.98 | 0.4691 | 0.4691 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane-Propane System., Industrial & Engineering Chemistry 3 (1950) 534-539. doi:10.1021/ie50483a037

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 27.58 | 0.0063 | 0.0276 | |
| 31.03 | 0.0249 | 0.0981 | |
| 34.48 | 0.0433 | 0.1550 | |
| 37.92 | 0.0622 | 0.2007 | |
| 41.37 | 0.0813 | 0.2392 | |
| 44.82 | 0.1002 | 0.2712 | |
| 48.26 | 0.1199 | 0.2983 | |
| 51.71 | 0.1402 | 0.3215 | |
| 55.16 | 0.1618 | 0.3414 | |
| 58.61 | 0.1820 | 0.3566 | |
| 62.05 | 0.2081 | 0.3656 | |
| 65.50 | 0.2375 | 0.3678 | |
| 68.95 | 0.2800 | 0.3558 | |
| 70.33 | 0.3228 | 0.3228 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane-Propane System., Industrial & Engineering Chemistry 3 (1950) 534-539. doi:10.1021/ie50483a037

**T / K = 360.93**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 37.92 | 0.0107 | 0.0280 | |
| 41.37 | 0.0333 | 0.0798 | |
| 44.82 | 0.0555 | 0.1208 | |
| 48.26 | 0.0786 | 0.1489 | |
| 49.99 | 0.0926 | 0.1570 | |
| 51.71 | 0.1120 | 0.1601 | |
| 52.88 | 0.1400 | 0.1400 | CRIT |

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**Isobaric phase equilibrium data**

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Watanabe, Kazuo - Kuroki, Masaaki - Ogura, Masao - Saito, Isao, Vapour-Liquid-Equilibrium of LNG, TEION KOGAKU (Journal of Cryogenics and Superconductivity Society of Japan) 6 (1969) 292-301. doi:10.2221/jcsj.4.292

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 223.15 | 0.0074 | 0.8142 |
| 213.15 | 0.0147 | 0.9144 |
| 203.15 | 0.0201 | 0.9380 |
| 193.15 | 0.0298 | 0.9533 |

Watanabe, Kazuo - Kuroki, Masaaki - Ogura, Masao - Saito, Isao, Vapour-Liquid-Equilibrium of LNG, TEION KOGAKU (Journal of Cryogenics and Superconductivity Society of Japan) 6 (1969) 292-301. doi:10.2221/jcsj.4.292

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 183.15 | 0.0311 | 0.9656 |
| 173.15 | 0.0465 | 0.9778 |
| 163.15 | 0.0587 | 0.9879 |
| 153.15 | 0.0853 | 0.9948 |
| 143.15 | 0.1158 | 0.9983 |

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**Enthalpy of mixing**

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Miller, R. C. - Staveley, L. A. K., Excess Enthalpies for Some Binary Liquid Mixtures of Low-Molecular-Weight Alkanes, Advances in Cryogenic Engineering (1960) 493-500.

**T / K =** **91.50**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 118.30 | 0.3053 |
| 137.50 | 0.3798 |
| 154.80 | 0.5013 |
| 155.30 | 0.5871 |
| 143.70 | 0.6889 |

Cutler, A. J. B. - Morrison, J. A., Excess thermodynamic functions for liquid mixtures of methane + propane, Transactions of the Faraday Society (1965) doi:10.1039/tf9656100429

**T / K =** **100.00**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 29.31 | 0.1000 |
| 54.43 | 0.2000 |
| 79.55 | 0.3000 |
| 100.48 | 0.4000 |
| 113.04 | 0.5000 |
| 121.42 | 0.6000 |
| 113.04 | 0.7000 |
| 83.74 | 0.8000 |
| 25.12 | 0.9000 |

Miller, R. C. - Staveley, L. A. K., Excess Enthalpies for Some Binary Liquid Mixtures of Low-Molecular-Weight Alkanes, Advances in Cryogenic Engineering (1960) 493-500.

**T / K =** **112.00**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 97.40 | 0.3019 |
| 119.70 | 0.4017 |
| 128.30 | 0.5048 |
| 128.40 | 0.6160 |
| 120.60 | 0.7022 |
| 85.70 | 0.8274 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K =** **243.20**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 20.00 | 0.2680 |
| 25.40 | 0.3910 |
| 27.40 | 0.4640 |
| 27.50 | 0.5270 |
| 25.30 | 0.5990 |
| 22.40 | 0.6780 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K =** **253.20**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 19.10 | 0.2800 |
| 22.70 | 0.4000 |
| 22.90 | 0.4670 |
| 23.20 | 0.5100 |
| 22.90 | 0.5790 |
| 22.60 | 0.6100 |
| 21.60 | 0.6620 |
| 18.40 | 0.7400 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K =** **263.60**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 12.40 | 0.2030 |
| 18.50 | 0.3610 |
| 19.50 | 0.4190 |
| 20.40 | 0.4860 |
| 20.60 | 0.5370 |
| 20.30 | 0.5910 |
| 18.90 | 0.6420 |
| 16.50 | 0.7030 |
| 12.00 | 0.7970 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of

Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K = 273.20**

**P / bar = 1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 10.90 | 0.1920 |
| 15.30 | 0.2990 |
| 18.30 | 0.4250 |
| 18.70 | 0.4960 |
| 17.70 | 0.6060 |
| 16.90 | 0.6510 |
| 15.30 | 0.7170 |
| 11.10 | 0.7870 |
| 10.90 | 0.8030 |
| 7.200 | 0.8830 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K = 281.20**

**P / bar = 1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 14.80 | 0.3590 |
| 16.50 | 0.4100 |
| 16.30 | 0.5620 |
| 16.10 | 0.5900 |
| 13.10 | 0.7360 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K = 290.70**

**P / bar = 1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 8.300 | 0.1550 |
| 9.700 | 0.2010 |
| 13.40 | 0.3440 |
| 13.80 | 0.3520 |
| 14.70 | 0.4190 |
| 15.20 | 0.5000 |
| 14.10 | 0.6190 |
| 12.50 | 0.6930 |
| 11.40 | 0.7080 |
| 10.70 | 0.7500 |
| 10.00 | 0.7530 |
| 9.100 | 0.7920 |
| 5.100 | 0.8920 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K = 302.20**

**P / bar = 1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 12.90 | 0.3590 |
| 13.30 | 0.4250 |
| 13.70 | 0.5040 |
| 13.40 | 0.5390 |
| 13.30 | 0.6070 |
| 12.10 | 0.6640 |
| 10.40 | 0.7300 |
| 6.300 | 0.8440 |

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**Heat capacity of mixing**

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Cutler, A. J. B. - Morrison, J. A., Excess thermodynamic functions for liquid mixtures of methane + propane, Transactions of the Faraday Society (1965) doi:10.1039/tf9656100429

**T / K = 100.00**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.6276 | 0.1000 |
| -0.8786 | 0.2000 |
| -0.9205 | 0.3000 |
| -0.7531 | 0.4000 |
| -0.4602 | 0.5000 |
| -0.1255 | 0.6000 |
| 0.1255 | 0.7000 |
| 0.2929 | 0.8000 |
| 0.2929 | 0.9000 |

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**Critical point**

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Roof, J. G. - Baron, J. D., Critical loci of binary mixtures of propane with methane, carbon dioxide, and nitrogen, Journal of Chemical & Engineering Data 3 (1967) 292-293. doi:10.1021/je60034a003

| T / K | P / bar | $x_1$ |
|---|---|---|
| 356.15 | 56.74 | 0.1700 |
| 344.82 | 66.95 | 0.2800 |
| 327.98 | 79.84 | 0.4200 |

| | | |
|---|---|---|
| 316.21 | 86.19 | 0.4900 |
| 304.98 | 91.22 | 0.5700 |

Sage, Bruce H. - Lacey, William N. - Schaafsma, Jan G., Phase Equilibria in Hydrocarbon Systems II. Methane-Propane System, Industrial & Engineering Chemistry 2 (1934) 214-217. doi:10.1021/ie50290a020

| T / K | P / bar | $x_1$ |
|---|---|---|
| 364.15 | 52.79 | 0.1000 |
| 354.35 | 61.40 | 0.2000 |
| 344.05 | 70.22 | 0.3000 |
| 332.45 | 79.84 | 0.4000 |
| 319.45 | 89.07 | 0.5000 |
| 304.25 | 96.97 | 0.6000 |
| 283.55 | 101.22 | 0.7000 |

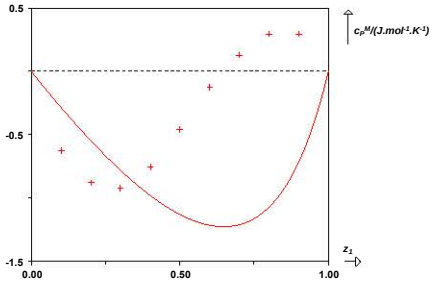
Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-propane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 4-9. doi:10.1021/je60052a019

| T / K | P / bar | $x_1$ |
|---|---|---|
| 213.71 | 65.10 | 0.9469 |
| 195.20 | 49.90 | 0.9856 |
| 192.30 | 47.47 | 0.9926 |

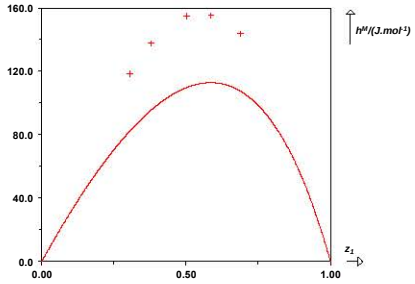
Akers, W. W. - Burns, J. F. - Fairchild, W. R., Low-Temperature Phase Equilibria: Methane-Propane System, Industrial & Engineering Chemistry 12 (1954) 2531-2534. doi:10.1021/ie50540a038

| T / K | P / bar | $x_1$ |
|---|---|---|
| 273.15 | 99.90 | 0.7450 |
| 226.48 | 77.20 | 0.9210 |
| 213.15 | 73.10 | 0.9450 |
| 194.82 | 47.60 | 0.9600 |

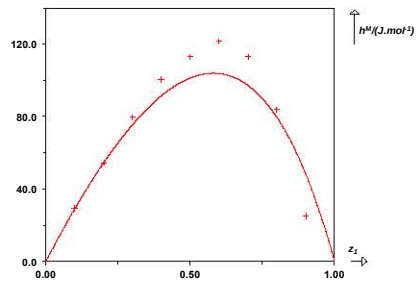
T/K = 100.00 - P/bar = 1.0132



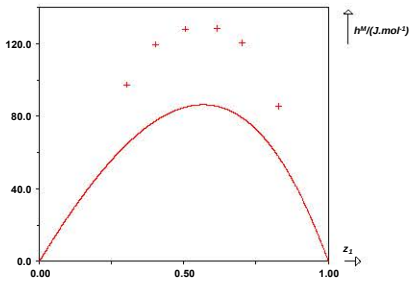

T/K = 91.50 - P/bar = 1.0132



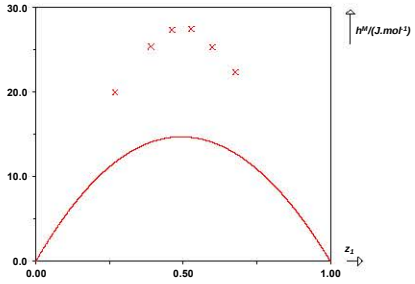

T/K = 100.00 - P/bar = 1.0132



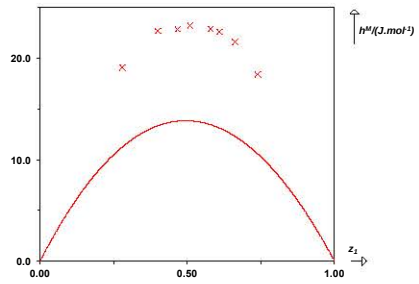

T/K = 112.00 - P/bar = 2.0923



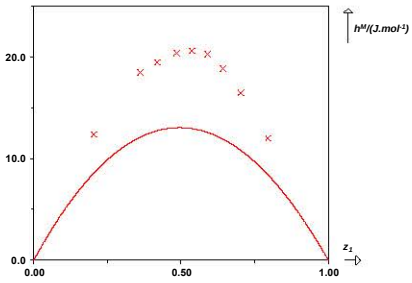

T/K = 243.20 - P/bar = 1.0132



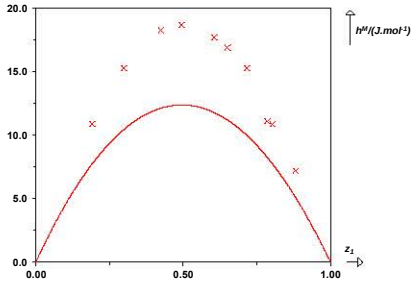

T/K = 253.20 - P/bar = 1.0132



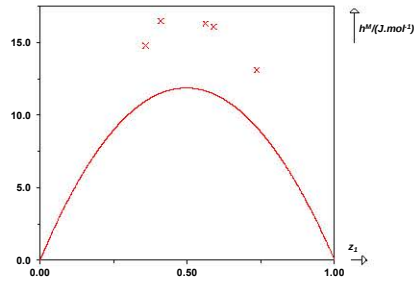

T/K = 263.60 - P/bar = 1.0132



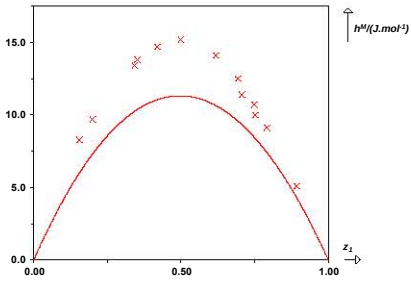

T/K = 273.20 - P/bar = 1.0132



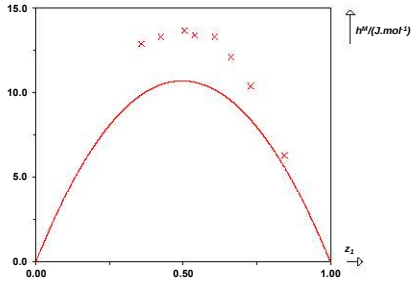

T/K = 281.20 - P/bar = 1.0132



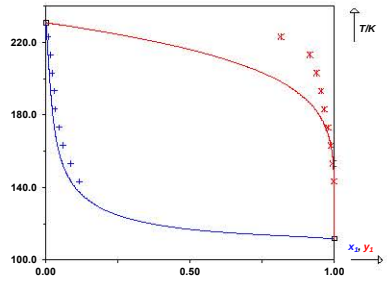

T/K = 290.70 - P/bar = 1.0132



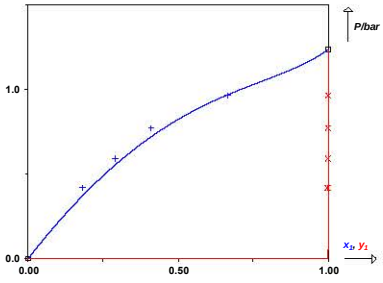

T/K = 302.20 - P/bar = 1.0132



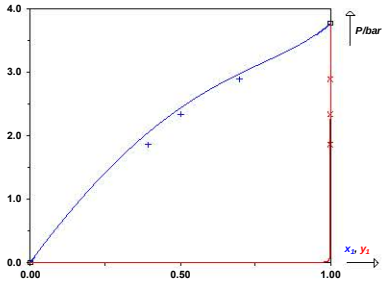

P/bar = 1.01320



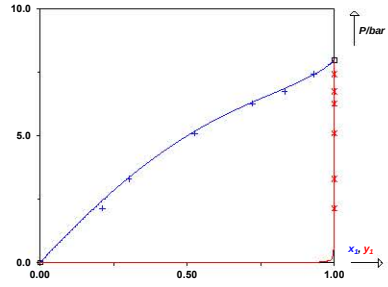

T/K = 114.10



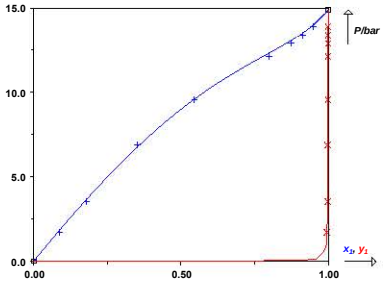

T/K = 130.37



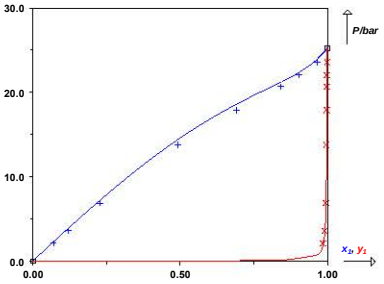

T/K = 144.26



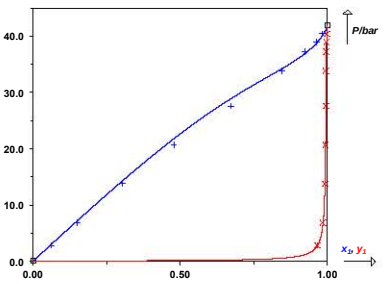
T/K = 158.15



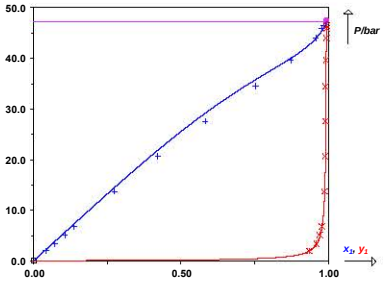

T/K = 172.04



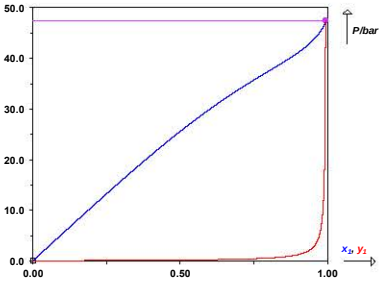

T/K = 187.43



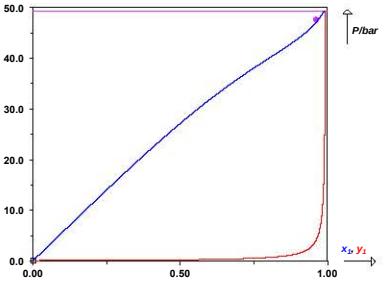

T/K = 192.26



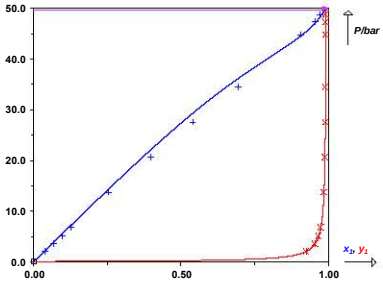

T/K = 192.30



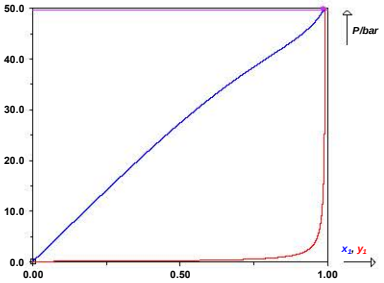

T/K = 194.82



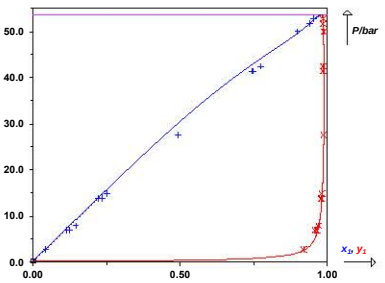

T/K = 195.15



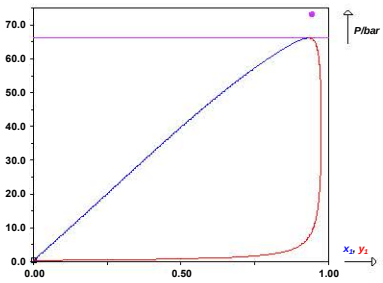

T/K = 195.20



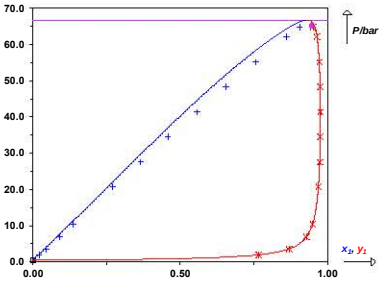

T/K = 199.82



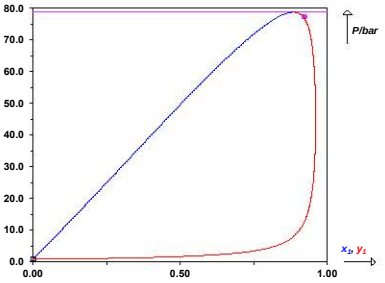

T/K = 213.15



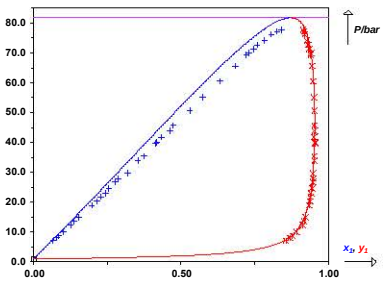

T/K = 213.71



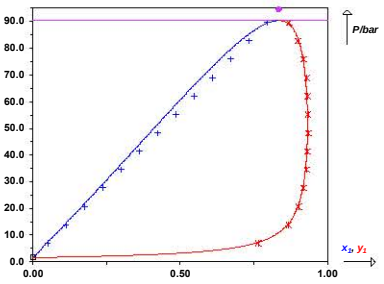

T/K = 226.48



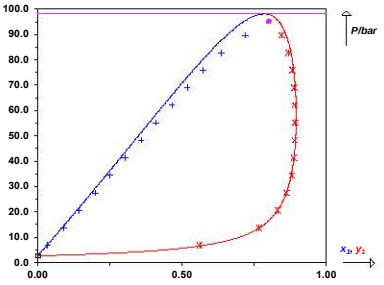

T/K = 230.00



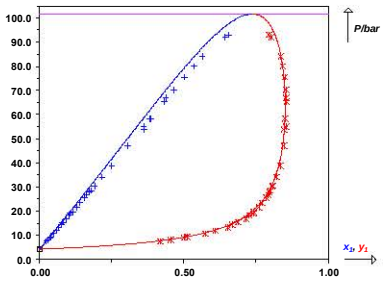

T/K = 241.48



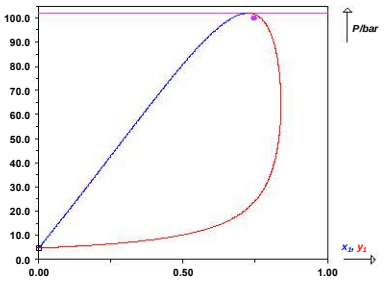

T/K = 256.48



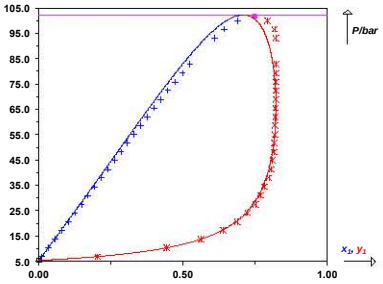
T/K = 270.00



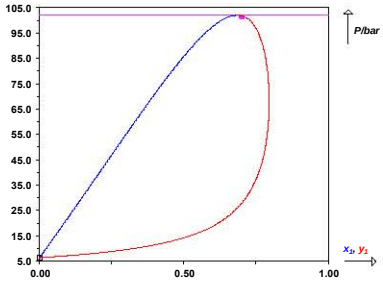

T/K = 273.15



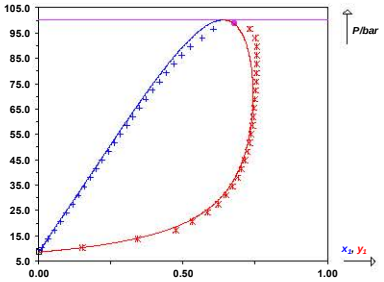

T/K = 277.59



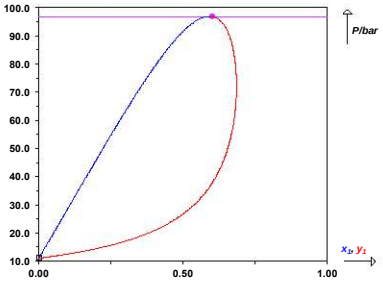

T/K = 283.55



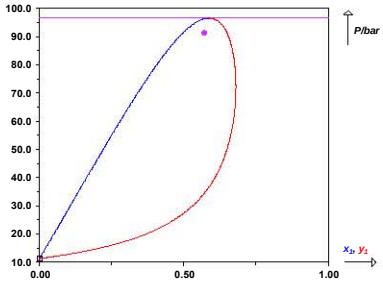

T/K = 294.26



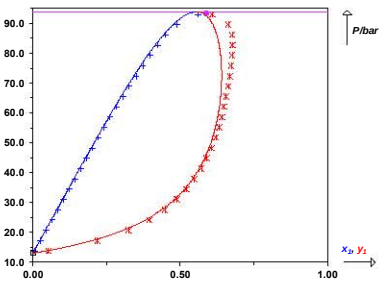

T/K = 304.25



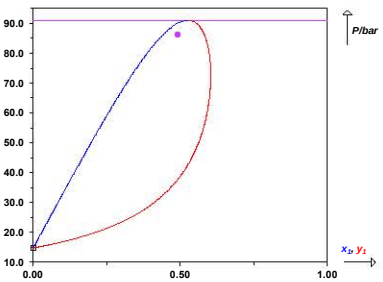

T/K = 304.98



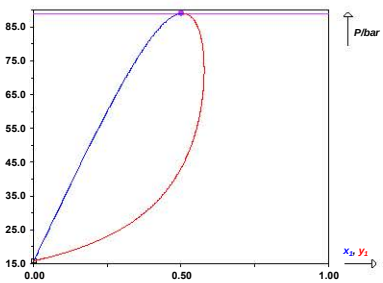

T/K = 310.93



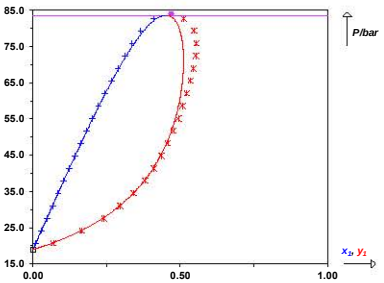

T/K = 316.21



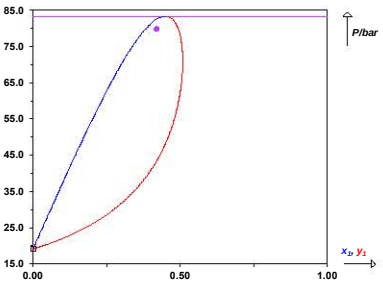

T/K = 319.45



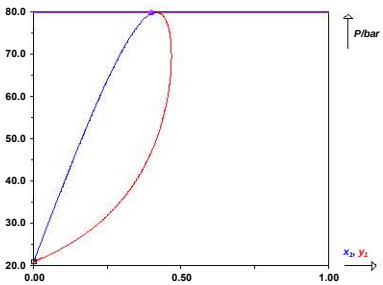

T/K = 327.59



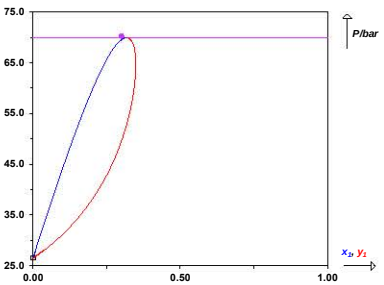

T/K = 327.98



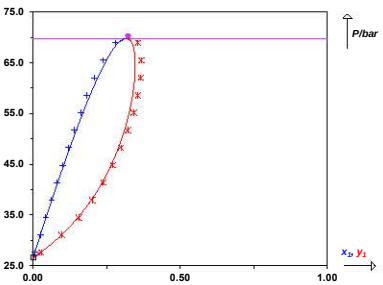

T/K = 332.45

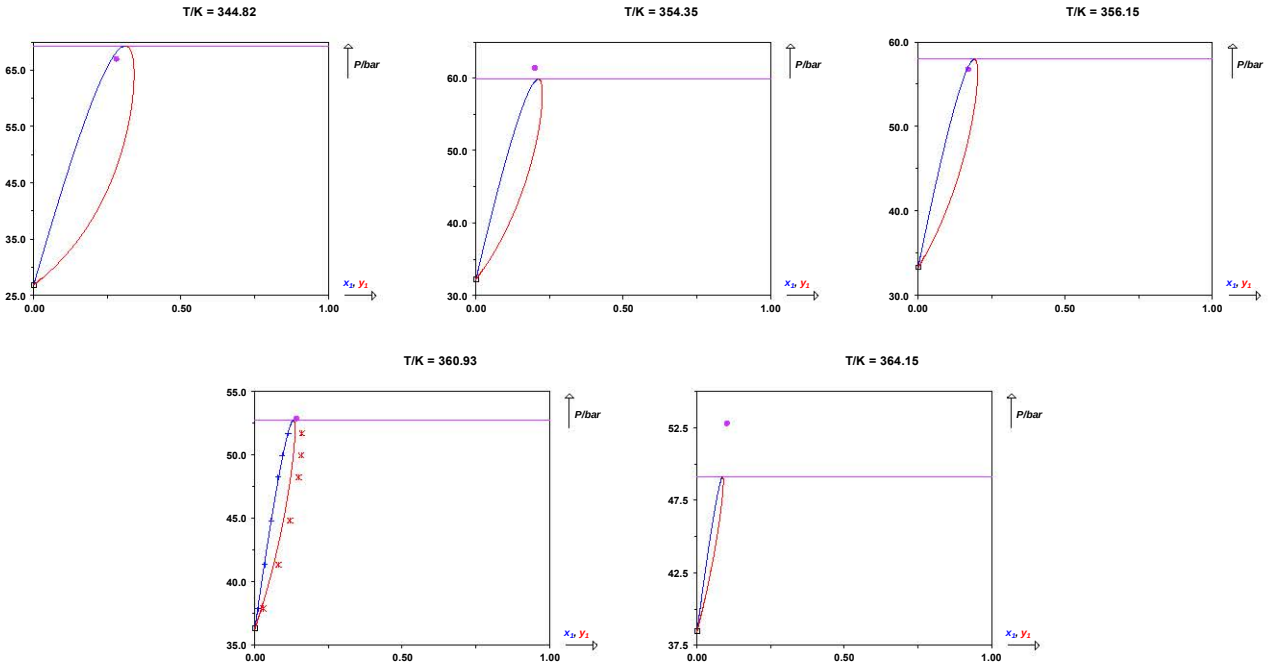



T/K = 344.05




T/K = 344.26




T/K = 344.82
P/bar
65.0
55.0
45.0
35.0
25.0
0.00
0.50
1.00
x1, y1
T/K = 354.35
P/bar
60.0
50.0
40.0
30.0
0.00
0.50
1.00
x1, y1
T/K = 356.15
P/bar
60.0
50.0
40.0
30.0
0.00
0.50
1.00
x1, y1
T/K = 360.93
P/bar
55.0
50.0
45.0
40.0
35.0
0.00
0.50
1.00
x1, y1
T/K = 364.15
P/bar
52.5
47.5
42.5
37.5
0.00
0.50
1.00
x1, y1

## METHANE (1) + n-HEXANE (2)

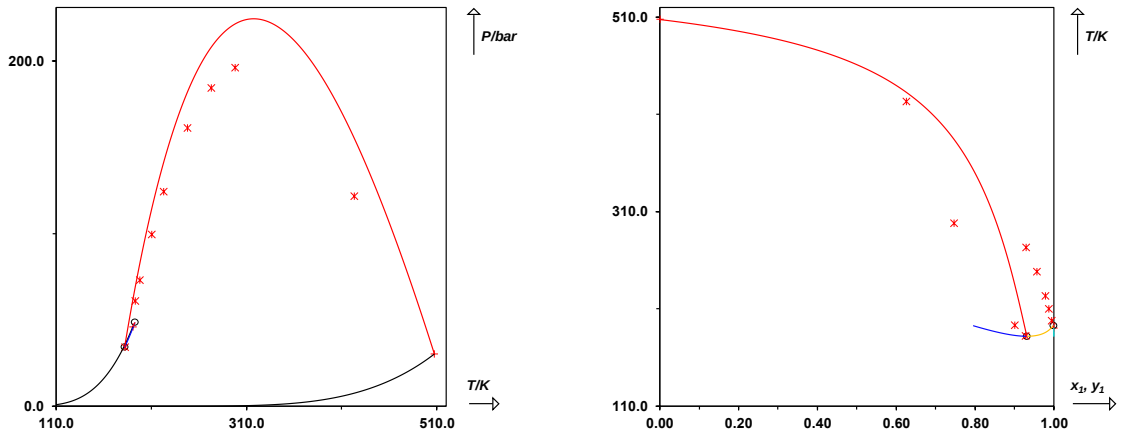
| | | |
|---|---|---|
| **CAS** | 74-82-8 | 110-54-3 |
| **InChiKey** | VNWKTOKETHGBQD-UHFFFAOYSA-N | VLKZOEOYAKHREP-UHFFFAOYSA-N |
| **$T_c$ / K** | 190.56 | 507.60 |
| **$P_c$ / bar** | 45.99 | 30.25 |
| **ω** | 0.012 | 0.301 |

Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 45.5
B/MPa = 15.6

*Deviations*
MAPE on x = 12 %
MAPE on y = 11 %
MAPE on $x_c$ = 130 %
MAPE on $P_c$ = 14 %
MAPE on $h^M$ = 40 %



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**Isothermal phase equilibrium data**

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Lin, Yueh-Neu - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-n-hexane system at low temperature, Journal of Chemical & Engineering Data 4 (1977) 402-408. doi:10.1021/je60075a007

**T / K = 186.23**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 38.54 | 0.8057 | 0.9505 |
| 39.99 | 0.8199 | 0.9412 |
| 41.37 | 0.8313 | 0.9335 |
| 42.20 | 0.8515 | 0.9246 |

Lin, Yueh-Neu - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-n-hexane system at low temperature, Journal of Chemical & Engineering Data 4 (1977) 402-408. doi:10.1021/je60075a007

**T / K = 190.50**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.379 | 0.0226 | 0.9999 |
| 1.724 | 0.0280 | 1.0000 |
| 6.895 | 0.1047 | 1.0000 |
| 20.68 | 0.3004 | 1.0000 |

Lin, Yueh-Neu - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-n-hexane system at low temperature, Journal of Chemical & Engineering Data 4 (1977) 402-408. doi:10.1021/je60075a007

**T / K = 193.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 47.71 | 0.7239 | 0.9864 | |
| 49.64 | 0.7415 | 0.9785 | |
| 51.02 | 0.7531 | 0.9716 | |
| 52.40 | 0.7649 | 0.9660 | |
| 55.16 | 0.7858 | 0.9522 | |
| 56.54 | 0.7949 | 0.9445 | |
| 57.92 | 0.8098 | 0.9377 | |
| 59.30 | 0.8278 | 0.9238 | |
| 60.88 | 0.9004 | 0.9004 | CRIT |

Lin, Yueh-Neu - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-n-hexane system at low temperature, Journal of Chemical & Engineering Data 4 (1977) 402-408. doi:10.1021/je60075a007

**T / K = 195.91**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 52.06 | 0.7177 | 0.9976 |
| 55.16 | 0.7425 | 0.9851 |
| 58.61 | 0.7701 | 0.9769 |
| 60.67 | 0.7809 | 0.9674 |
| 62.74 | 0.7950 | 0.9520 |
| 65.50 | 0.8151 | 0.9390 |
| 67.22 | 0.8416 | 0.9133 |

Lin, Yueh-Neu - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-n-hexane system at low temperature, Journal of Chemical & Engineering Data 4 (1977) 402-408. doi:10.1021/je60075a007

**T / K = 198.05**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 1.372 | 0.0195 | 0.9998 | |
| 1.724 | 0.0244 | 0.9999 | |
| 3.447 | 0.0474 | 0.9999 | |
| 6.895 | 0.0960 | 0.9999 | |
| 10.34 | 0.1390 | 1.0000 | |
| 13.79 | 0.1813 | 1.0000 | |
| 20.68 | 0.2660 | 0.9999 | |
| 27.58 | 0.3412 | 0.9999 | |
| 34.47 | 0.4225 | 0.9999 | |
| 41.37 | 0.5076 | 0.9998 | |
| 48.26 | 0.5936 | 0.9996 | |
| 55.16 | 0.6872 | 0.9979 | |
| 62.05 | 0.7596 | 0.9957 | |
| 68.95 | 0.8117 | 0.9943 | |
| 72.88 | 0.9936 | 0.9936 | CRIT |

Lin, Yueh-Neu - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-n-hexane system at low temperature, Journal of Chemical & Engineering Data 4 (1977) 402-408. doi:10.1021/je60075a007

**T / K = 210.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.393 | 0.0156 | 0.9995 |
| 1.738 | 0.0187 | 0.9996 |
| 3.461 | 0.0378 | 0.9998 |
| 6.909 | 0.0731 | 0.9999 |
| 10.36 | 0.1079 | 0.9999 |
| 13.80 | 0.1411 | 0.9999 |
| 20.70 | 0.2071 | 0.9999 |
| 27.59 | 0.2700 | 0.9999 |
| 41.37 | 0.3881 | 0.9998 |
| 55.16 | 0.5139 | 0.9994 |
| 68.95 | 0.6162 | 0.9973 |
| 82.74 | 0.7156 | 0.9918 |
| 96.53 | 0.8091 | 0.9882 |

| | | | |
|---|---|---|---|
| 99.49 | 0.9872 | 0.9872 | CRIT |

Lin, Yueh-Neu - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-n-hexane system at low temperature, Journal of Chemical & Engineering Data 4 (1977) 402-408. doi:10.1021/je60075a007

**T / K = 223.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 1.393 | 0.0141 | 0.9984 | |
| 1.738 | 0.0171 | 0.9987 | |
| 3.461 | 0.0337 | 0.9993 | |
| 6.909 | 0.0637 | 0.9996 | |
| 10.36 | 0.0921 | 0.9997 | |
| 13.80 | 0.1218 | 0.9998 | |
| 20.70 | 0.1771 | 0.9998 | |
| 27.59 | 0.2294 | 0.9998 | |
| 41.37 | 0.3282 | 0.9996 | |
| 55.16 | 0.4207 | 0.9993 | |
| 68.95 | 0.4952 | 0.9985 | |
| 82.74 | 0.5893 | 0.9961 | |
| 96.53 | 0.6518 | 0.9901 | |
| 103.42 | 0.7011 | 0.9871 | |
| 110.32 | 0.7423 | 0.9841 | |
| 117.21 | 0.7774 | 0.9816 | |
| 124.38 | 0.9784 | 0.9784 | CRIT |

Kandil, Mohamed E. - Thoma, Markus J. - Syed, Tauqir - Guo, Jerry - Graham, Brendan F. - Marsh, Kenneth N. - Huang, Stanley H. - May, Eric F., Vapor−Liquid Equilibria Measurements of the Methane + Pentane and Methane + Hexane Systems at Temperatures from (173 to 330) K and Pressures to 14 MPa, Journal of Chemical & Engineering Data 12 (2011) 4301-4309. doi:10.1021/je200101x

**T / K = 233.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 19.80 | 0.1820 | 0.9991 |
| 40.60 | 0.3140 | 0.9989 |
| 59.10 | 0.4150 | 0.9982 |
| 79.90 | 0.5170 | 0.9963 |
| 103.60 | 0.6470 | 0.9895 |
| 128.70 | 0.9590 | 0.9750 |

Lin, Yueh-Neu - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-n-hexane system at low temperature, Journal of Chemical & Engineering Data 4 (1977) 402-408. doi:10.1021/je60075a007

**T / K = 248.14**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.386 | 0.0095 | 0.9899 |
| 1.731 | 0.0115 | 0.9918 |
| 3.454 | 0.0232 | 0.9956 |
| 6.902 | 0.0464 | 0.9976 |
| 10.35 | 0.0688 | 0.9982 |
| 13.80 | 0.0900 | 0.9985 |
| 20.69 | 0.1340 | 0.9987 |
| 27.59 | 0.1819 | 0.9988 |
| 41.38 | 0.2595 | 0.9986 |
| 55.16 | 0.3347 | 0.9982 |
| 68.95 | 0.3998 | 0.9976 |
| 82.74 | 0.4672 | 0.9963 |
| 96.53 | 0.5252 | 0.9942 |
| 110.32 | 0.5804 | 0.9905 |
| 117.21 | 0.6123 | 0.9889 |
| 124.11 | 0.6382 | 0.9844 |
| 137.90 | 0.6937 | 0.9752 |
| 151.68 | 0.7601 | 0.9644 |
| 158.58 | 0.8191 | 0.9593 |
| 161.13 | 0.9564 | 0.9564 | CRIT |

Kandil, Mohamed E. - Thoma, Markus J. - Syed, Tauqir - Guo, Jerry - Graham, Brendan F. - Marsh, Kenneth N. - Huang, Stanley H. - May, Eric F., Vapor−Liquid Equilibria Measurements of the Methane + Pentane and Methane + Hexane Systems at Temperatures from (173 to 330) K and Pressures to 14 MPa, Journal of Chemical & Engineering Data 12 (2011) 4301-4309. doi:10.1021/je200101x

**T / K = 253.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.40 | 0.1520 | 0.9967 |
| 39.70 | 0.2590 | 0.9980 |
| 61.50 | 0.3610 | 0.9972 |
| 91.30 | 0.4770 | 0.9944 |
| 118.70 | 0.5750 | 0.9943 |

Lin, Yueh-Neu - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-n-hexane system at low temperature, Journal of Chemical & Engineering Data 4 (1977) 402-408. doi:10.1021/je60075a007

**T / K = 273.16**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.731 | 0.0097 | 0.9643 |
| 3.454 | 0.0196 | 0.9815 |
| 6.902 | 0.0387 | 0.9898 |
| 10.35 | 0.0567 | 0.9927 |
| 13.80 | 0.0744 | 0.9940 |
| 20.69 | 0.1116 | 0.9953 |
| 27.59 | 0.1469 | 0.9957 |
| 41.37 | 0.2127 | 0.9958 |

| | | | |
|---|---|---|---|
| 55.16 | 0.2742 | 0.9955 | |
| 68.95 | 0.3328 | 0.9947 | |
| 82.74 | 0.3886 | 0.9934 | |
| 96.53 | 0.4435 | 0.9917 | |
| 110.32 | 0.4924 | 0.9891 | |
| 124.11 | 0.5400 | 0.9849 | |
| 137.90 | 0.5933 | 0.9797 | |
| 151.68 | 0.6401 | 0.9692 | |
| 165.47 | 0.6949 | 0.9565 | |
| 175.82 | 0.7462 | 0.9400 | |
| 179.26 | 0.7758 | 0.9366 | |
| 182.71 | 0.8025 | 0.9348 | |
| 184.43 | 0.9290 | 0.9290 | CRIT |

Kandil, Mohamed E. - Thoma, Markus J. - Syed, Tauqir - Guo, Jerry - Graham, Brendan F. - Marsh, Kenneth N. - Huang, Stanley H. - May, Eric F., Vapor−Liquid Equilibria Measurements of the Methane + Pentane and Methane + Hexane Systems at Temperatures from (173 to 330) K and Pressures to 14 MPa, Journal of Chemical & Engineering Data 12 (2011) 4301-4309. doi:10.1021/je200101x

**T / K = 288.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 23.50 | 0.1360 | 0.9903 |
| 42.00 | 0.2210 | 0.9874 |
| 62.20 | 0.2990 | 0.9863 |
| 89.30 | 0.4000 | 0.9870 |
| 123.20 | 0.5160 | 0.9778 |

Stepanova, G.S. - Vybornova, Y.I., Phase equilibriums of methane-hexane system, Tr. Vses. Nauchno Issled. Inst. Prir. Gazov. (1962) 203-208.

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 98.17 | 0.4034 | 0.9889 |
| 124.99 | 0.5011 | 0.9829 |
| 138.52 | 0.5677 | 0.9778 |
| 167.29 | 0.6569 | 0.9639 |
| 184.33 | 0.7034 | 0.9525 |
| 192.22 | 0.7563 | 0.9207 |

Shim, Joosup - Kohn, J. P., Multiphase and Volumetric Equilibria of Methane-n-Hexane Binary System at Temperatures Between -110° and 150° C., Journal of Chemical & Engineering Data 1 (1962) 3-8. doi:10.1021/je60012a002

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.13 | 0.0490 | 0.9530 |
| 20.27 | 0.0978 | 0.9728 |
| 30.40 | 0.1450 | 0.9795 |
| 40.53 | 0.1890 | 0.9830 |
| 50.66 | 0.2316 | 0.9850 |
| 60.80 | 0.2710 | 0.9863 |
| 70.93 | 0.3090 | 0.9871 |
| 81.06 | 0.3447 | 0.9868 |
| 91.19 | 0.3810 | 0.9854 |
| 101.33 | 0.4125 | 0.9833 |
| 196.17 | 0.7466 | 0.7466 CRIT |

Kandil, Mohamed E. - Thoma, Markus J. - Syed, Tauqir - Guo, Jerry - Graham, Brendan F. - Marsh, Kenneth N. - Huang, Stanley H. - May, Eric F., Vapor−Liquid Equilibria Measurements of the Methane + Pentane and Methane + Hexane Systems at Temperatures from (173 to 330) K and Pressures to 14 MPa, Journal of Chemical & Engineering Data 12 (2011) 4301-4309. doi:10.1021/je200101x

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.70 | 0.1120 | 0.9832 |
| 58.70 | 0.2670 | 0.9801 |
| 83.90 | 0.3530 | 0.9818 |
| 110.70 | 0.4450 | 0.9771 |
| 141.90 | 0.5460 | 0.9830 |

Poston, R. S. - McKetta, J. J., Vapor-Liquid Equilibrium in the Methane-n-Hexane System., Journal of Chemical & Engineering Data 3 (1966) 362-363. doi:10.1021/je60030a021

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.46 | 0.1530 | 0.9690 |
| 68.93 | 0.2860 | 0.9800 |
| 103.39 | 0.4040 | 0.9790 |
| 137.85 | 0.5110 | 0.9700 |
| 172.32 | 0.6380 | 0.9690 |
| 186.10 | 0.6940 | 0.9700 |
| 190.59 | 0.7150 | 0.9680 |
| 196.10 | 0.7560 | 0.9640 |
| 194.73 | 0.7400 | 0.9620 |
| 197.83 | 0.7600 | 0.9570 |

Gunn, Robert D. - McKetta, John J. - Ata, Nassar, Measurement and prediction of high-pressure phase equilibria with a dilute component in the gas phase: The methane-n-hexane system, AIChE Journal 2 (1974) 347-353. doi:10.1002/aic.690200221

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.445 | 0.0152 | 0.8923 |

| | | |
|---|---|---|
| 6.890 | 0.0319 | 0.9451 |
| 10.35 | 0.0482 | 0.9606 |
| 13.79 | 0.0642 | 0.9696 |
| 17.24 | 0.0798 | 0.9728 |

Stepanova, G.S. - Vybornova, Y.I., Phase equilibriums of methane-hexane system, Tr. Vses. Nauchno Issled. Inst. Prir. Gazov. (1962) 203-208.

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 58.89 | 0.2433 | 0.9820 |
| 75.72 | 0.3042 | 0.9836 |
| 98.65 | 0.3997 | 0.9764 |
| 127.41 | 0.4819 | 0.9738 |
| 143.60 | 0.5354 | 0.9607 |
| 167.77 | 0.6142 | 0.9499 |
| 197.14 | 0.7236 | 0.9130 |

Kandil, Mohamed E. - Thoma, Markus J. - Syed, Tauqir - Guo, Jerry - Graham, Brendan F. - Marsh, Kenneth N. - Huang, Stanley H. - May, Eric F., Vapor−Liquid Equilibria Measurements of the Methane + Pentane and Methane + Hexane Systems at Temperatures from (173 to 330) K and Pressures to 14 MPa, Journal of Chemical & Engineering Data 12 (2011) 4301-4309. doi:10.1021/je200101x

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 24.30 | 0.1220 | 0.9717 |
| 51.10 | 0.2280 | 0.9772 |
| 77.50 | 0.3230 | 0.9756 |
| 111.80 | 0.4290 | 0.9679 |
| 142.10 | 0.5290 | 0.9783 |

Marteau, Ph. - Obriot, J. - Barreau, A. - Ruffier-Meray, V. - Behar, E., Experimental determination of the phase behavior of binary mixtures: methane-hexane and methane-benzene, Fluid Phase Equilibria 1-2 (1997) 285-305. doi:10.1016/S0378-3812(96)03125-1

**T / K = 323.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 140.10 | 0.5126 | 0.9580 |
| 150.10 | 0.5414 | 0.9511 |
| 158.80 | 0.5682 | 0.9477 |
| 159.10 | 0.5709 | 0.9497 |
| 170.40 | 0.6063 | 0.9368 |
| 180.10 | 0.6441 | 0.9216 |
| 190.00 | 0.6861 | 0.9164 |
| 195.00 | 0.7036 | 0.8885 |
| 197.30 | 0.7252 | 0.8768 |
| 199.80 | 0.7386 | 0.8572 |
| 200.40 | 0.7633 | 0.8532 |
| 201.10 | 0.7748 | 0.8416 |

Shim, Joosup - Kohn, J. P., Multiphase and Volumetric Equilibria of Methane-n-Hexane Binary System at Temperatures Between -110° and 150° C., Journal of Chemical & Engineering Data 1 (1962) 3-8. doi:10.1021/je60012a002

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.13 | 0.0422 | 0.9021 |
| 20.27 | 0.0860 | 0.9465 |
| 30.40 | 0.1290 | 0.9614 |
| 40.53 | 0.1690 | 0.9680 |
| 50.66 | 0.2080 | 0.9719 |
| 60.80 | 0.2458 | 0.9747 |
| 70.93 | 0.2820 | 0.9765 |
| 81.06 | 0.3186 | 0.9770 |
| 91.19 | 0.3540 | 0.9768 |
| 101.33 | 0.3850 | 0.9751 |

Poston, R. S. - McKetta, J. J., Vapor-Liquid Equilibrium in the Methane-n-Hexane System., Journal of Chemical & Engineering Data 3 (1966) 362-363. doi:10.1021/je60030a021

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.46 | 0.1350 | 0.9370 |
| 68.93 | 0.2580 | 0.9530 |
| 103.39 | 0.3710 | 0.9620 |
| 137.85 | 0.4850 | 0.9460 |
| 172.32 | 0.5940 | 0.9280 |
| 186.10 | 0.6680 | 0.9130 |
| 189.55 | 0.7010 | 0.9110 |
| 192.66 | 0.7030 | 0.8850 |

Gunn, Robert D. - McKetta, John J. - Ata, Nassar, Measurement and prediction of high-pressure phase equilibria with a dilute component in the gas phase: The methane-n-hexane system, AIChE Journal 2 (1974) 347-353. doi:10.1002/aic.690200221

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.445 | 0.0107 | 0.6791 |
| 6.890 | 0.0256 | 0.8281 |
| 10.35 | 0.0405 | 0.8830 |
| 13.79 | 0.0551 | 0.9097 |
| 17.24 | 0.0694 | 0.9257 |

Marteau, Ph. - Obriot, J. - Barreau, A. - Ruffier-Meray, V. - Behar, E., Experimental determination of the phase

behavior of binary mixtures: methane-hexane and methane-benzene, Fluid Phase Equilibria 1-2 (1997) 285-305. doi:10.1016/S0378-3812(96)03125-1

**T / K = 373.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 59.80 | 0.2169 | 0.9097 |
| 71.00 | 0.2517 | 0.9185 |
| 80.60 | 0.2868 | 0.9119 |
| 90.00 | 0.3094 | 0.9161 |
| 99.80 | 0.3408 | 0.9151 |
| 112.10 | 0.3753 | 0.9132 |
| 120.00 | 0.4038 | 0.9080 |
| 130.10 | 0.4362 | 0.9180 |
| 140.30 | 0.4715 | 0.8936 |
| 150.00 | 0.5013 | 0.8848 |
| 160.00 | 0.5397 | 0.8672 |
| 164.60 | 0.5596 | 0.8593 |
| 170.20 | 0.5878 | 0.8488 |
| 174.90 | 0.6085 | 0.8340 |
| 177.00 | 0.6178 | 0.8286 |
| 179.10 | 0.6286 | 0.8176 |
| 180.50 | 0.6438 | 0.8119 |
| 182.10 | 0.6565 | 0.8004 |
| 183.60 | 0.6807 | 0.7837 |
| 184.00 | 0.6953 | 0.7840 |
| 184.30 | 0.7109 | 0.7763 |

Shim, Joosup - Kohn, J. P., Multiphase and Volumetric Equilibria of Methane-n-Hexane Binary System at Temperatures Between -110° and 150° C., Journal of Chemical & Engineering Data 1 (1962) 3-8. doi:10.1021/je60012a002

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.13 | 0.0300 | 0.7875 |
| 20.27 | 0.0688 | 0.8316 |
| 30.40 | 0.1065 | 0.8760 |
| 40.53 | 0.1440 | 0.8970 |
| 50.66 | 0.1810 | 0.9082 |
| 60.80 | 0.2160 | 0.9158 |
| 70.93 | 0.2490 | 0.9224 |
| 81.06 | 0.2807 | 0.9280 |
| 91.19 | 0.3135 | 0.9321 |
| 101.33 | 0.3434 | 0.9340 |

Poston, R. S. - McKetta, J. J., Vapor-Liquid Equilibrium in the Methane-n-Hexane System., Journal of Chemical & Engineering Data 3 (1966) 362-363. doi:10.1021/je60030a021

**T / K = 377.55**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.46 | 0.1190 | 0.8710 |
| 68.93 | 0.2400 | 0.9110 |
| 103.39 | 0.3510 | 0.9080 |
| 137.85 | 0.4770 | 0.8950 |
| 172.32 | 0.6040 | 0.8610 |
| 175.08 | 0.6180 | 0.8220 |
| 177.84 | 0.6500 | 0.8170 |
| 180.25 | 0.6750 | 0.7840 |

Gunn, Robert D. - McKetta, John J. - Ata, Nassar, Measurement and prediction of high-pressure phase equilibria with a dilute component in the gas phase: The methane-n-hexane system, AIChE Journal 2 (1974) 347-353. doi:10.1002/aic.690200221

**T / K = 377.55**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.890 | 0.0164 | 0.5583 |
| 10.35 | 0.0299 | 0.6877 |
| 13.79 | 0.0431 | 0.7531 |
| 17.24 | 0.0563 | 0.7961 |

Poston, R. S. - McKetta, J. J., Vapor-Liquid Equilibrium in the Methane-n-Hexane System., Journal of Chemical & Engineering Data 3 (1966) 362-363. doi:10.1021/je60030a021

**T / K = 410.95**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.46 | 0.1030 | 0.7380 |
| 68.93 | 0.2230 | 0.8110 |
| 103.39 | 0.3450 | 0.8300 |
| 137.85 | 0.4770 | 0.8030 |
| 146.82 | 0.5280 | 0.7680 |
| 150.26 | 0.5560 | 0.7510 |
| 153.16 | 0.5980 | 0.7250 |

Gunn, Robert D. - McKetta, John J. - Ata, Nassar, Measurement and prediction of high-pressure phase equilibria with a dilute component in the gas phase: The methane-n-hexane system, AIChE Journal 2 (1974) 347-353. doi:10.1002/aic.690200221

**T / K = 410.95**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.79 | 0.0324 | 0.5185 |
| 17.24 | 0.0460 | 0.5999 |

Shim, Joosup - Kohn, J. P., Multiphase and Volumetric Equilibria of Methane-n-Hexane Binary System at Temperatures Between -110° and 150° C., Journal of Chemical & Engineering Data 1 (1962) 3-8. doi:10.1021/je60012a002

**T / K = 423.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 10.13 | 0.0110 | 0.4420 | |
| 20.27 | 0.0464 | 0.5625 | |
| 30.40 | 0.0826 | 0.6695 | |
| 40.53 | 0.1187 | 0.7220 | |
| 50.66 | 0.1553 | 0.7520 | |
| 60.80 | 0.1915 | 0.7675 | |
| 70.93 | 0.2278 | 0.7780 | |
| 81.06 | 0.2645 | 0.7800 | |
| 91.19 | 0.3040 | 0.7600 | |
| 101.33 | 0.3440 | 0.7380 | |
| 121.59 | 0.6250 | 0.6250 | CRIT |

Poston, R. S. - McKetta, J. J., Vapor-Liquid Equilibrium in the Methane-n-Hexane System., Journal of Chemical & Engineering Data 3 (1966) 362-363. doi:10.1021/je60030a021

**T / K = 444.25**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 25.09 | 0.0520 | 0.4380 |
| 34.46 | 0.0790 | 0.5220 |
| 68.93 | 0.2080 | 0.6540 |
| 103.39 | 0.3630 | 0.6600 |
| 108.56 | 0.3880 | 0.6580 |
| 112.56 | 0.4220 | 0.6410 |

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**Enthalpy of mixing**

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Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K = 343.20**

**P / bar = 1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 83.70 | 0.3040 |
| 91.40 | 0.3550 |
| 94.20 | 0.4210 |
| 99.30 | 0.4560 |
| 96.80 | 0.4780 |
| 98.20 | 0.5330 |
| 94.30 | 0.5950 |
| 82.40 | 0.6840 |
| 72.30 | 0.7500 |
| 56.30 | 0.8220 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K = 363.20**

**P / bar = 1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 70.70 | 0.2940 |
| 74.60 | 0.3500 |
| 80.00 | 0.4010 |
| 81.60 | 0.4250 |
| 82.10 | 0.5210 |
| 79.40 | 0.5560 |
| 77.00 | 0.6300 |
| 71.40 | 0.6750 |
| 63.20 | 0.7300 |
| 54.80 | 0.7840 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K = 407.70**

**P / bar = 1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 54.20 | 0.3660 |
| 54.60 | 0.3800 |
| 56.50 | 0.4130 |
| 57.00 | 0.4640 |
| 57.00 | 0.5390 |
| 55.30 | 0.5680 |
| 50.90 | 0.6240 |
| 44.50 | 0.7250 |

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**Critical point**

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Lin, Yueh-Neu - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-n-hexane system at low temperature, Journal of Chemical & Engineering Data 4 (1977) 402-408. doi:10.1021/je60075a007

| T / K | P / bar | $x_1$ |
|---|---|---|
| 182.46 | 34.15 | 0.9286 |

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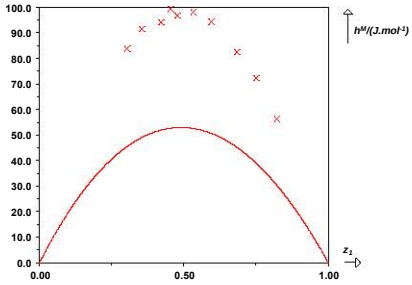
**Three-phase line**

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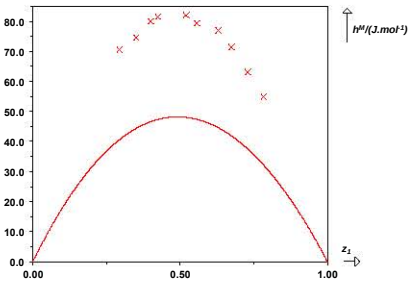
D.G. Elliott, Y.N. Lin, T.C. Chu, P.S. Chappelear, R. Kobayashi, K-values for the methane - n-butane, methane - n-pentane, and methane - n-hexane systems, GPA Research Report. (1976) 1–19.

| T / K | P / bar | $x_{1a}$ | $x_{1b}$ | $y_1$ |
|---|---|---|---|---|
| 193.150 | 47.712 | 0.7239 | 0.9864 | 0.9994 |
| 190.500 | 43.988 | 0.7438 | 0.9695 | 0.9996 |
| 186.230 | 38.542 | 0.8057 | 0.9505 | 0.9998 |
| 182.460 | 34.150 | 0.9286 | 0.9286 | 0.9995 |

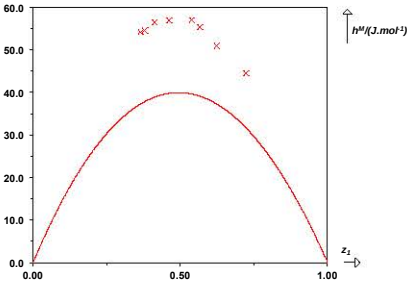
T/K = 343.20 - P/bar = 1.0132



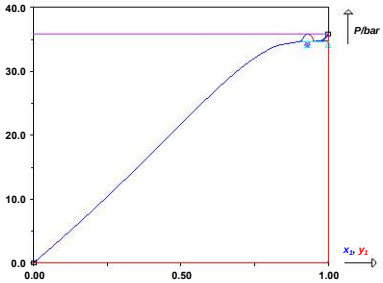

T/K = 363.20 - P/bar = 1.0132



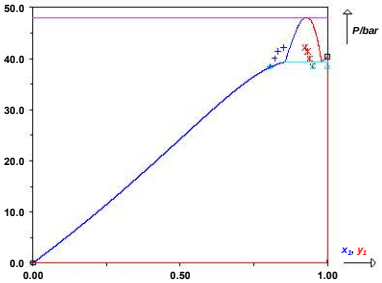

T/K = 407.70 - P/bar = 1.0132



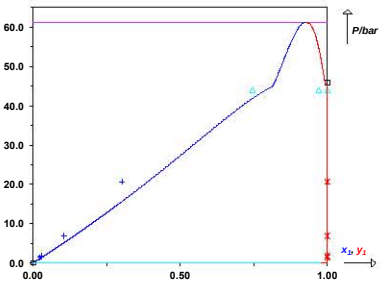

T/K = 182.46



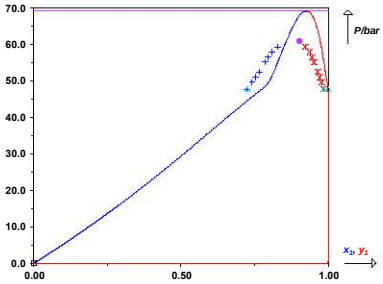

T/K = 186.23



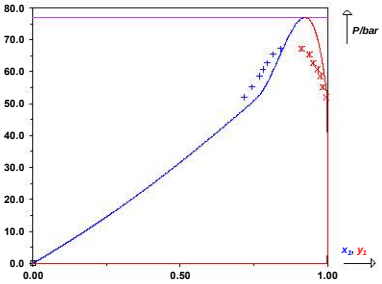

T/K = 190.50



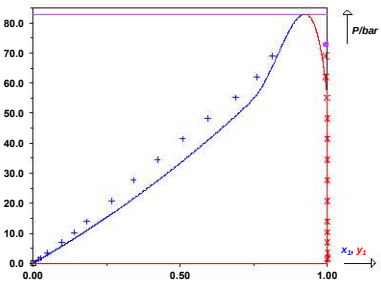

T/K = 193.15



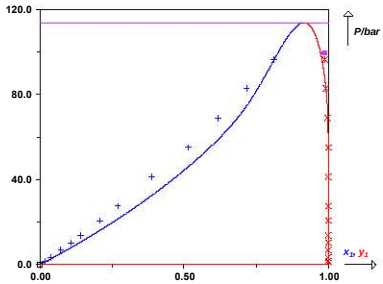

T/K = 195.91



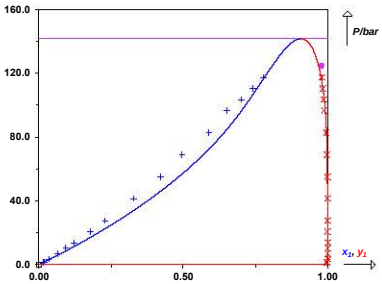

T/K = 198.05



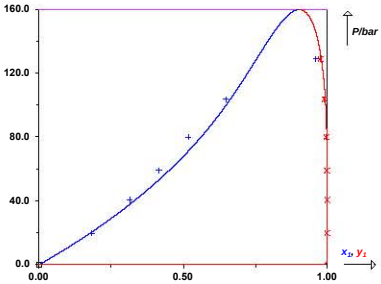

T/K = 210.15



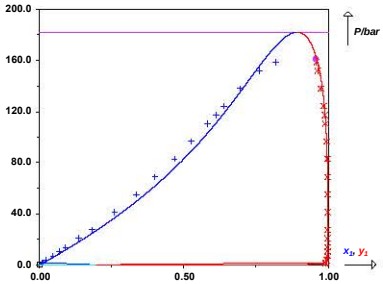

T/K = 223.15



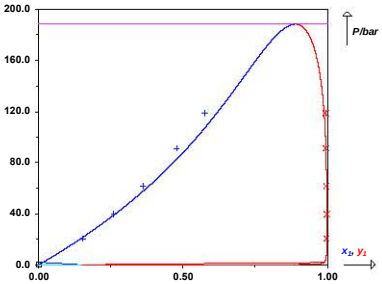

T/K = 233.15



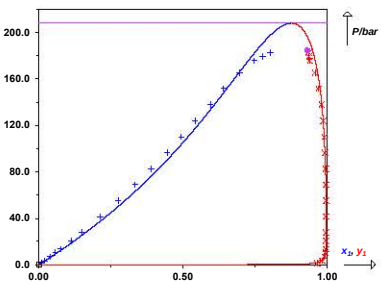

T/K = 248.14



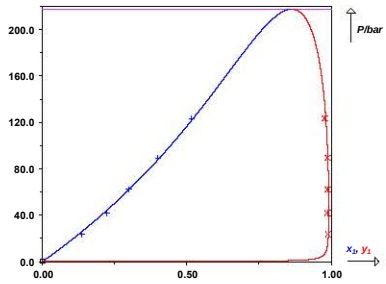

T/K = 253.15



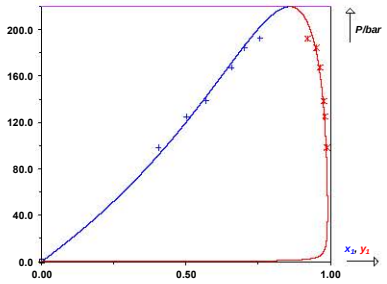

T/K = 273.16



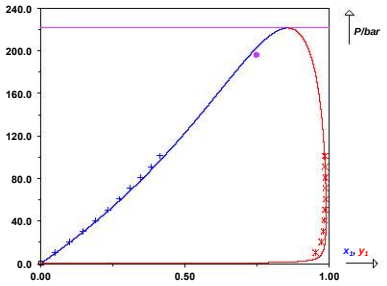
T/K = 288.15



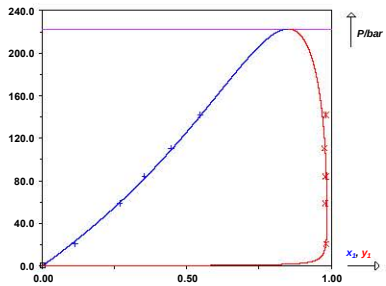

T/K = 293.15



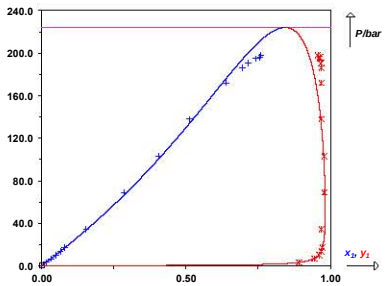

T/K = 298.15



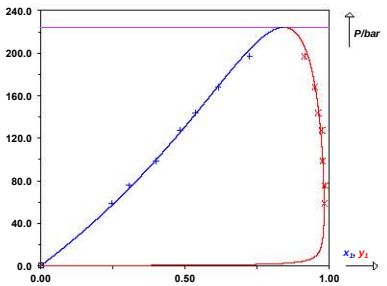

T/K = 303.15



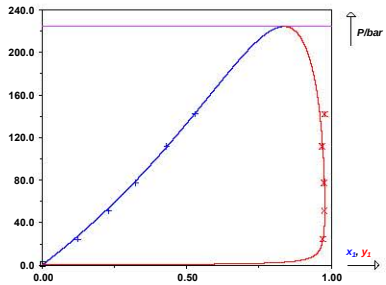

T/K = 310.93



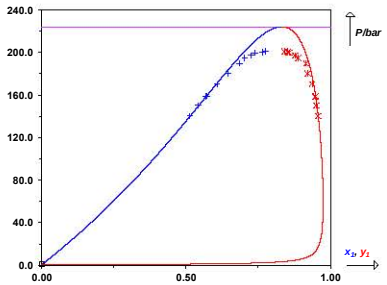

T/K = 313.15



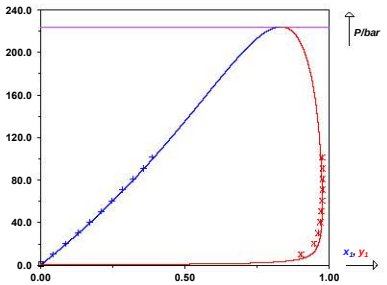

T/K = 318.15



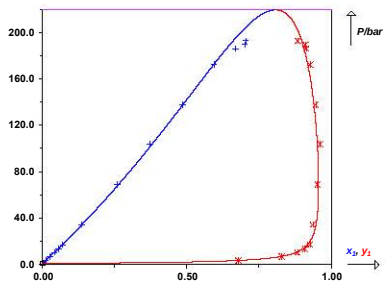

T/K = 323.00



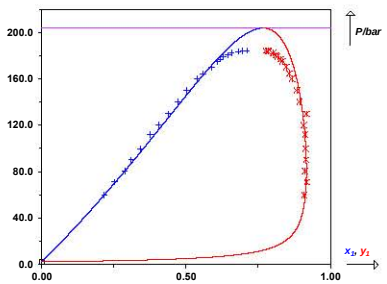

T/K = 323.15



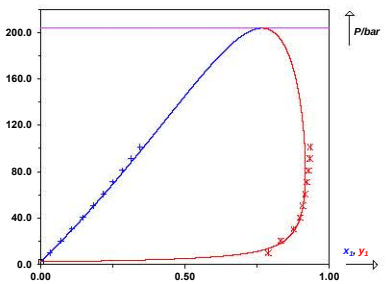

T/K = 344.26

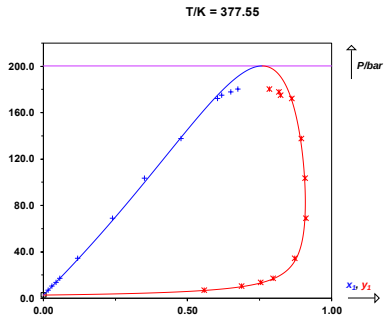


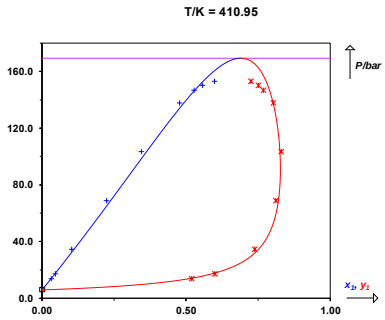

T/K = 373.00

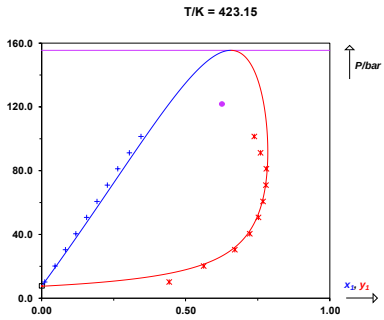


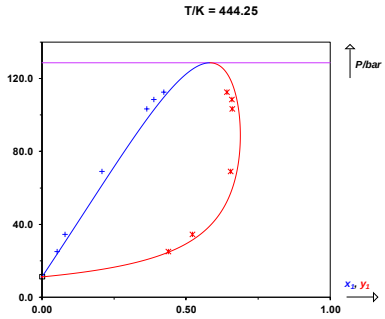

T/K = 373.15




T/K = 377.55
P/bar
200.0
160.0
120.0
80.0
40.0
0.0
0.00
0.50
1.00
$x_1, y_1$


T/K = 410.95
P/bar
160.0
120.0
80.0
40.0
0.0
0.00
0.50
1.00
$x_1, y_1$


T/K = 423.15
P/bar
160.0
120.0
80.0
40.0
0.0
0.00
0.50
1.00
$x_1, y_1$


T/K = 444.25
P/bar
120.0
80.0
40.0
0.0
0.00
0.50
1.00
$x_1, y_1$

## METHANE (1) + n-HEPTANE (2)

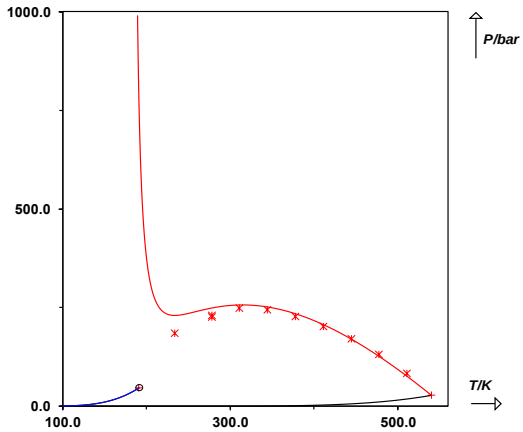
| | | |
|---|---|---|
| **CAS** | 74-82-8 | 142-82-5 |
| **InChiKey** | VNWKTOKETHGBQD-UHFFFAOYSA-N | IMNFDUFMRHMDMM-UHFFFAOYSA-N |
| **$T_c$ / K** | 190.56 | 540.20 |
| **$P_c$ / bar** | 45.99 | 27.40 |
| **ω** | 0.012 | 0.349 |

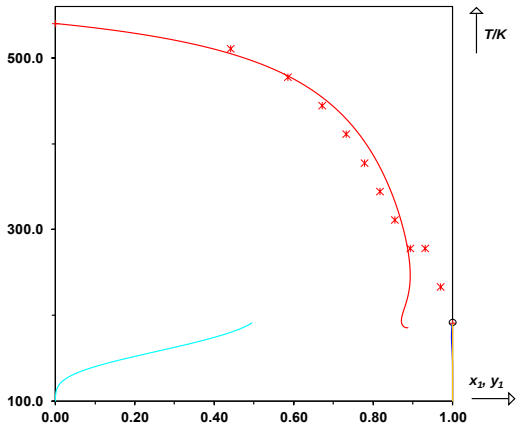
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 34.1
B/MPa = 151

*Deviations*
MAPE on x = 7.5 %
MAPE on y = 10 %
MAPE on $x_c$ = 22 %
MAPE on $P_c$ = 6.8 %
MAPE on $h^M$ = 40 %



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**Isothermal phase equilibrium data**

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Chang, Harry L. - Hurt, Lewis J. - Kobayashi, Riki, Vapor-liquid equilibria of light hydrocarbons at low temperatures and high pressures: The methane-n-heptane system, AIChE Journal 6 (1966) 1212-1216. doi:10.1002/aic.690120629

**T / K = 210.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 27.58 | 0.2630 | 0.9999 |
| 41.37 | 0.3780 | 0.9999 |
| 55.16 | 0.4765 | 0.9999 |
| 68.95 | 0.5549 | 0.9998 |
| 86.19 | 0.6480 | 0.9997 |
| 103.42 | 0.7210 | 0.9996 |
| 120.66 | 0.8030 | 0.9992 |
| 137.90 | 0.8911 | 0.9986 |

Chang, Harry L. - Hurt, Lewis J. - Kobayashi, Riki, Vapor-liquid equilibria of light hydrocarbons at low temperatures and high pressures: The methane-n-heptane system, AIChE Journal 6 (1966) 1212-1216. doi:10.1002/aic.690120629

**T / K = 222.04**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0628 | 0.9999 |
| 13.79 | 0.1235 | 0.9999 |
| 27.58 | 0.2322 | 0.9999 |
| 41.37 | 0.3255 | 0.9998 |
| 55.16 | 0.4117 | 0.9997 |
| 68.95 | 0.4921 | 0.9996 |
| 86.19 | 0.5720 | 0.9995 |
| 103.42 | 0.6542 | 0.9993 |
| 120.66 | 0.7280 | 0.9990 |
| 137.90 | 0.7949 | 0.9985 |
| 155.13 | 0.8819 | 0.9966 |

Chang, Harry L. - Hurt, Lewis J. - Kobayashi, Riki, Vapor-liquid equilibria of light hydrocarbons at low temperatures and high pressures: The methane-n-heptane system, AIChE Journal 6 (1966) 1212-1216. doi:10.1002/aic.690120629

**T / K = 233.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0556 | 0.9997 |
| 13.79 | 0.1163 | 0.9997 |
| 27.58 | 0.2081 | 0.9997 |
| 41.37 | 0.2990 | 0.9996 |
| 55.16 | 0.3728 | 0.9995 |
| 68.95 | 0.4481 | 0.9993 |
| 86.19 | 0.5160 | 0.9991 |
| 103.42 | 0.5789 | 0.9987 |
| 120.66 | 0.6549 | 0.9982 |
| 137.90 | 0.7375 | 0.9975 |
| 155.13 | 0.8150 | 0.9960 |
| 172.37 | 0.8880 | 0.9920 |

Chang, Harry L. - Hurt, Lewis J. - Kobayashi, Riki, Vapor-liquid equilibria of light hydrocarbons at low temperatures and high pressures: The methane-n-heptane system, AIChE Journal 6 (1966) 1212-1216. doi:10.1002/aic.690120629

**T / K = 244.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0490 | 0.9994 |
| 13.79 | 0.1033 | 0.9994 |
| 27.58 | 0.1883 | 0.9993 |
| 41.37 | 0.2668 | 0.9992 |
| 55.16 | 0.3412 | 0.9991 |
| 68.95 | 0.4078 | 0.9989 |
| 86.19 | 0.4784 | 0.9985 |
| 103.42 | 0.5389 | 0.9979 |
| 120.66 | 0.6058 | 0.9971 |
| 137.90 | 0.6658 | 0.9960 |
| 155.13 | 0.7219 | 0.9930 |
| 172.37 | 0.7813 | 0.9883 |
| 189.61 | 0.8634 | 0.9756 |

Chang, Harry L. - Hurt, Lewis J. - Kobayashi, Riki, Vapor-liquid equilibria of light hydrocarbons at low temperatures and high pressures: The methane-n-heptane system, AIChE Journal 6 (1966) 1212-1216. doi:10.1002/aic.690120629

**T / K = 255.37**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0445 | 0.9986 |
| 13.79 | 0.0901 | 0.9988 |
| 27.58 | 0.1744 | 0.9990 |
| 41.37 | 0.2490 | 0.9987 |
| 55.16 | 0.3160 | 0.9986 |
| 68.95 | 0.3772 | 0.9984 |
| 86.19 | 0.4452 | 0.9978 |
| 103.42 | 0.4966 | 0.9964 |
| 120.66 | 0.5570 | 0.9958 |
| 137.90 | 0.6169 | 0.9943 |
| 155.13 | 0.6659 | 0.9927 |
| 172.37 | 0.7183 | 0.9853 |
| 189.61 | 0.7789 | 0.9734 |
| 206.85 | 0.8585 | 0.9400 |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane- n-Heptane System, Industrial & Engineering Chemistry Chemical & Engineering Data Series 1 (1956) 29-42. doi:10.1021/i460001a007

**T / K = 277.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 13.79 | 0.0753 | 0.9964 | |
| 27.58 | 0.1445 | 0.9974 | |
| 41.37 | 0.2084 | 0.9971 | |
| 55.16 | 0.2670 | 0.9970 | |
| 68.95 | 0.3215 | 0.9966 | |
| 86.19 | 0.3840 | 0.9957 | |
| 103.42 | 0.4410 | 0.9940 | |
| 120.66 | 0.4930 | 0.9920 | |
| 137.90 | 0.5425 | 0.9890 | |
| 155.13 | 0.5900 | 0.9850 | |
| 172.37 | 0.6373 | 0.9780 | |
| 189.61 | 0.6870 | 0.9690 | |
| 206.85 | 0.7400 | 0.9530 | |
| 229.46 | 0.8940 | 0.8940 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane- n-Heptane System, Industrial & Engineering Chemistry Chemical & Engineering Data Series 1 (1956) 29-42. doi:10.1021/i460001a007

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 13.79 | 0.0640 | 0.9866 | |
| 27.58 | 0.1240 | 0.9905 | |
| 68.95 | 0.2842 | 0.9910 | |
| 86.19 | 0.3425 | 0.9900 | |
| 103.42 | 0.3963 | 0.9881 | |
| 120.66 | 0.4470 | 0.9850 | |
| 137.90 | 0.4950 | 0.9801 | |
| 155.13 | 0.5435 | 0.9748 | |
| 172.37 | 0.5905 | 0.9690 | |
| 189.61 | 0.6400 | 0.9620 | |
| 206.85 | 0.6910 | 0.9530 | |
| 241.31 | 0.8030 | 0.9050 | |
| 248.83 | 0.8550 | 0.8550 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane- n-Heptane System, Industrial & Engineering Chemistry Chemical & Engineering Data Series 1 (1956) 29-42. doi:10.1021/i460001a007

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 13.79 | 0.0565 | 0.9597 | |
| 27.58 | 0.1110 | 0.9733 | |
| 41.37 | 0.1623 | 0.9780 | |
| 55.16 | 0.2107 | 0.9798 | |
| 68.95 | 0.2567 | 0.9804 | |
| 86.19 | 0.3108 | 0.9795 | |
| 103.42 | 0.3620 | 0.9770 | |
| 120.66 | 0.4125 | 0.9742 | |
| 137.90 | 0.4620 | 0.9705 | |
| 155.13 | 0.5090 | 0.9656 | |
| 172.37 | 0.5580 | 0.9590 | |
| 189.61 | 0.6070 | 0.9490 | |
| 206.85 | 0.6610 | 0.9360 | |
| 241.31 | 0.7870 | 0.8595 | |
| 244.70 | 0.8170 | 0.8170 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane- n-Heptane System, Industrial & Engineering Chemistry Chemical & Engineering Data Series 1 (1956) 29-42. doi:10.1021/i460001a007

**T / K = 377.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 13.79 | 0.0494 | 0.8942 | |
| 27.58 | 0.1003 | 0.9305 | |
| 41.37 | 0.1492 | 0.9449 | |
| 55.16 | 0.1960 | 0.9517 | |
| 68.95 | 0.2410 | 0.9558 | |
| 86.19 | 0.2940 | 0.9566 | |
| 103.42 | 0.3450 | 0.9564 | |
| 120.66 | 0.3957 | 0.9532 | |
| 137.90 | 0.4457 | 0.9474 | |
| 155.13 | 0.4944 | 0.9392 | |
| 172.37 | 0.5450 | 0.9280 | |
| 189.61 | 0.5995 | 0.9120 | |
| 206.85 | 0.6615 | 0.8864 | |
| 227.39 | 0.7780 | 0.7780 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane- n-Heptane System, Industrial & Engineering Chemistry Chemical & Engineering Data Series 1 (1956) 29-42. doi:10.1021/i460001a007

**T / K = 410.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.79 | 0.0405 | 0.7481 |
| 27.58 | 0.0918 | 0.8628 |

| | | | |
|---|---|---|---|
| 41.37 | 0.1390 | 0.8894 | |
| 55.16 | 0.1850 | 0.9037 | |
| 68.95 | 0.2290 | 0.9100 | |
| 86.19 | 0.2810 | 0.9120 | |
| 103.42 | 0.3308 | 0.9107 | |
| 120.66 | 0.3810 | 0.9073 | |
| 137.90 | 0.4329 | 0.9000 | |
| 155.13 | 0.4880 | 0.8900 | |
| 172.37 | 0.5446 | 0.8660 | |
| 189.61 | 0.6150 | 0.8280 | |
| 201.81 | 0.7320 | 0.7320 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane- n-Heptane System, Industrial & Engineering Chemistry Chemical & Engineering Data Series 1 (1956) 29-42. doi:10.1021/i460001a007

**T / K = 444.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 13.79 | 0.0305 | 0.5100 | |
| 27.58 | 0.0840 | 0.7220 | |
| 41.37 | 0.1317 | 0.7750 | |
| 55.16 | 0.1786 | 0.8060 | |
| 68.95 | 0.2240 | 0.8260 | |
| 86.19 | 0.2780 | 0.8369 | |
| 103.42 | 0.3316 | 0.8360 | |
| 120.66 | 0.3850 | 0.8250 | |
| 137.90 | 0.4431 | 0.8040 | |
| 155.13 | 0.5165 | 0.7730 | |
| 170.23 | 0.6720 | 0.6720 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane- n-Heptane System, Industrial & Engineering Chemistry Chemical & Engineering Data Series 1 (1956) 29-42. doi:10.1021/i460001a007

**T / K = 477.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 13.79 | 0.0132 | 0.2060 | |
| 27.58 | 0.0670 | 0.5223 | |
| 41.37 | 0.1200 | 0.6210 | |
| 55.16 | 0.1740 | 0.6700 | |
| 68.95 | 0.2290 | 0.6930 | |
| 86.19 | 0.2980 | 0.6990 | |
| 103.42 | 0.3725 | 0.6940 | |
| 120.66 | 0.4620 | 0.6690 | |
| 131.41 | 0.5850 | 0.5850 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane- n-Heptane System, Industrial & Engineering Chemistry Chemical & Engineering Data Series 1 (1956) 29-42. doi:10.1021/i460001a007

**T / K = 510.93**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 27.58 | 0.0485 | 0.2640 | |
| 41.37 | 0.1205 | 0.4199 | |
| 55.16 | 0.1918 | 0.4670 | |
| 68.95 | 0.2730 | 0.4750 | |
| 83.15 | 0.4410 | 0.4410 | CRIT |

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**Enthalpy of mixing**

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Oscarson, J.L. - Coxam, J.Y. - Gillespie, S.E. - Izatt, R.M., Excess enthalpies of mixing methane with methanol, n-heptane, toluene and methylcyclohexane at 255.4 and 310.9 K and 13.8 MPa, Fluid Phase Equilibria 1-2 (1996) 161-174. doi:10.1016/0378-3812(95)02813-7

**T / K = 255.40**

**P / bar = 138.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -2.000 | 0.0226 |
| -44.00 | 0.0545 |
| -101.00 | 0.1014 |
| -147.00 | 0.1475 |
| -236.00 | 0.2051 |
| -295.00 | 0.2507 |
| -307.00 | 0.2530 |
| -369.00 | 0.3073 |
| -352.00 | 0.3076 |
| -454.00 | 0.3542 |
| -483.00 | 0.4070 |
| -559.00 | 0.4464 |
| -637.00 | 0.5020 |
| -691.00 | 0.5478 |
| -729.00 | 0.6019 |

Oscarson, J.L. - Coxam, J.Y. - Gillespie, S.E. - Izatt, R.M., Excess enthalpies of mixing methane with methanol, n-heptane, toluene and methylcyclohexane at 255.4 and 310.9 K and 13.8 MPa, Fluid Phase Equilibria 1-2 (1996) 161-174. doi:10.1016/0378-3812(95)02813-7

**T / K = 310.90**

**P / bar = 138.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -25.00 | 0.0196 |
| -53.00 | 0.0384 |

| | |
|---|---|
| -109.00 | 0.0736 |
| -112.00 | 0.0739 |
| -162.00 | 0.1065 |
| -198.00 | 0.1226 |
| -216.00 | 0.1372 |
| -257.00 | 0.1664 |
| -309.00 | 0.1926 |
| -354.00 | 0.2184 |
| -396.00 | 0.2421 |
| -430.00 | 0.2643 |
| -451.00 | 0.2844 |
| -499.00 | 0.3229 |
| -557.00 | 0.3585 |
| -577.00 | 0.3887 |
| -618.00 | 0.4181 |
| -656.00 | 0.4429 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

| | |
|---|---|
| **T / K =** | **389.20** |
| **P / bar =** | **1.013** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 98.70 | 0.3690 |
| 105.10 | 0.5240 |
| 101.90 | 0.5870 |
| 92.40 | 0.6610 |
| 68.90 | 0.7920 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

| | |
|---|---|
| **T / K =** | **405.70** |
| **P / bar =** | **1.013** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 94.60 | 0.5240 |
| 93.60 | 0.5580 |
| 88.40 | 0.6050 |
| 81.40 | 0.6640 |
| 69.50 | 0.7530 |

---

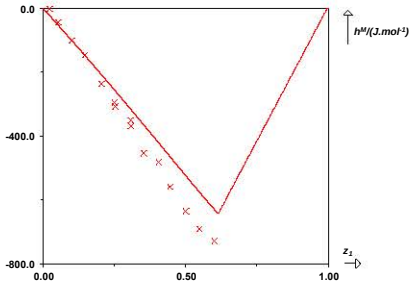
**Critical point**

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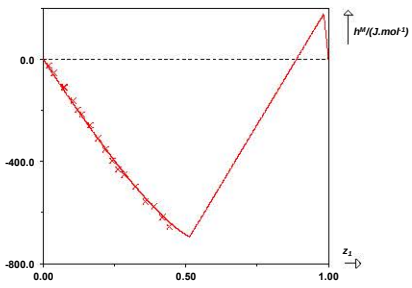
Chen, R.J.J. - Chappelear, P.S. - Kobayashi, R., Vapor Phase Data for the Binary Systems of Methane with n-Butane, n-Pentane, n-Hexane, and n-Heptane, GPA Research Report (1976) 1-14.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 233.15 | 184.43 | 0.9690 |

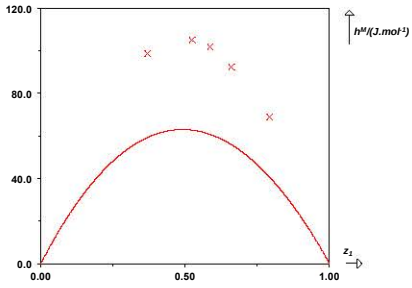
T/K = 255.40 - P/bar = 138.00



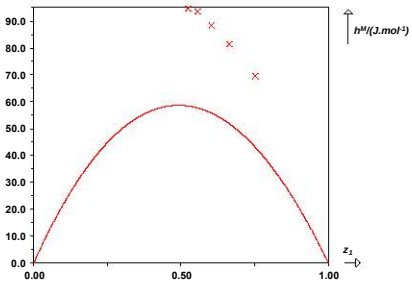

T/K = 310.90 - P/bar = 138.00



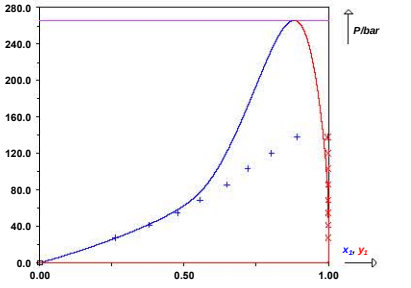

T/K = 389.20 - P/bar = 1.0132



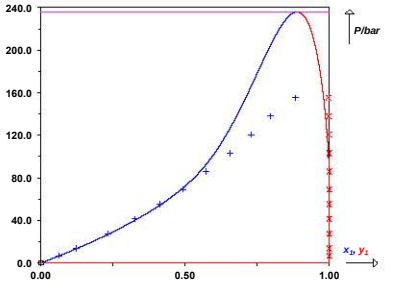

T/K = 405.70 - P/bar = 1.0132



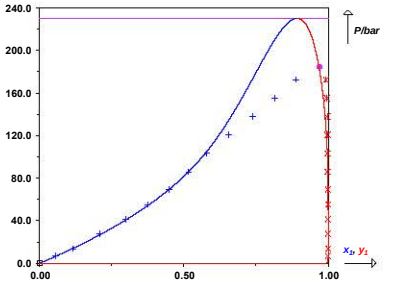

T/K = 210.93



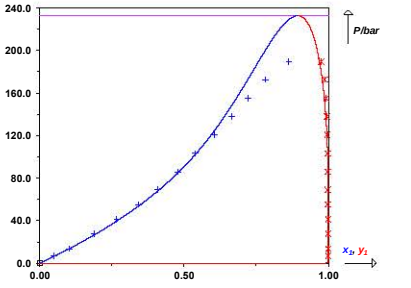

T/K = 222.04



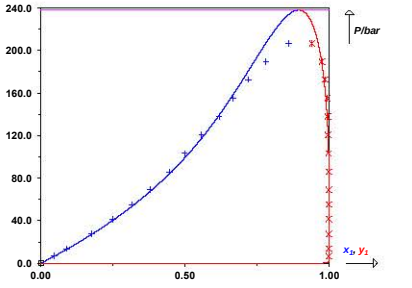

T/K = 233.15



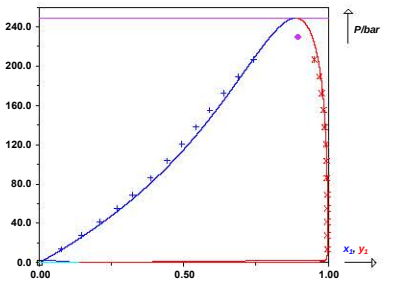

T/K = 244.26



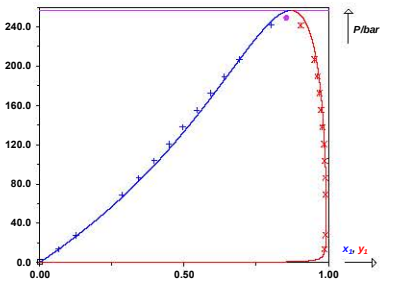

T/K = 255.37



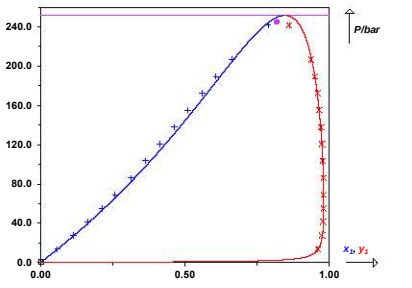

T/K = 277.59

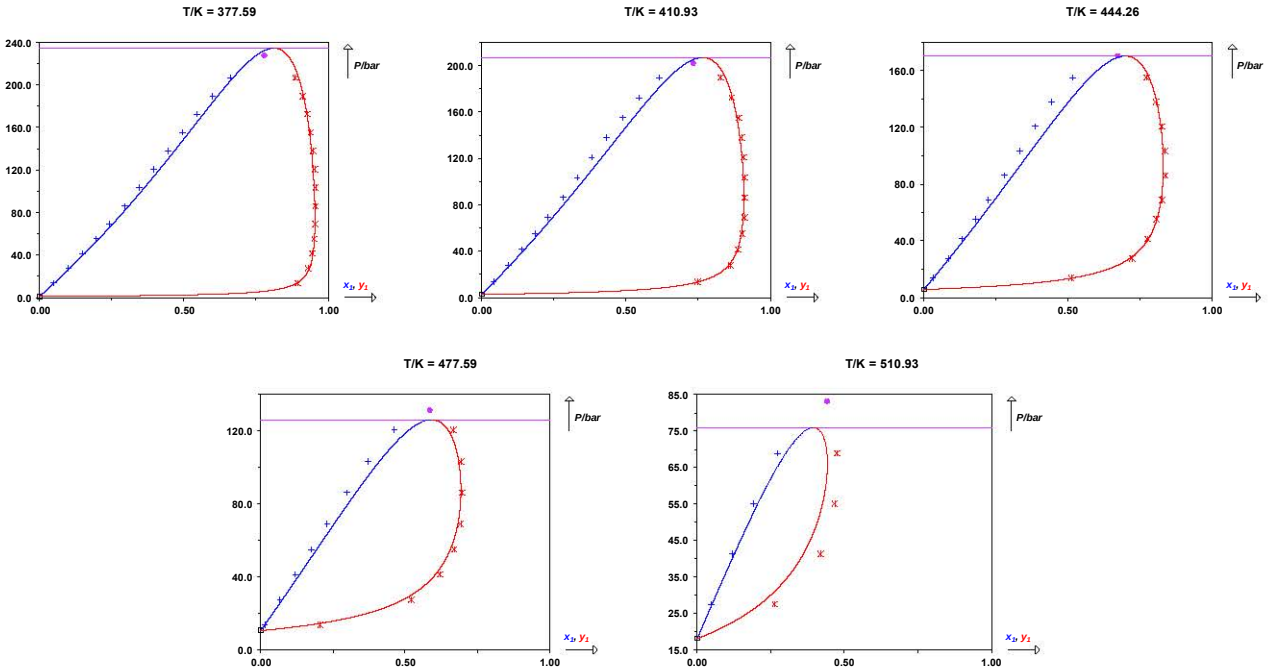



T/K = 310.93




T/K = 344.26




T/K = 377.59
P/bar
x1, y1
T/K = 410.93
P/bar
x1, y1
T/K = 444.26
P/bar
x1, y1
T/K = 477.59
P/bar
x1, y1
T/K = 510.93
P/bar
x1, y1

## NITROGEN (1) + ETHANE (2)

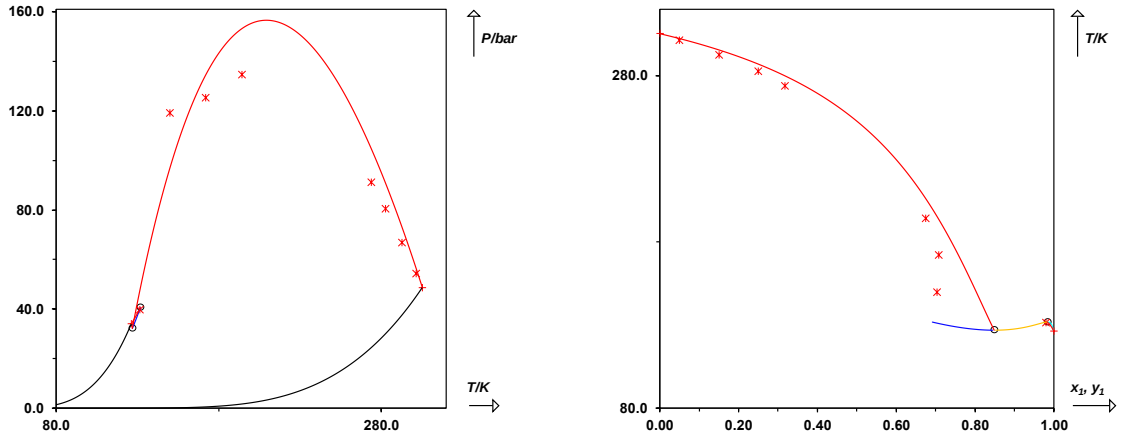
| | | |
|---|---|---|
| **CAS** | 7727-37-9 | 74-84-0 |
| **InChiKey** | MDFFNEOEWAXZRQ-UHFFFAOYSA-N | OTMSDBZUPAUEDD-UHFFFAOYSA-N |
| **$T_c$ / K** | 126.20 | 305.32 |
| **$P_c$ / bar** | 34.00 | 48.72 |
| **ω** | 0.038 | 0.099 |

Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 261
B/MPa = -62.7

*Deviations*
MAPE on x = 82 %
MAPE on y = 6.1 %
MAPE on $x_c$ = 58 %
MAPE on $P_c$ = 13 %
MAPE on $h^M$ = 180 %



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**Isothermal phase equilibrium data**

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Stryjek, Roman - Chappelear, Patsy S. - Kobayashi, Riki, Low-temperature vapor-liquid equilibriums of nitrogen-ethane system, Journal of Chemical & Engineering Data 4 (1974) 340-343. doi:10.1021/je60063a024

**T / K = 138.71**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.530 | 0.0188 | 0.9865 |
| 6.895 | 0.0387 | 0.9916 |
| 10.34 | 0.0579 | 0.9934 |
| 13.79 | 0.0776 | 0.9941 |
| 20.69 | 0.1192 | 0.9944 |
| 27.58 | 0.1637 | 0.9942 |
| 34.48 | 0.2120 | 0.9931 |
| 68.95 | 0.3897 | 0.9552 |
| 69.09 | 0.3740 | 0.9622 |

Stryjek, Roman - Chappelear, Patsy S. - Kobayashi, Riki, Low-temperature vapor-liquid equilibriums of nitrogen-ethane system, Journal of Chemical & Engineering Data 4 (1974) 340-343. doi:10.1021/je60063a024

**T / K = 149.82**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.447 | 0.0156 | 0.9604 | |
| 6.929 | 0.0318 | 0.9787 | |
| 10.34 | 0.0480 | 0.9841 | |
| 13.81 | 0.0640 | 0.9875 | |
| 20.69 | 0.0970 | 0.9894 | |
| 27.58 | 0.1343 | 0.9899 | |
| 34.48 | 0.1685 | 0.9883 | |
| 41.44 | 0.2058 | 0.9866 | |
| 55.50 | 0.2839 | 0.9810 | |
| 69.09 | 0.3531 | 0.9592 | |
| 119.14 | 0.7038 | 0.7038 | CRIT |

Stryjek, Roman - Chappelear, Patsy S. - Kobayashi, Riki, Low-temperature vapor-liquid equilibriums of nitrogen-ethane system, Journal of Chemical & Engineering Data 4 (1974) 340-343. doi:10.1021/je60063a024

**T / K = 172.04**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.620 | 0.0123 | 0.8449 | |
| 6.936 | 0.0232 | 0.9132 | |
| 13.72 | 0.0486 | 0.9475 | |
| 13.79 | 0.0485 | 0.9478 | |
| 27.58 | 0.0990 | 0.9637 | |
| 41.78 | 0.1552 | 0.9664 | |
| 55.30 | 0.2090 | 0.9621 | |
| 68.81 | 0.2689 | 0.9560 | |
| 90.39 | 0.3755 | 0.9277 | |
| 103.42 | 0.4327 | 0.9012 | |
| 120.66 | 0.5626 | 0.8138 | |
| 124.93 | 0.6341 | 0.7704 | |
| 125.35 | 0.7080 | 0.7080 | CRIT |

Stryjek, Roman - Chappelear, Patsy S. - Kobayashi, Riki, Low-temperature vapor-liquid equilibriums of nitrogen-ethane system, Journal of Chemical & Engineering Data 4 (1974) 340-343. doi:10.1021/je60063a024

**T / K = 194.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.516 | 0.0057 | 0.4862 | |
| 6.915 | 0.0161 | 0.7146 | |
| 13.79 | 0.0372 | 0.8360 | |
| 27.58 | 0.0808 | 0.8966 | |
| 41.51 | 0.1273 | 0.9126 | |
| 55.71 | 0.1756 | 0.9154 | |
| 69.09 | 0.2225 | 0.9126 | |
| 89.77 | 0.3024 | 0.8977 | |
| 97.56 | 0.3338 | 0.8885 | |
| 120.24 | 0.4534 | 0.8355 | |
| 121.35 | 0.4577 | 0.8304 | |
| 130.86 | 0.5510 | 0.7714 | |
| 134.18 | 0.6472 | 0.7144 | |
| 134.65 | 0.6746 | 0.6746 | CRIT |

Grausø, Louis - Fredenslund, Aage - Mollerup, Jørgen, Vapour-liquid equilibrium data for the systems C2H6 + N2, C2H4 + N2, C3H8 + N2, and C3H6 + N2, Fluid Phase Equilibria 1 (1977) 13-26. doi:10.1016/0378-3812(77)80022-8

**T / K = 200.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.657 | 0.0137 | 0.6389 |
| 10.43 | 0.0264 | 0.7533 |
| 21.17 | 0.0647 | 0.8568 |
| 41.54 | 0.1360 | 0.9029 |
| 60.99 | 0.2063 | 0.9064 |
| 80.48 | 0.2764 | 0.8981 |
| 102.42 | 0.3751 | 0.8716 |
| 124.79 | 0.5112 | 0.8116 |
| 131.95 | 0.5728 | 0.7620 |

Brown, T.S. - Sloan, E.D. - Kidnay, A.J., Vapor-liquid equilibria in the nitrogen + carbon dioxide + ethane

system, Fluid Phase Equilibria (1989) 299-313. doi:10.1016/0378-3812(89)80372-3

**T / K = 220.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.07 | 0.0160 | 0.4638 |
| 17.45 | 0.0356 | 0.6584 |
| 24.16 | 0.0552 | 0.7332 |
| 37.62 | 0.0952 | 0.7961 |
| 44.87 | 0.1168 | 0.8116 |
| 51.79 | 0.1394 | 0.8221 |
| 58.29 | 0.1582 | 0.8264 |
| 65.62 | 0.1838 | 0.8298 |
| 72.96 | 0.2077 | 0.8286 |
| 79.45 | 0.2326 | 0.8276 |
| 86.64 | 0.2572 | 0.8225 |
| 92.61 | 0.2810 | 0.8173 |
| 105.10 | 0.3310 | 0.7982 |
| 119.80 | 0.4080 | 0.7592 |

Grausø, Louis - Fredenslund, Aage - Mollerup, Jørgen, Vapour-liquid equilibrium data for the systems C2H6 + N2, C2H4 + N2, C3H8 + N2, and C3H6 + N2, Fluid Phase Equilibria 1 (1977) 13-26. doi:10.1016/0378-3812(77)80022-8

**T / K = 230.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.54 | 0.0094 | 0.2927 |
| 15.70 | 0.0240 | 0.4889 |
| 21.56 | 0.0399 | 0.6029 |
| 34.52 | 0.0776 | 0.7129 |
| 54.05 | 0.1372 | 0.7660 |
| 80.72 | 0.2265 | 0.7796 |
| 101.77 | 0.3120 | 0.7566 |
| 119.58 | 0.4110 | 0.7047 |
| 124.76 | 0.4543 | 0.6650 |

Zeck, S. - Knapp, H., Vapor—liquid and vapor—liquid—liquid phase equilibria for binary and ternary systems for nitrogen, ethane and methanol: Experiment and data reduction, Fluid Phase Equilibria 3 (1986) 303-322. doi:10.1016/0378-3812(86)80006-1

**T / K = 240.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 18.69 | 0.0252 | 0.4103 |
| 25.00 | 0.0433 | 0.5262 |
| 34.12 | 0.0698 | 0.6145 |
| 43.10 | 0.0968 | 0.6627 |
| 50.00 | 0.1187 | 0.6854 |
| 58.20 | 0.1442 | 0.7033 |
| 67.00 | 0.1731 | 0.7129 |
| 75.00 | 0.2006 | 0.7167 |

Zeck, S. - Knapp, H., Vapor—liquid and vapor—liquid—liquid phase equilibria for binary and ternary systems for nitrogen, ethane and methanol: Experiment and data reduction, Fluid Phase Equilibria 3 (1986) 303-322. doi:10.1016/0378-3812(86)80006-1

**T / K = 260.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 25.00 | 0.0221 | 0.2404 |
| 33.54 | 0.0468 | 0.3761 |
| 40.97 | 0.0692 | 0.4481 |
| 50.00 | 0.0971 | 0.5017 |
| 57.00 | 0.1202 | 0.5291 |
| 66.00 | 0.1504 | 0.5507 |
| 75.00 | 0.1830 | 0.5608 |

Grausø, Louis - Fredenslund, Aage - Mollerup, Jørgen, Vapour-liquid equilibrium data for the systems C2H6 + N2, C2H4 + N2, C3H8 + N2, and C3H6 + N2, Fluid Phase Equilibria 1 (1977) 13-26. doi:10.1016/0378-3812(77)80022-8

**T / K = 260.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 25.72 | 0.0235 | 0.2562 |
| 31.15 | 0.0393 | 0.3478 |
| 44.83 | 0.0796 | 0.4753 |
| 56.46 | 0.1160 | 0.5287 |
| 71.06 | 0.1647 | 0.5576 |
| 88.49 | 0.2373 | 0.5558 |
| 100.55 | 0.3077 | 0.5209 |

Gupta, Mukesh K. - Gardner, Glenn C. - Hegarty, Michael J. - Kidnay, Arthur J., Liquid-vapor equilibriums for the N2 + CH4 + C2H6 system from 260 to 280 K, Journal of Chemical & Engineering Data 4 (1980) 313-318. doi:10.1021/je60087a016

**T / K = 260.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 18.34 | 0.0036 | 0.0523 |
| 20.86 | 0.0106 | 0.1375 |
| 35.83 | 0.0541 | 0.4065 |
| 45.48 | 0.0828 | 0.4823 |
| 65.91 | 0.1494 | 0.5541 |
| 76.20 | 0.1873 | 0.5653 |
| 85.39 | 0.2258 | 0.5632 |
| 95.04 | 0.2714 | 0.5473 |

Brown, T.S. - Sloan, E.D. - Kidnay, A.J., Vapor-liquid equilibria in the nitrogen + carbon dioxide + ethane system, Fluid Phase Equilibria (1989) 299-313. doi:10.1016/0378-3812(89)80372-3

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 32.22 | 0.0282 | 0.2216 |
| 40.80 | 0.0508 | 0.3184 |
| 54.47 | 0.0985 | 0.4159 |
| 86.40 | 0.2282 | 0.4499 |
| 89.94 | 0.2510 | 0.4378 |
| 93.04 | 0.2758 | 0.4186 |
| 94.15 | 0.2900 | 0.4044 |
| 94.65 | 0.2944 | 0.3939 |
| 94.90 | 0.2995 | 0.3902 |

Gupta, Mukesh K. - Gardner, Glenn C. - Hegarty, Michael J. - Kidnay, Arthur J., Liquid-vapor equilibriums for the N2 + CH4 + C2H6 system from 260 to 280 K, Journal of Chemical & Engineering Data 4 (1980) 313-318. doi:10.1021/je60087a016

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 23.81 | 0.0051 | 0.0521 |
| 24.67 | 0.0077 | 0.0770 |
| 25.46 | 0.0098 | 0.0942 |
| 28.02 | 0.0157 | 0.1489 |
| 29.01 | 0.0193 | 0.1698 |
| 30.40 | 0.0233 | 0.1889 |
| 34.98 | 0.0359 | 0.2636 |
| 35.16 | 0.0382 | 0.2646 |
| 35.73 | 0.0390 | 0.2668 |
| 37.80 | 0.0435 | 0.2938 |
| 40.93 | 0.0543 | 0.3216 |
| 41.74 | 0.0554 | 0.3339 |
| 41.07 | 0.0563 | 0.3321 |
| 48.05 | 0.0687 | 0.3811 |
| 46.10 | 0.0696 | 0.3618 |
| 50.98 | 0.0848 | 0.3921 |
| 54.18 | 0.0951 | 0.4156 |
| 55.93 | 0.0989 | 0.4127 |
| 58.47 | 0.1076 | 0.4290 |
| 60.98 | 0.1165 | 0.4291 |
| 71.36 | 0.1555 | 0.4545 |
| 81.57 | 0.2030 | 0.4631 |
| 82.50 | 0.2079 | 0.4611 |
| 91.00 | 0.2572 | 0.4652 |

Gupta, Mukesh K. - Gardner, Glenn C. - Hegarty, Michael J. - Kidnay, Arthur J., Liquid-vapor equilibriums for the N2 + CH4 + C2H6 system from 260 to 280 K, Journal of Chemical & Engineering Data 4 (1980) 313-318. doi:10.1021/je60087a016

**T / K = 280.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 29.89 | 0.0061 | 0.0437 |
| 31.13 | 0.0097 | 0.0684 |
| 32.22 | 0.0128 | 0.0866 |
| 36.71 | 0.0265 | 0.1558 |
| 40.85 | 0.0394 | 0.2047 |
| 45.95 | 0.0556 | 0.2511 |
| 50.66 | 0.0709 | 0.2835 |
| 52.38 | 0.0767 | 0.2943 |
| 56.63 | 0.0921 | 0.3167 |
| 61.00 | 0.1078 | 0.3331 |
| 65.86 | 0.1277 | 0.3463 |
| 66.17 | 0.1284 | 0.3471 |
| 72.63 | 0.1570 | 0.3542 |
| 75.99 | 0.1743 | 0.3521 |
| 77.92 | 0.1852 | 0.3484 |
| 81.31 | 0.2088 | 0.3360 |
| 81.97 | 0.2162 | 0.3339 |
| 83.34 | 0.2311 | 0.3177 |

Grausø, Louis - Fredenslund, Aage - Mollerup, Jørgen, Vapour-liquid equilibrium data for the systems C2H6 + N2, C2H4 + N2, C3H8 + N2, and C3H6 + N2, Fluid Phase Equilibria 1 (1977) 13-26. doi:10.1016/0378-3812(77)80022-8

**T / K = 290.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 42.68 | 0.0242 | 0.0970 |
| 49.54 | 0.0464 | 0.1586 |
| 55.49 | 0.0709 | 0.1940 |
| 61.30 | 0.0936 | 0.2163 |
| 68.32 | 0.1322 | 0.2196 |
| 70.18 | 0.1594 | 0.2115 |

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**Isobaric phase equilibrium data**

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Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 13.79**

| T / K | $y_1$ |
|---|---|
| 249.93 | 0.0498 |
| 244.93 | 0.1501 |
| 236.87 | 0.3169 |
| 224.21 | 0.5018 |
| 211.54 | 0.7000 |

| | |
|---|---|
| 194.48 | 0.8506 |
| 172.71 | 0.9505 |
| 153.21 | 0.9802 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 13.79**

| T / K | $x_1$ |
|---|---|
| 116.54 | 0.1501 |
| 112.37 | 0.2002 |
| 109.09 | 0.9802 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 24.13**

| T / K | $y_1$ |
|---|---|
| 270.59 | 0.0498 |
| 264.37 | 0.1501 |
| 254.26 | 0.3169 |
| 239.48 | 0.5018 |
| 223.87 | 0.7000 |
| 204.04 | 0.8506 |
| 178.98 | 0.9505 |
| 159.15 | 0.9802 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 24.13**

| T / K | $x_1$ |
|---|---|
| 228.71 | 0.0498 |
| 136.98 | 0.1501 |
| 127.71 | 0.2002 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 24.13**

| T / K | $x_1$ |
|---|---|
| 122.37 | 0.2493 |
| 119.71 | 0.9802 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 27.58**

| T / K | $y_1$ |
|---|---|
| 275.82 | 0.0498 |
| 269.32 | 0.1501 |
| 258.43 | 0.3169 |
| 243.87 | 0.5018 |
| 226.76 | 0.7000 |
| 206.21 | 0.8506 |
| 181.09 | 0.9490 |
| 180.32 | 0.9505 |
| 160.26 | 0.9802 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 27.58**

| T / K | $x_1$ |
|---|---|
| 240.65 | 0.0498 |
| 143.82 | 0.1501 |
| 132.32 | 0.2002 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 27.58**

| T / K | $x_1$ |
|---|---|
| 126.15 | 0.2493 |
| 122.43 | 0.9802 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 31.03**

| T / K | $y_1$ |
|---|---|
| 280.71 | 0.0498 |

| | |
|---|---|
| 273.71 | 0.1501 |
| 262.09 | 0.3169 |
| 247.21 | 0.5018 |
| 229.26 | 0.7000 |
| 208.09 | 0.8506 |
| 182.65 | 0.9490 |
| 181.32 | 0.9505 |
| 160.93 | 0.9802 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 31.03**

| T / K | $x_1$ |
|---|---|
| 251.04 | 0.0498 |
| 151.15 | 0.1501 |
| 137.04 | 0.2002 |
| 129.87 | 0.2493 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 34.47**

| T / K | $x_1$ |
|---|---|
| 285.15 | 0.0498 |
| 277.59 | 0.1501 |
| 265.43 | 0.3169 |
| 250.26 | 0.5018 |
| 231.48 | 0.7000 |
| 209.65 | 0.8506 |
| 183.71 | 0.9490 |
| 182.04 | 0.9505 |
| 161.37 | 0.9802 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 34.47**

| T / K | $x_1$ |
|---|---|
| 260.04 | 0.0498 |
| 158.76 | 0.1501 |
| 141.93 | 0.2002 |
| 133.43 | 0.2493 |
| 127.54 | 0.9802 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 37.92**

| T / K | $x_1$ |
|---|---|
| 289.15 | 0.0498 |
| 281.09 | 0.1501 |
| 268.54 | 0.3169 |
| 253.21 | 0.5018 |
| 233.37 | 0.7000 |
| 210.98 | 0.8506 |
| 184.43 | 0.9490 |
| 182.54 | 0.9505 |
| 161.59 | 0.9802 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 37.92**

| T / K | $x_1$ |
|---|---|
| 267.71 | 0.0498 |
| 166.82 | 0.1501 |
| 147.15 | 0.2002 |
| 137.09 | 0.2493 |
| 130.09 | 0.9802 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 41.37**

| T / K | $x_1$ |
|---|---|
| 292.76 | 0.0498 |
| 284.21 | 0.1501 |
| 271.26 | 0.3169 |
| 255.32 | 0.5018 |
| 235.09 | 0.7000 |
| 212.15 | 0.8506 |
| 184.54 | 0.9490 |
| 182.82 | 0.9505 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 41.37**

| T / K | $x_1$ |
|---|---|
| 274.54 | 0.0498 |
| 175.71 | 0.1501 |
| 152.59 | 0.2002 |
| 141.37 | 0.2493 |
| 133.21 | 0.3169 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 44.82**

| T / K | $x_1$ |
|---|---|
| 295.93 | 0.0498 |
| 286.98 | 0.1501 |
| 273.65 | 0.3169 |
| 257.26 | 0.5018 |
| 236.54 | 0.7000 |
| 213.09 | 0.8506 |
| 184.71 | 0.9490 |
| 182.98 | 0.9505 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 44.82**

| T / K | $x_1$ |
|---|---|
| 280.82 | 0.0498 |
| 186.32 | 0.1501 |
| 158.76 | 0.2002 |
| 145.54 | 0.2493 |
| 136.32 | 0.3169 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 48.26**

| T / K | $x_1$ |
|---|---|
| 298.82 | 0.0498 |
| 289.48 | 0.1501 |
| 275.76 | 0.3169 |
| 259.04 | 0.5018 |
| 237.82 | 0.7000 |
| 213.93 | 0.8506 |
| 184.76 | 0.9490 |
| 182.98 | 0.9505 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 48.26**

| T / K | $x_1$ |
|---|---|
| 286.87 | 0.0498 |
| 198.26 | 0.1501 |
| 165.76 | 0.2002 |
| 149.59 | 0.2493 |
| 139.37 | 0.3169 |

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**Enthalpy of mixing**

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Guedes, Henrique J.R - Zollweg, John A - Filipe, Eduardo J.M - Martins, Luís F.G - Calado, Jorge C.G, Thermodynamics of liquid (nitrogen + ethane), The Journal of Chemical Thermodynamics 5 (2002) 669-678. doi:10.1006/jcht.2001.0936

**T / K = 92.10**

**P / bar = 7.900**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 79.50 | 0.0500 |
| 86.60 | 0.0550 |
| 108.60 | 0.0760 |
| 118.50 | 0.0840 |
| 145.70 | 0.0850 |
| 174.40 | 0.1120 |
| 178.00 | 0.1300 |
| 171.90 | 0.1920 |
| 168.30 | 0.2500 |
| 167.60 | 0.3010 |
| 148.30 | 0.3980 |
| 132.70 | 0.4780 |
| 129.50 | 0.4990 |
| 132.50 | 0.5120 |
| 122.50 | 0.5730 |
| 126.70 | 0.5830 |

| | |
|---|---|
| 111.70 | 0.6100 |
| 109.30 | 0.6860 |
| 99.40 | 0.7350 |
| 93.50 | 0.8010 |
| 82.00 | 0.8370 |
| 76.30 | 0.9080 |
| 65.50 | 0.9500 |
| 66.20 | 0.9600 |
| 52.70 | 0.9700 |
| 45.00 | 0.9760 |
| 38.70 | 0.9860 |
| 22.60 | 0.9980 |

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**Critical point**

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Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 301.46 | 54.36 | 0.0498 |
| 292.59 | 66.88 | 0.1501 |
| 282.65 | 80.43 | 0.2493 |
| 273.97 | 91.07 | 0.3169 |
| 131.48 | 39.65 | 0.9802 |

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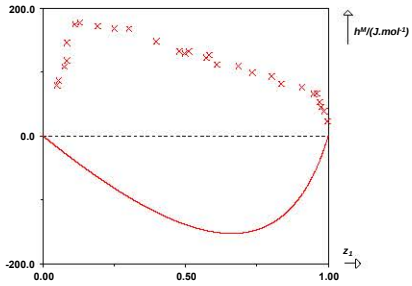
**Three-phase line**

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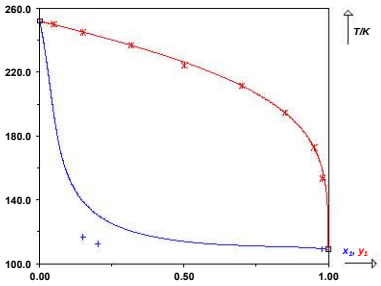
P. Yu, I.M. - Elshayal, B.C.-Y. - Lu, Liquid-liquid-vapor equilibria in the nitrogen-methane-ethane system, The Canadian Journal of Chemical Engineering. 47 (1969) 495–498. doi:10.1002/cjce.5450470516.

| T / K | P / bar | $x_{1a}$ | $x_{1b}$ | $y_1$ |
|---|---|---|---|---|
| 133.26 | 40.75 | 0.3018 | 0.9797 | 0.9873 |
| 132.54 | 40.54 | 0.2962 | 0.9565 | 0.9868 |
| 130.09 | 36.86 | 0.2963 | 0.9347 | 0.9935 |
| 129.81 | 37.41 | 0.2954 | 0.9353 | 0.9935 |
| 128.93 | 35.78 | 0.3261 | 0.9570 | 0.9942 |
| 128.43 | 34.33 | 0.2929 | 0.9430 | 0.9941 |
| 124.87 | 29.87 | 0.2925 | 0.9343 | 0.9931 |
| 122.04 | 26.03 | 0.2846 | 0.9374 | 0.9997 |
| 119.26 | 23.71 | 0.2695 | 0.9398 | 0.9921 |
| 116.48 | 20.99 | 0.2599 | 0.9219 | 0.9978 |
| 116.48 | 21.01 | 0.2608 | 0.9426 | 0.9972 |
| 115.31 | 18.67 | 0.2582 | 0.9431 | 0.9997 |
| 113.70 | 18.50 | 0.2548 | 0.9444 | 0.9999 |
| 113.70 | 17.96 | 0.2549 | 0.9429 | 0.9999 |

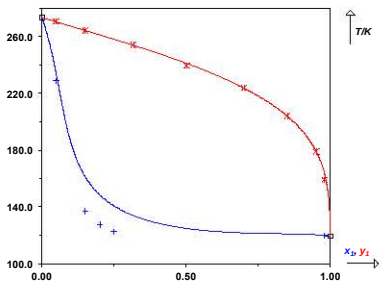
T/K = 92.10 - P/bar = 7.900



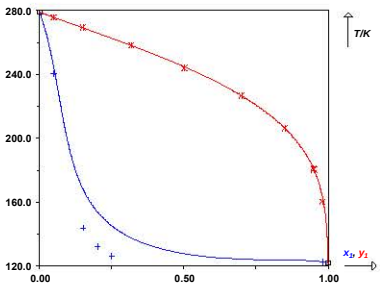

P/bar = 13.79000



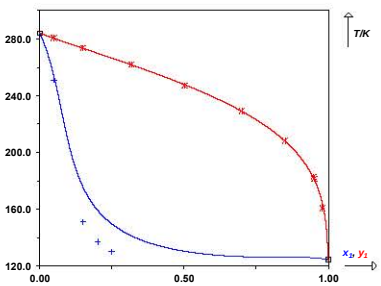

P/bar = 24.13200



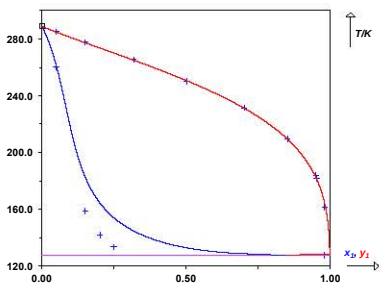

P/bar = 27.57900



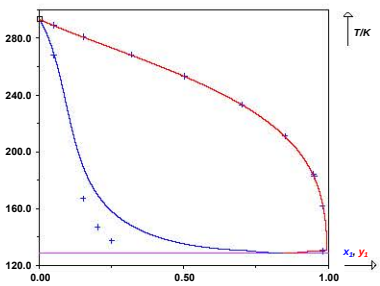

P/bar = 31.02600



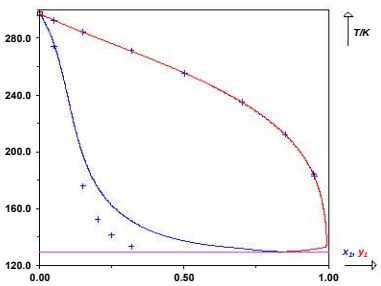

P/bar = 34.47400



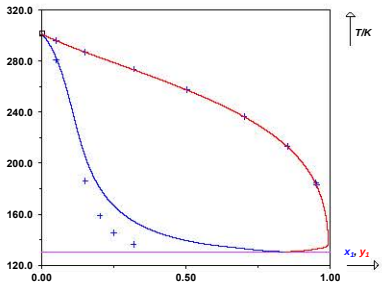

P/bar = 37.92100



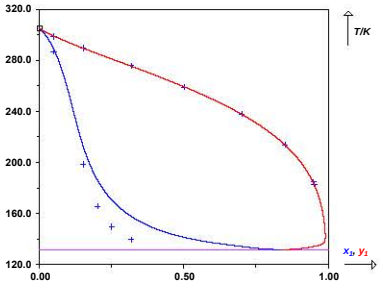

P/bar = 41.36800



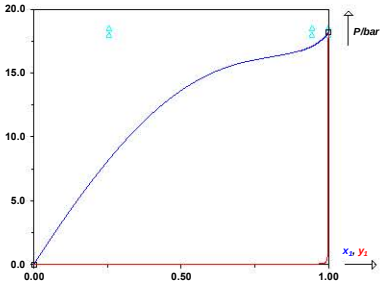

P/bar = 44.81600



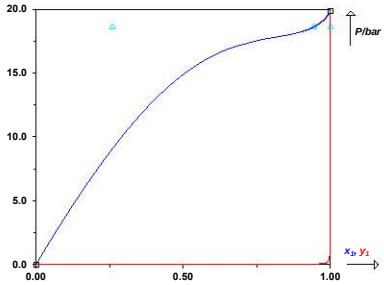

P/bar = 48.26300



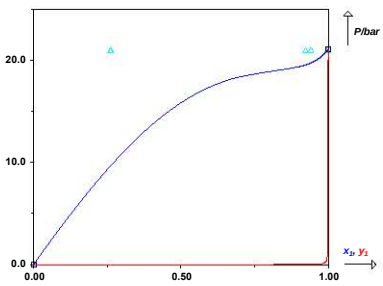

T/K = 113.70



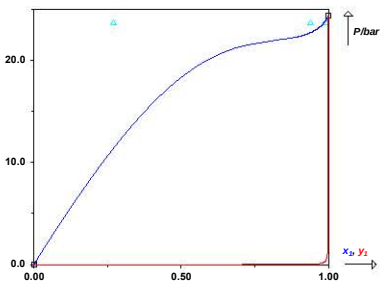

T/K = 115.31



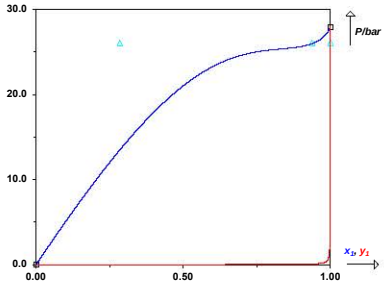

T/K = 116.48



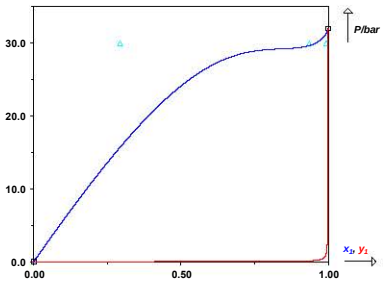

T/K = 119.26



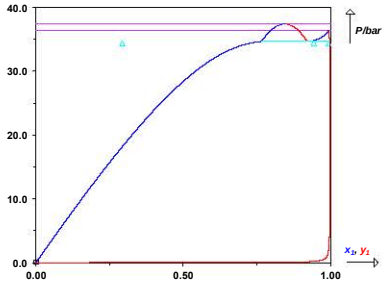

T/K = 122.04



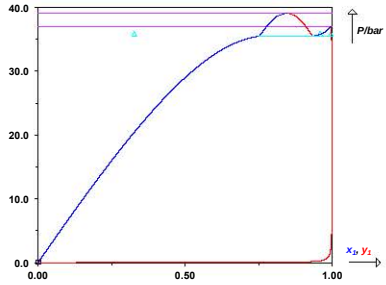
T/K = 124.87



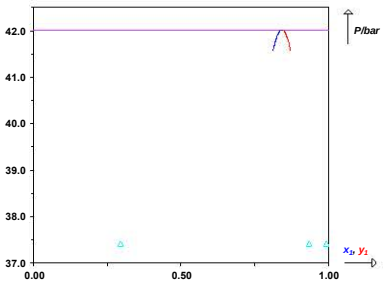

T/K = 128.43



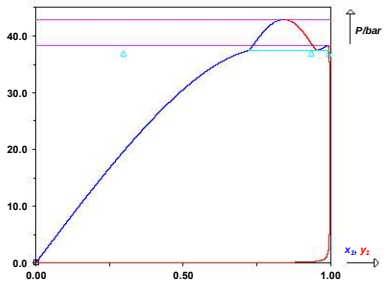

T/K = 128.93



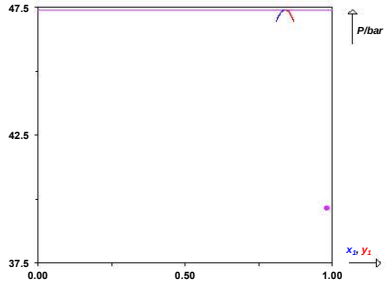

T/K = 129.81



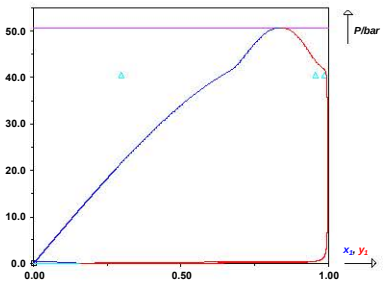

T/K = 130.09



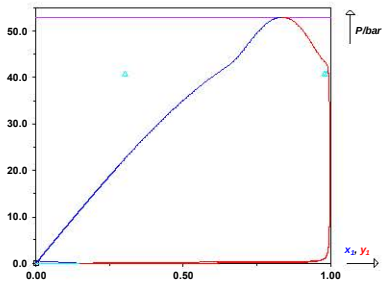

T/K = 131.48



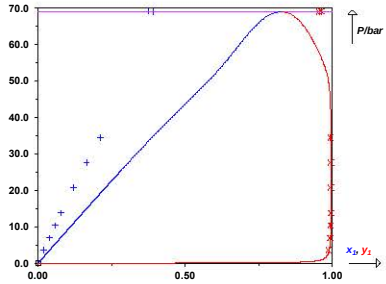

T/K = 132.54



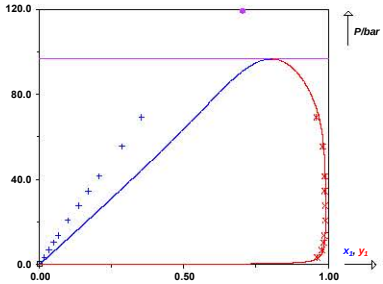

T/K = 133.26



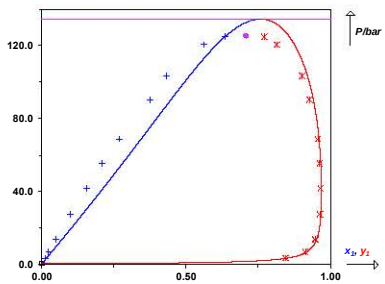

T/K = 138.71



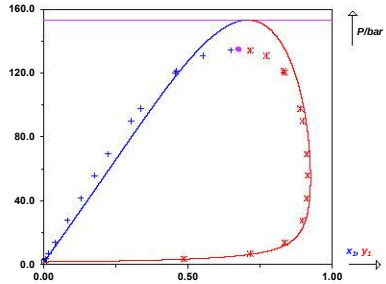

T/K = 149.82



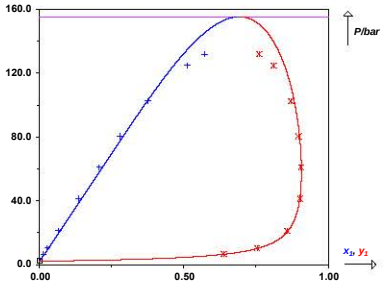

T/K = 172.04



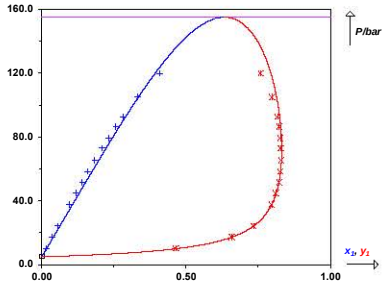

T/K = 194.26



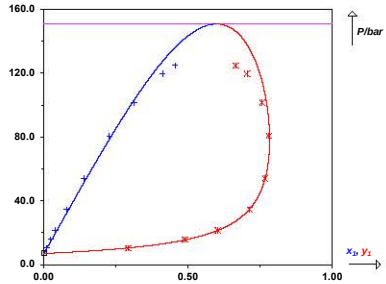

T/K = 200.00

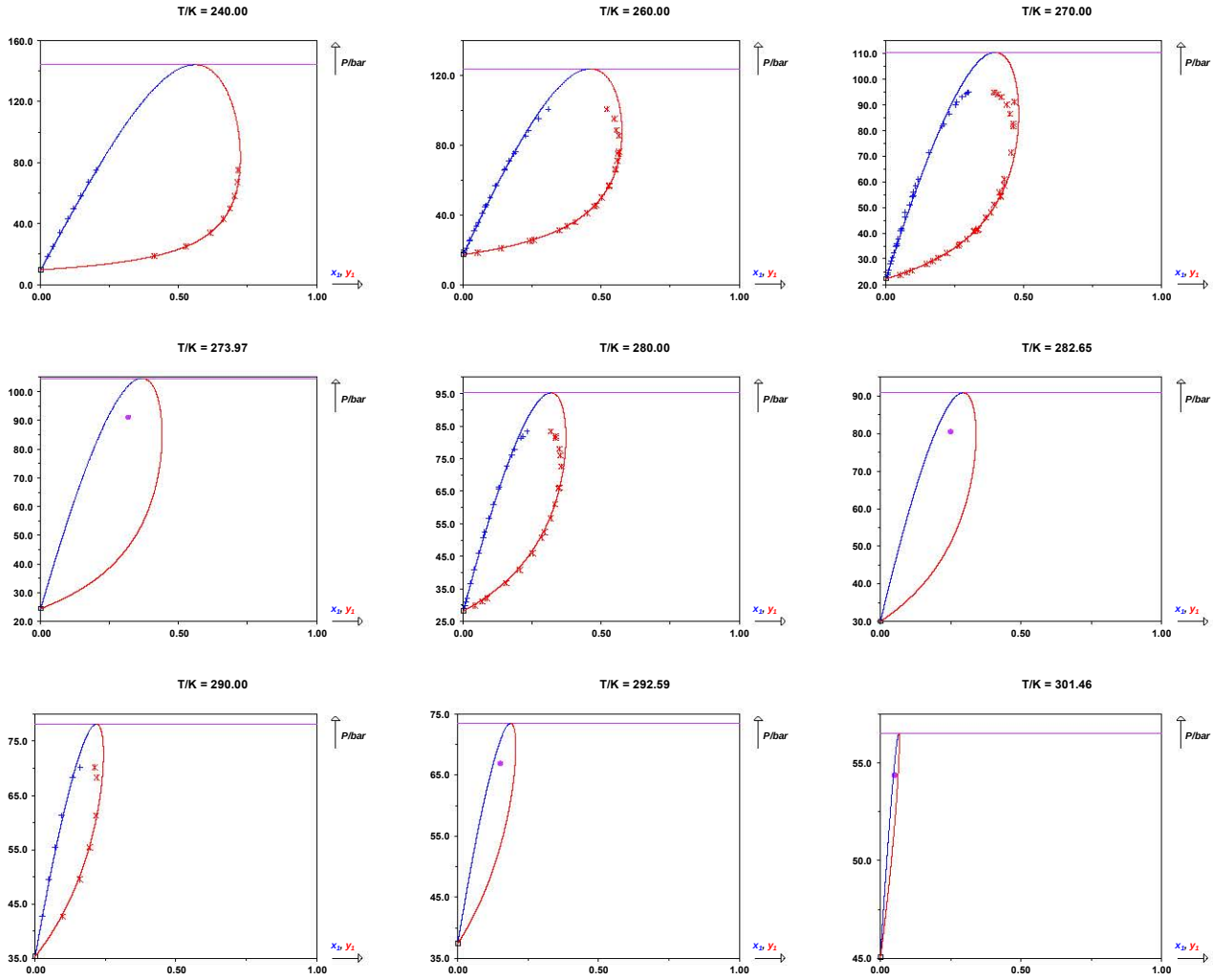



T/K = 220.00




T/K = 230.00




T/K = 240.00
T/K = 260.00
T/K = 270.00
T/K = 273.97
T/K = 280.00
T/K = 282.65
T/K = 290.00
T/K = 292.59
T/K = 301.46
P/bar
x₁, y₁

## METHANE (1) + n-DECANE (2)

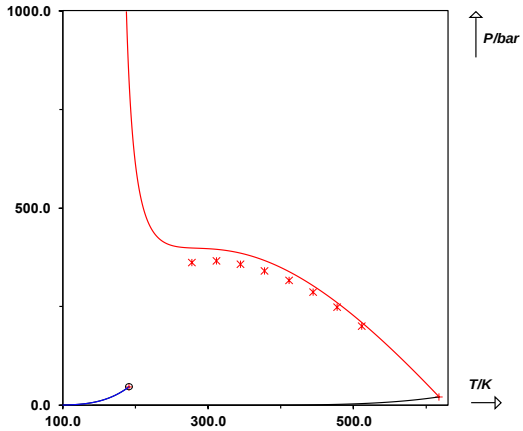
| | | |
|---|---|---|
| **CAS** | 74-82-8 | 124-18-5 |
| **InChiKey** | VNWKTOKETHGBQD-UHFFFAOYSA-N | DIOQZVSQGTUSAI-UHFFFAOYSA-N |
| **$T_c$ / K** | 190.56 | 617.70 |
| **$P_c$ / bar** | 45.99 | 21.10 |
| **ω** | 0.012 | 0.492 |

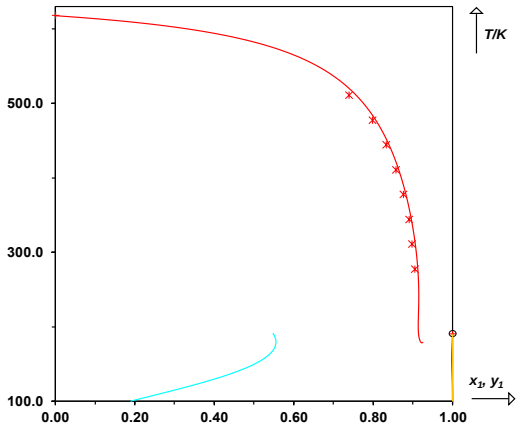
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 62.2
B/MPa = 140

*Deviations*
MAPE on x = 3.0 %
MAPE on y = 7.4 %
MAPE on $x_c$ = 3.4 %
MAPE on $P_c$ = 7.0 %



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**Isothermal phase equilibrium data**

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Koonce, K. T. - Kobayashi, Riki., A Method for Determining the Solubility of Gases in Relatively Nonvolatile Liquids: Solubility of Methane in n-Decane., Journal of Chemical & Engineering Data 4 (1964) 490-494. doi:10.1021/je60023a004

**T / K = 244.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 16.00 | 0.1103 | 0.9990 |
| 21.19 | 0.1453 | 0.9997 |
| 31.88 | 0.2061 | 0.9996 |

Koonce, K. T. - Kobayashi, Riki., A Method for Determining the Solubility of Gases in Relatively Nonvolatile Liquids: Solubility of Methane in n-Decane., Journal of Chemical & Engineering Data 4 (1964) 490-494. doi:10.1021/je60023a004

**T / K = 255.37**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.65 | 0.0982 | 0.9997 |
| 22.02 | 0.1356 | 0.9994 |
| 29.93 | 0.1783 | 0.9990 |
| 41.69 | 0.2402 | 0.9992 |
| 63.19 | 0.3248 | 0.9994 |

Koonce, K. T. - Kobayashi, Riki., A Method for Determining the Solubility of Gases in Relatively Nonvolatile Liquids: Solubility of Methane in n-Decane., Journal of Chemical & Engineering Data 4 (1964) 490-494. doi:10.1021/je60023a004

**T / K = 266.48**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 46.28 | 0.2433 | 1.0000 |
| 66.87 | 0.3185 | 0.9990 |

Koonce, K. T. - Kobayashi, Riki., A Method for Determining the Solubility of Gases in Relatively Nonvolatile Liquids: Solubility of Methane in n-Decane., Journal of Chemical & Engineering Data 4 (1964) 490-494. doi:10.1021/je60023a004

**T / K = 277.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 17.34 | 0.0947 | 0.9991 |
| 22.66 | 0.1243 | 0.9994 |
| 28.27 | 0.1498 | 0.9992 |
| 37.70 | 0.1923 | 1.0000 |
| 52.19 | 0.2525 | 0.9999 |
| 63.83 | 0.2901 | 0.9990 |

Lentz, H. - Nuennerich, P., Die Bestimmung der Zusammensetzung koexistierender Phasen binärer Mischungen aus Nodenlinien und Volumen, Chem. Ing. Tech. (2001) 1162-1164. doi:10.1002/1522-2640(200109)73:9<1162::AID-CITE1162>3.0.CO;2-4

**T / K = 300.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 150.00 | 0.4910 | 0.9984 |
| 200.00 | 0.5720 | 0.9957 |
| 250.00 | 0.6550 | 0.9914 |
| 300.00 | 0.7250 | 0.9790 |

Reamer, H. H. - Olds, R. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 12 (1942) 1526-1531. doi:10.1021/ie50396a025

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 1.379 | 0.0070 | 0.9961 | |
| 2.758 | 0.0141 | 0.9979 | |
| 4.137 | 0.0210 | 0.9985 | |
| 5.516 | 0.0278 | 0.9988 | |
| 6.895 | 0.0345 | 0.9990 | |
| 13.79 | 0.0666 | 0.9993 | |
| 27.58 | 0.1251 | 0.9994 | |
| 41.37 | 0.1773 | 0.9994 | |
| 55.16 | 0.2243 | 0.9994 | |
| 68.95 | 0.2679 | 0.9993 | |
| 86.19 | 0.3178 | 0.9991 | |
| 103.42 | 0.3637 | 0.9989 | |
| 120.66 | 0.4069 | 0.9986 | |
| 137.90 | 0.4469 | 0.9981 | |
| 155.13 | 0.4842 | 0.9974 | |
| 172.37 | 0.5183 | 0.9965 | |
| 189.61 | 0.5507 | 0.9955 | |
| 206.85 | 0.5827 | 0.9942 | |
| 224.07 | 0.6111 | 0.9926 | |
| 241.31 | 0.6370 | 0.9906 | |
| 258.55 | 0.6629 | 0.9877 | |
| 275.79 | 0.6870 | 0.9837 | |
| 293.03 | 0.7124 | 0.9788 | |
| 310.27 | 0.7378 | 0.9721 | |
| 327.51 | 0.7682 | 0.9636 | |
| 344.74 | 0.8064 | 0.9514 | |
| 361.98 | 0.8609 | 0.9276 | |
| 366.11 | 0.8979 | 0.8979 | CRIT |

Lavender, H.M. - Sage, B.H. - Lacey, W.N., Gas-liquid equilibrium constants, methane-decane system, Oil Gas J. (1940) 48-49.

| **T / K =** | **310.93** | |
|---|---|---|
| P / bar | $x_1$ | $y_1$ |
| 1.014 | 0.0052 | 0.9952 |
| 3.447 | 0.0176 | 0.9985 |
| 6.895 | 0.0347 | 0.9992 |
| 17.24 | 0.0830 | 0.9996 |
| 68.95 | 0.2576 | 0.9996 |
| 86.18 | 0.3021 | 0.9995 |
| 103.42 | 0.3489 | 0.9994 |
| 120.66 | 0.3940 | 0.9992 |
| 137.90 | 0.4379 | 0.9990 |
| 1.014 | 0.0046 | 0.9724 |
| 3.447 | 0.0157 | 0.9916 |
| 6.895 | 0.0312 | 0.9957 |
| 17.24 | 0.0749 | 0.9980 |
| 34.47 | 0.1399 | 0.9988 |
| 51.71 | 0.1937 | 0.9989 |
| 68.95 | 0.2387 | 0.9988 |
| 86.18 | 0.2815 | 0.9987 |
| 103.42 | 0.3240 | 0.9983 |
| 120.66 | 0.3662 | 0.9979 |
| 137.90 | 0.4087 | 0.9976 |

Reamer, H. H. - Olds, R. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 12 (1942) 1526-1531. doi:10.1021/ie50396a025

| **T / K =** | **344.26** | | |
|---|---|---|---|
| P / bar | $x_1$ | $y_1$ | |
| 1.379 | 0.0062 | 0.9792 | |
| 2.758 | 0.0125 | 0.9891 | |
| 4.137 | 0.0186 | 0.9924 | |
| 5.516 | 0.0247 | 0.9940 | |
| 6.895 | 0.0308 | 0.9950 | |
| 13.79 | 0.0600 | 0.9970 | |
| 27.58 | 0.1139 | 0.9980 | |
| 68.95 | 0.2496 | 0.9980 | |
| 86.19 | 0.2983 | 0.9977 | |
| 103.42 | 0.3429 | 0.9973 | |
| 120.66 | 0.3847 | 0.9969 | |
| 137.90 | 0.4234 | 0.9963 | |
| 155.13 | 0.4596 | 0.9956 | |
| 172.37 | 0.4943 | 0.9945 | |
| 189.61 | 0.5272 | 0.9932 | |
| 206.85 | 0.5593 | 0.9915 | |
| 224.07 | 0.5908 | 0.9892 | |
| 241.31 | 0.6202 | 0.9863 | |
| 258.55 | 0.6498 | 0.9826 | |
| 275.79 | 0.6796 | 0.9779 | |
| 293.03 | 0.7107 | 0.9721 | |
| 310.27 | 0.7441 | 0.9647 | |
| 327.51 | 0.7795 | 0.9541 | |
| 344.74 | 0.8240 | 0.9364 | |
| 357.70 | 0.8911 | 0.8911 | CRIT |

Reamer, H. H. - Olds, R. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 12 (1942) 1526-1531. doi:10.1021/ie50396a025

| **T / K =** | **377.59** | | |
|---|---|---|---|
| P / bar | $x_1$ | $y_1$ | |
| 1.379 | 0.0052 | 0.9172 | |
| 2.758 | 0.0109 | 0.9570 | |
| 4.137 | 0.0165 | 0.9703 | |
| 5.516 | 0.0220 | 0.9769 | |
| 6.895 | 0.0275 | 0.9811 | |
| 13.79 | 0.0543 | 0.9890 | |
| 27.58 | 0.1045 | 0.9931 | |
| 41.37 | 0.1510 | 0.9942 | |
| 55.16 | 0.1945 | 0.9945 | |
| 68.95 | 0.2352 | 0.9947 | |
| 86.19 | 0.2825 | 0.9945 | |
| 103.42 | 0.3275 | 0.9941 | |
| 120.66 | 0.3700 | 0.9933 | |
| 137.90 | 0.4091 | 0.9921 | |
| 155.13 | 0.4460 | 0.9907 | |
| 172.37 | 0.4804 | 0.9889 | |
| 189.61 | 0.5139 | 0.9867 | |
| 206.85 | 0.5462 | 0.9841 | |
| 224.07 | 0.5795 | 0.9809 | |
| 241.31 | 0.6124 | 0.9770 | |
| 258.55 | 0.6442 | 0.9716 | |
| 275.79 | 0.6782 | 0.9657 | |
| 293.03 | 0.7150 | 0.9576 | |
| 310.27 | 0.7550 | 0.9467 | |
| 327.51 | 0.8064 | 0.9273 | |
| 340.26 | 0.8767 | 0.8767 | CRIT |

Lavender, H.M. - Sage, B.H. - Lacey, W.N., Gas-liquid equilibrium constants, methane-decane system, Oil Gas J. (1940) 48-49.

| **T / K =** | **344.26** |
|---|---|
| P / bar | $x_1$ |

Lavender, H.M. - Sage, B.H. - Lacey, W.N., Gas-liquid equilibrium constants, methane-decane system, Oil Gas J. (1940) 48-49.

| **T / K =** | **377.59** |
|---|---|

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.014 | 0.0038 | 0.8830 |
| 3.447 | 0.0141 | 0.9654 |
| 6.895 | 0.0283 | 0.9822 |
| 17.24 | 0.0689 | 0.9927 |
| 34.47 | 0.1299 | 0.9954 |
| 51.71 | 0.1804 | 0.9960 |
| 68.95 | 0.2228 | 0.9960 |
| 86.18 | 0.2643 | 0.9957 |
| 103.42 | 0.3064 | 0.9952 |
| 120.66 | 0.3485 | 0.9937 |
| 137.90 | 0.3906 | 0.9937 |

Reamer, H. H. - Olds, R. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 12 (1942) 1526-1531. doi:10.1021/ie50396a025

**T / K = 410.93**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 1.379 | 0.0039 | 0.7384 | |
| 2.758 | 0.0092 | 0.8654 | |
| 4.137 | 0.0143 | 0.9073 | |
| 5.516 | 0.0194 | 0.9282 | |
| 6.895 | 0.0245 | 0.9411 | |
| 13.79 | 0.0496 | 0.9665 | |
| 27.58 | 0.0974 | 0.9798 | |
| 41.37 | 0.1425 | 0.9842 | |
| 55.16 | 0.1852 | 0.9862 | |
| 68.95 | 0.2256 | 0.9870 | |
| 86.19 | 0.2738 | 0.9874 | |
| 103.42 | 0.3191 | 0.9870 | |
| 120.66 | 0.3623 | 0.9859 | |
| 137.90 | 0.4027 | 0.9845 | |
| 155.13 | 0.4411 | 0.9819 | |
| 172.37 | 0.4779 | 0.9787 | |
| 206.85 | 0.5476 | 0.9715 | |
| 224.07 | 0.5827 | 0.9669 | |
| 241.31 | 0.6168 | 0.9608 | |
| 258.55 | 0.6523 | 0.9531 | |
| 275.79 | 0.6912 | 0.9430 | |
| 293.03 | 0.7369 | 0.9279 | |
| 310.27 | 0.8009 | 0.8950 | |
| 315.78 | 0.8574 | 0.8574 | CRIT |

Reamer, H. H. - Olds, R. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 12 (1942) 1526-1531. doi:10.1021/ie50396a025

**T / K = 444.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 1.379 | 0.0017 | 0.3187 | |
| 2.758 | 0.0067 | 0.6493 | |
| 4.137 | 0.0117 | 0.7594 | |
| 5.516 | 0.0167 | 0.8154 | |
| 6.895 | 0.0217 | 0.8489 | |
| 13.79 | 0.0460 | 0.9150 | |
| 27.58 | 0.0932 | 0.9511 | |
| 41.37 | 0.1380 | 0.9627 | |
| 55.16 | 0.1807 | 0.9673 | |
| 68.95 | 0.2213 | 0.9692 | |
| 86.19 | 0.2698 | 0.9702 | |
| 103.42 | 0.3163 | 0.9699 | |
| 120.66 | 0.3605 | 0.9683 | |
| 137.90 | 0.4025 | 0.9656 | |
| 155.13 | 0.4434 | 0.9622 | |
| 172.37 | 0.4827 | 0.9580 | |
| 189.61 | 0.5224 | 0.9536 | |
| 206.85 | 0.5607 | 0.9477 | |
| 224.07 | 0.6005 | 0.9401 | |
| 241.31 | 0.6435 | 0.9326 | |
| 258.55 | 0.6831 | 0.9125 | |
| 275.79 | 0.7358 | 0.8823 | |
| 287.03 | 0.8333 | 0.8333 | CRIT |

Reamer, H. H. - Olds, R. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 12 (1942) 1526-1531. doi:10.1021/ie50396a025

**T / K = 477.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.758 | 0.0023 | 0.2124 |
| 4.137 | 0.0075 | 0.4645 |
| 5.516 | 0.0127 | 0.5906 |
| 6.895 | 0.0179 | 0.6662 |
| 13.79 | 0.0439 | 0.8160 |
| 27.58 | 0.0926 | 0.8940 |
| 41.37 | 0.1390 | 0.9189 |
| 55.16 | 0.1835 | 0.9306 |
| 68.95 | 0.2258 | 0.9357 |
| 86.19 | 0.2758 | 0.9381 |
| 103.42 | 0.3234 | 0.9389 |
| 120.66 | 0.3678 | 0.9379 |
| 137.90 | 0.4119 | 0.9351 |
| 155.13 | 0.4555 | 0.9301 |
| 172.37 | 0.4983 | 0.9227 |
| 189.61 | 0.5427 | 0.9136 |
| 206.85 | 0.5912 | 0.9030 |
| 224.07 | 0.6467 | 0.8848 |
| 241.31 | 0.7214 | 0.8517 |

| | | | |
|---|---|---|---|
| 248.56 | 0.7979 | 0.7979 | CRIT |

Reamer, H. H. - Olds, R. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 12 (1942) 1526-1531. doi:10.1021/ie50396a025

**T / K = 510.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.516 | 0.0046 | 0.1828 |
| 6.895 | 0.0104 | 0.3335 |
| 13.79 | 0.0392 | 0.6409 |
| 27.58 | 0.0937 | 0.7929 |
| 41.37 | 0.1452 | 0.8468 |
| 55.16 | 0.1933 | 0.8700 |
| 68.95 | 0.2378 | 0.8802 |
| 86.19 | 0.2895 | 0.8858 |
| 103.42 | 0.3374 | 0.8872 |
| 120.66 | 0.3837 | 0.8861 |
| 137.90 | 0.4280 | 0.8813 |
| 155.13 | 0.4763 | 0.8713 |
| 172.37 | 0.5379 | 0.8533 |
| 189.61 | 0.6157 | 0.8204 |
| 200.71 | 0.7390 | 0.7390 | CRIT |

Lin, Ho-Mu - Sebastian, Herbert M. - Simnick, James J. - Chao, Kwang-Chu, Gas-liquid equilibrium in binary mixtures of methane with N-decane, benzene, and toluene, Journal of Chemical & Engineering Data 2 (1979) 146-149. doi:10.1021/je60081a004

**T / K = 542.75**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 30.50 | 0.0946 | 0.6795 |
| 50.98 | 0.1706 | 0.7638 |
| 101.38 | 0.3508 | 0.8051 |
| 126.68 | 0.4440 | 0.7901 |
| 151.43 | 0.6682 | 0.7116 |

Lin, Ho-Mu - Sebastian, Herbert M. - Simnick, James J. - Chao, Kwang-Chu, Gas-liquid equilibrium in binary mixtures of methane with N-decane, benzene, and toluene, Journal of Chemical & Engineering Data 2 (1979) 146-149. doi:10.1021/je60081a004

**T / K = 563.25**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 30.37 | 0.0911 | 0.5528 |
| 50.70 | 0.1744 | 0.6690 |
| 75.87 | 0.2744 | 0.7118 |
| 100.97 | 0.3817 | 0.7055 |
| 111.45 | 0.4399 | 0.6835 |
| 116.14 | 0.4652 | 0.6604 |

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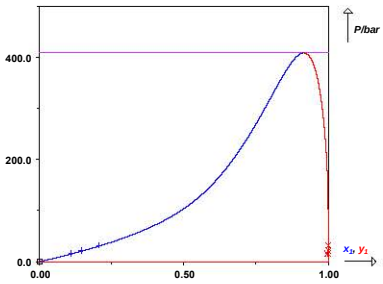
**Critical point**

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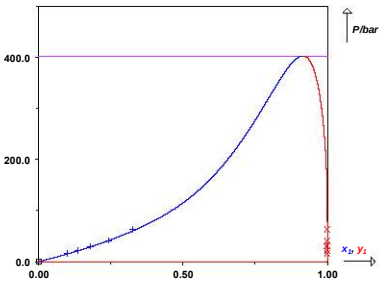
Wiese, H. C. - Reamer, H. H. - Sage, B. H., Phase equilibriums in hydrocarbon systems. Phase behavior in the methane-propane-n-decane system, Journal of Chemical & Engineering Data 1 (1970) 75-82. doi:10.1021/je60044a018

| T / K | P / bar | $x_1$ |
|---|---|---|
| 277.59 | 361.29 | 0.9050 |

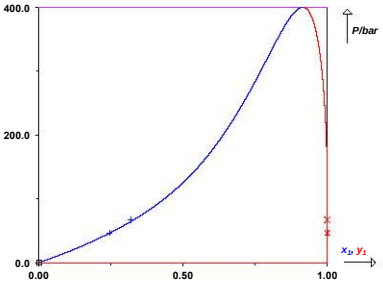
T/K = 244.26



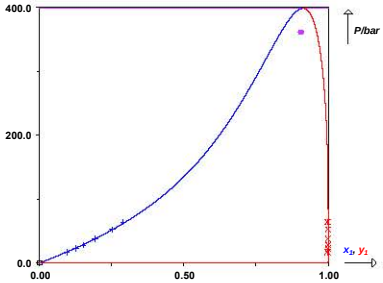

T/K = 255.37



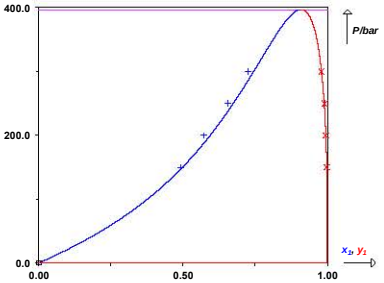

T/K = 266.48



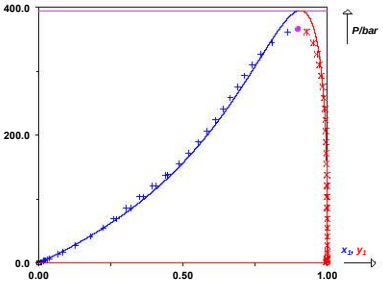

T/K = 277.59



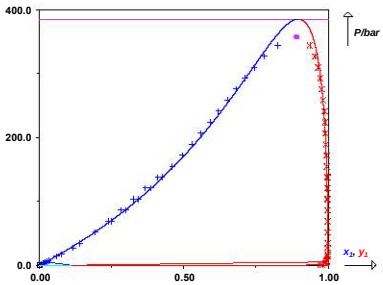

T/K = 300.00



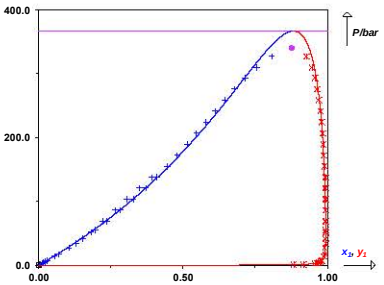

T/K = 310.93



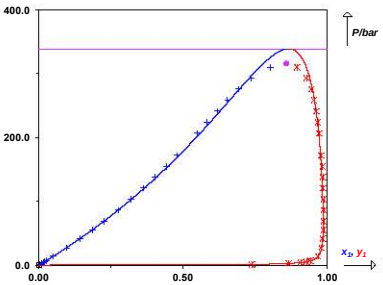

T/K = 344.26



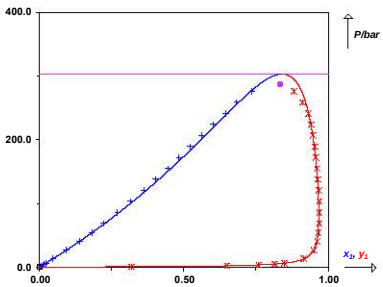

T/K = 377.59



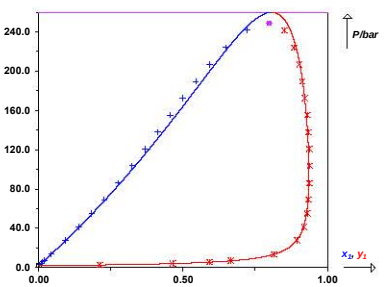

T/K = 410.93



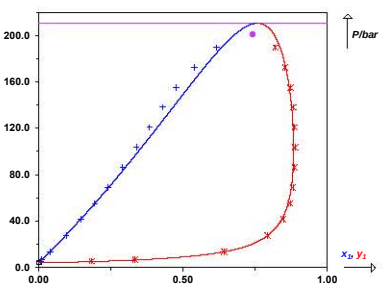

T/K = 444.26



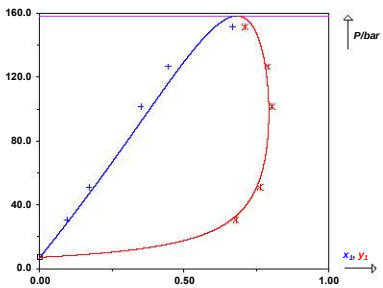

T/K = 477.59



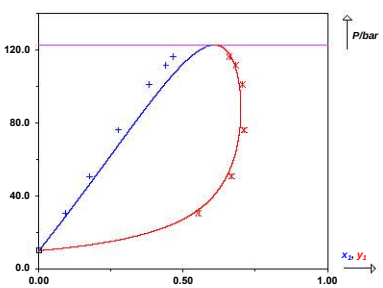

T/K = 510.93




T/K = 542.75




T/K = 563.25



## ETHANE (1) + n-HEPTANE (2)

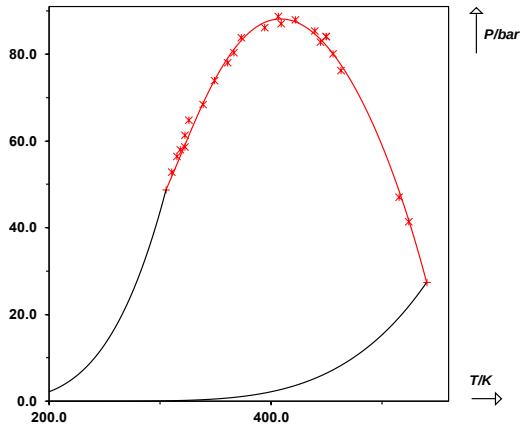
| | | |
|---|---|---|
| **CAS** | 74-84-0 | 142-82-5 |
| **InChiKey** | OTMSDBZUPAUEDD-UHFFFAOYSA-N | IMNFDUFMRHMDMM-UHFFFAOYSA-N |
| **$T_c$ / K** | 305.32 | 540.20 |
| **$P_c$ / bar** | 48.72 | 27.40 |
| **ω** | 0.099 | 0.349 |

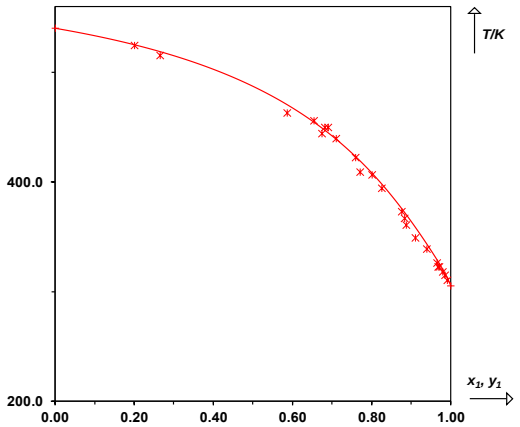
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 1.4
B/MPa = -9.79

*Deviations*
MAPE on x = 76 %
MAPE on y = 5.6 %
MAPE on $x_c$ = 6.4 %
MAPE on $P_c$ = 1.6 %



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**Isobaric phase equilibrium data**

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Kay, W. B., Liquid-Vapor Phase Equilibrium Relations in the Ethane-n-Heptane System, Industrial & Engineering Chemistry 4 (1938) 459-465. doi:10.1021/ie50340a023

**P / bar = 27.58**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 285.35 | 0.9000 | 0.9980 |
| 292.55 | 0.8000 | 0.9960 |
| 300.95 | 0.7000 | 0.9950 |
| 312.55 | 0.6000 | 0.9930 |
| 328.45 | 0.5000 | 0.9870 |
| 350.35 | 0.4000 | 0.9700 |
| 384.55 | 0.3000 | 0.9190 |
| 434.25 | 0.2000 | 0.7640 |
| 497.35 | 0.1000 | 0.3420 |

Kay, W. B., Liquid-Vapor Phase Equilibrium Relations in the Ethane-n-Heptane System, Industrial & Engineering Chemistry 4 (1938) 459-465. doi:10.1021/ie50340a023

**P / bar = 41.37**

| T / K | $x_1$ |
|---|---|
| 524.26 | 0.2000 |
| 523.15 | 0.2380 |
| 522.04 | 0.2530 |
| 519.26 | 0.2800 |
| 517.04 | 0.3000 |
| 505.37 | 0.4000 |
| 492.04 | 0.5000 |
| 477.59 | 0.6000 |
| 460.93 | 0.7000 |
| 437.59 | 0.8000 |
| 402.04 | 0.9000 |
| 373.15 | 0.9500 |
| 355.93 | 0.9700 |
| 344.26 | 0.9800 |
| 328.15 | 0.9900 |

Kay, W. B., Liquid-Vapor Phase Equilibrium Relations in the Ethane-n-Heptane System, Industrial & Engineering Chemistry 4 (1938) 459-465. doi:10.1021/ie50340a023

**P / bar = 41.37**

| T / K | $x_1$ |
|---|---|
| 524.26 | 0.2000 |
| 523.70 | 0.1850 |
| 522.04 | 0.1790 |
| 519.26 | 0.1770 |
| 505.37 | 0.1930 |
| 500.37 | 0.2000 |
| 469.26 | 0.2500 |
| 442.59 | 0.3000 |
| 418.15 | 0.3500 |
| 397.59 | 0.4000 |
| 365.37 | 0.5000 |
| 343.15 | 0.6000 |
| 327.59 | 0.7000 |
| 316.48 | 0.8000 |
| 306.76 | 0.9000 |

Kay, W. B., Liquid-Vapor Phase Equilibrium Relations in the Ethane-n-Heptane System, Industrial & Engineering Chemistry 4 (1938) 459-465. doi:10.1021/ie50340a023

**P / bar = 55.16**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 323.75 | 0.9000 | 0.9827 |
| 335.95 | 0.8000 | 0.9850 |
| 351.45 | 0.7000 | 0.9720 |
| 371.45 | 0.6000 | 0.9520 |
| 397.05 | 0.5000 | 0.9160 |
| 433.15 | 0.4000 | 0.8290 |
| 474.85 | 0.3400 | 0.6540 |

Kay, W. B., Liquid-Vapor Phase Equilibrium Relations in the Ethane-n-Heptane System, Industrial & Engineering Chemistry 4 (1938) 459-465. doi:10.1021/ie50340a023

**P / bar = 68.95**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 342.55 | 0.9000 | 0.9461 |
| 347.55 | 0.8500 | 0.9598 |
| 355.35 | 0.8000 | 0.9580 |
| 376.45 | 0.7000 | 0.9382 |
| 401.45 | 0.6000 | 0.9017 |
| 441.45 | 0.5000 | 0.8000 |
| 479.25 | 0.5000 | 0.5740 |
| 480.35 | 0.5100 | 0.5550 |

Kay, W. B., Liquid-Vapor Phase Equilibrium Relations in the Ethane-n-Heptane System, Industrial & Engineering Chemistry 4 (1938) 459-465. doi:10.1021/ie50340a023

**P / bar = 82.74**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 374.85 | 0.8500 | 0.8775 |
| 380.95 | 0.8000 | 0.8930 |

| | | |
|---|---|---|
| 392.55 | 0.7500 | 0.8830 |
| 407.55 | 0.7000 | 0.8540 |
| 425.95 | 0.6500 | 0.8000 |
| 442.05 | 0.6400 | 0.7130 |

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**Critical point**

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Cota, H. M. - Thodos, George, Critical Temperatures and Critical Pressures of Hydrocarbon Mixtures. Methane Ethane-n-Butane System., Journal of Chemical & Engineering Data 1 (1962) 62-65. doi:10.1021/je60012a018

| T / K | P / bar | $x_1$ |
|---|---|---|
| 449.82 | 84.05 | 0.6900 |
| 422.04 | 87.91 | 0.7600 |

Mehra, V. S. - Thodos, George, Vapor-Liquid Equilibrium in the Ethane-n-Heptane System., Journal of Chemical & Engineering Data 3 (1965) 211-214. doi:10.1021/je60026a001

| T / K | P / bar | $x_1$ |
|---|---|---|
| 338.71 | 68.33 | 0.9390 |
| 366.48 | 80.32 | 0.8830 |
| 394.26 | 86.19 | 0.8250 |

Ekiner, Okan - Thodos, George, Critical temperatures and pressures of the ethane-n-heptane system, The Canadian Journal of Chemical Engineering 4 (1965) 205-208. doi:10.1002/cjce.5450430411

| T / K | P / bar | $x_1$ |
|---|---|---|
| 348.98 | 73.84 | 0.9112 |
| 372.87 | 83.77 | 0.8760 |
| 406.48 | 88.74 | 0.8014 |
| 439.54 | 85.36 | 0.7104 |
| 455.93 | 80.12 | 0.6550 |

Mehra, Vinod S. - Thodos, George., Vapor-liquid equilibrium constants for the ethane-butane-n-heptane system at 300° and 350°F, Journal of Chemical & Engineering Data 2 (1968) 155-160. doi:10.1021/je60037a004

| T / K | P / bar | $x_1$ |
|---|---|---|
| 449.82 | 84.05 | 0.6810 |

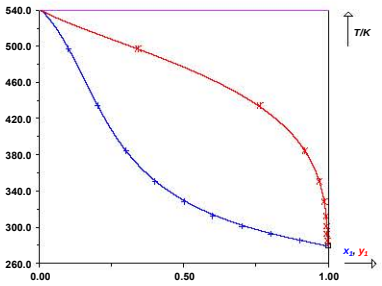
Singh, Harcharan - Lucien, Frank P. - Foster, Neil R., Critical Properties for Binary Mixtures of Ethane Containing Low Concentrations of n-Alkane, Journal of Chemical & Engineering Data 1 (2000) 131-135. doi:10.1021/je990220w

| T / K | P / bar | $x_1$ |
|---|---|---|
| 310.40 | 52.80 | 0.9913 |
| 315.00 | 56.40 | 0.9849 |
| 318.00 | 57.90 | 0.9798 |
| 322.40 | 61.30 | 0.9713 |
| 325.80 | 64.80 | 0.9650 |

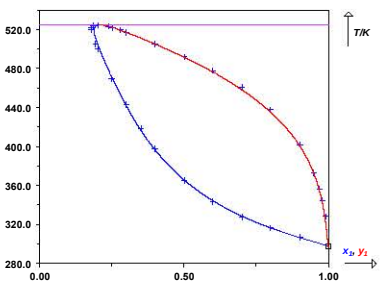
Kay, W. B., Liquid-Vapor Phase Equilibrium Relations in the Ethane-n-Heptane System, Industrial & Engineering Chemistry 4 (1938) 459-465. doi:10.1021/ie50340a023

| T / K | P / bar | $x_1$ |
|---|---|---|
| 515.48 | 47.02 | 0.2654 |
| 463.09 | 76.26 | 0.5871 |
| 409.15 | 87.08 | 0.7709 |
| 360.82 | 78.05 | 0.8871 |
| 322.21 | 58.61 | 0.9685 |
| 524.26 | 41.37 | 0.2000 |
| 444.25 | 82.74 | 0.6750 |

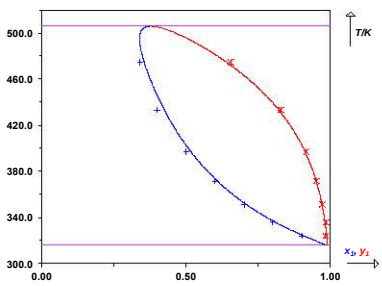
P/bar = 27.58000



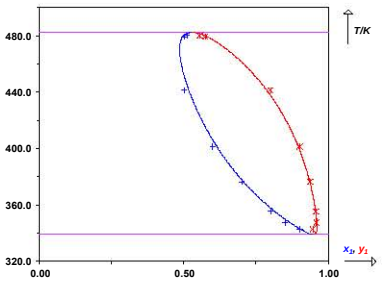

P/bar = 41.36800



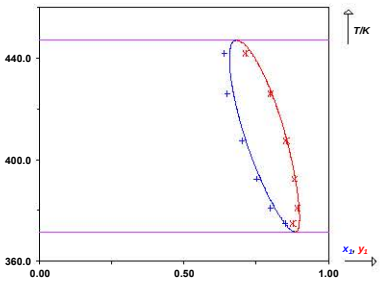

P/bar = 55.16100



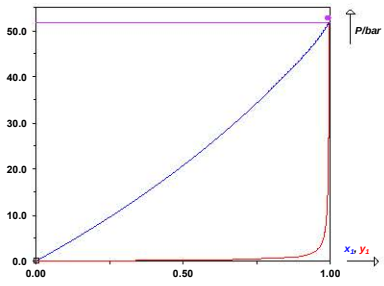

P/bar = 68.95100



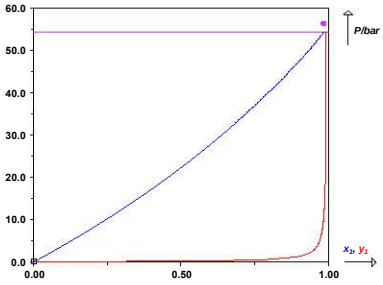

P/bar = 82.74100



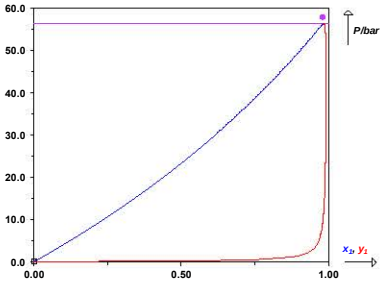

T/K = 310.40



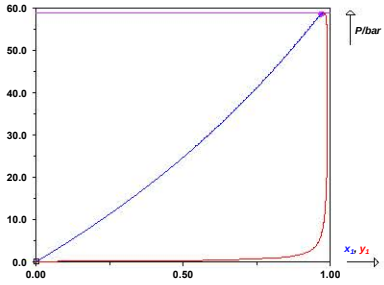

T/K = 315.00



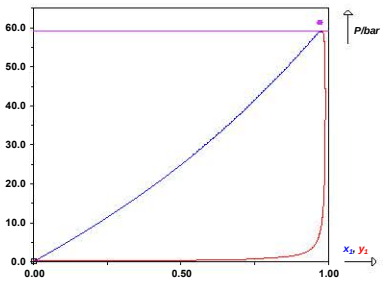

T/K = 318.00



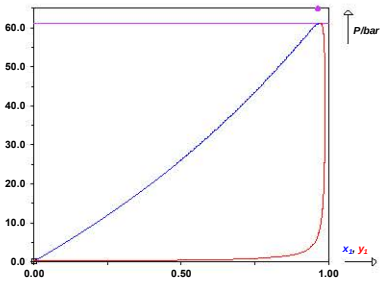

T/K = 322.21



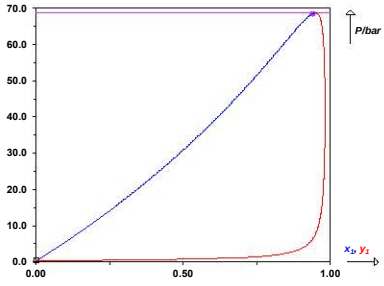

T/K = 322.40



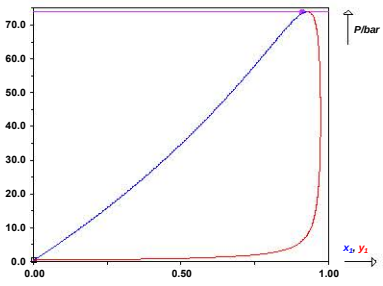

T/K = 325.80



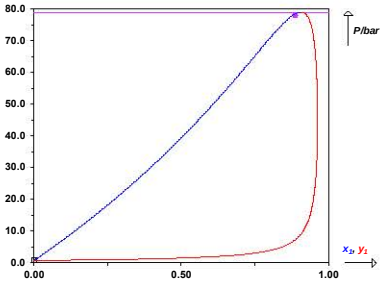

T/K = 338.71



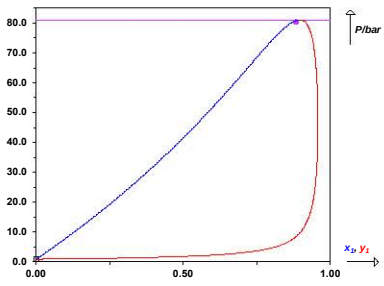

T/K = 348.98



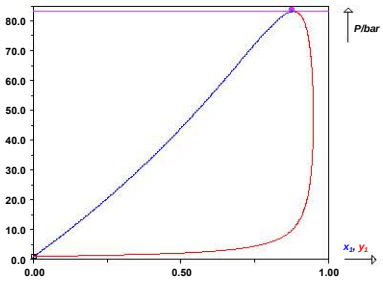

T/K = 360.82



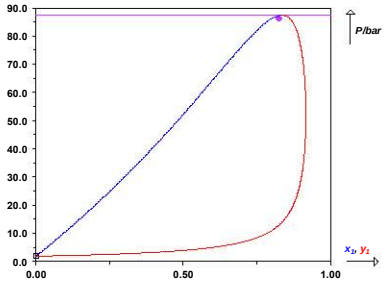

T/K = 366.48



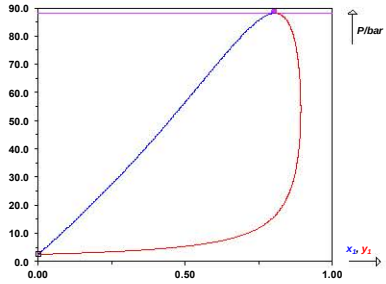
T/K = 372.87



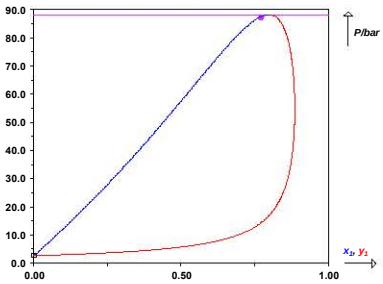

T/K = 394.26



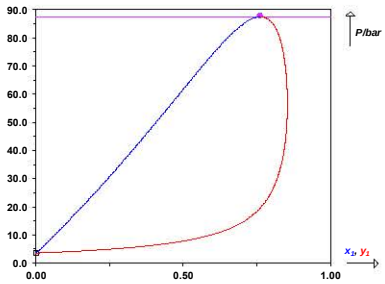

T/K = 406.48



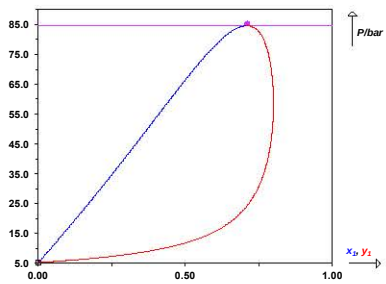

T/K = 409.15



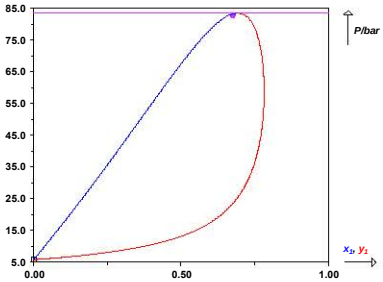

T/K = 422.04



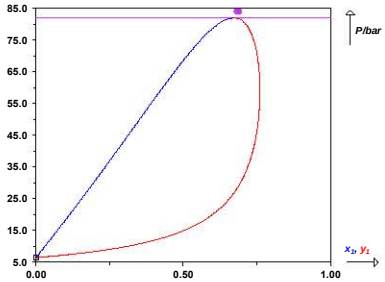

T/K = 439.54



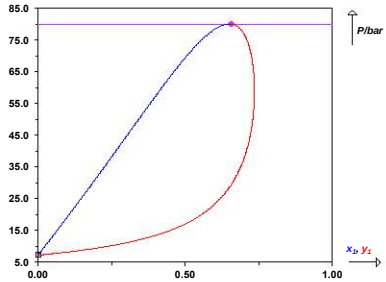

T/K = 444.25



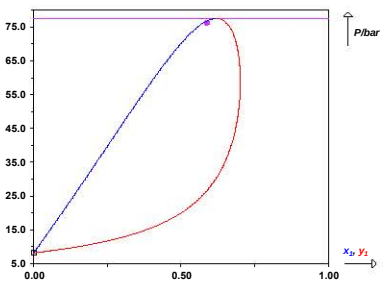

T/K = 449.82



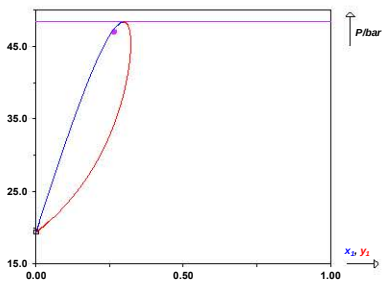

T/K = 455.93



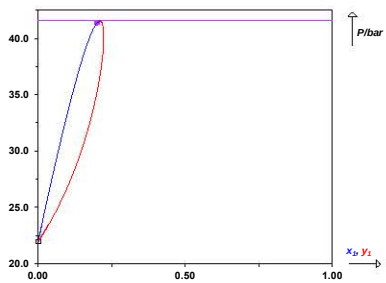

T/K = 463.09




T/K = 515.48




T/K = 524.26



## NITROGEN (1) + n-PENTANE (2)

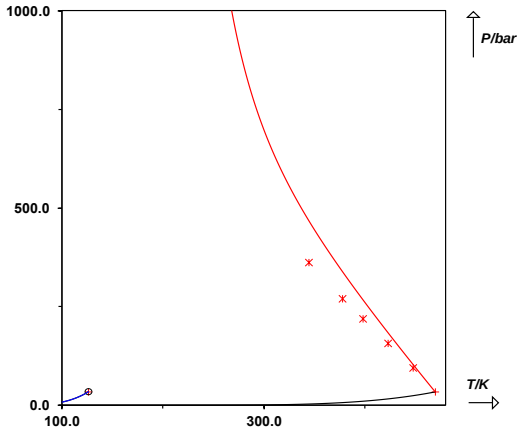
| | | |
|---|---|---|
| **CAS** | 7727-37-9 | 109-66-0 |
| **InChiKey** | MDFFNEOEWAXZRQ-UHFFFAOYSA-N | OFBQJSOFQDEBGM-UHFFFAOYSA-N |
| **$T_c$ / K** | 126.20 | 469.70 |
| **$P_c$ / bar** | 34.00 | 33.70 |
| **ω** | 0.038 | 0.252 |

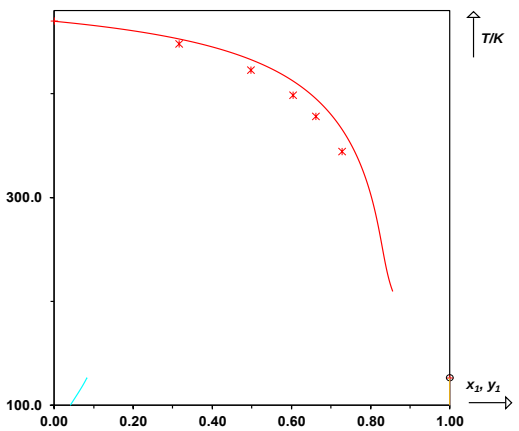
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 204
B/MPa = 342

*Deviations*
MAPE on x = 7.7 %
MAPE on y = 9.3 %
MAPE on $x_c$ = 10 %
MAPE on $P_c$ = 21 %



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**Isothermal phase equilibrium data**

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Kurata, F. - Swift, G.W., Experimental Measurements of Vapor-Liquid Equilibrium Data for the Ethane - Carbon Dioxide and Nitrogen - n-Pentane Binary Systems, GPA Research Report (1971) 1-10.

**T / K = 144.30**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 24.19 | 0.0538 | 0.9763 |
| 33.05 | 0.0684 | 0.9864 |
| 45.11 | 0.0865 | 0.9944 |
| 58.04 | 0.0995 | 0.9961 |

Kurata, F. - Swift, G.W., Experimental Measurements of Vapor-Liquid Equilibrium Data for the Ethane - Carbon Dioxide and Nitrogen - n-Pentane Binary Systems, GPA Research Report (1971) 1-10.

**T / K = 172.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.63 | 0.0698 | 0.9781 |
| 64.31 | 0.1083 | 0.9949 |
| 102.72 | 0.1533 | 0.9975 |
| 141.86 | 0.1761 | 0.9979 |

Kurata, F. - Swift, G.W., Experimental Measurements of Vapor-Liquid Equilibrium Data for the Ethane - Carbon Dioxide and Nitrogen - n-Pentane Binary Systems, GPA Research Report (1971) 1-10.

**T / K = 199.80**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 63.68 | 0.1148 | 0.9928 |
| 136.29 | 0.1963 | 0.9969 |
| 237.34 | 0.2916 | 0.9964 |
| 310.71 | 0.3333 | 0.9949 |

Kurata, F. - Swift, G.W., Experimental Measurements of Vapor-Liquid Equilibrium Data for the Ethane - Carbon Dioxide and Nitrogen - n-Pentane Binary Systems, GPA Research Report (1971) 1-10.

**T / K = 227.60**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 270.03 | 0.3387 | 0.9928 |
| 200.14 | 0.2847 | 0.9949 |
| 210.61 | 0.2962 | 0.9944 |
| 142.16 | 0.2264 | 0.9952 |
| 66.96 | 0.1240 | 0.9910 |

Kurata, F. - Swift, G.W., Experimental Measurements of Vapor-Liquid Equilibrium Data for the Ethane - Carbon Dioxide and Nitrogen - n-Pentane Binary Systems, GPA Research Report (1971) 1-10.

**T / K = 255.40**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 279.06 | 0.3900 | 0.9900 |
| 219.76 | 0.3233 | 0.9914 |
| 145.87 | 0.2441 | 0.9930 |
| 73.51 | 0.1390 | 0.9908 |
| 76.59 | 0.1424 | 0.9906 |

Kalra, Harish - Robinson, Donald B. - Besserer, George J., The equilibrium phase properties of the nitrogen-n-pentane system, Journal of Chemical & Engineering Data 2 (1977) 215-218. doi:10.1021/je60073a023

**T / K = 277.43**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 16.62 | 0.0250 | 0.9810 |
| 41.44 | 0.0550 | 0.9900 |
| 172.64 | 0.2230 | 0.9870 |
| 207.26 | 0.2510 | 0.9850 |

Kalra, Harish - Robinson, Donald B. - Besserer, George J., The equilibrium phase properties of the nitrogen-n-pentane system, Journal of Chemical & Engineering Data 2 (1977) 215-218. doi:10.1021/je60073a023

**T / K = 310.71**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.503 | 0.0027 | 0.5770 |
| 4.502 | 0.0055 | 0.7570 |
| 7.791 | 0.0110 | 0.8560 |
| 13.72 | 0.0200 | 0.9130 |
| 21.37 | 0.0310 | 0.9400 |
| 29.03 | 0.0430 | 0.9500 |
| 41.30 | 0.0610 | 0.9600 |
| 63.57 | 0.0950 | 0.9680 |
| 125.62 | 0.1850 | 0.9690 |
| 153.20 | 0.2230 | 0.9670 |
| 180.92 | 0.2580 | 0.9640 |
| 207.53 | 0.2880 | 0.9610 |

Silva-Oliver, Guadalupe - Eliosa-Jiménez, Gaudencio - García-Sánchez, Fernando - Avendaño-Gómez, Juan R., High-pressure vapor–liquid equilibria in the nitrogen–n-pentane system, Fluid Phase Equilibria 1-2 (2006) 37-48. doi:10.1016/j.fluid.2006.09.018

**T / K = 344.30**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 16.70 | 0.0213 | 0.7845 |
| 33.10 | 0.0478 | 0.8849 |
| 43.80 | 0.0652 | 0.9078 |
| 66.50 | 0.1002 | 0.9292 |
| 94.20 | 0.1427 | 0.9353 |
| 124.70 | 0.1907 | 0.9364 |

| | | |
|---|---|---|
| 164.10 | 0.2524 | 0.9328 |
| 209.80 | 0.3266 | 0.9233 |
| 252.40 | 0.3921 | 0.9082 |
| 301.60 | 0.4867 | 0.8781 |
| 344.80 | 0.5960 | 0.8218 |
| 354.70 | 0.6341 | 0.7923 |

Silva-Oliver, Guadalupe - Eliosa-Jiménez, Gaudencio - García-Sánchez, Fernando - Avendaño-Gómez, Juan R., High-pressure vapor–liquid equilibria in the nitrogen–n-pentane system, Fluid Phase Equilibria 1-2 (2006) 37-48. doi:10.1016/j.fluid.2006.09.018

**T / K = 377.90**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 17.10 | 0.0179 | 0.5334 |
| 21.60 | 0.0259 | 0.6269 |
| 30.90 | 0.0431 | 0.7285 |
| 54.10 | 0.0856 | 0.8190 |
| 88.70 | 0.1496 | 0.8625 |
| 126.00 | 0.2180 | 0.8688 |
| 164.90 | 0.2934 | 0.8590 |
| 197.00 | 0.3640 | 0.8470 |
| 210.40 | 0.3911 | 0.8368 |
| 225.10 | 0.4239 | 0.8224 |
| 241.50 | 0.4729 | 0.8014 |
| 257.60 | 0.5352 | 0.7686 |
| 263.60 | 0.5626 | 0.7449 |
| 266.10 | 0.5855 | 0.7277 |

Silva-Oliver, Guadalupe - Eliosa-Jiménez, Gaudencio - García-Sánchez, Fernando - Avendaño-Gómez, Juan R., High-pressure vapor–liquid equilibria in the nitrogen–n-pentane system, Fluid Phase Equilibria 1-2 (2006) 37-48. doi:10.1016/j.fluid.2006.09.018

**T / K = 398.30**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 17.00 | 0.0138 | 0.3503 |
| 19.70 | 0.0189 | 0.4272 |
| 23.10 | 0.0258 | 0.4967 |
| 28.00 | 0.0356 | 0.5718 |
| 39.00 | 0.0589 | 0.6651 |
| 48.10 | 0.0769 | 0.7093 |
| 68.10 | 0.1172 | 0.7644 |
| 88.10 | 0.1600 | 0.7823 |
| 107.10 | 0.1994 | 0.7938 |
| 127.10 | 0.2443 | 0.7956 |
| 147.60 | 0.2927 | 0.7898 |
| 166.90 | 0.3378 | 0.7769 |
| 182.40 | 0.3879 | 0.7585 |
| 197.00 | 0.4323 | 0.7377 |
| 208.10 | 0.4806 | 0.7087 |
| 212.30 | 0.5030 | 0.6838 |

Silva-Oliver, Guadalupe - Eliosa-Jiménez, Gaudencio - García-Sánchez, Fernando - Avendaño-Gómez, Juan R., High-pressure vapor–liquid equilibria in the nitrogen–n-pentane system, Fluid Phase Equilibria 1-2 (2006) 37-48. doi:10.1016/j.fluid.2006.09.018

**T / K = 422.70**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 19.90 | 0.0100 | 0.1663 |
| 23.20 | 0.0175 | 0.2577 |
| 28.20 | 0.0293 | 0.3535 |
| 33.10 | 0.0402 | 0.4216 |
| 42.50 | 0.0624 | 0.5146 |
| 53.10 | 0.0875 | 0.5730 |
| 68.10 | 0.1241 | 0.6244 |
| 83.90 | 0.1633 | 0.6533 |
| 96.60 | 0.1979 | 0.6632 |
| 111.60 | 0.2402 | 0.6627 |
| 126.70 | 0.2864 | 0.6535 |
| 136.40 | 0.3237 | 0.6411 |
| 142.60 | 0.3551 | 0.6216 |
| 149.20 | 0.3854 | 0.5989 |
| 152.30 | 0.4034 | 0.5787 |

Silva-Oliver, Guadalupe - Eliosa-Jiménez, Gaudencio - García-Sánchez, Fernando - Avendaño-Gómez, Juan R., High-pressure vapor–liquid equilibria in the nitrogen–n-pentane system, Fluid Phase Equilibria 1-2 (2006) 37-48. doi:10.1016/j.fluid.2006.09.018

**T / K = 447.90**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 28.70 | 0.0131 | 0.1035 |
| 33.70 | 0.0271 | 0.1833 |
| 37.00 | 0.0370 | 0.2270 |
| 42.60 | 0.0527 | 0.2762 |
| 47.30 | 0.0667 | 0.3109 |
| 51.20 | 0.0798 | 0.3383 |
| 56.40 | 0.0960 | 0.3702 |
| 63.90 | 0.1215 | 0.3970 |
| 67.60 | 0.1353 | 0.4062 |
| 71.90 | 0.1534 | 0.4132 |
| 76.60 | 0.1718 | 0.4175 |
| 81.90 | 0.1957 | 0.4183 |
| 87.60 | 0.2279 | 0.4054 |
| 92.00 | 0.2579 | 0.3888 |

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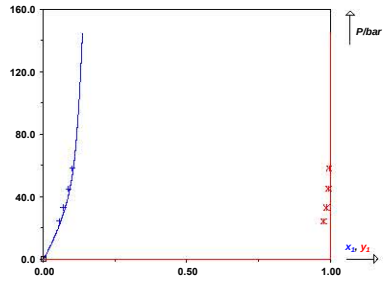
**Critical point**

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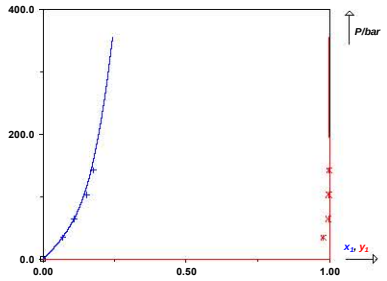
Rai, R.N. - Reddi, R.S.B., Thermal, solid–liquid equilibrium, crystallization, and microstructural studies of organic monotectic alloy: 4,4′-Dibromobiphenyl–succinonitrile, Thermochimica Acta 1-2 (2009) 13-17. doi:10.1016/j.tca.2009.06.012

| T / K | P / bar | $x_1$ |
|---|---|---|
| 344.30 | 361.60 | 0.7275 |
| 377.90 | 269.70 | 0.6612 |
| 398.30 | 218.60 | 0.6032 |
| 422.70 | 156.80 | 0.4967 |
| 447.90 | 94.40 | 0.3162 |

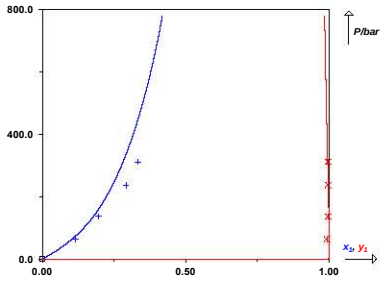
T/K = 144.30



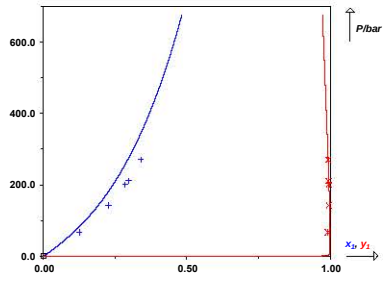

T/K = 172.00



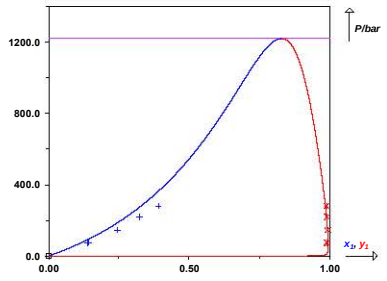

T/K = 199.80



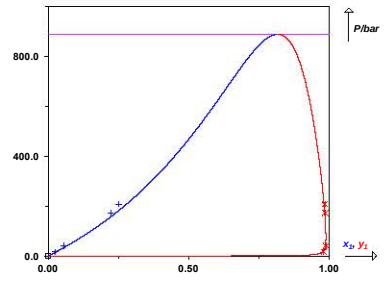

T/K = 227.60



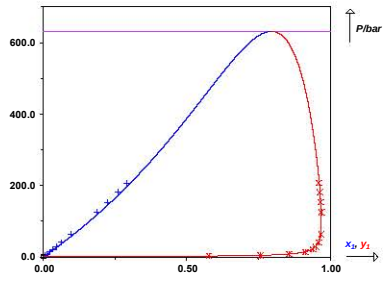

T/K = 255.40



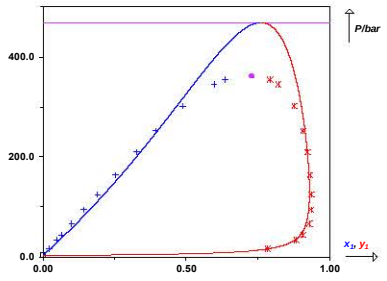

T/K = 277.43



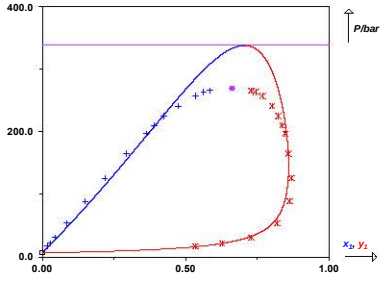

T/K = 310.71



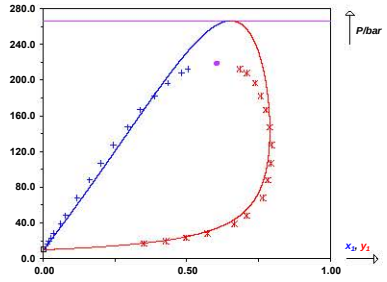

T/K = 344.30



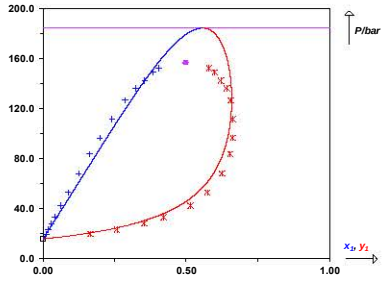

T/K = 377.90



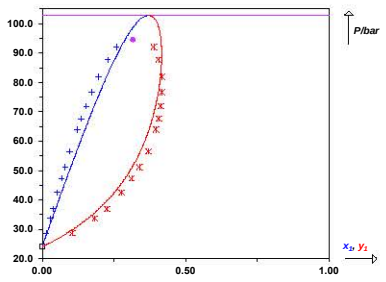

T/K = 398.30




T/K = 422.70




T/K = 447.90



## NITROGEN (1) + n-DECANE (2)

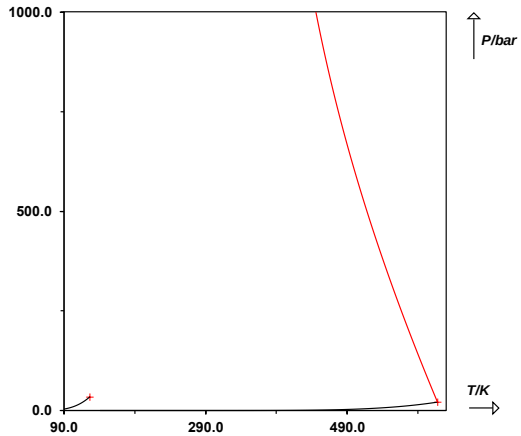
| | | |
|---|---|---|
| **CAS** | 7727-37-9 | 124-18-5 |
| **InChiKey** | MDFFNEOEWAXZRQ-UHFFFAOYSA-N | DIOQZVSQGTUSAI-UHFFFAOYSA-N |
| **$T_c$ / K** | 126.20 | 617.70 |
| **$P_c$ / bar** | 34.00 | 21.10 |
| **ω** | 0.038 | 0.492 |

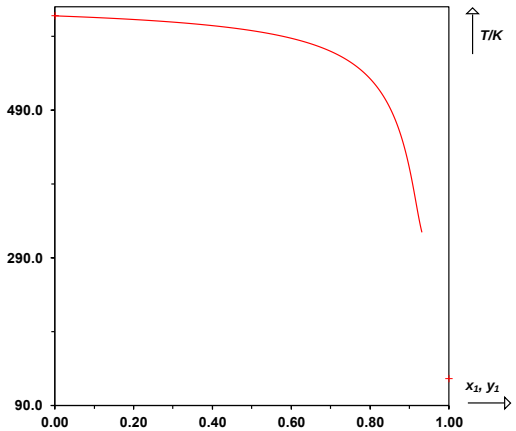
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 221
B/MPa = 442

*Deviations*
MAPE on x = 6.5 %
MAPE on y = 9.3 %



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**Isothermal phase equilibrium data**

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Azarnoosh, A. - McKetta, J. J., Nitrogen-n-Decane System in the Two-Phase Region., Journal of Chemical & Engineering Data 4 (1963) 494-496. doi:10.1021/je60019a005

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.48 | 0.0482 | 0.9977 |
| 46.89 | 0.0665 | 0.9993 |
| 51.71 | 0.0710 | 0.9998 |
| 55.16 | 0.0763 | 0.9997 |
| 68.95 | 0.0930 | 0.9997 |
| 93.08 | 0.1242 | 0.9997 |
| 131.00 | 0.1715 | 0.9992 |
| 144.79 | 0.1875 | 0.9997 |
| 172.37 | 0.2130 | 0.9992 |
| 182.70 | 0.2280 | 0.9998 |
| 248.21 | 0.2822 | 0.9993 |
| 293.03 | 0.3180 | 0.9986 |
| 344.74 | 0.3550 | 0.9968 |

García-Sánchez, Fernando - Eliosa-Jiménez, Gaudencio - Silva-Oliver, Guadalupe - García-Flores, Blanca E., Vapor-Liquid Equilibrium Data for the Nitrogen + n-Decane System from (344 to 563) K and at Pressures up to 50 MPa, Journal of Chemical & Engineering Data 5 (2009) 1560-1568. doi:10.1021/je800881t

**T / K = 344.60**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 14.60 | 0.0195 | 0.9953 |
| 21.20 | 0.0263 | 0.9968 |
| 29.90 | 0.0365 | 0.9975 |
| 49.90 | 0.0592 | 0.9981 |
| 69.90 | 0.0838 | 0.9983 |
| 94.00 | 0.1097 | 0.9984 |
| 120.30 | 0.1343 | 0.9983 |
| 144.40 | 0.1580 | 0.9982 |
| 170.00 | 0.1812 | 0.9980 |
| 196.30 | 0.2025 | 0.9978 |
| 222.30 | 0.2264 | 0.9976 |
| 244.90 | 0.2420 | 0.9974 |
| 270.10 | 0.2630 | 0.9971 |
| 296.10 | 0.2838 | 0.9968 |
| 320.60 | 0.2982 | 0.9965 |
| 346.10 | 0.3162 | 0.9962 |
| 370.90 | 0.3341 | 0.9959 |
| 395.80 | 0.3467 | 0.9955 |
| 420.30 | 0.3617 | 0.9950 |
| 444.30 | 0.3777 | 0.9945 |
| 470.10 | 0.3902 | 0.9941 |
| 487.80 | 0.3985 | 0.9936 |
| 499.10 | 0.4036 | 0.9932 |

García-Sánchez, Fernando - Eliosa-Jiménez, Gaudencio - Silva-Oliver, Guadalupe - García-Flores, Blanca E., Vapor-Liquid Equilibrium Data for the Nitrogen + n-Decane System from (344 to 563) K and at Pressures up to 50 MPa, Journal of Chemical & Engineering Data 5 (2009) 1560-1568. doi:10.1021/je800881t

**T / K = 377.40**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 22.30 | 0.0307 | 0.9932 |
| 45.50 | 0.0601 | 0.9958 |
| 50.10 | 0.0659 | 0.9960 |
| 69.70 | 0.0902 | 0.9963 |
| 94.80 | 0.1195 | 0.9965 |
| 119.80 | 0.1480 | 0.9964 |
| 144.60 | 0.1748 | 0.9963 |
| 169.80 | 0.2009 | 0.9961 |
| 194.40 | 0.2235 | 0.9958 |
| 219.90 | 0.2474 | 0.9955 |
| 244.60 | 0.2682 | 0.9950 |
| 269.60 | 0.2891 | 0.9945 |
| 295.40 | 0.3106 | 0.9940 |
| 320.40 | 0.3322 | 0.9935 |
| 344.40 | 0.3483 | 0.9932 |
| 370.20 | 0.3679 | 0.9927 |
| 395.00 | 0.3863 | 0.9920 |
| 420.20 | 0.4061 | 0.9913 |
| 440.10 | 0.4205 | 0.9907 |
| 468.90 | 0.4417 | 0.9896 |
| 482.70 | 0.4480 | 0.9887 |
| 495.60 | 0.4580 | 0.9882 |

García-Sánchez, Fernando - Eliosa-Jiménez, Gaudencio - Silva-Oliver, Guadalupe - García-Flores, Blanca E., Vapor-Liquid Equilibrium Data for the Nitrogen + n-Decane System from (344 to 563) K and at Pressures up to 50 MPa, Journal of Chemical & Engineering Data 5 (2009) 1560-1568. doi:10.1021/je800881t

**T / K = 410.90**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 19.40 | 0.0352 | 0.9823 |
| 32.10 | 0.0564 | 0.9877 |
| 46.20 | 0.0759 | 0.9899 |
| 54.80 | 0.0876 | 0.9906 |
| 73.90 | 0.1145 | 0.9915 |
| 96.20 | 0.1428 | 0.9917 |

| | | |
|---|---|---|
| 120.70 | 0.1729 | 0.9916 |
| 143.70 | 0.2003 | 0.9915 |
| 170.70 | 0.2317 | 0.9912 |
| 195.80 | 0.2563 | 0.9905 |
| 219.90 | 0.2808 | 0.9900 |
| 246.80 | 0.3078 | 0.9893 |
| 268.70 | 0.3295 | 0.9887 |
| 294.60 | 0.3546 | 0.9877 |
| 321.30 | 0.3786 | 0.9870 |
| 344.70 | 0.3974 | 0.9864 |
| 370.10 | 0.4189 | 0.9852 |
| 393.50 | 0.4391 | 0.9840 |
| 420.10 | 0.4611 | 0.9819 |
| 444.10 | 0.4815 | 0.9808 |
| 470.40 | 0.5046 | 0.9796 |
| 495.00 | 0.5234 | 0.9778 |
| 503.20 | 0.5300 | 0.9771 |

García-Sánchez, Fernando - Eliosa-Jiménez, Gaudencio - Silva-Oliver, Guadalupe - García-Flores, Blanca E., Vapor-Liquid Equilibrium Data for the Nitrogen + n-Decane System from (344 to 563) K and at Pressures up to 50 MPa, Journal of Chemical & Engineering Data 5 (2009) 1560-1568. doi:10.1021/je800881t

**T / K = 463.70**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 18.30 | 0.0384 | 0.9299 |
| 22.50 | 0.0461 | 0.9385 |
| 31.90 | 0.0634 | 0.9513 |
| 45.10 | 0.0855 | 0.9604 |
| 53.10 | 0.0993 | 0.9632 |
| 69.90 | 0.1263 | 0.9673 |
| 94.60 | 0.1643 | 0.9709 |
| 120.70 | 0.2001 | 0.9725 |
| 144.80 | 0.2351 | 0.9726 |
| 219.10 | 0.3315 | 0.9705 |
| 244.60 | 0.3656 | 0.9688 |
| 270.60 | 0.3939 | 0.9673 |
| 294.30 | 0.4254 | 0.9653 |
| 319.60 | 0.4544 | 0.9629 |
| 345.80 | 0.4851 | 0.9611 |
| 369.80 | 0.5149 | 0.9578 |
| 395.40 | 0.5433 | 0.9532 |
| 421.00 | 0.5728 | 0.9502 |
| 444.60 | 0.5999 | 0.9464 |
| 472.70 | 0.6285 | 0.9381 |
| 498.40 | 0.6553 | 0.9313 |

García-Sánchez, Fernando - Eliosa-Jiménez, Gaudencio - Silva-Oliver, Guadalupe - García-Flores, Blanca E., Vapor-Liquid Equilibrium Data for the Nitrogen + n-Decane System from (344 to 563) K and at Pressures up to 50 MPa, Journal of Chemical & Engineering Data 5 (2009) 1560-1568. doi:10.1021/je800881t

**T / K = 503.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.20 | 0.0279 | 0.7515 |
| 21.40 | 0.0406 | 0.8122 |
| 27.50 | 0.0535 | 0.8477 |
| 36.40 | 0.0705 | 0.8779 |
| 45.30 | 0.0878 | 0.8957 |
| 56.10 | 0.1072 | 0.9084 |
| 69.80 | 0.1317 | 0.9179 |
| 94.90 | 0.1758 | 0.9289 |
| 119.50 | 0.2192 | 0.9358 |
| 191.20 | 0.3370 | 0.9387 |
| 219.30 | 0.3802 | 0.9368 |
| 243.80 | 0.4186 | 0.9339 |
| 267.40 | 0.4561 | 0.9309 |
| 296.00 | 0.5012 | 0.9239 |
| 320.50 | 0.5409 | 0.9161 |
| 348.80 | 0.5878 | 0.9001 |
| 372.50 | 0.6317 | 0.8849 |
| 402.20 | 0.7053 | 0.8487 |

García-Sánchez, Fernando - Eliosa-Jiménez, Gaudencio - Silva-Oliver, Guadalupe - García-Flores, Blanca E., Vapor-Liquid Equilibrium Data for the Nitrogen + n-Decane System from (344 to 563) K and at Pressures up to 50 MPa, Journal of Chemical & Engineering Data 5 (2009) 1560-1568. doi:10.1021/je800881t

**T / K = 533.50**

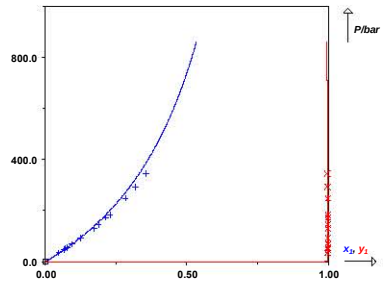
| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.40 | 0.0152 | 0.4458 |
| 14.90 | 0.0260 | 0.5759 |
| 21.00 | 0.0402 | 0.6677 |
| 26.80 | 0.0525 | 0.7204 |
| 36.50 | 0.0735 | 0.7755 |
| 45.50 | 0.0938 | 0.8069 |
| 55.50 | 0.1167 | 0.8322 |
| 69.50 | 0.1452 | 0.8538 |
| 93.70 | 0.1955 | 0.8752 |
| 119.50 | 0.2464 | 0.8872 |
| 144.80 | 0.2984 | 0.8899 |
| 169.60 | 0.3452 | 0.8905 |
| 195.10 | 0.3949 | 0.8854 |
| 220.80 | 0.4455 | 0.8766 |
| 244.80 | 0.4988 | 0.8655 |
| 270.30 | 0.5610 | 0.8445 |
| 296.60 | 0.6239 | 0.7848 |

García-Sánchez, Fernando - Eliosa-Jiménez, Gaudencio - Silva-Oliver, Guadalupe - García-Flores, Blanca E., Vapor-Liquid Equilibrium Data for the Nitrogen + n-Decane System from (344 to 563) K and at Pressures up to 50 MPa, Journal of Chemical & Engineering Data 5 (2009) 1560-1568. doi:10.1021/je800881t

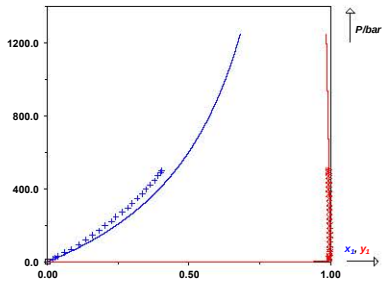
**T / K = 563.10**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.30 | 0.0212 | 0.3473 |
| 21.40 | 0.0371 | 0.4794 |
| 26.60 | 0.0526 | 0.5604 |
| 35.00 | 0.0735 | 0.6402 |
| 45.40 | 0.0997 | 0.6895 |
| 56.20 | 0.1275 | 0.7179 |
| 70.10 | 0.1632 | 0.7488 |
| 95.00 | 0.2265 | 0.7808 |
| 119.40 | 0.2891 | 0.7975 |
| 144.90 | 0.3566 | 0.7964 |
| 157.20 | 0.3945 | 0.7900 |
| 170.00 | 0.4305 | 0.7766 |
| 190.50 | 0.5000 | 0.7375 |
| 196.40 | 0.5373 | 0.7120 |

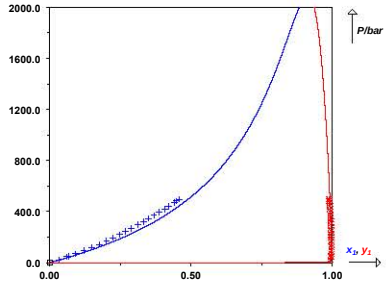
T/K = 310.93



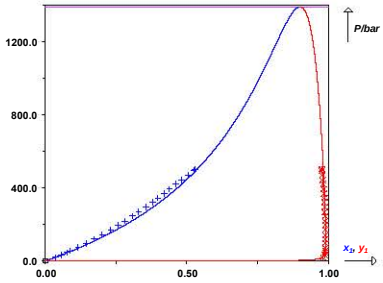

T/K = 344.60



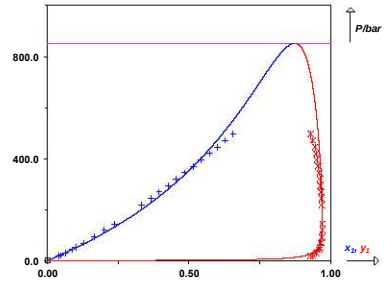

T/K = 377.40



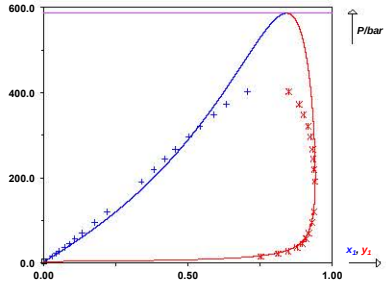

T/K = 410.90



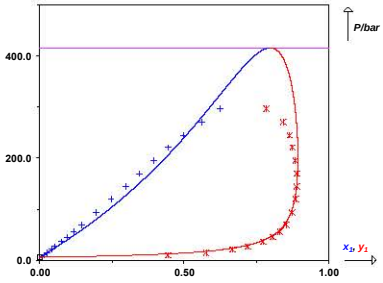

T/K = 463.70



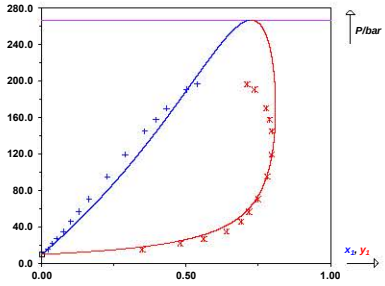

T/K = 503.00




T/K = 533.50




T/K = 563.10



## n-HEXANE (1) + CYCLOHEXANE (2)

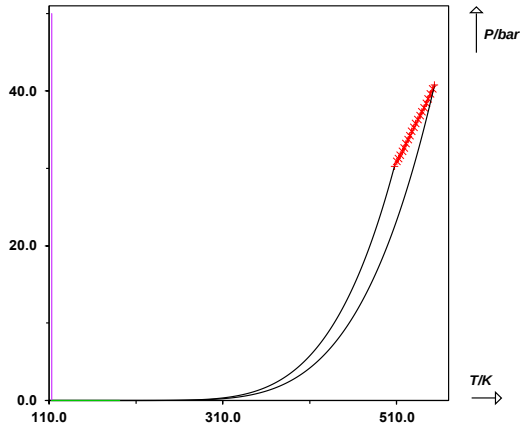
| | | |
|---|---|---|
| **CAS** | 110-54-3 | 110-82-7 |
| **InChiKey** | VLKZOEOYAKHREP-UHFFFAOYSA-N | XDTMQSROBMDMFD-UHFFFAOYSA-N |
| **$T_c$ / K** | 507.6 | 553.8 |
| **$P_c$ / bar** | 30.25 | 40.8 |
| **ω** | 0.301 | 0.208 |

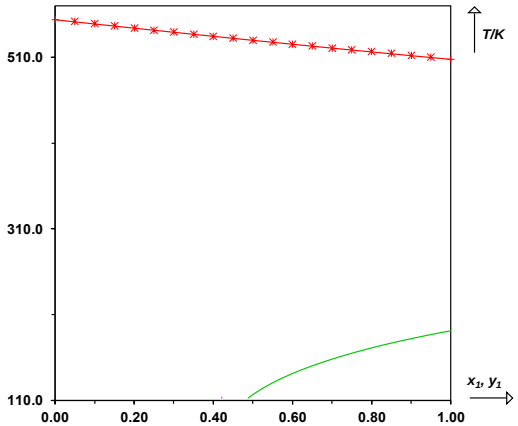
Ideal

**PPR78 results**

*Parameters*
A/MPa = 16.3
B/MPa = 45.6

*Deviations*
MAPE on x = 12 %
MAPE on y = 13 %
MAPE on $x_c$ = 2.2 %
MAPE on $P_c$ = 0.26 %
MAPE on $h^M$ = 7.8 %
MAPE on $c_P{}^M$ = 10 %



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**Isothermal phase equilibrium data**

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Martin, MI - Youings, Jc, Vapour pressures and excess Gibbs free energies of cyclohexane + n-hexane, + n-heptane and + n-octane at 298. 15 K, Australian Journal of Chemistry 10 (1980) doi:10.1071/CH9802133

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1320 | 0.0180 | 0.0330 |
| 0.1339 | 0.0361 | 0.0635 |
| 0.1355 | 0.0531 | 0.0905 |
| 0.1371 | 0.0695 | 0.1159 |
| 0.1382 | 0.0811 | 0.1332 |
| 0.1394 | 0.0944 | 0.1523 |
| 0.1434 | 0.1397 | 0.2152 |
| 0.1480 | 0.1946 | 0.2853 |
| 0.1517 | 0.2406 | 0.3400 |
| 0.1550 | 0.2824 | 0.3872 |
| 0.1578 | 0.3197 | 0.4276 |
| 0.1603 | 0.3527 | 0.4620 |
| 0.1625 | 0.3830 | 0.4924 |
| 0.1631 | 0.3951 | 0.5037 |
| 0.1639 | 0.4031 | 0.5122 |
| 0.1642 | 0.4109 | 0.5190 |
| 0.1664 | 0.4405 | 0.5476 |
| 0.1681 | 0.4661 | 0.5716 |
| 0.1702 | 0.4959 | 0.5989 |
| 0.1724 | 0.5294 | 0.6289 |
| 0.1749 | 0.5672 | 0.6622 |
| 0.1777 | 0.6089 | 0.6981 |
| 0.1809 | 0.6591 | 0.7401 |
| 0.1837 | 0.7039 | 0.7769 |
| 0.1872 | 0.7585 | 0.8205 |
| 0.1912 | 0.8243 | 0.8712 |
| 0.1946 | 0.8793 | 0.9123 |
| 0.1958 | 0.8987 | 0.9266 |
| 0.1970 | 0.9187 | 0.9411 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2121 | 0.0823 | 0.1306 |
| 0.2240 | 0.1762 | 0.2571 |
| 0.2240 | 0.1763 | 0.2574 |
| 0.2351 | 0.2724 | 0.3705 |
| 0.2359 | 0.2780 | 0.3769 |
| 0.2454 | 0.3673 | 0.4713 |
| 0.2542 | 0.4513 | 0.5538 |
| 0.2547 | 0.4559 | 0.5582 |
| 0.2634 | 0.5432 | 0.6384 |
| 0.2637 | 0.5460 | 0.6409 |
| 0.2724 | 0.6361 | 0.7189 |
| 0.2812 | 0.7286 | 0.7947 |
| 0.2895 | 0.8197 | 0.8661 |
| 0.2985 | 0.9194 | 0.9412 |

Susarev, M.P. - Chen, S.T., Calculation of vapor-liquid equilibrium in ternary systems from the data on binary systems. The system benzene-n-hexane-cyclohexane, Russ. J. Phys. Chem. 8 (1963) 938-943.

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.7733 | 0.1250 | 0.1790 |
| 0.8161 | 0.2500 | 0.3360 |
| 0.8567 | 0.3750 | 0.4650 |
| 0.9003 | 0.5000 | 0.5900 |
| 0.9402 | 0.6250 | 0.7080 |
| 0.9797 | 0.7420 | 0.8060 |
| 1.008 | 0.8750 | 0.9010 |

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**Isobaric phase equilibrium data**

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Ridgway, Kenneth - Butler, Paul Alexander, Physical properties of the ternary system benzene-cyclohexane-hexane, Journal of Chemical & Engineering Data 4 (1967) 509-515. doi:10.1021/je60035a012

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 352.65 | 0.0820 | 0.1210 |
| 352.15 | 0.1210 | 0.1670 |
| 351.35 | 0.1670 | 0.2260 |
| 350.50 | 0.2260 | 0.3000 |
| 349.90 | 0.2700 | 0.3530 |
| 349.55 | 0.3000 | 0.3840 |
| 348.85 | 0.3530 | 0.4380 |
| 348.55 | 0.3840 | 0.4680 |
| 347.85 | 0.4380 | 0.5230 |
| 346.85 | 0.5230 | 0.6020 |
| 346.05 | 0.5910 | 0.6710 |
| 345.20 | 0.6710 | 0.7400 |
| 344.55 | 0.7400 | 0.7920 |
| 344.00 | 0.7970 | 0.8400 |

| | | |
|---|---|---|
| 343.55 | 0.8400 | 0.8770 |
| 343.20 | 0.8770 | 0.9040 |

Myers, H.S., [Vapor-liquid] equilibrium for naphthenes and paraffins, Pet. Refiner 3 (1957) 175-178.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 353.75 | 0.0080 | 0.0180 |
| 353.50 | 0.0190 | 0.0320 |
| 353.15 | 0.0450 | 0.0700 |
| 352.90 | 0.0630 | 0.0975 |
| 352.45 | 0.0935 | 0.1350 |
| 351.80 | 0.1330 | 0.1870 |
| 351.15 | 0.1815 | 0.2470 |
| 350.30 | 0.2385 | 0.3160 |
| 349.65 | 0.2870 | 0.3730 |
| 349.20 | 0.3180 | 0.4000 |
| 348.50 | 0.3690 | 0.4575 |
| 347.95 | 0.4145 | 0.5050 |
| 347.65 | 0.4425 | 0.5335 |
| 347.40 | 0.4620 | 0.5530 |
| 346.90 | 0.4980 | 0.5835 |
| 346.75 | 0.5155 | 0.5995 |
| 346.55 | 0.5355 | 0.6175 |
| 346.40 | 0.5490 | 0.6300 |
| 345.90 | 0.5955 | 0.6730 |
| 345.25 | 0.6545 | 0.7240 |
| 344.85 | 0.6925 | 0.7575 |
| 344.55 | 0.7240 | 0.7860 |
| 344.10 | 0.7570 | 0.8080 |
| 344.05 | 0.7685 | 0.8180 |
| 343.95 | 0.7770 | 0.8295 |
| 343.70 | 0.8070 | 0.8520 |
| 343.50 | 0.8310 | 0.8715 |
| 343.30 | 0.8500 | 0.8830 |
| 343.10 | 0.8735 | 0.9020 |
| 342.90 | 0.9000 | 0.9260 |
| 342.50 | 0.9350 | 0.9500 |
| 342.20 | 0.9690 | 0.9760 |

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**Enthalpy of mixing**

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Siddiqi, M.A. - Lucas, K., An isothermal high-pressure flow calorimeter the excess enthalpy of (cyclohexane + n-hexane) at different pressures at 288.15, 298.15, and 313.15 K, The Journal of Chemical Thermodynamics 12 (1982) 1183-1190. doi:10.1016/0021-9614(82)90042-8

**T / K = 288.15**

**P / bar = 150.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 170.20 | 0.1750 |
| 194.00 | 0.2200 |
| 214.80 | 0.2660 |
| 231.30 | 0.3130 |
| 240.10 | 0.3610 |
| 241.60 | 0.4590 |
| 237.00 | 0.5090 |
| 226.40 | 0.5600 |
| 190.60 | 0.6640 |

Ewing, M.B - Marsh, K.N, The enthalpy of mixing of n-hexane + cyclohexane at 288.15 and 318.15 K, The Journal of Chemical Thermodynamics 2 (1970) 295-296. doi:10.1016/0021-9614(70)90094-7

**T / K = 288.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 9.170 | 0.0071 |
| 25.15 | 0.0199 |
| 49.39 | 0.0406 |
| 89.88 | 0.0793 |
| 121.91 | 0.1150 |
| 147.30 | 0.1482 |
| 167.34 | 0.1787 |
| 183.28 | 0.2073 |
| 195.96 | 0.2339 |
| 210.17 | 0.2707 |
| 220.06 | 0.3040 |
| 226.75 | 0.3345 |
| 231.07 | 0.3624 |
| 234.05 | 0.3962 |
| 234.85 | 0.4265 |
| 233.85 | 0.4515 |
| 233.47 | 0.4518 |
| 234.03 | 0.4540 |
| 231.67 | 0.4791 |
| 231.46 | 0.4794 |
| 227.79 | 0.5106 |
| 227.66 | 0.5109 |
| 221.54 | 0.5462 |
| 221.35 | 0.5466 |
| 214.73 | 0.5766 |
| 214.50 | 0.5767 |
| 205.51 | 0.6104 |
| 205.24 | 0.6107 |
| 193.21 | 0.6484 |
| 192.98 | 0.6487 |

| | |
|---|---|
| 176.96 | 0.6915 |
| 176.79 | 0.6917 |
| 163.32 | 0.7235 |
| 163.23 | 0.7238 |
| 147.03 | 0.7587 |
| 146.96 | 0.7589 |
| 127.42 | 0.7974 |
| 127.36 | 0.7976 |
| 103.79 | 0.8404 |
| 103.85 | 0.8405 |
| 75.21 | 0.8882 |
| 75.28 | 0.8883 |
| 40.50 | 0.9418 |
| 40.69 | 0.9418 |
| 20.63 | 0.9711 |
| 20.46 | 0.9711 |
| 7.340 | 0.9898 |
| 7.140 | 0.9898 |

Siddiqi, M.A. - Lucas, K., An isothermal high-pressure flow calorimeter the excess enthalpy of (cyclohexane + n-hexane) at different pressures at 288.15, 298.15, and 313.15 K, The Journal of Chemical Thermodynamics 12 (1982) 1183-1190. doi:10.1016/0021-9614(82)90042-8

**T / K = 298.15**

**P / bar = 150.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 160.30 | 0.1750 |
| 185.50 | 0.2200 |
| 203.50 | 0.2660 |
| 226.10 | 0.3610 |
| 230.10 | 0.4090 |
| 230.40 | 0.4590 |
| 215.80 | 0.5600 |
| 211.80 | 0.5730 |
| 201.00 | 0.6110 |
| 165.20 | 0.7180 |

Christensen, J.J. - Izatt, R.M. - Eatough, D.J. - Hansen, L.D., The effect of pressure on the excess enthalpies of cyclohexane + n-hexane at 298.15 K, The Journal of Chemical Thermodynamics 1 (1978) 25-34. doi:10.1016/0021-9614(78)90145-3

**T / K = 298.15**

**P / bar = 69.81**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 90.23 | 0.0829 |
| 115.15 | 0.1117 |
| 124.59 | 0.1255 |
| 146.59 | 0.1553 |
| 151.83 | 0.1629 |
| 150.72 | 0.1630 |
| 154.65 | 0.1690 |
| 176.62 | 0.2063 |
| 178.62 | 0.2133 |
| 190.74 | 0.2360 |
| 195.11 | 0.2486 |
| 195.55 | 0.2506 |
| 198.52 | 0.2585 |
| 210.09 | 0.2992 |
| 213.11 | 0.3045 |
| 217.03 | 0.3233 |
| 219.52 | 0.3386 |
| 220.16 | 0.3411 |
| 220.72 | 0.3477 |
| 221.67 | 0.3516 |
| 225.98 | 0.3818 |
| 225.30 | 0.3995 |
| 227.11 | 0.4314 |
| 226.00 | 0.4354 |
| 225.30 | 0.4485 |
| 221.27 | 0.4985 |
| 217.73 | 0.5268 |
| 218.24 | 0.5293 |
| 213.50 | 0.5495 |
| 207.14 | 0.5782 |
| 200.84 | 0.6016 |
| 192.25 | 0.6316 |
| 191.94 | 0.6346 |
| 190.88 | 0.6355 |
| 184.66 | 0.6549 |
| 173.90 | 0.6812 |
| 163.82 | 0.7093 |
| 148.66 | 0.7414 |
| 148.75 | 0.7424 |
| 148.79 | 0.7437 |
| 148.71 | 0.7453 |
| 139.65 | 0.7649 |
| 111.30 | 0.8217 |
| 78.16 | 0.8798 |

Heintz, A. - Lichtenthaler, R. N., An Isothermal Flow Calorimeter for Pressures to 600 bar, Berichte der Bunsengesellschaft für physikalische Chemie 8 (1979) 853-856. doi:10.1002/bbpc.19790830816

**T / K = 298.15**

**P / bar = 150.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|

| | |
|---|---|
| 136.80 | 0.1430 |
| 158.70 | 0.1690 |
| 182.00 | 0.2130 |
| 230.00 | 0.4530 |
| 204.90 | 0.6080 |
| 160.90 | 0.7140 |

Siddiqi, M.A. - Lucas, K., An isothermal high-pressure flow calorimeter the excess enthalpy of (cyclohexane + n-hexane) at different pressures at 288.15, 298.15, and 313.15 K, The Journal of Chemical Thermodynamics 12 (1982) 1183-1190. doi:10.1016/0021-9614(82)90042-8

**T / K = 313.15**

**P / bar = 150.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 140.50 | 0.1750 |
| 164.10 | 0.2200 |
| 182.20 | 0.2660 |
| 196.20 | 0.3130 |
| 205.20 | 0.3610 |
| 213.50 | 0.4590 |
| 209.70 | 0.5090 |
| 202.00 | 0.5600 |
| 190.80 | 0.6110 |
| 175.10 | 0.6640 |
| 154.90 | 0.7180 |

Siddiqi, M.A. - Lucas, K., An isothermal high-pressure flow calorimeter the excess enthalpy of (cyclohexane + n-hexane) at different pressures at 288.15, 298.15, and 313.15 K, The Journal of Chemical Thermodynamics 12 (1982) 1183-1190. doi:10.1016/0021-9614(82)90042-8

**T / K = 313.15**

**P / bar = 1.0000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 149.80 | 0.7180 |
| 169.30 | 0.6640 |
| 183.00 | 0.6110 |
| 194.80 | 0.5600 |
| 202.50 | 0.5090 |
| 206.00 | 0.4590 |
| 200.30 | 0.3610 |
| 190.60 | 0.3130 |
| 177.70 | 0.2660 |
| 158.30 | 0.2200 |
| 136.90 | 0.1750 |

Gmehling, J. - Meents, B., Excess enthalpy. Cyclohexane-hexane system, Int. Data Ser. Sel. Data Mixtures Ser. A 3 (1992)

**T / K = 332.65**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 16.19 | 0.0186 |
| 40.28 | 0.0468 |
| 73.05 | 0.0944 |
| 105.27 | 0.1430 |
| 128.67 | 0.1925 |
| 145.16 | 0.2429 |
| 160.47 | 0.2944 |
| 164.89 | 0.3468 |
| 173.92 | 0.4003 |
| 172.90 | 0.4548 |
| 172.78 | 0.4548 |
| 171.13 | 0.4548 |
| 171.25 | 0.5105 |
| 159.41 | 0.5673 |
| 151.35 | 0.6253 |
| 133.41 | 0.6845 |
| 115.82 | 0.7449 |
| 95.42 | 0.8066 |
| 62.94 | 0.8697 |
| 36.96 | 0.9341 |
| 18.17 | 0.9735 |

Gmehling, J. - Krentscher, B., Excess enthalpies of 12 binary liquid mixtures containing cyclohexane at elevated temperatures and pressures (up to 416 K and 1.9 MPa), ELDATA Int. Electron. J. Phys.-Chem. Data 3 (1995) 181-190.

**T / K = 413.21**

**P / bar = 11.34**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 33.01 | 0.0846 |
| 56.67 | 0.1721 |
| 72.17 | 0.2627 |
| 80.68 | 0.3566 |
| 80.90 | 0.4540 |
| 77.08 | 0.5550 |
| 65.89 | 0.6599 |
| 47.97 | 0.7688 |
| 24.84 | 0.8821 |

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**Heat capacity of mixing**

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Saito, Akemi - Tanaka, Reiji, Excess volumes and heat capacities of binary mixtures formed from cyclohexane, hexane, and heptane at 298.15 K, The Journal of Chemical Thermodynamics 7 (1988) 859-865. doi:10.1016/0021-9614(88)90075-4

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.2730 | 0.0394 |
| -0.4700 | 0.0712 |
| -0.9960 | 0.1792 |
| -1.127 | 0.6701 |
| -0.8830 | 0.7638 |
| -0.5830 | 0.8535 |
| -0.1950 | 0.9533 |
| -0.4550 | 0.0686 |
| -0.7320 | 0.1194 |
| -0.9250 | 0.1627 |
| -1.106 | 0.2129 |
| -1.234 | 0.2600 |
| -1.326 | 0.3093 |
| -1.397 | 0.3757 |
| -1.419 | 0.4145 |
| -1.417 | 0.4573 |
| -1.356 | 0.5367 |
| -1.225 | 0.6228 |
| -0.7600 | 0.8027 |
| -0.4180 | 0.9006 |

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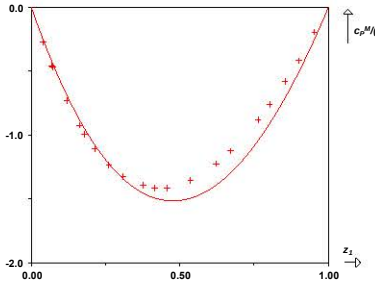
**Critical point**

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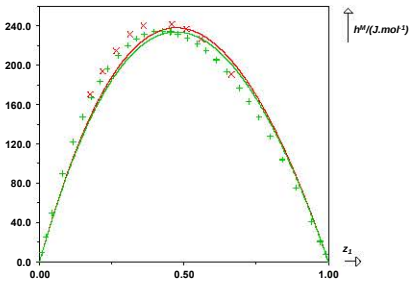
Hissong, D.W. - Kay, W.B., Critical properties of hydrocarbons. II. Correlational studies, Proc. Am. Pet. Inst. Refin. Dep. (1968) 397-463.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 510.18 | 30.88 | 0.9500 |
| 512.37 | 31.25 | 0.9000 |
| 514.47 | 31.72 | 0.8500 |
| 516.59 | 32.17 | 0.8000 |
| 518.75 | 32.66 | 0.7500 |
| 520.95 | 33.17 | 0.7000 |
| 523.18 | 33.70 | 0.6500 |
| 525.40 | 34.24 | 0.6000 |
| 527.62 | 34.76 | 0.5500 |
| 529.83 | 35.28 | 0.5000 |
| 532.15 | 35.79 | 0.4500 |
| 534.50 | 36.29 | 0.4000 |
| 536.87 | 36.80 | 0.3500 |
| 539.25 | 37.31 | 0.3000 |
| 541.69 | 37.85 | 0.2500 |
| 544.15 | 38.40 | 0.2000 |
| 546.65 | 38.99 | 0.1500 |
| 549.12 | 39.60 | 0.1000 |
| 551.60 | 40.25 | 0.0500 |

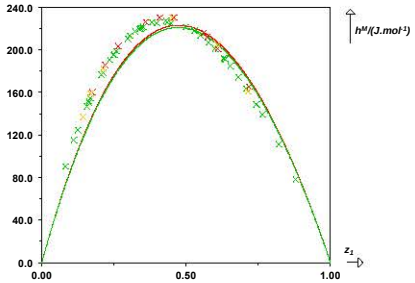
T/K = 298.15 - P/bar = 1.0132



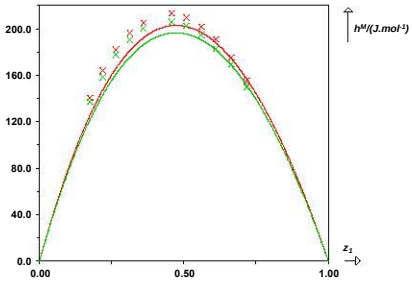

T/K = 288.15 - P/bar = 150.00 1.0132



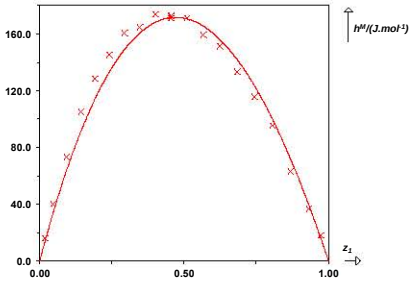

T/K = 298.15 - P/bar = 150.00 69.8100 150.00



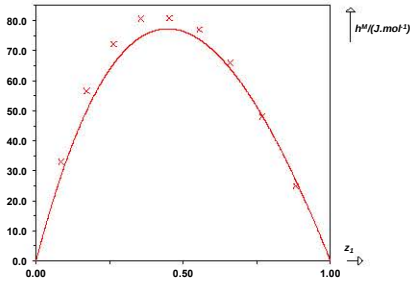

T/K = 313.15 - P/bar = 150.00 1.00



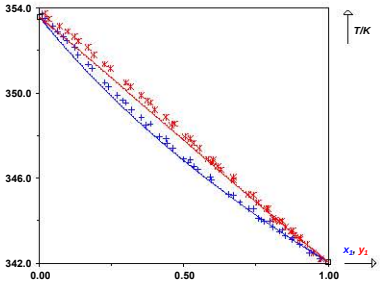

T/K = 332.65 - P/bar = 4.00



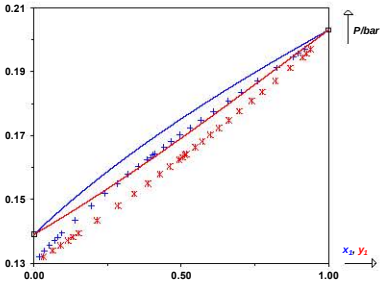

T/K = 413.21 - P/bar = 11.3400



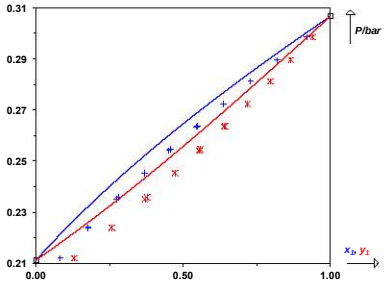

P/bar = 1.01330



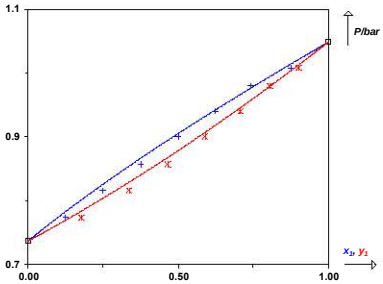

T/K = 298.15



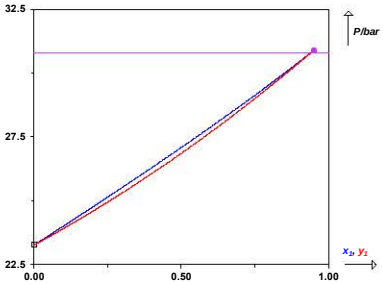

T/K = 308.15



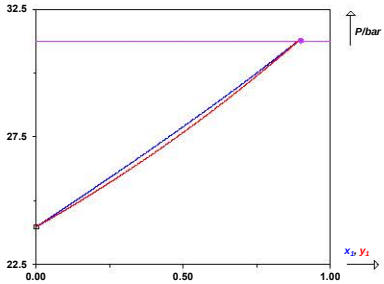

T/K = 343.15



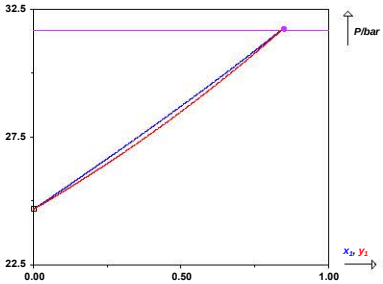

T/K = 510.18



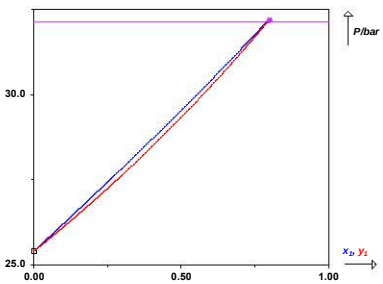

T/K = 512.37



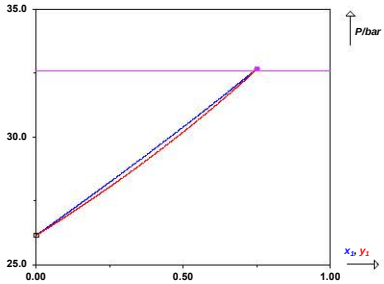

T/K = 514.47



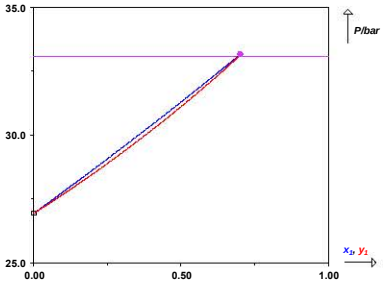

T/K = 516.59



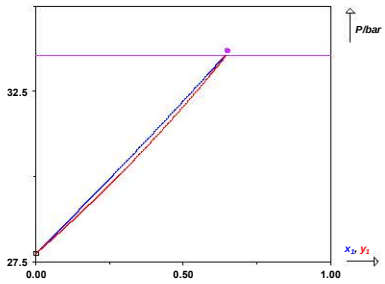

T/K = 518.75



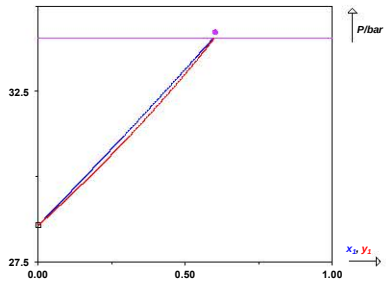
T/K = 520.95



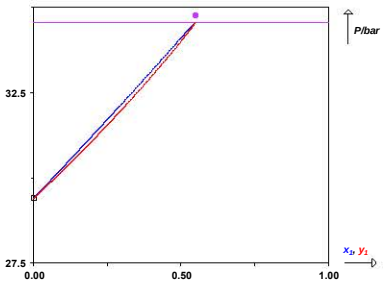

T/K = 523.18



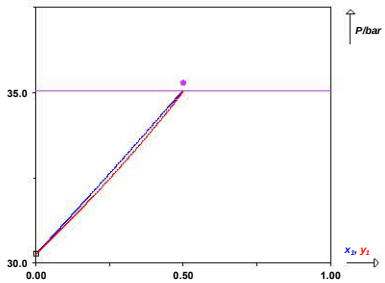

T/K = 525.40



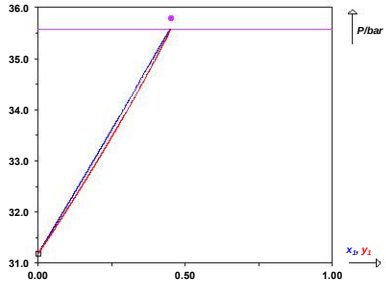

T/K = 527.62



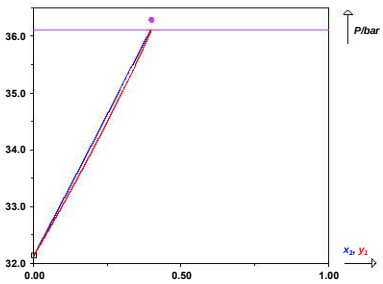

T/K = 529.83



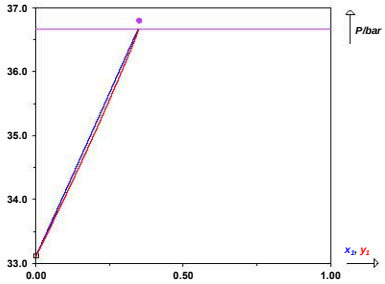

T/K = 532.15



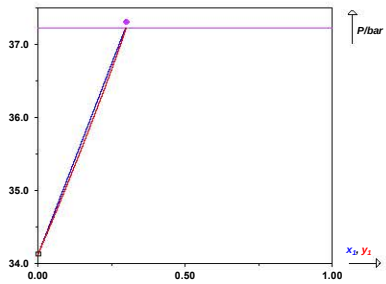

T/K = 534.50



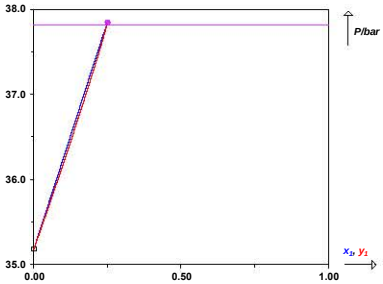

T/K = 536.87



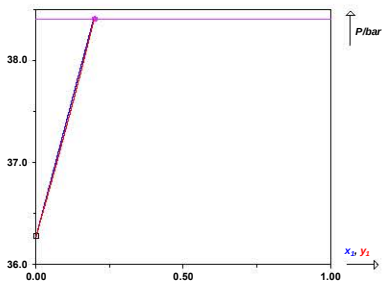

T/K = 539.25



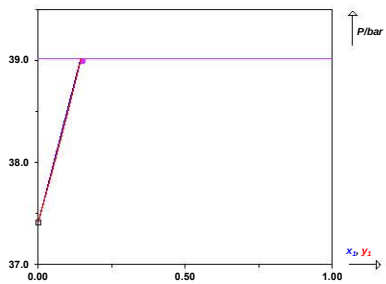

T/K = 541.69



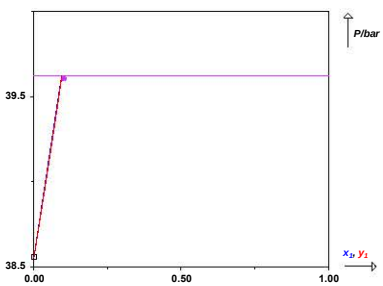

T/K = 544.15



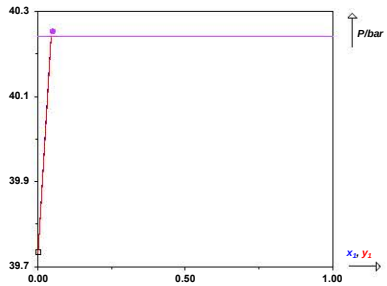

T/K = 546.65




T/K = 549.12




T/K = 551.60



## BENZENE (1) + TOLUENE (2)

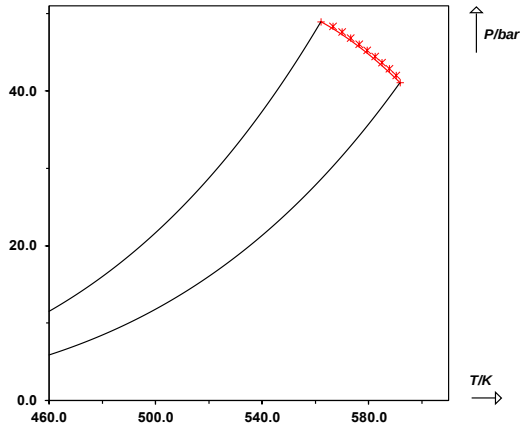
| | | |
|---|---|---|
| **CAS** | 71-43-2 | 108-88-3 |
| **InChiKey** | UHOVQNZJYSORNB-UHFFFAOYSA-N | YXFVVABEGXRONW-UHFFFAOYSA-N |
| **$T_c$ / K** | 562.05 | 591.75 |
| **$P_c$ / bar** | 48.95 | 41.08 |
| **ω** | 0.210 | 0.264 |

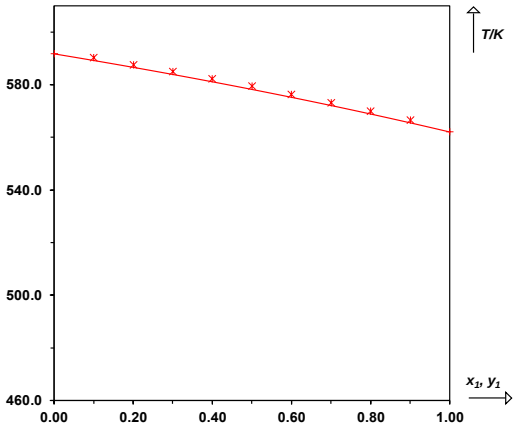
Ideal

**PPR78 results**

*Parameters*
A/MPa = 7.35
B/MPa = 16.3

*Deviations*
MAPE on x = 3.9 %
MAPE on y = 3.6 %
MAPE on $x_c$ = 10 %
MAPE on $P_c$ = 0.73 %
MAPE on $h^M$ = 5.3 %
MAPE on $c_P^M$ = 5.6 %



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**Isothermal phase equilibrium data**

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Kassmann, K.-D. - Knapp, H., Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Benzene, Toluene and n-Butyraldehyde, Berichte der Bunsengesellschaft für physikalische Chemie 5 (1986) 452-458. doi:10.1002/bbpc.19860900514

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0854 | 0.0401 | 0.1128 |
| 0.0952 | 0.0992 | 0.2514 |
| 0.1197 | 0.2484 | 0.5020 |
| 0.1309 | 0.3094 | 0.5839 |
| 0.1335 | 0.3315 | 0.6012 |
| 0.1431 | 0.3854 | 0.6599 |
| 0.1561 | 0.4673 | 0.7273 |
| 0.1678 | 0.5398 | 0.7801 |
| 0.1812 | 0.6209 | 0.8312 |
| 0.1962 | 0.7068 | 0.8797 |
| 0.2089 | 0.7899 | 0.9181 |
| 0.2208 | 0.8616 | 0.9490 |
| 0.2328 | 0.9352 | 0.9773 |

Kassmann, K.-D. - Knapp, H., Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Benzene, Toluene and n-Butyraldehyde, Berichte der Bunsengesellschaft für physikalische Chemie 5 (1986) 452-458. doi:10.1002/bbpc.19860900514

**T / K = 334.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2157 | 0.0622 | 0.1535 |
| 0.2333 | 0.1140 | 0.2589 |
| 0.2517 | 0.1680 | 0.3516 |
| 0.2752 | 0.2334 | 0.4519 |
| 0.2996 | 0.3003 | 0.5390 |
| 0.3121 | 0.3368 | 0.5802 |
| 0.3433 | 0.4288 | 0.6683 |
| 0.3620 | 0.4799 | 0.7128 |
| 0.3999 | 0.5873 | 0.7949 |
| 0.4233 | 0.6571 | 0.8372 |
| 0.4692 | 0.7891 | 0.9091 |
| 0.4856 | 0.8374 | 0.9332 |
| 0.5065 | 0.8981 | 0.9574 |
| 0.5235 | 0.9478 | 0.9810 |

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**Isobaric phase equilibrium data**

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Saito, S., Separation of hydrocarbons. 2. Vapor-liquid equilibriums of normal paraffin-aromatic systems, Asahi Garasu Kogyo Gijutsu Shoreikai Kenkyu Hokoku (1969) 397-407.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 381.85 | 0.0520 | 0.1100 |
| 380.35 | 0.0830 | 0.1720 |
| 379.05 | 0.1190 | 0.2380 |
| 378.25 | 0.1410 | 0.2740 |
| 377.05 | 0.1730 | 0.3220 |
| 375.95 | 0.1940 | 0.3600 |
| 374.65 | 0.2240 | 0.4020 |
| 373.75 | 0.2530 | 0.4340 |
| 372.15 | 0.2990 | 0.5010 |
| 371.45 | 0.3140 | 0.5230 |
| 369.75 | 0.3660 | 0.5810 |
| 367.85 | 0.4330 | 0.6430 |
| 365.85 | 0.5020 | 0.7060 |
| 363.85 | 0.5710 | 0.7610 |
| 362.25 | 0.6210 | 0.8010 |
| 360.25 | 0.7050 | 0.8530 |
| 358.45 | 0.7690 | 0.8890 |
| 357.35 | 0.8200 | 0.9190 |
| 356.25 | 0.8790 | 0.9460 |
| 354.95 | 0.9310 | 0.9680 |
| 354.45 | 0.9610 | 0.9830 |

Zhangli Jin - Aibao Hu - Kunyuan Liu, VLE of Binary and Ternary Systems for BTX Mixtures, Chemical Engineering (China) (1991)

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 382.65 | 0.0333 | 0.0714 |
| 380.58 | 0.0780 | 0.1625 |
| 379.05 | 0.1136 | 0.2323 |
| 375.25 | 0.2056 | 0.3757 |
| 373.35 | 0.2588 | 0.4511 |
| 371.34 | 0.3179 | 0.5240 |
| 369.59 | 0.3731 | 0.5858 |
| 368.88 | 0.3952 | 0.6049 |
| 366.64 | 0.4616 | 0.6761 |
| 364.40 | 0.5326 | 0.7375 |
| 362.28 | 0.6125 | 0.7935 |
| 360.62 | 0.6742 | 0.8353 |
| 359.65 | 0.7193 | 0.8622 |
| 358.00 | 0.7832 | 0.9002 |
| 355.97 | 0.8732 | 0.9430 |
| 354.68 | 0.9315 | 0.9700 |

| | | |
|---|---|---|
| 353.67 | 0.9767 | 0.9900 |

Schuberth, Horst, Phasengleichgewichtsmessungen. II. Vorausberechnung von Gleichgewichtsdaten dampfförmig-flüssig idealer binärer Systeme und Prüfung derselben mittels einer neuen Gleichgewichtsapparatur, Journal für Praktische Chemie 2 (1958) 129-138. doi:10.1002/prac.19580060209

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 378.90 | 0.1070 | 0.2190 |
| 374.90 | 0.2070 | 0.3810 |
| 371.40 | 0.3030 | 0.5090 |
| 368.40 | 0.3930 | 0.6090 |
| 365.60 | 0.4860 | 0.6960 |
| 363.00 | 0.5780 | 0.7690 |
| 360.50 | 0.6730 | 0.8350 |
| 358.10 | 0.7730 | 0.8930 |
| 355.80 | 0.8750 | 0.9450 |

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**Enthalpy of mixing**

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Baud, E., Thermal analysis of binary mixtures, Bull. Soc. Chim. Fr. (1915) 329-345.

**T / K = 290.65**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 65.11 | 0.3240 |
| 75.33 | 0.4900 |
| 70.34 | 0.6000 |
| 56.13 | 0.7500 |
| 35.92 | 0.8570 |

Hsu, Kuei-Yen - Lawrence Clever, H, The excess enthalpies of the 15 binary mixtures formed from cyclohexane, benzene, toluene, 1,4-dimethylbenzene, 1,2,4-trimethylbenzene, and 1,3,5-trimethylbenzene at 298.15 K, The Journal of Chemical Thermodynamics 5 (1975) 435-442. doi:10.1016/0021-9614(75)90273-6

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 30.00 | 0.1374 |
| 46.23 | 0.2369 |
| 62.55 | 0.3785 |
| 66.99 | 0.4593 |
| 67.40 | 0.5443 |
| 65.02 | 0.6268 |
| 58.99 | 0.7009 |
| 49.54 | 0.7663 |
| 32.38 | 0.8650 |

Murakami, S. - Lam, V.T. - Benson, G.C., The thermodynamic properties of binary aromatic systems II. Excess enthalpies and volumes of benzene + toluene and toluene + isomeric xylene mixtures at 25 °C, The Journal of Chemical Thermodynamics 4 (1969) 397-407. doi:10.1016/0021-9614(69)90070-6

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 9.600 | 0.0393 |
| 19.10 | 0.0804 |
| 28.00 | 0.1248 |
| 37.20 | 0.1746 |
| 45.00 | 0.2227 |
| 52.60 | 0.2783 |
| 58.60 | 0.3383 |
| 63.60 | 0.3938 |
| 66.20 | 0.4395 |
| 67.80 | 0.4668 |
| 67.80 | 0.4890 |
| 68.40 | 0.5065 |
| 68.10 | 0.5317 |
| 68.10 | 0.5474 |
| 67.70 | 0.5719 |
| 66.80 | 0.5920 |
| 66.20 | 0.6090 |
| 64.20 | 0.6390 |
| 60.40 | 0.6839 |
| 54.90 | 0.7311 |
| 47.70 | 0.7848 |
| 40.80 | 0.8262 |
| 32.20 | 0.8705 |
| 23.40 | 0.9101 |
| 12.80 | 0.9533 |

Diaz Pena, M. - Menduina, C., Semicontinuous calorimeter for measuring heats of mixing, An. Quim. (1973) 857-868.

**T / K = 323.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 10.00 | 0.0358 |
| 17.00 | 0.0709 |
| 23.00 | 0.1040 |
| 28.00 | 0.1351 |
| 32.00 | 0.1630 |
| 35.00 | 0.1866 |

| | |
|---|---|
| 38.00 | 0.2112 |
| 40.00 | 0.2336 |
| 43.00 | 0.2559 |
| 45.00 | 0.2783 |
| 46.00 | 0.2970 |
| 48.00 | 0.3137 |
| 49.00 | 0.3313 |
| 50.00 | 0.3487 |
| 50.00 | 0.3655 |
| 51.00 | 0.3817 |
| 52.00 | 0.3974 |
| 52.00 | 0.4092 |
| 52.00 | 0.4206 |
| 52.00 | 0.4315 |
| 52.00 | 0.4399 |
| 52.00 | 0.5132 |
| 52.00 | 0.5412 |
| 51.00 | 0.5725 |
| 51.00 | 0.6073 |
| 50.00 | 0.6456 |
| 49.00 | 0.6887 |
| 44.00 | 0.7382 |
| 38.00 | 0.7955 |
| 29.00 | 0.8618 |
| 14.00 | 0.9411 |

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**Heat capacity of mixing**

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Fortier, Jean Luc - Benson, George C., Heat capacities of some binary aromatic hydrocarbon mixtures containing benzene or toluene, Journal of Chemical & Engineering Data 1 (1979) 34-37. doi:10.1021/je60080a015

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.1160 | 0.1127 |
| -0.2030 | 0.2055 |
| -0.2510 | 0.2937 |
| -0.3000 | 0.4070 |
| -0.3150 | 0.5006 |
| -0.3020 | 0.5946 |
| -0.2650 | 0.7031 |
| -0.2000 | 0.7968 |
| -0.1020 | 0.8930 |

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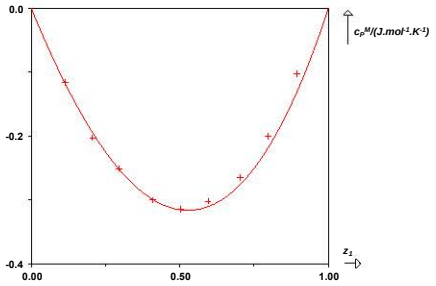
**Critical point**

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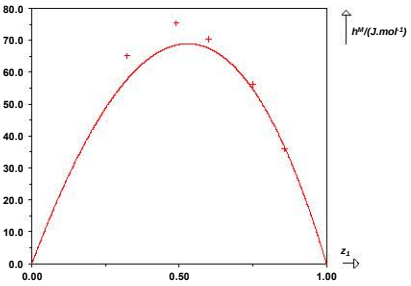
Kay, W.B. - Hissong, D., The critical properties of hydrocarbons. I. Simple mixtures, Proc. Am. Pet. Inst. Refin. Dep. (1967) 653-722.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 566.55 | 48.37 | 0.9000 |
| 569.95 | 47.61 | 0.8000 |
| 573.15 | 46.82 | 0.7000 |
| 576.35 | 46.04 | 0.6000 |
| 579.45 | 45.26 | 0.5000 |
| 582.35 | 44.46 | 0.4000 |
| 585.05 | 43.66 | 0.3000 |
| 587.65 | 42.84 | 0.2000 |
| 590.25 | 42.01 | 0.1000 |

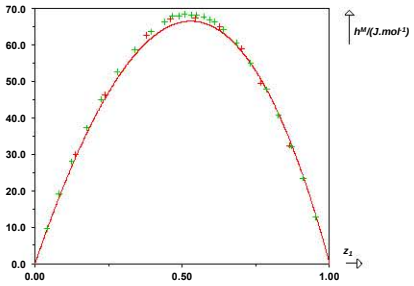
T/K = 298.15 - P/bar = 1.0132



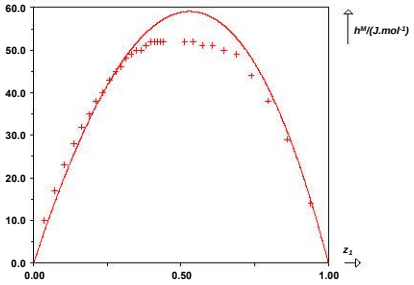

T/K = 290.65 - P/bar = 1.0132



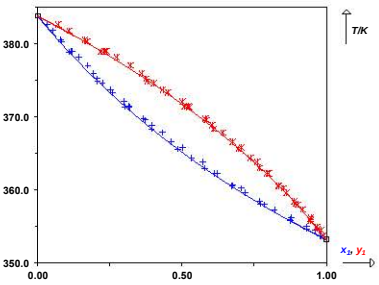

T/K = 298.15 - P/bar = 1.0132 1.0132



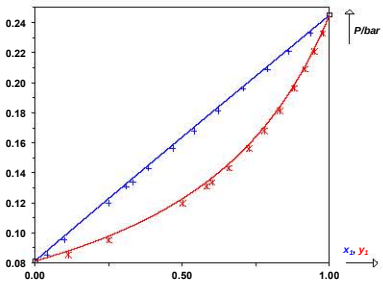

T/K = 323.15 - P/bar = 1.0132



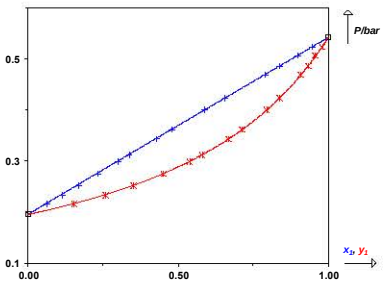

P/bar = 1.01330



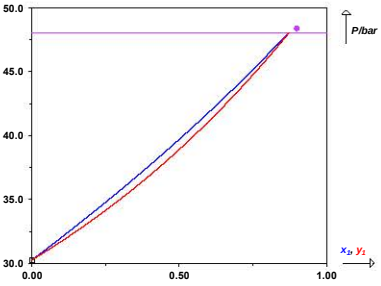

T/K = 313.15



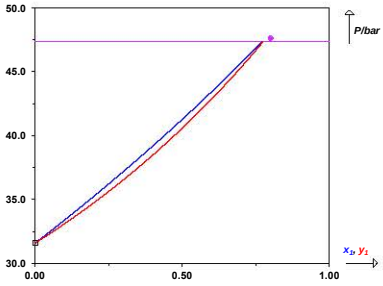

T/K = 334.15



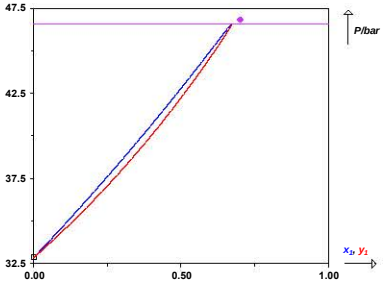

T/K = 566.55



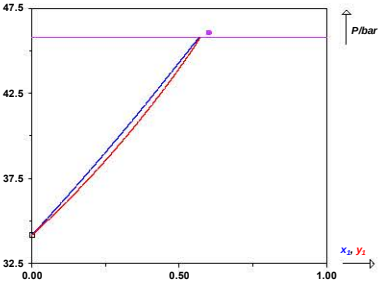

T/K = 569.95



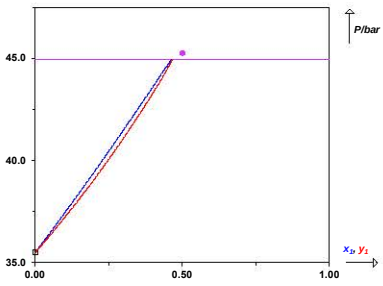

T/K = 573.15



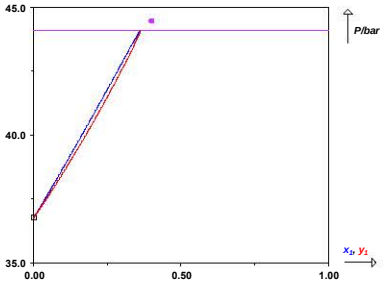

T/K = 576.35



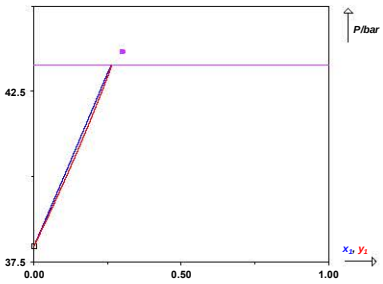

T/K = 579.45



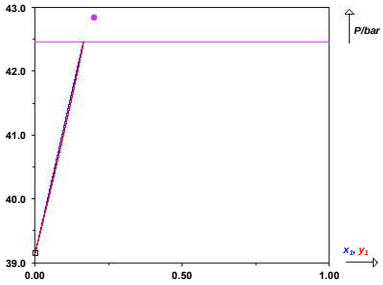
T/K = 582.35



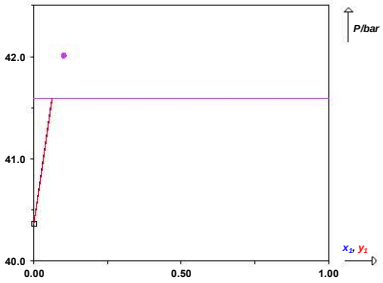

T/K = 585.05




T/K = 587.65




T/K = 590.25



## PROPANE (1) + ISOPENTANE (2)

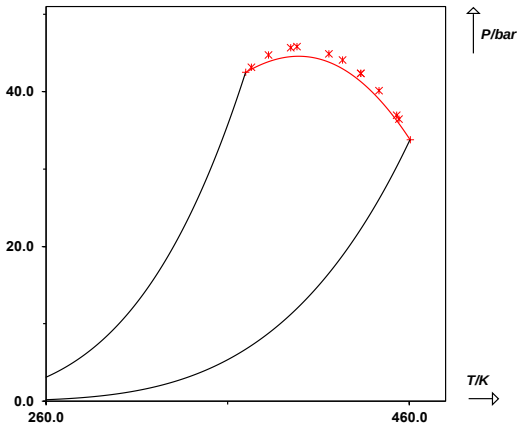
| | | |
|---|---|---|
| **CAS** | 74-98-6 | 78-78-4 |
| **InChiKey** | ATUOYWHBWRKTHZ-UHFFFAOYSA-N | QWTDNUCVQCZILF-UHFFFAOYSA-N |
| **$T_c$ / K** | 369.83 | 460.40 |
| **$P_c$ / bar** | 42.48 | 33.80 |
| **ω** | 0.152 | 0.228 |

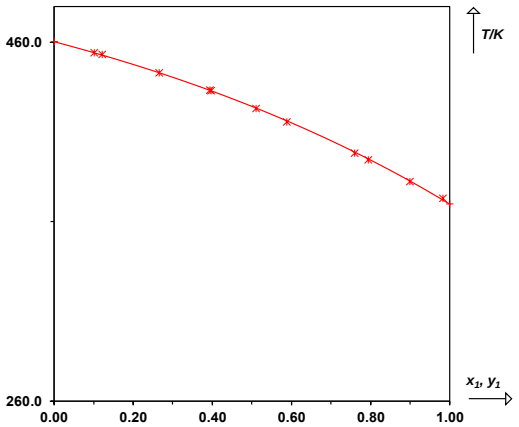
Ideal

**PPR78 results**

*Parameters*
A/MPa = 18.4
B/MPa = -3.78

*Deviations*
MAPE on x = 3.2 %
MAPE on y = 3.2 %
MAPE on $x_c$ = 3 %
MAPE on $P_c$ = 2.1 %



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**Isothermal phase equilibrium data**

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Vaughan, William E. - Collins, Frank C., P-V-T-x Relations of the System Propane-Isopentane, Industrial & Engineering Chemistry 7 (1942) 885-890. doi:10.1021/ie50391a027

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5068 | 0.0350 | 0.3510 |
| 0.7598 | 0.0880 | 0.4980 |
| 1.014 | 0.1580 | 0.7030 |
| 1.216 | 0.2120 | 0.7640 |
| 1.520 | 0.2740 | 0.8210 |
| 2.026 | 0.3900 | 0.8840 |
| 3.040 | 0.6210 | 0.9496 |
| 4.053 | 0.8500 | 0.9845 |

Vaughan, William E. - Collins, Frank C., P-V-T-x Relations of the System Propane-Isopentane, Industrial & Engineering Chemistry 7 (1942) 885-890. doi:10.1021/ie50391a027

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.520 | 0.0740 | 0.4040 |
| 2.026 | 0.1370 | 0.5810 |
| 2.533 | 0.1980 | 0.6860 |
| 3.040 | 0.2610 | 0.7540 |
| 4.053 | 0.3820 | 0.8430 |
| 5.066 | 0.5010 | 0.8970 |
| 7.093 | 0.7340 | 0.9590 |

Vaughan, William E. - Collins, Frank C., P-V-T-x Relations of the System Propane-Isopentane, Industrial & Engineering Chemistry 7 (1942) 885-890. doi:10.1021/ie50391a027

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.040 | 0.0780 | 0.3680 |
| 4.053 | 0.1500 | 0.5460 |
| 5.066 | 0.2210 | 0.6550 |
| 7.093 | 0.3580 | 0.7820 |
| 10.13 | 0.5620 | 0.8860 |
| 13.17 | 0.7610 | 0.9481 |
| 15.20 | 0.8970 | 0.9787 |

Vaughan, William E. - Collins, Frank C., P-V-T-x Relations of the System Propane-Isopentane, Industrial & Engineering Chemistry 7 (1942) 885-890. doi:10.1021/ie50391a027

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.066 | 0.0460 | 0.1970 |
| 7.093 | 0.1470 | 0.4660 |
| 8.612 | 0.2180 | 0.5810 |
| 10.13 | 0.2900 | 0.6650 |
| 13.17 | 0.4230 | 0.7730 |
| 15.20 | 0.5090 | 0.8220 |
| 20.27 | 0.7110 | 0.9070 |
| 25.33 | 0.8940 | 0.9662 |

Vaughan, William E. - Collins, Frank C., P-V-T-x Relations of the System Propane-Isopentane, Industrial & Engineering Chemistry 7 (1942) 885-890. doi:10.1021/ie50391a027

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 8.612 | 0.0490 | 0.1530 | |
| 10.13 | 0.0970 | 0.2830 | |
| 13.17 | 0.1950 | 0.4960 | |
| 15.20 | 0.2570 | 0.5770 | |
| 20.27 | 0.4140 | 0.7130 | |
| 25.33 | 0.5580 | 0.7990 | |
| 30.40 | 0.6940 | 0.8630 | |
| 32.42 | 0.7450 | 0.8840 | |
| 35.46 | 0.8200 | 0.9140 | |
| 37.49 | 0.8650 | 0.9330 | |
| 39.52 | 0.9095 | 0.9510 | |
| 40.53 | 0.9310 | 0.9600 | |
| 41.54 | 0.9520 | 0.9695 | |
| 42.56 | 0.9710 | 0.9785 | |
| 43.11 | 0.9830 | 0.9830 | CRIT |

Vaughan, William E. - Collins, Frank C., P-V-T-x Relations of the System Propane-Isopentane, Industrial & Engineering Chemistry 7 (1942) 885-890. doi:10.1021/ie50391a027

**T / K = 398.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.20 | 0.0810 | 0.2110 |
| 20.27 | 0.2050 | 0.4310 |
| 25.33 | 0.3230 | 0.5630 |
| 30.40 | 0.4370 | 0.6520 |
| 32.42 | 0.4790 | 0.6790 |
| 35.46 | 0.5390 | 0.7150 |
| 37.49 | 0.5770 | 0.7350 |
| 39.52 | 0.6130 | 0.7530 |
| 40.53 | 0.6310 | 0.7620 |
| 41.54 | 0.6490 | 0.7690 |
| 42.56 | 0.6690 | 0.7760 |
| 43.57 | 0.6910 | 0.7810 |

| | | | |
|---|---|---|---|
| 44.58 | 0.7150 | 0.7900 | |
| 45.80 | 0.7600 | 0.7600 | CRIT |

Vaughan, William E. - Collins, Frank C., P-V-T-x Relations of the System Propane-Isopentane, Industrial & Engineering Chemistry 7 (1942) 885-890. doi:10.1021/ie50391a027

**T / K = 423.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 20.27 | 0.0350 | 0.0810 | |
| 25.33 | 0.1310 | 0.2550 | |
| 30.40 | 0.2260 | 0.3760 | |
| 32.42 | 0.2640 | 0.4150 | |
| 35.46 | 0.3200 | 0.4670 | |
| 37.49 | 0.3590 | 0.4940 | |
| 39.52 | 0.3980 | 0.5170 | |
| 40.53 | 0.4170 | 0.5250 | |
| 41.54 | 0.4380 | 0.5300 | |
| 42.56 | 0.4600 | 0.5310 | |
| 43.57 | 0.4840 | 0.5250 | |
| 44.08 | 0.5100 | 0.5100 | CRIT |

Vaughan, William E. - Collins, Frank C., P-V-T-x Relations of the System Propane-Isopentane, Industrial & Engineering Chemistry 7 (1942) 885-890. doi:10.1021/ie50391a027

**T / K = 433.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 25.33 | 0.0620 | 0.1230 | |
| 30.40 | 0.1510 | 0.2570 | |
| 32.42 | 0.1880 | 0.2990 | |
| 35.46 | 0.2420 | 0.3530 | |
| 37.49 | 0.2790 | 0.3820 | |
| 39.52 | 0.3200 | 0.4030 | |
| 40.53 | 0.3420 | 0.4090 | |
| 41.54 | 0.3650 | 0.4110 | |
| 42.35 | 0.3960 | 0.3960 | CRIT |

Vaughan, William E. - Collins, Frank C., P-V-T-x Relations of the System Propane-Isopentane, Industrial & Engineering Chemistry 7 (1942) 885-890. doi:10.1021/ie50391a027

**T / K = 443.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 30.40 | 0.0770 | 0.1320 | |
| 32.42 | 0.1110 | 0.1770 | |
| 35.46 | 0.1650 | 0.2350 | |
| 37.49 | 0.2040 | 0.2610 | |
| 39.52 | 0.2470 | 0.2750 | |
| 40.13 | 0.2650 | 0.2650 | CRIT |

Vaughan, William E. - Collins, Frank C., P-V-T-x Relations of the System Propane-Isopentane, Industrial & Engineering Chemistry 7 (1942) 885-890. doi:10.1021/ie50391a027

**T / K = 453.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 32.42 | 0.0380 | 0.0570 | |
| 35.46 | 0.0900 | 0.1150 | |
| 36.98 | 0.1220 | 0.1220 | CRIT |

---

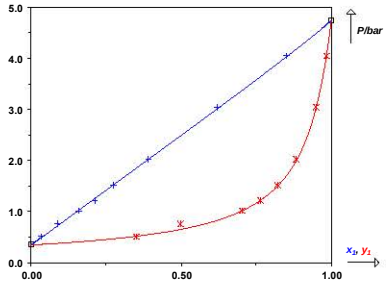
**Critical point**

---

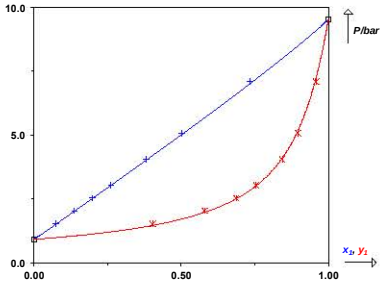
Vaughan, William E. - Collins, Frank C., P-V-T-x Relations of the System Propane-Isopentane, Industrial & Engineering Chemistry 7 (1942) 885-890. doi:10.1021/ie50391a027

| T / K | P / bar | $x_1$ |
|---|---|---|
| 382.45 | 44.74 | 0.8990 |
| 394.55 | 45.70 | 0.7940 |
| 415.55 | 44.89 | 0.5880 |
| 433.35 | 42.33 | 0.3930 |
| 454.25 | 36.43 | 0.1010 |

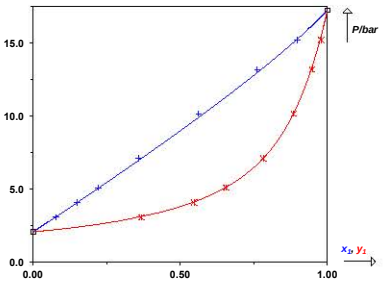
T/K = 273.15



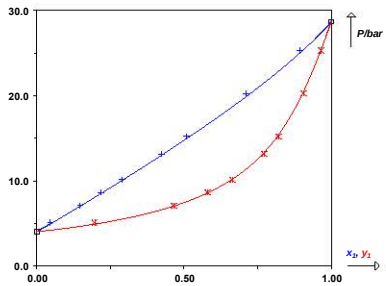

T/K = 298.15



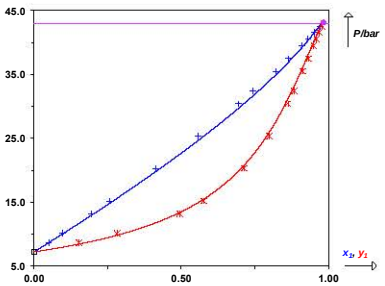

T/K = 323.15



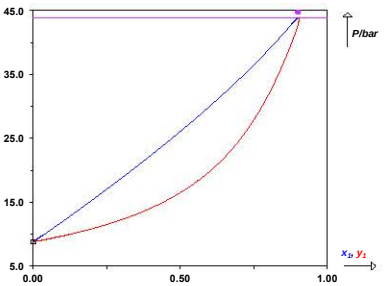

T/K = 348.15



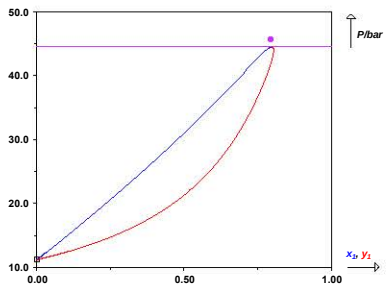

T/K = 373.15



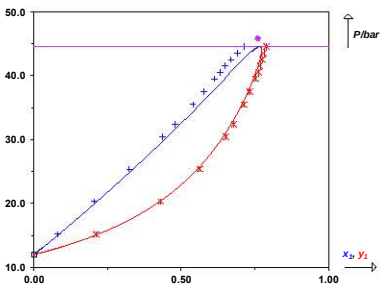

T/K = 382.45



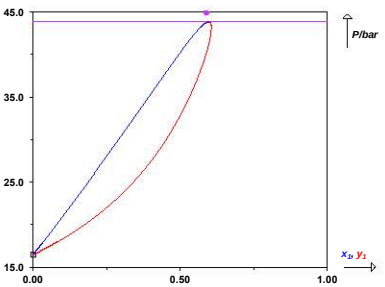

T/K = 394.55



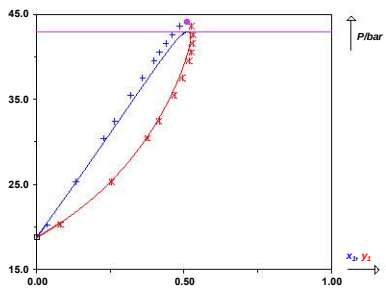

T/K = 398.15



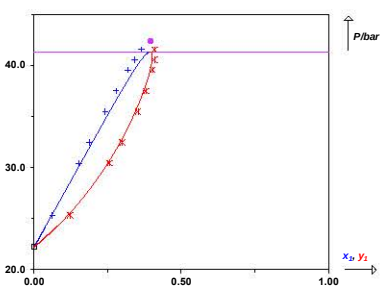

T/K = 415.55



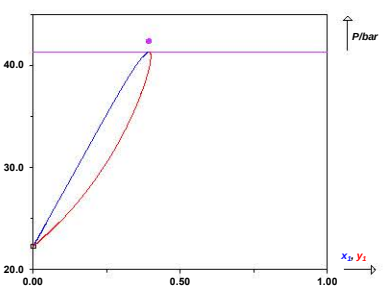

T/K = 423.15



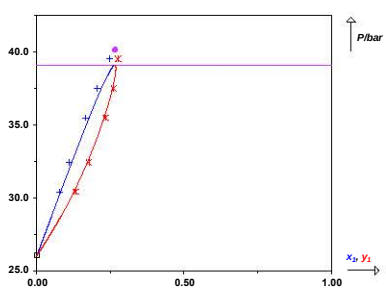

T/K = 433.15



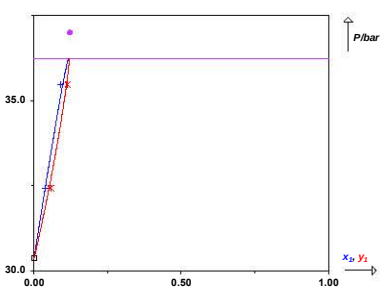

T/K = 433.35



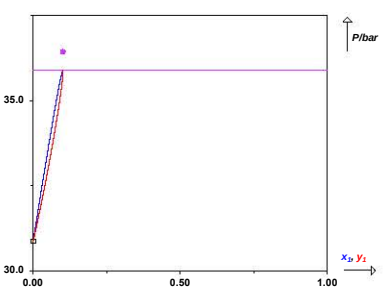

T/K = 443.15




T/K = 453.15




T/K = 454.25



## CYCLOHEXANE (1) + METHYLCYCLOHEXANE (2)

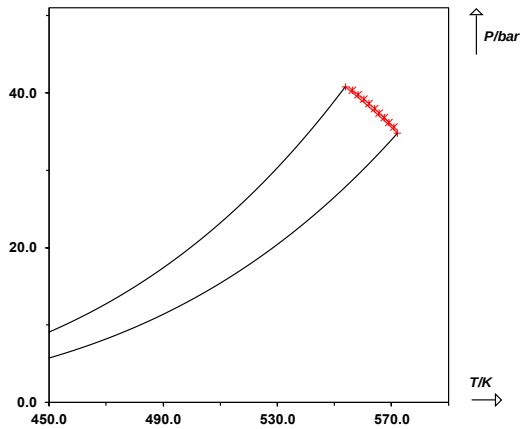
| | | |
|---|---|---|
| **CAS** | 110-82-7 | 108-87-2 |
| **InChiKey** | XDTMQSROBMDMFD-UHFFFAOYSA-N | UAEPNZWRGJTJPN-UHFFFAOYSA-N |
| **$T_c$ / K** | 553.80 | 572.10 |
| **$P_c$ / bar** | 40.80 | 34.80 |
| **ω** | 0.208 | 0.236 |

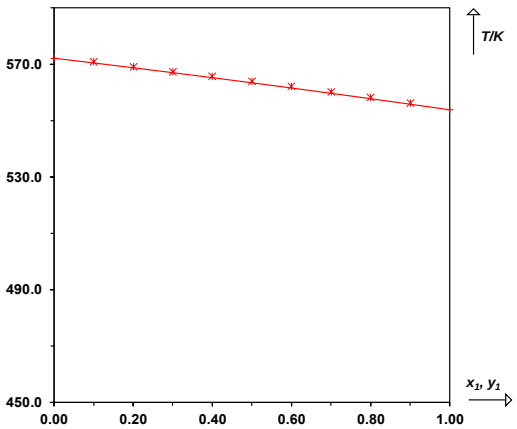
Ideal

**PPR78 results**

*Parameters*
A/MPa = 1.7
B/MPa = -0.0011

*Deviations*
MAPE on x = 14 %
MAPE on y = 14 %
MAPE on $x_c$ = 7.4 %
MAPE on $P_c$ = 0.9 %
MAPE on $h^M$ = 97 %
MAPE on $c_P^M$ = 98 %



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**Isothermal phase equilibrium data**

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Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1065 | 0.0814 | 0.1535 |
| 0.1165 | 0.1767 | 0.3055 |
| 0.1258 | 0.2668 | 0.4263 |
| 0.1352 | 0.3587 | 0.5325 |
| 0.1445 | 0.4489 | 0.6235 |
| 0.1535 | 0.5371 | 0.7017 |
| 0.1596 | 0.5977 | 0.7503 |
| 0.1627 | 0.6283 | 0.7735 |
| 0.1706 | 0.7056 | 0.8285 |
| 0.1803 | 0.8007 | 0.8898 |
| 0.1903 | 0.8995 | 0.9472 |
| 0.1924 | 0.9197 | 0.9582 |
| 0.1965 | 0.9596 | 0.9794 |

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**Isobaric phase equilibrium data**

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Zhang, X. - Zheng, Y. - Zhao, W., Measurement and correlation of vapor liquid equilibrium data for benzene cyclohexane methyl cyclohexane DMF systems, Natural Gas Chemical Industry 5 (1997) 52-55.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 373.30 | 0.0256 | 0.0431 |
| 371.70 | 0.0833 | 0.1351 |
| 370.90 | 0.1183 | 0.1962 |
| 370.50 | 0.1398 | 0.2137 |
| 369.00 | 0.2006 | 0.2966 |
| 367.90 | 0.2420 | 0.3519 |
| 367.20 | 0.2719 | 0.3918 |
| 366.60 | 0.2975 | 0.4228 |
| 366.00 | 0.3286 | 0.4576 |
| 365.40 | 0.3580 | 0.4925 |
| 364.90 | 0.3850 | 0.5195 |
| 362.80 | 0.4867 | 0.6209 |
| 360.80 | 0.5825 | 0.7098 |
| 359.60 | 0.6512 | 0.7689 |
| 358.40 | 0.7190 | 0.8182 |
| 357.90 | 0.7551 | 0.8432 |
| 357.30 | 0.7874 | 0.8676 |
| 356.80 | 0.8132 | 0.8839 |
| 356.30 | 0.8466 | 0.9077 |
| 355.80 | 0.8765 | 0.9263 |
| 355.50 | 0.8977 | 0.9381 |
| 355.10 | 0.9207 | 0.9528 |
| 354.80 | 0.9369 | 0.9640 |
| 354.50 | 0.9568 | 0.9752 |
| 354.40 | 0.9658 | 0.9811 |

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**Enthalpy of mixing**

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Howell, P.J. - Skillerne de Bristowe, B.J. - Stubley, D., Enthalpies of mixing of pentafluorobenzene with some hydrocarbons, The Journal of Chemical Thermodynamics 2 (1972) 225-231. doi:10.1016/0021-9614(72)90060-2

**T / K = 293.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 5.090 | 0.0473 |
| 9.090 | 0.0928 |
| 12.21 | 0.1320 |
| 18.41 | 0.2645 |
| 18.77 | 0.3402 |
| 15.76 | 0.5262 |
| 2.670 | 0.8018 |
| 0.3600 | 0.9302 |
| 0.4400 | 0.9303 |
| 0.3800 | 0.9557 |
| 0.8000 | 0.9624 |
| 0.7900 | 0.9712 |
| 0.9900 | 0.9714 |

Ott, J.B. - Marsh, K.N. - Stokes, R.H., Excess enthalpies, excess Gibbs free energies, and excess volumes for (cyclohexane + n-hexane), and excess Gibbs free energies and excess volumes for (cyclohexane + methylcyclohexane) at 298.15 and 308.15 K, The Journal of Chemical Thermodynamics 12 (1980) 1139-1148. doi:10.1016/S0021-9614(80)80006-1

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 3.530 | 0.0342 |
| 6.540 | 0.0664 |
| 11.20 | 0.1247 |
| 14.44 | 0.1762 |
| 16.73 | 0.2219 |
| 18.27 | 0.2626 |

| | |
|---|---|
| 19.41 | 0.3081 |
| 19.97 | 0.3484 |
| 20.11 | 0.3842 |
| 19.96 | 0.4161 |
| 19.55 | 0.4505 |
| 18.92 | 0.4810 |
| 18.46 | 0.4996 |
| 18.28 | 0.5069 |
| 17.97 | 0.5167 |
| 17.63 | 0.5274 |
| 17.42 | 0.5328 |
| 16.97 | 0.5459 |
| 16.66 | 0.5551 |
| 16.21 | 0.5657 |
| 15.91 | 0.5753 |
| 15.27 | 0.5869 |
| 14.22 | 0.6097 |
| 13.07 | 0.6339 |
| 11.70 | 0.6615 |
| 10.20 | 0.6907 |
| 8.560 | 0.7227 |
| 6.820 | 0.7578 |
| 4.920 | 0.7963 |
| 3.410 | 0.8299 |
| 2.040 | 0.8666 |
| 0.8300 | 0.9072 |
| 0.0300 | 0.9515 |

Ott, J.B. - Marsh, K.N. - Stokes, R.H., Excess enthalpies, excess Gibbs free energies, and excess volumes for (cyclohexane + n-hexane), and excess Gibbs free energies and excess volumes for (cyclohexane + methylcyclohexane) at 298.15 and 308.15 K, The Journal of Chemical Thermodynamics 12 (1980) 1139-1148. doi:10.1016/S0021-9614(80)80006-1

**T / K =** **308.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 3.640 | 0.0344 |
| 6.770 | 0.0664 |
| 11.78 | 0.1248 |
| 15.44 | 0.1764 |
| 18.10 | 0.2222 |
| 20.01 | 0.2629 |
| 21.58 | 0.3085 |
| 22.51 | 0.3488 |
| 22.98 | 0.3846 |
| 23.12 | 0.4165 |
| 23.02 | 0.4455 |
| 22.68 | 0.4765 |
| 22.30 | 0.4999 |
| 22.35 | 0.5060 |
| 21.97 | 0.5171 |
| 21.87 | 0.5263 |
| 21.59 | 0.5332 |
| 21.23 | 0.5489 |
| 20.97 | 0.5555 |
| 20.69 | 0.5648 |
| 20.32 | 0.5756 |
| 20.07 | 0.5815 |
| 19.37 | 0.5995 |
| 18.14 | 0.6286 |
| 16.66 | 0.6607 |
| 15.20 | 0.6899 |
| 13.49 | 0.7218 |
| 11.54 | 0.7569 |
| 9.390 | 0.7957 |
| 7.530 | 0.8295 |
| 5.560 | 0.8666 |
| 3.570 | 0.9068 |
| 1.660 | 0.9513 |
| 0.7800 | 0.9751 |

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**Heat capacity of mixing**

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Tamura, Katsutoshi, Excess heat capacities of the mixtures containing methylcyclohexane at 298.15 K, Fluid Phase Equilibria 1-2 (2001) 303-312. doi:10.1016/S0378-3812(01)00407-1

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.0900 | 0.0500 |
| -0.1800 | 0.1000 |
| -0.2300 | 0.1500 |
| -0.2800 | 0.2000 |
| -0.2600 | 0.2500 |
| -0.2300 | 0.3000 |
| -0.1600 | 0.3500 |
| -0.1200 | 0.4000 |
| -0.0300 | 0.4500 |
| 0.0200 | 0.5000 |
| 0.0800 | 0.5500 |
| 0.1500 | 0.6000 |
| 0.2200 | 0.6500 |
| 0.2600 | 0.7000 |

| | |
|---|---|
| 0.2700 | 0.7500 |
| 0.2800 | 0.8000 |
| 0.2300 | 0.8500 |
| 0.1900 | 0.9000 |
| 0.1000 | 0.9500 |
| 0.0200 | 0.9750 |

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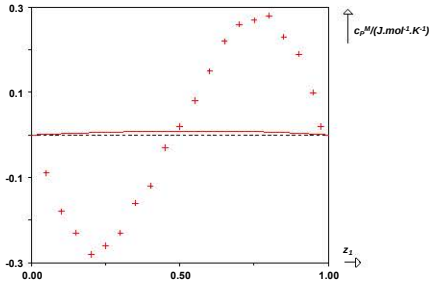
**Critical point**

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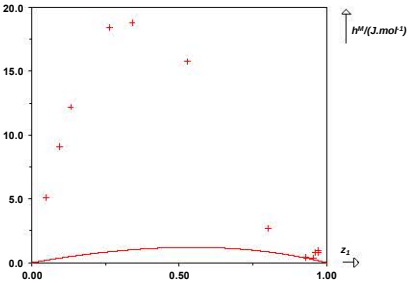
Kay, W.B. - Hissong, D., The critical properties of hydrocarbons. I. Simple mixtures, Proc. Am. Pet. Inst. Refin. Dep. (1967) 653-722.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 570.75 | 35.59 | 0.1000 |
| 569.05 | 36.19 | 0.2000 |
| 567.35 | 36.79 | 0.3000 |
| 565.65 | 37.38 | 0.4000 |
| 563.95 | 37.98 | 0.5000 |
| 562.05 | 38.58 | 0.6000 |
| 560.15 | 39.18 | 0.7000 |
| 558.25 | 39.77 | 0.8000 |
| 556.25 | 40.36 | 0.9000 |

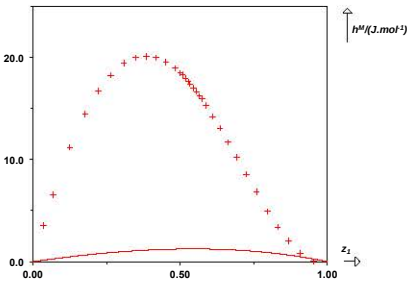
T/K = 298.15 - P/bar = 1.0132



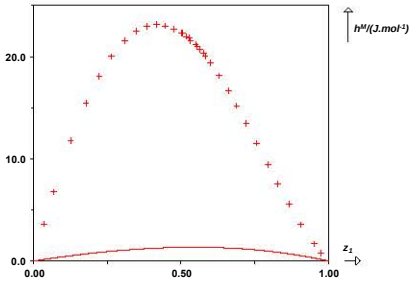

T/K = 293.15 - P/bar = 1.0132



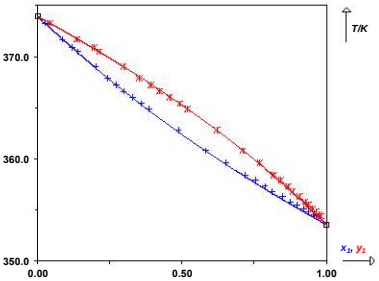

T/K = 298.15 - P/bar = 1.0132



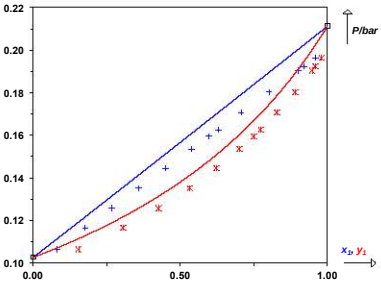

T/K = 308.15 - P/bar = 1.0132



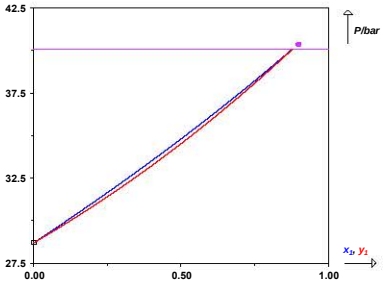

P/bar = 1.01300



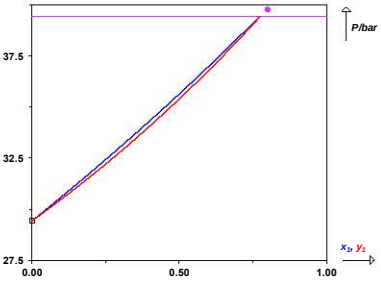

T/K = 308.15



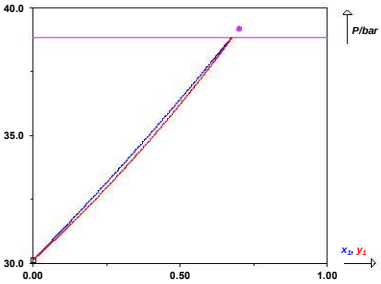

T/K = 556.25



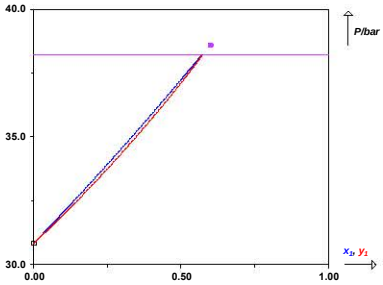

T/K = 558.25



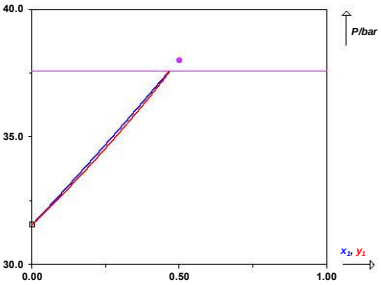

T/K = 560.15



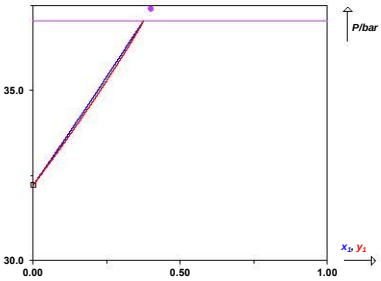

T/K = 562.05



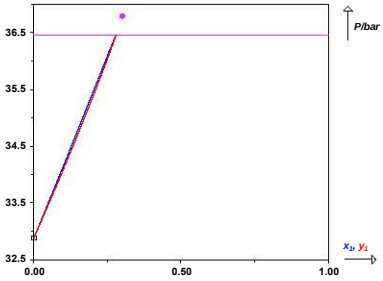

T/K = 563.95



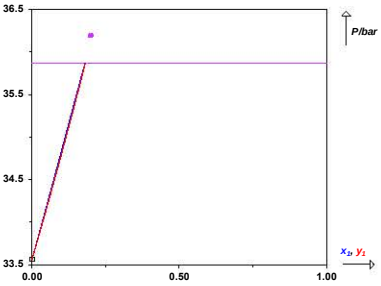

T/K = 565.65



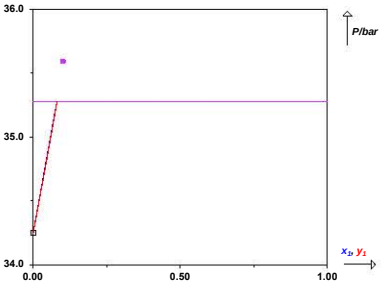

T/K = 567.35




T/K = 569.05




T/K = 570.75



## ETHANE (1) + PROPANE (2)

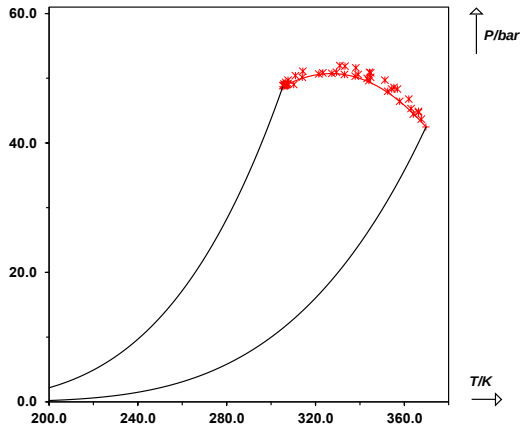
| | | |
|---|---|---|
| **CAS** | 74-84-0 | 74-98-6 |
| **InChiKey** | OTMSDBZUPAUEDD-UHFFFAOYSA-N | ATUOYWHBWRKTHZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 305.32 | 369.83 |
| **$P_c$ / bar** | 48.72 | 42.48 |
| **ω** | 0.099 | 0.152 |

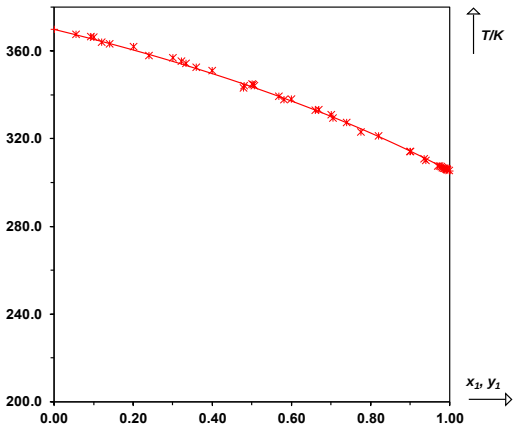
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 1.26
B/MPa = 4.9

*Deviations*
MAPE on x = 4.3 %
MAPE on y = 6.1 %
MAPE on $x_c$ = 4.4 %
MAPE on $P_c$ = 1.2 %
MAPE on $h^M$ = 51 %



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**Isothermal phase equilibrium data**

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Djordjevich, Ljubomir - Budenholzer, R. A., Vapor-liquid equilibrium data for ethane-propane system at low temperatures, Journal of Chemical & Engineering Data 1 (1970) 10-12. doi:10.1021/je60044a020

**T / K = 127.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0002 | 0.0061 | 0.3310 |
| 0.0007 | 0.0520 | 0.7875 |
| 0.0013 | 0.1180 | 0.8980 |
| 0.0023 | 0.2144 | 0.9569 |
| 0.0030 | 0.2840 | 0.9725 |
| 0.0040 | 0.3840 | 0.9820 |
| 0.0048 | 0.4664 | 0.9860 |
| 0.0054 | 0.5300 | 0.9890 |
| 0.0072 | 0.7060 | 0.9940 |
| 0.0080 | 0.7850 | 0.9950 |
| 0.0088 | 0.8650 | 0.9968 |
| 0.0093 | 0.9175 | 0.9980 |

Hirata, M. - Suda, S. - Hakuta, T. - Nagahama, K., Light hydrocarbon vapor-liquid equilibria, Mem. Fac. Technol. Tokyo Metropol. Univ. (1969) 103-122.

**T / K = 196.85**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2440 | 0.0380 | 0.2710 |
| 0.3506 | 0.1100 | 0.5630 |
| 0.4400 | 0.1640 | 0.6780 |
| 0.5800 | 0.2430 | 0.7710 |
| 0.6893 | 0.3020 | 0.8110 |
| 0.8039 | 0.3620 | 0.8530 |
| 1.053 | 0.5120 | 0.9230 |
| 1.236 | 0.6110 | 0.9500 |
| 1.367 | 0.6920 | 0.9620 |
| 1.452 | 0.7500 | 0.9720 |
| 1.632 | 0.8550 | 0.9850 |
| 1.805 | 0.9600 | 0.9960 |

Hirata, M. - Suda, S. - Hakuta, T. - Nagahama, K., Light hydrocarbon vapor-liquid equilibria, Mem. Fac. Technol. Tokyo Metropol. Univ. (1969) 103-122.

**T / K = 202.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2840 | 0.0290 | 0.2270 |
| 0.3226 | 0.0500 | 0.3410 |
| 0.4213 | 0.1050 | 0.5080 |
| 0.5626 | 0.1710 | 0.6530 |
| 0.8626 | 0.3150 | 0.8070 |
| 1.019 | 0.4000 | 0.8560 |
| 1.149 | 0.4550 | 0.8900 |
| 1.269 | 0.5160 | 0.9120 |
| 1.461 | 0.6000 | 0.9350 |
| 1.669 | 0.6780 | 0.9560 |
| 1.849 | 0.7490 | 0.9690 |
| 2.116 | 0.8700 | 0.9870 |
| 2.320 | 0.9580 | 0.9960 |

Skripka, V.G. - Nikitina, I.E. - Zhdanovich, L.A. - Sirotin, A.G. - Ben'yaminovich, O.A., Liquid-vapor phase equilibriums at low temperatures in binary systems formed by components of natural gas, Gazov. Promst. 1 (1970) 35-36.

**T / K = 213.15**

| P / bar | $y_1$ |
|---|---|
| 0.4609 | 0.0500 |
| 0.6276 | 0.2000 |
| 0.8532 | 0.4000 |
| 1.079 | 0.6000 |
| 1.471 | 0.8000 |
| 2.648 | 0.9500 |

Skripka, V.G. - Nikitina, I.E. - Zhdanovich, L.A. - Sirotin, A.G. - Ben'yaminovich, O.A., Liquid-vapor phase equilibriums at low temperatures in binary systems formed by components of natural gas, Gazov. Promst. 1 (1970) 35-36.

**T / K = 213.15**

| P / bar | $x_1$ |
|---|---|
| 0.5590 | 0.0500 |
| 1.000 | 0.2000 |
| 1.677 | 0.4000 |
| 2.393 | 0.6000 |
| 3.119 | 0.8000 |
| 3.609 | 0.9500 |

Blanc, Claude J. - Setier, Jean Claude B., Vapor-liquid equilibria for the ethane-propane system at low temperature, Journal of Chemical & Engineering Data 2 (1988) 111-115. doi:10.1021/je00052a015

**T / K = 225.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.7820 | 0.0006 | 0.0045 |
| 0.9930 | 0.0440 | 0.2730 |
| 1.001 | 0.0447 | 0.2799 |
| 1.218 | 0.0906 | 0.4404 |
| 1.227 | 0.0936 | 0.4501 |
| 1.239 | 0.0950 | 0.4623 |
| 1.911 | 0.2305 | 0.6865 |
| 1.928 | 0.2357 | 0.6882 |

| | | |
|---|---|---|
| 2.130 | 0.2844 | 0.7370 |
| 2.216 | 0.2943 | 0.7694 |
| 2.235 | 0.2969 | 0.7704 |
| 2.334 | 0.3305 | 0.7871 |
| 2.786 | 0.4294 | 0.8394 |
| 2.799 | 0.4213 | 0.8439 |
| 3.351 | 0.5339 | 0.8908 |
| 3.363 | 0.5314 | 0.8920 |
| 3.586 | 0.5752 | 0.9096 |
| 3.600 | 0.5762 | 0.9055 |
| 4.688 | 0.7766 | 0.9590 |
| 4.703 | 0.7822 | 0.9613 |

Skripka, V.G. - Nikitina, I.E. - Zhdanovich, L.A. - Sirotin, A.G. - Ben'yaminovich, O.A., Liquid-vapor phase equilibriums at low temperatures in binary systems formed by components of natural gas, Gazov. Promst. 1 (1970) 35-36.

**T / K = 233.15**

| P / bar | $y_1$ |
|---|---|
| 1.216 | 0.0500 |
| 1.373 | 0.2000 |
| 1.628 | 0.4000 |
| 2.197 | 0.6000 |
| 3.501 | 0.8000 |
| 6.080 | 0.9500 |

Skripka, V.G. - Nikitina, I.E. - Zhdanovich, L.A. - Sirotin, A.G. - Ben'yaminovich, O.A., Liquid-vapor phase equilibriums at low temperatures in binary systems formed by components of natural gas, Gazov. Promst. 1 (1970) 35-36.

**T / K = 233.15**

| P / bar | $x_1$ |
|---|---|
| 1.412 | 0.0500 |
| 2.295 | 0.2000 |
| 3.501 | 0.4000 |
| 4.786 | 0.6000 |
| 6.296 | 0.8000 |
| 7.424 | 0.9500 |

Blanc, Claude J. - Setier, Jean Claude B., Vapor-liquid equilibria for the ethane-propane system at low temperature, Journal of Chemical & Engineering Data 2 (1988) 111-115. doi:10.1021/je00052a015

**T / K = 245.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.320 | 0.0633 | 0.3072 |
| 2.337 | 0.0647 | 0.3194 |
| 2.358 | 0.0667 | 0.3255 |
| 2.548 | 0.0917 | 0.3640 |
| 2.581 | 0.0955 | 0.3559 |
| 2.624 | 0.1004 | 0.4216 |
| 2.648 | 0.1031 | 0.4350 |
| 3.395 | 0.1939 | 0.5796 |
| 3.461 | 0.2027 | 0.5925 |
| 3.510 | 0.2041 | 0.5996 |
| 4.394 | 0.3079 | 0.7206 |
| 4.475 | 0.3167 | 0.7226 |
| 4.538 | 0.3178 | 0.7309 |
| 5.370 | 0.4202 | 0.8016 |
| 5.466 | 0.4280 | 0.8060 |
| 5.535 | 0.4303 | 0.8115 |
| 6.548 | 0.5435 | 0.8663 |
| 6.616 | 0.5497 | 0.8706 |
| 6.678 | 0.5519 | 0.8709 |
| 9.349 | 0.8339 | 0.9563 |
| 9.722 | 0.8756 | 0.9668 |
| 9.725 | 0.8733 | 0.9664 |
| 9.730 | 0.8774 | 0.9674 |
| 10.03 | 0.9014 | 0.9749 |
| 10.08 | 0.9059 | 0.9762 |
| 10.11 | 0.9084 | 0.9767 |

Blanc, Claude J. - Setier, Jean Claude B., Vapor-liquid equilibria for the ethane-propane system at low temperature, Journal of Chemical & Engineering Data 2 (1988) 111-115. doi:10.1021/je00052a015

**T / K = 255.40**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.634 | 0.0953 | 0.3380 |
| 3.637 | 0.0946 | 0.3389 |
| 4.282 | 0.1534 | 0.4648 |
| 4.289 | 0.1536 | 0.4670 |
| 5.197 | 0.2376 | 0.5986 |
| 5.210 | 0.2371 | 0.6015 |
| 5.797 | 0.2923 | 0.6589 |
| 5.807 | 0.2929 | 0.6604 |
| 5.821 | 0.2916 | 0.6593 |
| 6.669 | 0.3672 | 0.7279 |
| 6.679 | 0.3675 | 0.7299 |
| 6.712 | 0.3692 | 0.7294 |
| 7.649 | 0.4494 | 0.7876 |
| 7.664 | 0.4491 | 0.7878 |
| 7.822 | 0.4643 | 0.7985 |
| 7.945 | 0.4760 | 0.8048 |
| 9.330 | 0.5871 | 0.8613 |
| 9.387 | 0.5921 | 0.8632 |
| 9.927 | 0.6325 | 0.8814 |
| 9.942 | 0.6339 | 0.8839 |

| | | |
|---|---|---|
| 10.06 | 0.6376 | 0.8846 |
| 11.11 | 0.7246 | 0.9167 |
| 12.08 | 0.7955 | 0.9405 |
| 12.08 | 0.7982 | 0.9415 |
| 12.12 | 0.7983 | 0.9406 |
| 13.21 | 0.8780 | 0.9642 |
| 13.23 | 0.8782 | 0.9634 |

Clark, Alisdair Q - Stead, Keith, (Vapour + liquid) phase equilibria of binary, ternary, and quaternary mixtures of CH4, C2H6, C3H8, C4H10, and CO2, The Journal of Chemical Thermodynamics 4 (1988) 413-427. doi:10.1016/0021-9614(88)90178-4

**T / K = 260.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.620 | 0.0600 | 0.1700 |
| 5.017 | 0.1680 | 0.4520 |
| 6.336 | 0.2830 | 0.6120 |
| 9.366 | 0.5010 | 0.7840 |
| 11.56 | 0.6720 | 0.8990 |
| 14.10 | 0.8550 | 0.9680 |
| 15.37 | 0.9290 | 0.9800 |

Hirata, M. - Suda, S. - Hakuta, T. - Nagahama, K., Light hydrocarbon vapor-liquid equilibria, Mem. Fac. Technol. Tokyo Metropol. Univ. (1969) 103-122.

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.034 | 0.1692 | 0.4140 |
| 9.032 | 0.2889 | 0.5628 |
| 10.95 | 0.3968 | 0.6702 |
| 15.05 | 0.6372 | 0.8419 |
| 16.84 | 0.7117 | 0.8814 |

Kahre, LeRoy C., Liquid density of light hydrocarbon mixtures, Journal of Chemical & Engineering Data 3 (1973) 267-270. doi:10.1021/je60058a030

**T / K = 288.75**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.656 | 0.1078 | 0.2795 |
| 11.68 | 0.2003 | 0.4376 |
| 14.22 | 0.3094 | 0.5750 |
| 16.52 | 0.4037 | 0.6659 |
| 18.61 | 0.4855 | 0.7290 |
| 19.79 | 0.5346 | 0.7621 |
| 22.00 | 0.6209 | 0.8134 |
| 23.62 | 0.6810 | 0.8463 |
| 26.82 | 0.7867 | 0.9009 |
| 29.20 | 0.8635 | 0.9365 |

Pöll, Heinrich - Huemer, Hans - Moser, Franz, Eine Apparatur zur Bestimmung von Dampf-Flüssigkeits-Gleichgewichten unter erhöhtem Druck, Monatshefte für Chemie 5 (1980) 1159-1164. doi:10.1007/BF00909673

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 12.96 | 0.1034 | 0.2430 |
| 15.11 | 0.1807 | 0.3789 |
| 16.80 | 0.2375 | 0.4574 |
| 20.04 | 0.3426 | 0.5958 |
| 20.86 | 0.3717 | 0.6101 |
| 27.31 | 0.5493 | 0.7613 |
| 31.48 | 0.6577 | 0.8186 |
| 39.39 | 0.8557 | 0.9119 |
| 42.17 | 0.9216 | 0.9551 |

Miksovsky, J. - Wichterle, I., Liquid-vapor equilibrium. LXX. Vapor -liquid equilibriums in the ethane-propane system at high pressures, Collect. Czech. Chem. Commun. 2 (1975) 365-370. doi:10.1135/cccc19750365

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.59 | 0.0245 | 0.0689 |
| 12.26 | 0.0538 | 0.1409 |
| 13.98 | 0.1244 | 0.2890 |
| 15.94 | 0.1748 | 0.3848 |
| 19.89 | 0.3217 | 0.5602 |
| 23.77 | 0.4392 | 0.6641 |
| 30.23 | 0.6180 | 0.7837 |
| 33.79 | 0.7085 | 0.8332 |
| 37.63 | 0.8075 | 0.8881 |
| 41.05 | 0.8813 | 0.9280 |
| 42.43 | 0.9124 | 0.9459 |

Miksovsky, J. - Wichterle, I., Liquid-vapor equilibrium. LXX. Vapor -liquid equilibriums in the ethane-propane system at high pressures, Collect. Czech. Chem. Commun. 2 (1975) 365-370. doi:10.1135/cccc19750365

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 43.55 | 0.9374 | 0.9597 |
| 44.55 | 0.9527 | 0.9686 |
| 45.47 | 0.9759 | 0.9838 |
| 45.52 | 0.9763 | 0.9838 |
| 46.20 | 0.9908 | 0.9935 |
| 46.42 | 0.9947 | 0.9961 |
| 46.44 | 0.9948 | 0.9962 |

Matschke, D. E. - Thodos, G., Vapor-liquid equilibriums for the ethane-propane system, J. Chem. Eng. Data 2 (1962) 232-234. doi:10.1021/je60013a022

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 13.79 | 0.0313 | 0.0789 | |
| 17.24 | 0.1490 | 0.3100 | |
| 20.68 | 0.2550 | 0.4550 | |
| 24.13 | 0.3530 | 0.5580 | |
| 27.58 | 0.4470 | 0.6380 | |
| 31.03 | 0.5350 | 0.7040 | |
| 34.47 | 0.6220 | 0.7640 | |
| 37.92 | 0.7050 | 0.8160 | |
| 41.37 | 0.7810 | 0.8610 | |
| 44.82 | 0.8430 | 0.8940 | |
| 48.26 | 0.8950 | 0.9220 | |
| 50.44 | 0.9350 | 0.9350 | CRIT |

Miksovsky, J. - Wichterle, I., Liquid-vapor equilibrium. LXX. Vapor -liquid equilibriums in the ethane-propane system at high pressures, Collect. Czech. Chem. Commun. 2 (1975) 365-370. doi:10.1135/cccc19750365

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 18.12 | 0.0271 | 0.0600 | |
| 19.51 | 0.0665 | 0.1385 | |
| 20.03 | 0.0778 | 0.1599 | |
| 21.33 | 0.1097 | 0.2168 | |
| 22.79 | 0.1466 | 0.2661 | |
| 26.08 | 0.2287 | 0.3779 | |
| 26.54 | 0.2363 | 0.3877 | |
| 27.68 | 0.2660 | 0.4208 | |
| 30.07 | 0.3217 | 0.4848 | |
| 34.33 | 0.4278 | 0.5870 | |
| 37.56 | 0.5015 | 0.6460 | |
| 41.14 | 0.5653 | 0.6967 | |
| 45.94 | 0.6666 | 0.7576 | |
| 47.90 | 0.7035 | 0.7715 | |
| 49.38 | 0.7332 | 0.7786 | |
| 50.16 | 0.7504 | 0.7823 | |
| 50.59 | 0.7586 | 0.7810 | |
| 50.78 | 0.7621 | 0.7765 | |
| 50.87 | 0.7755 | 0.7755 | CRIT |

Matschke, D. E. - Thodos, G., Vapor-liquid equilibriums for the ethane-propane system, J. Chem. Eng. Data 2 (1962) 232-234. doi:10.1021/je60013a022

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 24.13 | 0.0711 | 0.1400 | |
| 27.58 | 0.1520 | 0.2670 | |
| 31.03 | 0.2300 | 0.3670 | |
| 34.47 | 0.3050 | 0.4480 | |
| 37.92 | 0.3780 | 0.5150 | |
| 41.37 | 0.4480 | 0.5730 | |
| 44.82 | 0.5150 | 0.6180 | |
| 48.26 | 0.5810 | 0.6550 | |
| 49.99 | 0.6130 | 0.6720 | |
| 51.71 | 0.6520 | 0.6700 | |
| 51.85 | 0.6685 | 0.6685 | CRIT |

Matschke, D. E. - Thodos, G., Vapor-liquid equilibriums for the ethane-propane system, J. Chem. Eng. Data 2 (1962) 232-234. doi:10.1021/je60013a022

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 27.58 | 0.0253 | 0.0480 | |
| 31.03 | 0.1040 | 0.1760 | |
| 34.47 | 0.1740 | 0.2700 | |
| 37.92 | 0.2410 | 0.3430 | |
| 41.37 | 0.3050 | 0.4030 | |
| 44.82 | 0.3690 | 0.4570 | |
| 48.26 | 0.4320 | 0.5020 | |
| 49.99 | 0.4630 | 0.5160 | |
| 50.88 | 0.5060 | 0.5060 | CRIT |

Matschke, D. E. - Thodos, G., Vapor-liquid equilibriums for the ethane-propane system, J. Chem. Eng. Data 2 (1962) 232-234. doi:10.1021/je60013a022

**T / K = 355.37**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 34.47 | 0.0356 | 0.0570 | |
| 36.20 | 0.0693 | 0.1060 | |
| 37.92 | 0.1020 | 0.1490 | |
| 39.65 | 0.1350 | 0.1880 | |
| 41.37 | 0.1680 | 0.2250 | |
| 43.09 | 0.2010 | 0.2620 | |
| 44.82 | 0.2350 | 0.2940 | |
| 46.54 | 0.2700 | 0.3240 | |
| 48.26 | 0.3090 | 0.3310 | |
| 48.61 | 0.3215 | 0.3215 | CRIT |

Miksovsky, J. - Wichterle, I., Liquid-vapor equilibrium. LXX. Vapor -liquid equilibriums in the ethane-propane system at high pressures, Collect. Czech. Chem. Commun. 2 (1975) 365-370. doi:10.1135/cccc19750365

**T / K = 363.16**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|

| | | | |
|---|---|---|---|
| 38.40 | 0.0116 | 0.0173 | |
| 38.99 | 0.0214 | 0.0307 | |
| 39.97 | 0.0395 | 0.0543 | |
| 41.02 | 0.0566 | 0.0746 | |
| 41.88 | 0.0716 | 0.0912 | |
| 43.68 | 0.1017 | 0.1216 | |
| 44.74 | 0.1224 | 0.1367 | |
| 45.26 | 0.1333 | 0.1405 | |
| 45.34 | 0.1402 | 0.1402 | CRIT |

Matschke, D. E. - Thodos, G., Vapor-liquid equilibriums for the ethane-propane system, J. Chem. Eng. Data 2 (1962) 232-234. doi:10.1021/je60013a022

**T / K = 366.48**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 39.99 | 0.0065 | 0.0095 | |
| 40.68 | 0.0193 | 0.0275 | |
| 41.37 | 0.0320 | 0.0446 | |
| 42.06 | 0.0445 | 0.0602 | |
| 42.75 | 0.0566 | 0.0742 | |
| 43.44 | 0.0682 | 0.0869 | |
| 44.13 | 0.0791 | 0.0949 | |
| 44.47 | 0.0846 | 0.0953 | |
| 44.71 | 0.0930 | 0.0930 | CRIT |

Miksovsky, J. - Wichterle, I., Liquid-vapor equilibrium. LXX. Vapor -liquid equilibriums in the ethane-propane system at high pressures, Collect. Czech. Chem. Commun. 2 (1975) 365-370. doi:10.1135/cccc19750365

**T / K = 367.66**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 41.14 | 0.0056 | 0.0076 | |
| 41.86 | 0.0179 | 0.0233 | |
| 42.46 | 0.0279 | 0.0346 | |
| 43.20 | 0.0413 | 0.0472 | |
| 43.56 | 0.0492 | 0.0531 | |
| 43.71 | 0.0552 | 0.0552 | CRIT |

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**Enthalpy of mixing**

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Ott, J.B. - Brown, P.R. - Moore, J.D. - Lewellen, A.C., Excess molar enthalpies and excess molar volumes for (propane + ethane) over the temperature range from 273.15 K to 373.15 K and the pressure range from 5 MPa to 15 MPa, The Journal of Chemical Thermodynamics 2 (1997) 149-178. doi:10.1006/jcht.1996.0144

**T / K = 273.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -8.000 | 0.0351 |
| -18.00 | 0.0701 |
| -39.00 | 0.1570 |
| -46.00 | 0.1915 |
| -63.00 | 0.2602 |
| -70.00 | 0.3114 |
| -77.00 | 0.3453 |
| -82.00 | 0.3961 |
| -88.00 | 0.4297 |
| -91.00 | 0.4633 |
| -95.00 | 0.5134 |
| -97.00 | 0.5466 |
| -98.00 | 0.5963 |
| -98.00 | 0.6293 |
| -92.00 | 0.7111 |
| -88.00 | 0.7437 |
| -79.00 | 0.7923 |
| -70.00 | 0.8246 |
| -54.00 | 0.8727 |
| -42.00 | 0.9047 |
| -18.00 | 0.9525 |
| -3.000 | 0.9842 |

Ott, J.B. - Brown, P.R. - Moore, J.D. - Lewellen, A.C., Excess molar enthalpies and excess molar volumes for (propane + ethane) over the temperature range from 273.15 K to 373.15 K and the pressure range from 5 MPa to 15 MPa, The Journal of Chemical Thermodynamics 2 (1997) 149-178. doi:10.1006/jcht.1996.0144

**T / K = 323.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -158.00 | 0.0344 |
| -369.00 | 0.0687 |
| -581.00 | 0.1030 |
| -839.00 | 0.1542 |
| -1036.0 | 0.1883 |
| -1203.0 | 0.2223 |
| -1464.0 | 0.2562 |
| -1660.0 | 0.3069 |
| -1851.0 | 0.3407 |
| -2154.0 | 0.3911 |
| -2289.0 | 0.4247 |
| -2426.0 | 0.4581 |
| -2624.0 | 0.5082 |
| -2756.0 | 0.5415 |
| -2944.0 | 0.5913 |

| | |
|---|---|
| -2963.0 | 0.6244 |
| -2991.0 | 0.6574 |
| -2963.0 | 0.6904 |
| -2843.0 | 0.7069 |
| -2692.0 | 0.7233 |
| -2368.0 | 0.7397 |
| -2045.0 | 0.7561 |
| -1026.0 | 0.7725 |
| -293.00 | 0.7889 |
| -5.000 | 0.8052 |
| 264.00 | 0.8215 |
| 284.00 | 0.8378 |
| 353.00 | 0.8541 |
| 350.00 | 0.9029 |
| 202.00 | 0.9515 |
| 61.00 | 0.9839 |

Ott, J.B. - Brown, P.R. - Moore, J.D. - Lewellen, A.C., Excess molar enthalpies and excess molar volumes for (propane + ethane) over the temperature range from 273.15 K to 373.15 K and the pressure range from 5 MPa to 15 MPa, The Journal of Chemical Thermodynamics 2 (1997) 149-178. doi:10.1006/jcht.1996.0144

**T / K = 363.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -29.00 | 0.0171 |
| -52.00 | 0.0343 |
| -72.00 | 0.0514 |
| -78.00 | 0.0685 |
| -74.00 | 0.1026 |
| -52.00 | 0.1197 |
| 80.00 | 0.1537 |
| 153.00 | 0.1707 |
| 442.00 | 0.1877 |
| 954.00 | 0.2046 |
| 1435.0 | 0.2216 |
| 2461.0 | 0.2723 |
| 2965.0 | 0.3061 |
| 3276.0 | 0.3566 |
| 3305.0 | 0.3901 |
| 3272.0 | 0.4237 |
| 3157.0 | 0.4738 |
| 3032.0 | 0.5072 |
| 2904.0 | 0.5405 |
| 2677.0 | 0.5903 |
| 2502.0 | 0.6234 |
| 2225.0 | 0.6730 |
| 2035.0 | 0.7060 |
| 1702.0 | 0.7553 |
| 1502.0 | 0.7882 |
| 1280.0 | 0.8209 |
| 1016.0 | 0.8700 |
| 756.00 | 0.9026 |
| 87.00 | 0.9838 |

Ott, J.B. - Brown, P.R. - Moore, J.D. - Lewellen, A.C., Excess molar enthalpies and excess molar volumes for (propane + ethane) over the temperature range from 273.15 K to 373.15 K and the pressure range from 5 MPa to 15 MPa, The Journal of Chemical Thermodynamics 2 (1997) 149-178. doi:10.1006/jcht.1996.0144

**T / K = 373.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 287.00 | 0.0344 |
| 1072.0 | 0.0687 |
| 1326.0 | 0.0859 |
| 2117.0 | 0.1201 |
| 2390.0 | 0.1542 |
| 2683.0 | 0.1883 |
| 2829.0 | 0.2223 |
| 2938.0 | 0.2562 |
| 2936.0 | 0.3069 |
| 2870.0 | 0.3407 |
| 2733.0 | 0.3911 |
| 2654.0 | 0.4247 |
| 2546.0 | 0.4581 |
| 2273.0 | 0.5082 |
| 2222.0 | 0.5415 |
| 1963.0 | 0.5913 |
| 1868.0 | 0.6244 |
| 1649.0 | 0.6574 |
| 1452.0 | 0.7069 |
| 1269.0 | 0.7397 |
| 1067.0 | 0.7889 |
| 802.00 | 0.8215 |
| 616.00 | 0.8704 |
| 394.00 | 0.9029 |
| 214.00 | 0.9515 |
| 33.00 | 0.9839 |

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**Critical point**

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Horstmann, Sven - Fischer, Kai - Gmehling, Jürgen, Experimental determination of critical data of mixtures

and their relevance for the development of thermodynamic models, Chemical Engineering Science 24 (2001) 6905-6913. doi:10.1016/S0009-2509(01)00332-3

| T / K | P / bar | $x_1$ |
|---|---|---|
| 363.96 | 44.47 | 0.1202 |
| 358.00 | 46.47 | 0.2398 |
| 352.45 | 47.98 | 0.3598 |
| 344.06 | 49.60 | 0.4803 |
| 337.91 | 50.30 | 0.5807 |
| 333.05 | 50.61 | 0.6603 |
| 327.48 | 50.76 | 0.7389 |
| 321.38 | 50.65 | 0.8205 |
| 314.10 | 50.17 | 0.8997 |

Matschke, D. E. - Thodos, G., Vapor-liquid equilibriums for the ethane-propane system, J. Chem. Eng. Data 2 (1962) 232-234. doi:10.1021/je60013a022

| T / K | P / bar | $x_1$ |
|---|---|---|
| 366.39 | 44.89 | 0.1000 |
| 361.94 | 46.75 | 0.2000 |
| 356.78 | 48.33 | 0.3000 |
| 351.11 | 49.71 | 0.4000 |
| 344.89 | 50.81 | 0.5000 |
| 338.17 | 51.57 | 0.6000 |
| 330.89 | 51.92 | 0.7000 |
| 314.22 | 51.09 | 0.9000 |

Van Poolen, Lambert J. - Holcomb, Cynthia D., Critical temperatures, pressures, and densities for the mixtures CO2–C3H8, CO2–nC4H10, C2H6–C3H8, and C3H8–nC4H10, Fluid Phase Equilibria 2 (1999) 157-168. doi:10.1016/S0378-3812(99)00275-7

| T / K | P / bar | $x_1$ |
|---|---|---|
| 310.18 | 48.99 | 0.9400 |
| 329.46 | 50.92 | 0.7050 |
| 339.24 | 50.61 | 0.5686 |
| 344.72 | 50.16 | 0.5031 |
| 354.37 | 48.35 | 0.3331 |

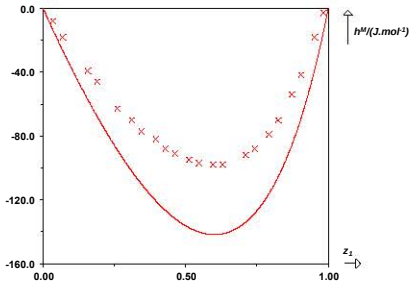
Uchytil, Petr - Wichterle, Ivan, Liquid-vapour critical region of the most volatile component of a ternary system. I. Vapour-liquid equilibria in the ethane - propane - n-butane system, Fluid Phase Equilibria 2 (1983) 209-217. doi:10.1016/0378-3812(83)80153-8

| T / K | P / bar | $x_1$ |
|---|---|---|
| 305.81 | 48.82 | 0.9946 |
| 305.97 | 48.88 | 0.9932 |
| 306.19 | 48.95 | 0.9911 |
| 306.29 | 48.96 | 0.9897 |
| 306.54 | 49.01 | 0.9864 |
| 306.88 | 49.06 | 0.9818 |
| 307.20 | 49.13 | 0.9784 |
| 307.60 | 49.21 | 0.9734 |

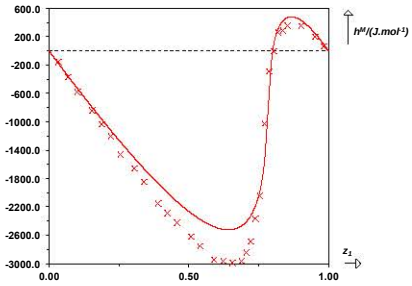
Miksovsky, J. - Wichterle, I., Liquid-vapor equilibrium. LXX. Vapor -liquid equilibriums in the ethane-propane system at high pressures, Collect. Czech. Chem. Commun. 2 (1975) 365-370. doi:10.1135/cccc19750365

| T / K | P / bar | $x_1$ |
|---|---|---|
| 343.17 | 49.96 | 0.4783 |
| 305.40 | 48.81 | 0.9986 |
| 305.93 | 49.11 | 0.9920 |
| 306.50 | 49.38 | 0.9839 |
| 307.55 | 49.71 | 0.9697 |

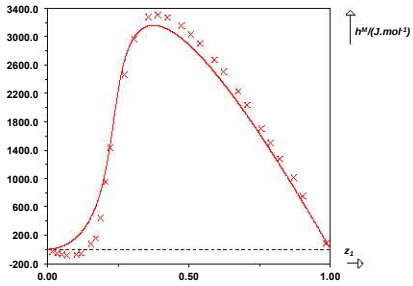
T/K = 273.15 - P/bar = 50.00



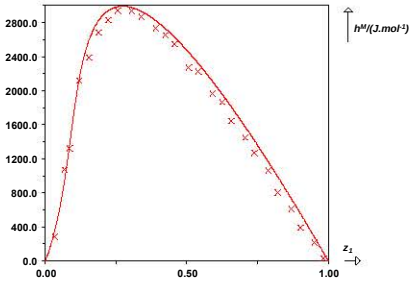

T/K = 323.15 - P/bar = 50.00



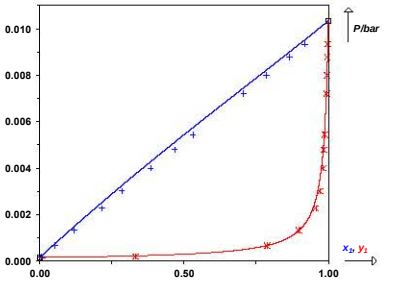

T/K = 363.15 - P/bar = 50.00



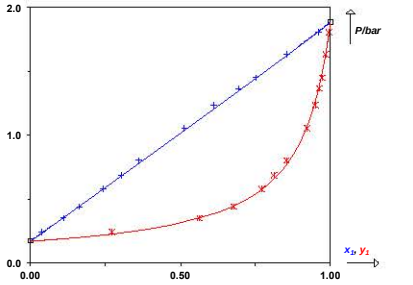

T/K = 373.15 - P/bar = 50.00



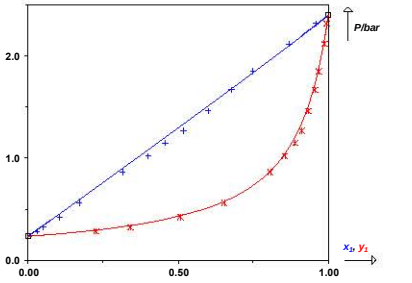

T/K = 127.59



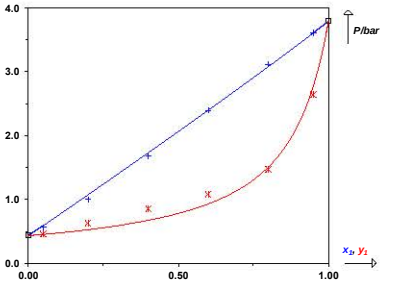

T/K = 196.85



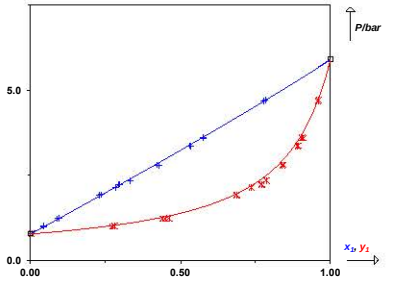

T/K = 202.15



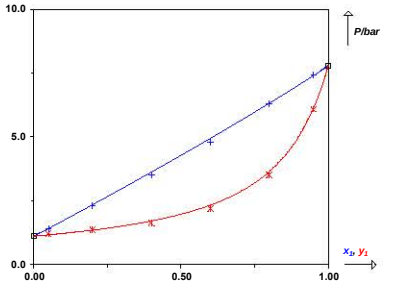

T/K = 213.15



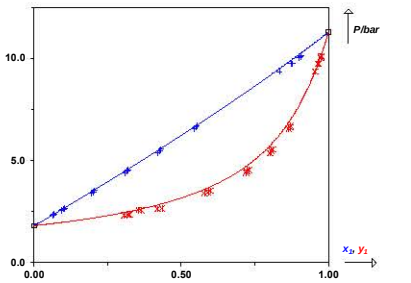

T/K = 225.00



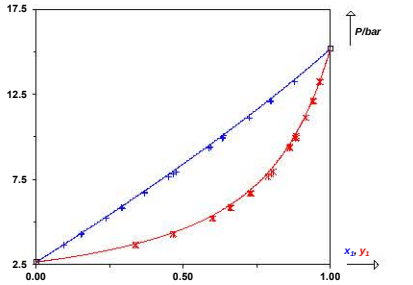

T/K = 233.15



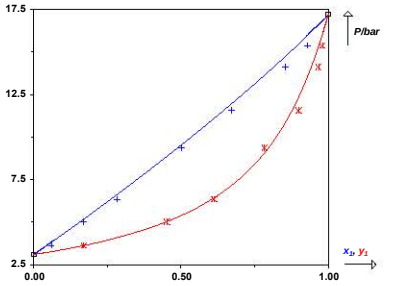

T/K = 245.00



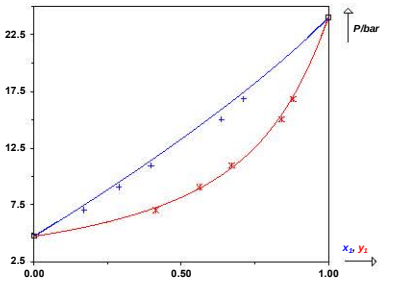

T/K = 255.40



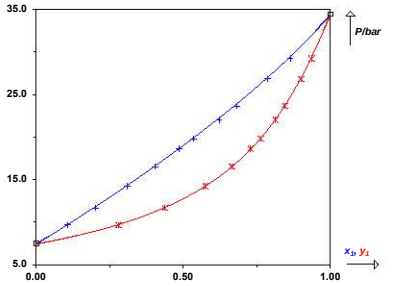

T/K = 260.00



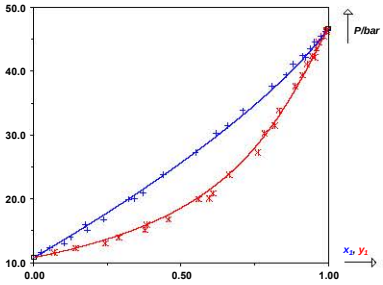

T/K = 273.15



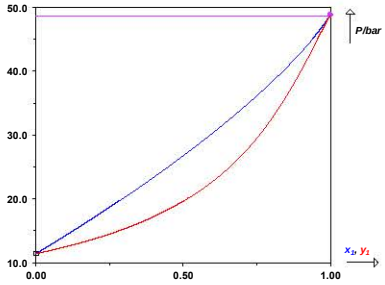

T/K = 288.75



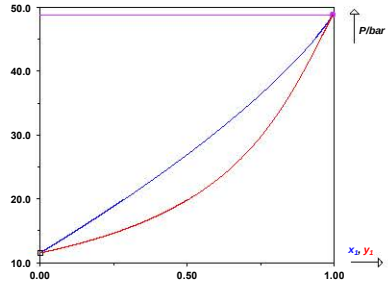
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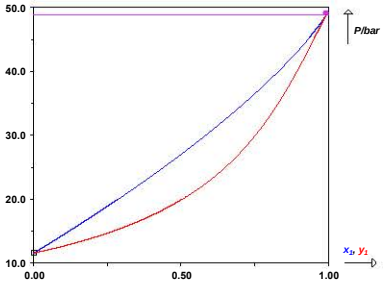

T/K = 305.40



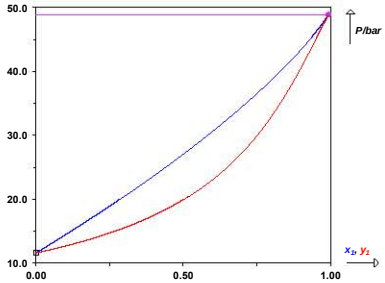

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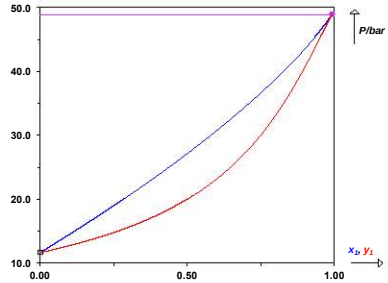

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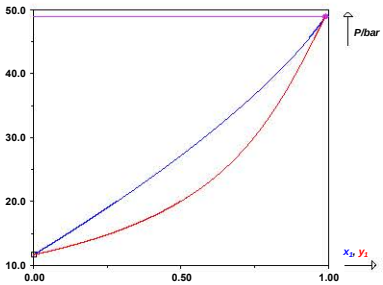

T/K = 305.97



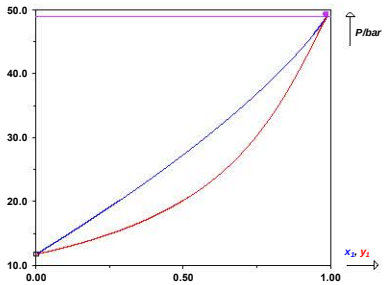

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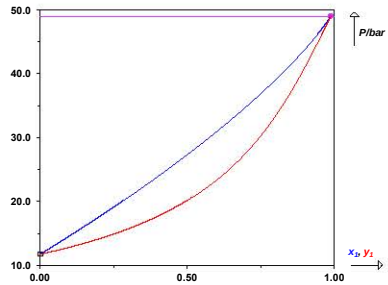

T/K = 306.29



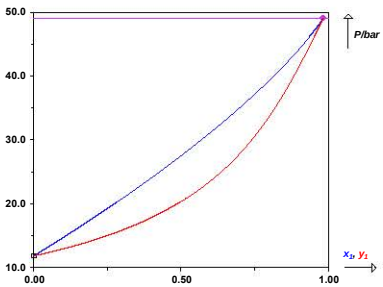

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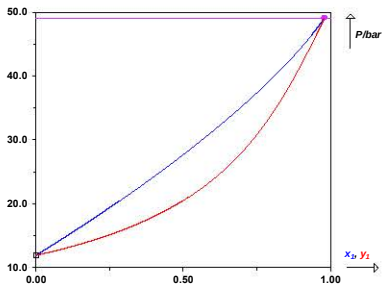

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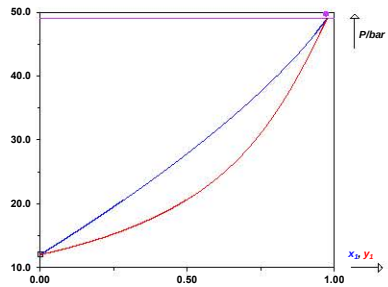

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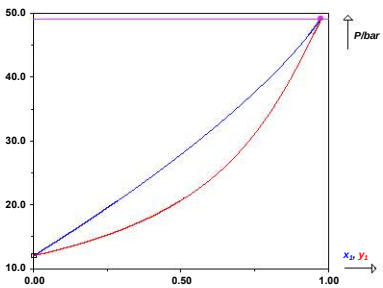

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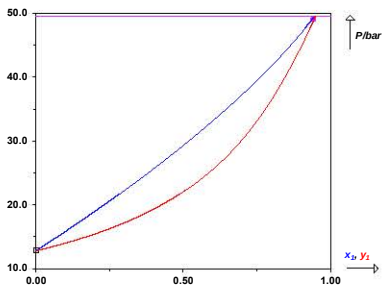

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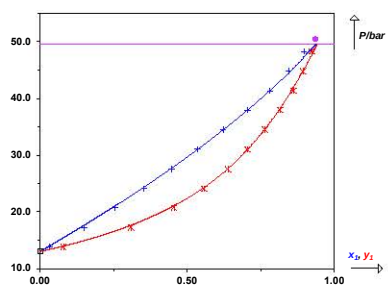

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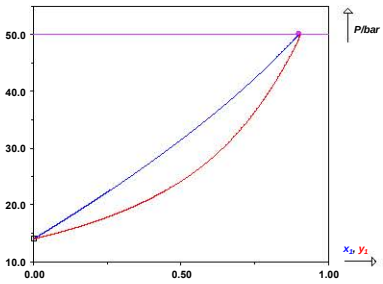

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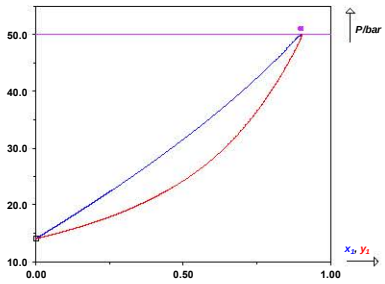

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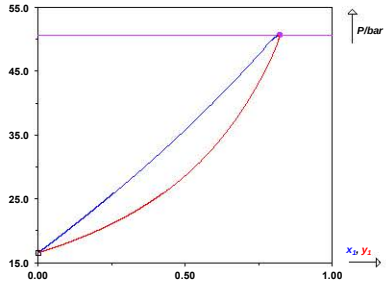
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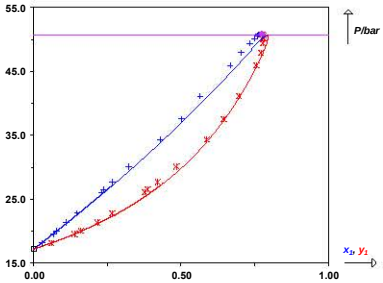

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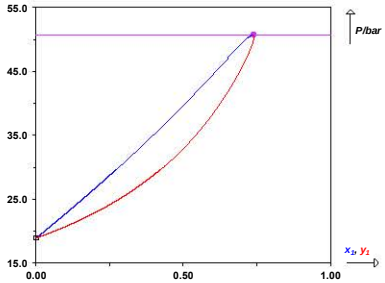

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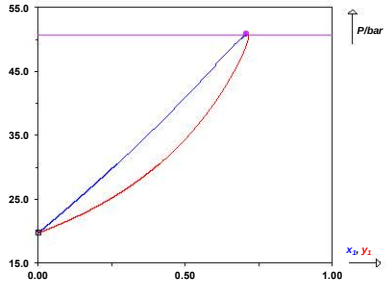

T/K = 323.15



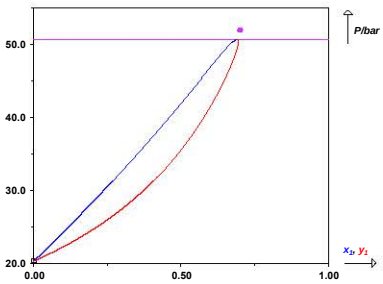

T/K = 327.48



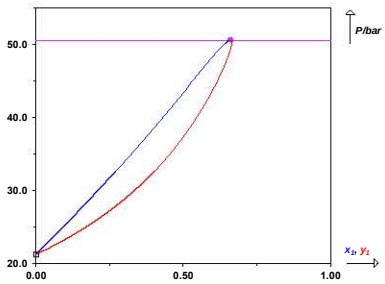

T/K = 329.46



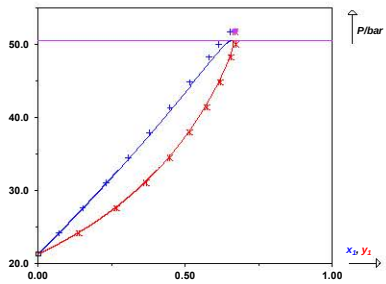

T/K = 330.89



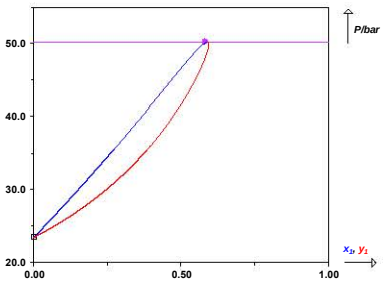

T/K = 333.05



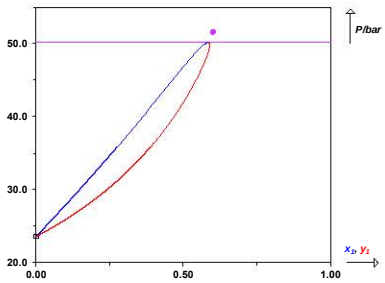

T/K = 333.15



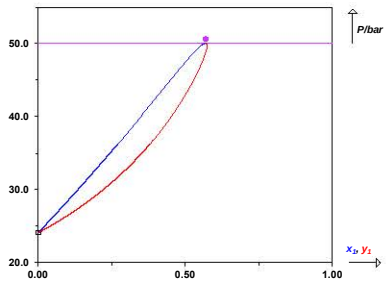

T/K = 337.91



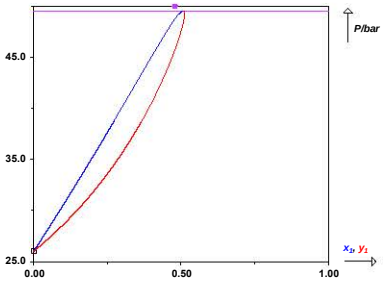

T/K = 338.17



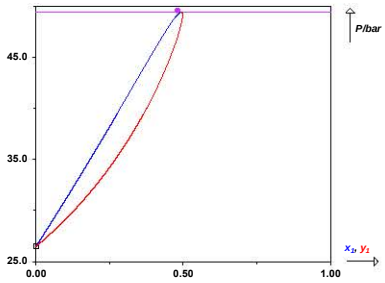

T/K = 339.24



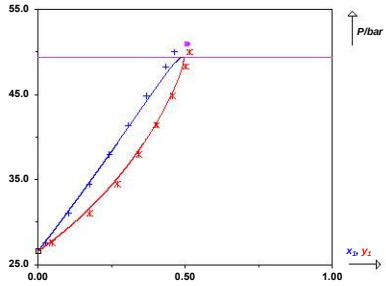

T/K = 343.17



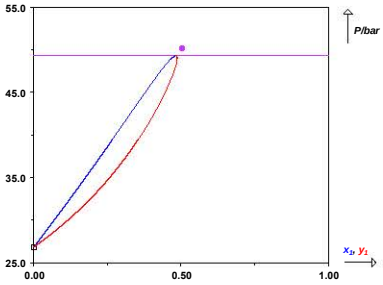

T/K = 344.06



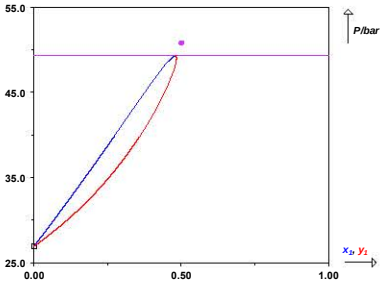

T/K = 344.26



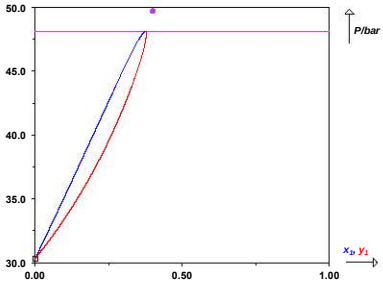
T/K = 344.72



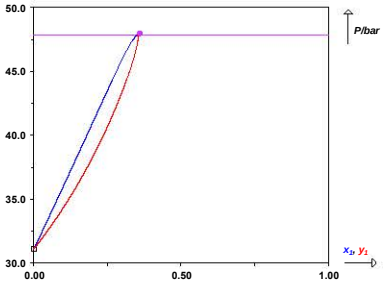

T/K = 344.89



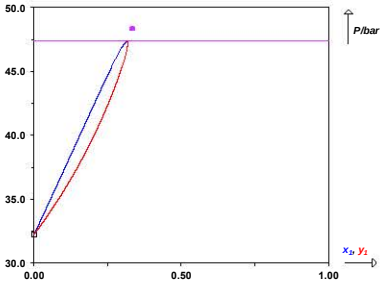

T/K = 351.11



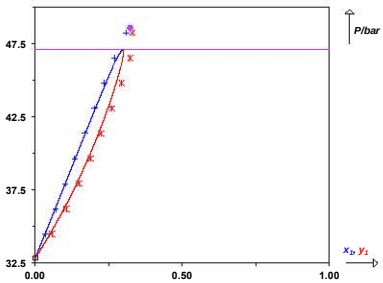

T/K = 352.45



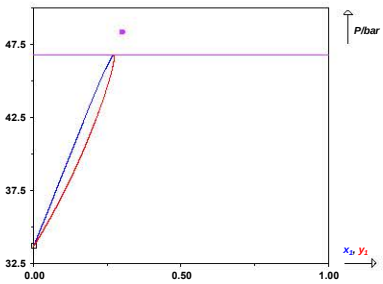

T/K = 354.37



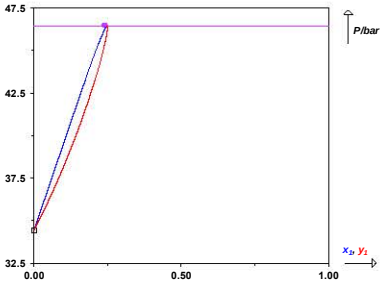

T/K = 355.37



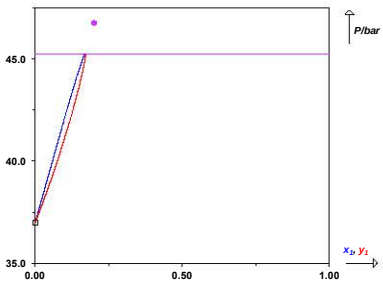

T/K = 356.78



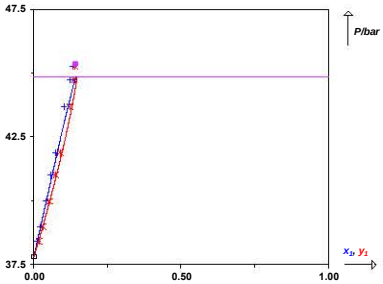

T/K = 358.00



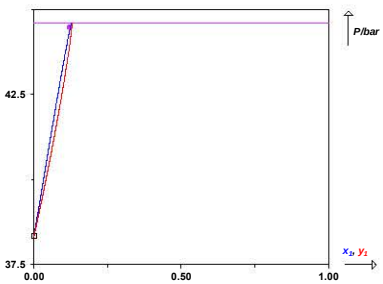

T/K = 361.94



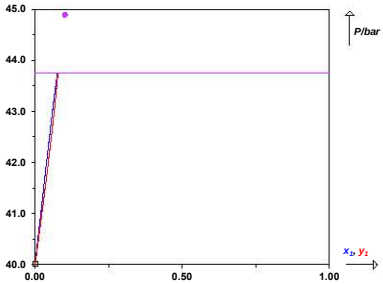

T/K = 363.16



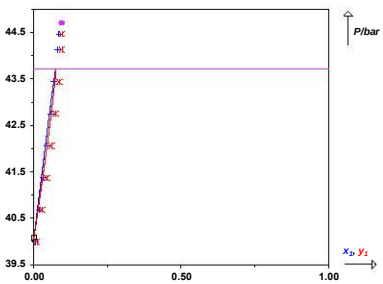

T/K = 363.96



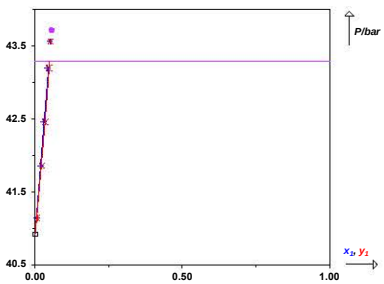

T/K = 366.39




T/K = 366.48




T/K = 367.66



## METHANE (1) + n-BUTANE (2)

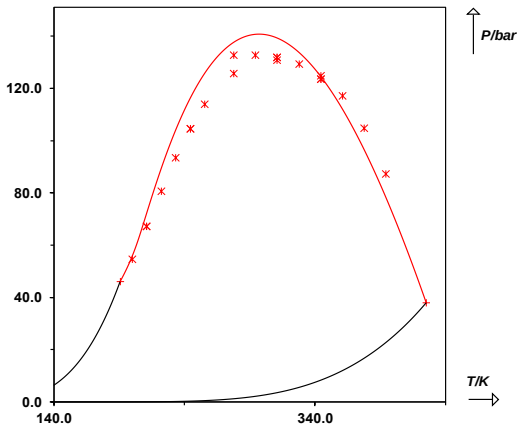
| | | |
|---|---|---|
| **CAS** | 74-82-8 | 106-97-8 |
| **InChiKey** | VNWKTOKETHGBQD-UHFFFAOYSA-N | IJDNQMDRQITEOD-UHFFFAOYSA-N |
| **$T_c$ / K** | 190.56 | 425.12 |
| **$P_c$ / bar** | 45.99 | 37.96 |
| **ω** | 0.012 | 0.200 |

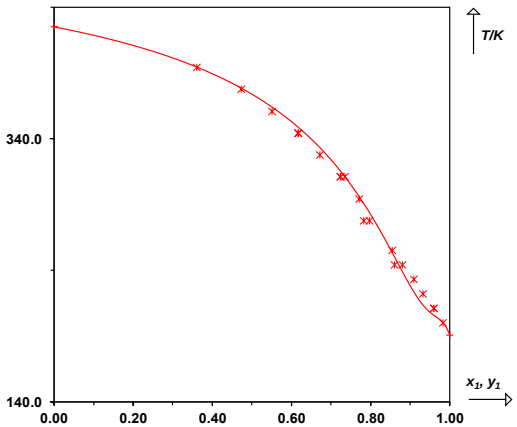
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 49.8
B/MPa = 18.5

*Deviations*
MAPE on x = 5.5 %
MAPE on y = 4 %
MAPE on $x_c$ = 6.1 %
MAPE on $P_c$ = 6.5 %
MAPE on $h^M$ = 46 %



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**Isothermal phase equilibrium data**

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Kahre, LeRoy C., Low-temperature K data for methane-butane, Journal of Chemical & Engineering Data 1 (1974) 67-71. doi:10.1021/je60060a014

**T / K = 166.48**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.379 | 0.0470 | 0.9994 |
| 3.378 | 0.1160 | 0.9997 |
| 6.895 | 0.2510 | 0.9998 |
| 10.20 | 0.3790 | 0.9999 |
| 13.72 | 0.5450 | 0.9999 |
| 17.17 | 0.7530 | 0.9999 |
| 18.75 | 0.8970 | 0.9999 |
| 19.51 | 0.9500 | 0.9999 |

Kahre, LeRoy C., Low-temperature K data for methane-butane, Journal of Chemical & Engineering Data 1 (1974) 67-71. doi:10.1021/je60060a014

**T / K = 177.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.379 | 0.0360 | 0.9981 |
| 3.447 | 0.0910 | 0.9992 |
| 6.895 | 0.1800 | 0.9995 |
| 13.79 | 0.3600 | 0.9996 |
| 20.62 | 0.5730 | 0.9997 |
| 24.41 | 0.7320 | 0.9997 |
| 26.61 | 0.8750 | 0.9997 |
| 27.86 | 0.9340 | 0.9997 |

Kahre, LeRoy C., Low-temperature K data for methane-butane, Journal of Chemical & Engineering Data 1 (1974) 67-71. doi:10.1021/je60060a014

**T / K = 185.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.379 | 0.0280 | 0.9956 |
| 3.447 | 0.0690 | 0.9981 |
| 6.895 | 0.1440 | 0.9989 |
| 13.79 | 0.2900 | 0.9993 |
| 20.62 | 0.4440 | 0.9993 |
| 27.51 | 0.6080 | 0.9993 |
| 30.96 | 0.7280 | 0.9992 |
| 34.41 | 0.8710 | 0.9991 |
| 37.85 | 0.9720 | 0.9993 |

Kahre, LeRoy C., Low-temperature K data for methane-butane, Journal of Chemical & Engineering Data 1 (1974) 67-71. doi:10.1021/je60060a014

**T / K = 194.09**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.379 | 0.0250 | 0.9917 |
| 2.758 | 0.0510 | 0.9955 |
| 5.585 | 0.1030 | 0.9975 |
| 6.895 | 0.1300 | 0.9979 |
| 13.79 | 0.2480 | 0.9986 |
| 27.51 | 0.5000 | 0.9988 |
| 41.03 | 0.8300 | 0.9980 |
| 43.23 | 0.8960 | 0.9977 |
| 44.75 | 0.9300 | 0.9975 |
| 46.68 | 0.9680 | 0.9972 |

Elliot, Douglas G. - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of methane-butane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1974) 71-77. doi:10.1021/je60060a015

**T / K = 199.88**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.80 | 0.2267 | 0.9976 |
| 20.71 | 0.3261 | 0.9979 |
| 27.58 | 0.4267 | 0.9980 |
| 34.47 | 0.5322 | 0.9977 |
| 41.37 | 0.6591 | 0.9971 |
| 48.26 | 0.8296 | 0.9958 |
| 51.71 | 0.9257 | 0.9944 |

Kahre, LeRoy C., Low-temperature K data for methane-butane, Journal of Chemical & Engineering Data 1 (1974) 67-71. doi:10.1021/je60060a014

**T / K = 210.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.379 | 0.0190 | 0.9690 |
| 2.758 | 0.0380 | 0.9840 |
| 5.516 | 0.0770 | 0.9913 |
| 8.274 | 0.1110 | 0.9936 |
| 11.03 | 0.1480 | 0.9948 |
| 13.79 | 0.1840 | 0.9955 |
| 27.51 | 0.3610 | 0.9965 |
| 41.30 | 0.5320 | 0.9959 |
| 55.02 | 0.7210 | 0.9934 |
| 67.09 | 0.9330 | 0.9802 |

Elliot, Douglas G. - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of methane-butane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1974) 71-77. doi:10.1021/je60060a015

**T / K = 222.07**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.909 | 0.0820 | 0.9840 |

| | | |
|---|---|---|
| 13.81 | 0.1586 | 0.9903 |
| 27.58 | 0.2981 | 0.9930 |
| 41.37 | 0.4284 | 0.9926 |
| 55.16 | 0.5564 | 0.9905 |
| 68.95 | 0.7056 | 0.9843 |
| 75.84 | 0.8001 | 0.9774 |
| 79.29 | 0.8637 | 0.9648 |

Elliot, Douglas G. - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of methane-butane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1974) 71-77. doi:10.1021/je60060a015

**T / K = 233.18**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 6.915 | 0.0721 | 0.9703 | |
| 13.81 | 0.1400 | 0.9827 | |
| 27.58 | 0.2655 | 0.9878 | |
| 41.37 | 0.3739 | 0.9882 | |
| 55.16 | 0.4804 | 0.9868 | |
| 68.95 | 0.5875 | 0.9822 | |
| 82.74 | 0.6948 | 0.9705 | |
| 89.63 | 0.7886 | 0.9608 | |
| 93.08 | 0.8549 | 0.9318 | |
| 93.42 | 0.9097 | 0.9097 | CRIT |

Elliot, Douglas G. - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of methane-butane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1974) 71-77. doi:10.1021/je60060a015

**T / K = 244.28**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 6.909 | 0.0630 | 0.9488 | |
| 13.81 | 0.1237 | 0.9703 | |
| 27.58 | 0.2335 | 0.9801 | |
| 41.37 | 0.3325 | 0.9818 | |
| 55.16 | 0.4223 | 0.9809 | |
| 68.95 | 0.5101 | 0.9772 | |
| 82.74 | 0.6062 | 0.9688 | |
| 96.53 | 0.7189 | 0.9498 | |
| 103.42 | 0.8059 | 0.9150 | |
| 104.46 | 0.8805 | 0.8805 | CRIT |

Elliot, Douglas G. - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of methane-butane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1974) 71-77. doi:10.1021/je60060a015

**T / K = 255.38**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.475 | 0.0257 | 0.8370 | |
| 6.922 | 0.0559 | 0.9161 | |
| 13.81 | 0.1124 | 0.9516 | |
| 20.71 | 0.1643 | 0.9639 | |
| 27.58 | 0.2135 | 0.9689 | |
| 34.48 | 0.2580 | 0.9716 | |
| 48.26 | 0.3455 | 0.9729 | |
| 55.16 | 0.3905 | 0.9728 | |
| 68.95 | 0.4651 | 0.9696 | |
| 82.74 | 0.5466 | 0.9625 | |
| 96.53 | 0.6326 | 0.9499 | |
| 110.32 | 0.7498 | 0.9175 | |
| 113.90 | 0.8543 | 0.8543 | CRIT |

Elliot, Douglas G. - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of methane-butane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1974) 71-77. doi:10.1021/je60060a015

**T / K = 277.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.922 | 0.0426 | 0.7960 |
| 13.82 | 0.0899 | 0.8900 |
| 20.71 | 0.1339 | 0.9176 |
| 27.58 | 0.1759 | 0.9313 |
| 34.48 | 0.2152 | 0.9385 |
| 41.37 | 0.2536 | 0.9425 |
| 55.16 | 0.3262 | 0.9469 |
| 68.95 | 0.3976 | 0.9459 |
| 82.74 | 0.4651 | 0.9390 |
| 96.53 | 0.5331 | 0.9294 |
| 110.32 | 0.6078 | 0.9100 |
| 117.21 | 0.6558 | 0.8967 |
| 124.11 | 0.7278 | 0.8460 |

Wiese, H. C. - Jacobs, Joan - Sage, B. H., Phase equilibriums in the hydrocarbon systems. Phase behavior in the methane-propane-n-butane system, Journal of Chemical & Engineering Data 1 (1970) 82-91. doi:10.1021/je60044a021

**T / K = 277.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 13.79 | 0.0808 | 0.8888 | |
| 34.47 | 0.1913 | 0.9369 | |
| 68.95 | 0.3651 | 0.9461 | |
| 86.18 | 0.4513 | 0.9407 | |
| 103.42 | 0.5390 | 0.9262 | |
| 117.21 | 0.6194 | 0.9044 | |
| 132.59 | 0.7970 | 0.7970 | CRIT |

Sage, R. H. - Hicks, B. L. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 8 (1940) 1085-1092. doi:10.1021/ie50368a014

**T / K = 294.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 2.758 | 0.0036 | 0.2103 | |
| 4.137 | 0.0111 | 0.4593 | |
| 5.516 | 0.0186 | 0.5843 | |
| 6.895 | 0.0263 | 0.6600 | |
| 10.34 | 0.0452 | 0.7591 | |
| 13.79 | 0.0639 | 0.8088 | |
| 20.69 | 0.1011 | 0.8587 | |
| 27.58 | 0.1380 | 0.8831 | |
| 34.48 | 0.1744 | 0.8978 | |
| 41.37 | 0.2106 | 0.9074 | |
| 55.16 | 0.2804 | 0.9174 | |
| 68.95 | 0.3490 | 0.9202 | |
| 82.74 | 0.4162 | 0.9178 | |
| 86.19 | 0.4305 | 0.9162 | |
| 96.53 | 0.4775 | 0.9087 | |
| 103.42 | 0.5101 | 0.9026 | |
| 110.32 | 0.5451 | 0.8942 | |
| 117.21 | 0.5863 | 0.8827 | |
| 120.66 | 0.6105 | 0.8750 | |
| 124.11 | 0.6375 | 0.8652 | |
| 127.55 | 0.6700 | 0.8511 | |
| 131.00 | 0.7152 | 0.8253 | |
| 132.59 | 0.7712 | 0.7712 | CRIT |

Rigas, T. J. - Mason, D. F. - Thodos, George, Vapor-Liquid Equilibria. Microsampling Technique Applied to a New Variable-Volume Cell, Industrial & Engineering Chemistry 9 (1958) 1297-1300. doi:10.1021/ie50585a039

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 66.19 | 0.3110 | 0.8790 | |
| 81.70 | 0.3880 | 0.8780 | |
| 98.73 | 0.4760 | 0.8680 | |
| 111.49 | 0.5370 | 0.8500 | |
| 116.66 | 0.5580 | 0.8330 | |
| 126.38 | 0.6580 | 0.8060 | |
| 128.31 | 0.6770 | 0.7860 | |
| 130.66 | 0.7350 | 0.7350 | CRIT |

Sage, R. H. - Hicks, B. L. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 8 (1940) 1085-1092. doi:10.1021/ie50368a014

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 4.137 | 0.0029 | 0.1335 | |
| 5.516 | 0.0104 | 0.3369 | |
| 6.895 | 0.0175 | 0.4596 | |
| 10.34 | 0.0353 | 0.6225 | |
| 13.79 | 0.0530 | 0.7027 | |
| 20.69 | 0.0872 | 0.7827 | |
| 27.58 | 0.1216 | 0.8239 | |
| 34.48 | 0.1556 | 0.8473 | |
| 41.37 | 0.1889 | 0.8623 | |
| 55.16 | 0.2540 | 0.8775 | |
| 68.95 | 0.3171 | 0.8809 | |
| 82.74 | 0.3810 | 0.8799 | |
| 86.19 | 0.3974 | 0.8786 | |
| 96.53 | 0.4465 | 0.8731 | |
| 103.42 | 0.4799 | 0.8665 | |
| 110.32 | 0.5168 | 0.8570 | |
| 117.21 | 0.5586 | 0.8440 | |
| 120.66 | 0.5837 | 0.8349 | |
| 124.11 | 0.6110 | 0.8227 | |
| 127.55 | 0.6435 | 0.8053 | |
| 131.00 | 0.7032 | 0.7709 | |
| 131.83 | 0.7236 | 0.7236 | CRIT |

Sage, R. H. - Hicks, B. L. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 8 (1940) 1085-1092. doi:10.1021/ie50368a014

**T / K = 327.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 6.895 | 0.0065 | 0.1790 | |
| 10.34 | 0.0235 | 0.4301 | |
| 13.79 | 0.0404 | 0.5531 | |
| 20.69 | 0.0734 | 0.6777 | |
| 27.58 | 0.1060 | 0.7390 | |
| 34.48 | 0.1382 | 0.7745 | |
| 41.37 | 0.1697 | 0.7966 | |
| 55.16 | 0.2319 | 0.8193 | |
| 68.95 | 0.2934 | 0.8270 | |
| 82.74 | 0.3557 | 0.8283 | |
| 86.19 | 0.3716 | 0.8275 | |
| 96.53 | 0.4194 | 0.8218 | |
| 103.42 | 0.4521 | 0.8146 | |
| 110.32 | 0.4888 | 0.8042 | |
| 117.21 | 0.5284 | 0.7864 | |
| 120.66 | 0.5549 | 0.7739 | |
| 124.11 | 0.5796 | 0.7566 | |
| 127.55 | 0.6229 | 0.7294 | |
| 129.35 | 0.6718 | 0.6718 | CRIT |

Sage, R. H. - Hicks, B. L. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 8 (1940) 1085-1092. doi:10.1021/ie50368a014

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 10.34 | 0.0090 | 0.1722 | |
| 13.79 | 0.0242 | 0.3518 | |
| 20.69 | 0.0573 | 0.5318 | |
| 27.58 | 0.0885 | 0.6233 | |
| 34.48 | 0.1201 | 0.6766 | |
| 41.37 | 0.1513 | 0.7098 | |
| 55.16 | 0.2119 | 0.7451 | |
| 68.95 | 0.2739 | 0.7574 | |
| 82.74 | 0.3328 | 0.7594 | |
| 86.19 | 0.3482 | 0.7588 | |
| 96.53 | 0.3978 | 0.7528 | |
| 103.42 | 0.4329 | 0.7439 | |
| 110.32 | 0.4696 | 0.7285 | |
| 117.21 | 0.5104 | 0.7037 | |
| 120.66 | 0.5425 | 0.6831 | |
| 124.11 | 0.5683 | 0.6440 | |
| 124.80 | 0.6165 | 0.6165 | CRIT |

Sage, R. H. - Hicks, B. L. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 8 (1940) 1085-1092. doi:10.1021/ie50368a014

**T / K = 360.93**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 13.79 | 0.0079 | 0.1110 | |
| 20.69 | 0.0387 | 0.3626 | |
| 27.58 | 0.0695 | 0.4849 | |
| 34.48 | 0.1005 | 0.5580 | |
| 41.37 | 0.1309 | 0.6037 | |
| 55.16 | 0.1916 | 0.6529 | |
| 68.95 | 0.2521 | 0.6718 | |
| 82.74 | 0.3154 | 0.6745 | |
| 86.19 | 0.3319 | 0.6734 | |
| 96.53 | 0.3861 | 0.6645 | |
| 103.42 | 0.4263 | 0.6518 | |
| 110.32 | 0.4685 | 0.6266 | |
| 113.76 | 0.4918 | 0.6054 | |
| 117.07 | 0.5503 | 0.5503 | CRIT |

Sage, R. H. - Hicks, B. L. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 8 (1940) 1085-1092. doi:10.1021/ie50368a014

**T / K = 377.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 20.69 | 0.0175 | 0.1599 | |
| 27.58 | 0.0476 | 0.3242 | |
| 34.48 | 0.0783 | 0.4201 | |
| 41.37 | 0.1094 | 0.4799 | |
| 55.16 | 0.1722 | 0.5428 | |
| 68.95 | 0.2356 | 0.5630 | |
| 82.74 | 0.3012 | 0.5613 | |
| 86.19 | 0.3190 | 0.5583 | |
| 89.63 | 0.3363 | 0.5530 | |
| 96.53 | 0.3819 | 0.5370 | |
| 99.97 | 0.4038 | 0.5228 | |
| 103.42 | 0.4376 | 0.4987 | |
| 104.80 | 0.4721 | 0.4721 | CRIT |

Sage, R. H. - Hicks, B. L. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems, Industrial & Engineering Chemistry 8 (1940) 1085-1092. doi:10.1021/ie50368a014

**T / K = 394.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 27.58 | 0.0218 | 0.1418 | |
| 34.48 | 0.0530 | 0.2650 | |
| 41.37 | 0.0850 | 0.3411 | |
| 55.16 | 0.1519 | 0.4148 | |
| 68.95 | 0.2192 | 0.4327 | |
| 75.84 | 0.2638 | 0.4294 | |
| 82.74 | 0.3021 | 0.4101 | |
| 86.19 | 0.3396 | 0.3851 | |
| 87.15 | 0.3602 | 0.3602 | CRIT |

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**Enthalpy of mixing**

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Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K = 277.00**

**P / bar = 1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 32.50 | 0.2090 |
| 36.90 | 0.2730 |
| 43.00 | 0.3330 |
| 49.90 | 0.4270 |
| 51.20 | 0.4760 |
| 49.20 | 0.5690 |
| 47.10 | 0.6100 |

| | |
|---|---|
| 41.80 | 0.6740 |
| 36.70 | 0.7300 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

| **T / K =** | **284.20** |
|---|---|
| **P / bar =** | **1.013** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 35.60 | 0.2850 |
| 42.20 | 0.3800 |
| 45.40 | 0.4470 |
| 43.00 | 0.6000 |
| 41.40 | 0.6350 |
| 38.70 | 0.6790 |
| 35.20 | 0.7400 |
| 27.30 | 0.7960 |

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**Critical point**

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Wiese, H. C. - Jacobs, Joan - Sage, B. H., Phase equilibriums in the hydrocarbon systems. Phase behavior in the methane-propane-n-butane system, Journal of Chemical & Engineering Data 1 (1970) 82-91. doi:10.1021/je60044a021

| T / K | P / bar | $x_1$ |
|---|---|---|
| 344.26 | 123.55 | 0.6165 |

Elliott, D.G. - Lin, Y.N. - Chu, T.C. - Chappelear, P.S. - Kobayashi, R., K-values for the methane - n-butane, methane - n-pentane, and methane - n-hexane systems, GPA Research Report (1976) 1-19.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 277.59 | 125.62 | 0.7828 |
| 244.28 | 104.46 | 0.8605 |
| 222.07 | 80.60 | 0.9326 |
| 210.94 | 67.09 | 0.9591 |
| 199.88 | 54.61 | 0.9829 |

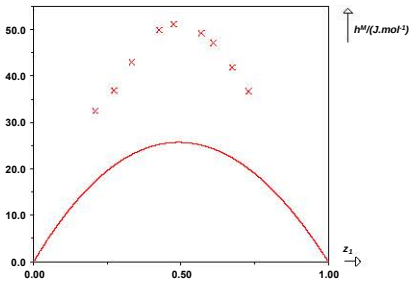
Elliot, Douglas G. - Chen, Roger J. J. - Chappelear, Patsy S. - Kobayashi, Riki, Vapor-liquid equilibrium of methane-butane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1974) 71-77. doi:10.1021/je60060a015

| T / K | P / bar | $x_1$ |
|---|---|---|
| 210.94 | 67.09 | 0.9591 |

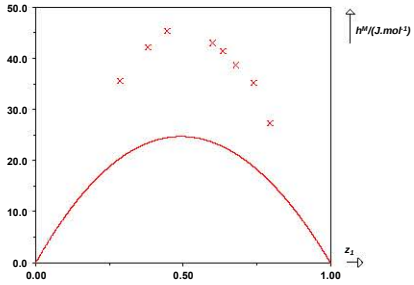
Wiese, H. C. - Jacobs, Joan - Sage, B. H., Phase equilibriums in the hydrocarbon systems. Phase behavior in the methane-propane-n-butane system, Journal of Chemical & Engineering Data 1 (1970) 82-91. doi:10.1021/je60044a021

| T / K | P / bar | $x_1$ |
|---|---|---|
| 310.93 | 131.83 | 0.7236 |
| 344.26 | 123.55 | 0.6165 |

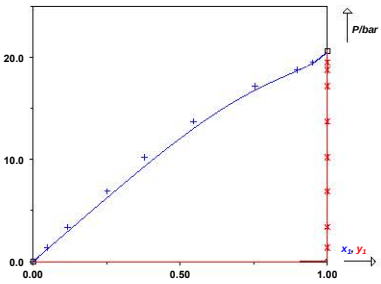
T/K = 277.00 - P/bar = 1.0132



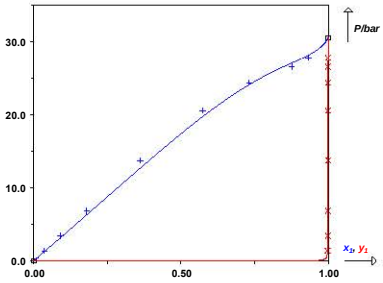

T/K = 284.20 - P/bar = 1.0132



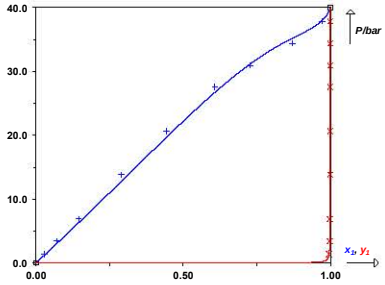

T/K = 166.48



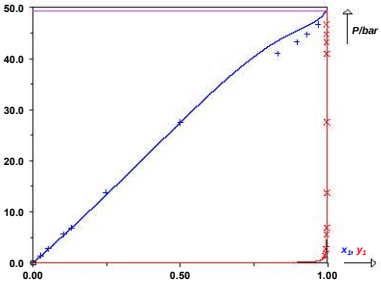

T/K = 177.59



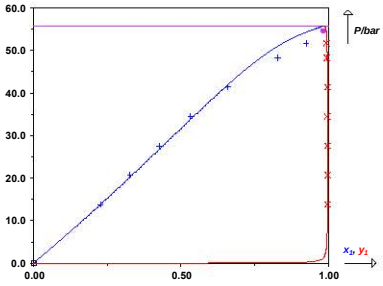

T/K = 185.93



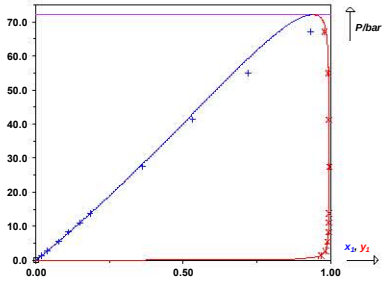

T/K = 194.09



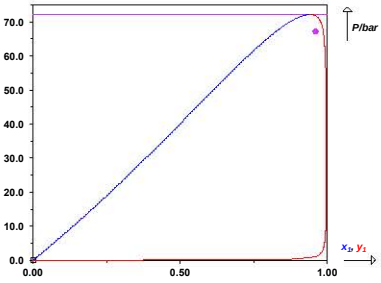

T/K = 199.88



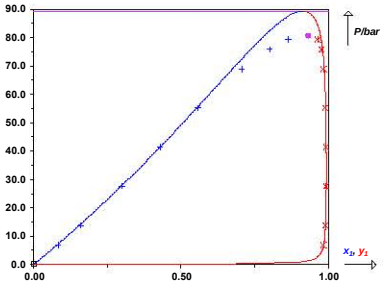

T/K = 210.93



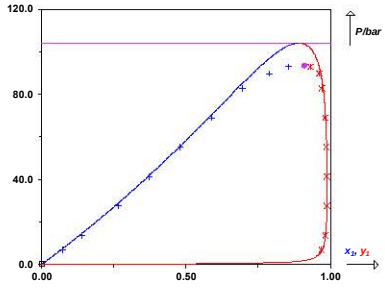

T/K = 210.94



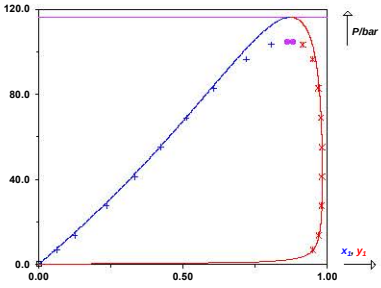

T/K = 222.07



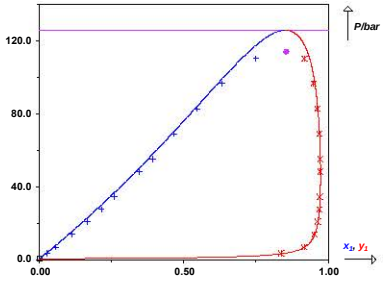

T/K = 233.18



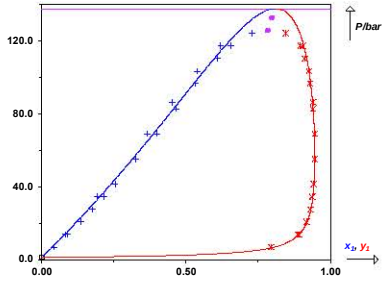

T/K = 244.28



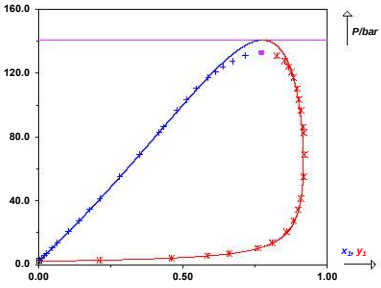

T/K = 255.38

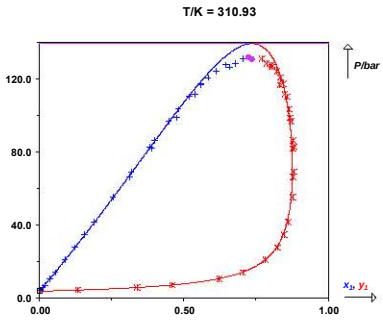


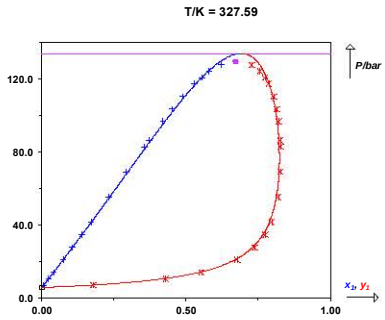

T/K = 277.59

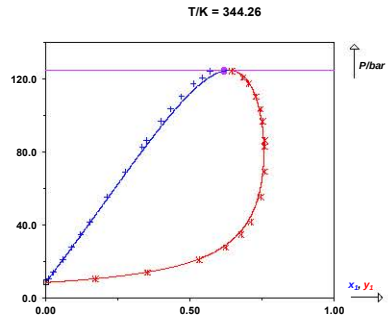


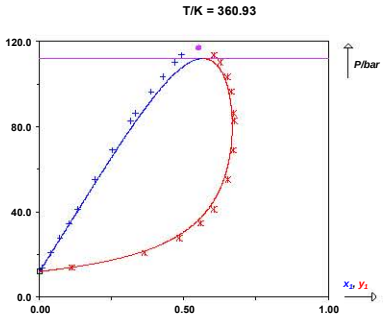

T/K = 294.26

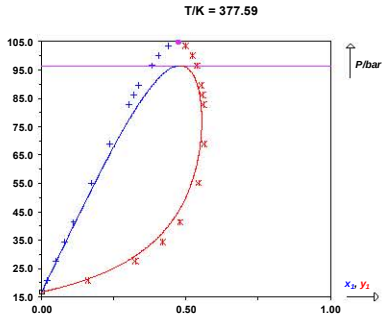


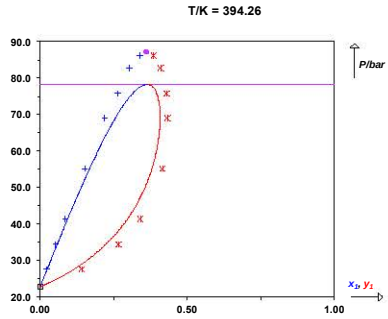

T/K = 310.93
P/bar
120.0
80.0
40.0
0.0
0.00
0.50
1.00
x1, y1


T/K = 327.59
P/bar
120.0
80.0
40.0
0.0
0.00
0.50
1.00
x1, y1


T/K = 344.26
P/bar
120.0
80.0
40.0
0.0
0.00
0.50
1.00
x1, y1


T/K = 360.93
P/bar
120.0
80.0
40.0
0.0
0.00
0.50
1.00
x1, y1


T/K = 377.59
P/bar
105.0
95.0
85.0
75.0
65.0
55.0
45.0
35.0
25.0
15.0
0.00
0.50
1.00
x1, y1


T/K = 394.26
P/bar
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
0.00
0.50
1.00
x1, y1

## ARGON (1) + METHANE (2)

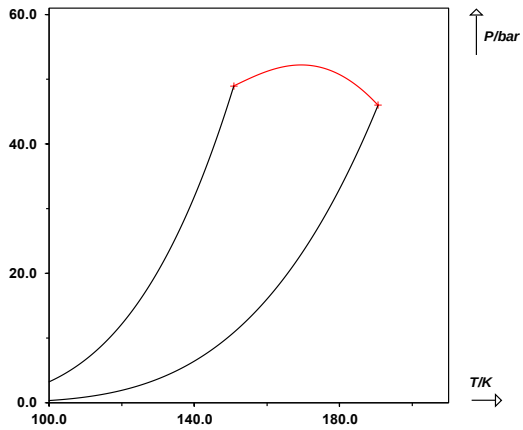
| | | |
|---|---|---|
| **CAS** | 7440-37-1 | 74-82-8 |
| **InChiKey** | XKRFYHLGVUSROY-UHFFFAOYSA-N | VNWKTOKETHGBQD-UHFFFAOYSA-N |
| **$T_c$ / K** | 150.86 | 190.56 |
| **$P_c$ / bar** | 48.98 | 45.99 |
| **ω** | 0.000 | 0.012 |

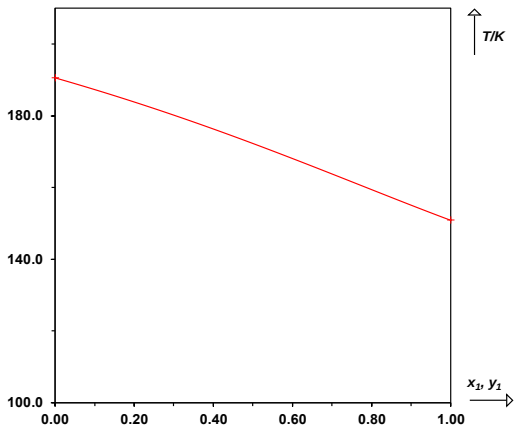
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 55.7
B/MPa = 77.2

*Deviations*
MAPE on x = 4.6 %
MAPE on y = 5.3 %
MAPE on $h^M$ = 43 %



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**Isothermal phase equilibrium data**

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Sprow, F. B. - Prausnitz, J. M., Vapor-Liquid equilibria for five cryogenic mixtures, AIChE Journal 4 (1966) 780-784. doi:10.1002/aic.690120427

**T / K = 90.67**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2671 | 0.0832 | 0.5950 |
| 0.3238 | 0.1170 | 0.6770 |
| 0.4606 | 0.2040 | 0.7920 |
| 0.5829 | 0.2890 | 0.8480 |
| 0.7426 | 0.4110 | 0.8980 |
| 0.8597 | 0.5080 | 0.9240 |
| 1.092 | 0.7120 | 0.9610 |
| 1.252 | 0.8520 | 0.9800 |
| 1.324 | 0.9130 | 0.9880 |

Calado, J. C. G. - Staveley, L. A. K., Excess Gibbs Energy of Argon-Methane Liquid Mixtures at 115.77°K, The Journal of Chemical Physics 9 (1972) 4718-4719. doi:10.1063/1.1677927

**T / K = 115.77**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.124 | 0.1812 | 0.6069 |
| 3.909 | 0.2790 | 0.7116 |
| 4.964 | 0.4098 | 0.8022 |
| 5.385 | 0.4632 | 0.8294 |
| 5.738 | 0.5139 | 0.8511 |
| 6.857 | 0.6603 | 0.9048 |
| 7.555 | 0.7538 | 0.9333 |
| 7.762 | 0.8049 | 0.9477 |

Shatskaya, L.V. - Zhirnova, N.A., Liquid-vapor phase equilibriums in two-component systems at low temperatures. I. Argon-methane system, Russ. J. Phys. Chem. 2 (1976) 298-298.

**T / K = 123.05**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.040 | 0.0487 | 0.2340 |
| 4.053 | 0.1240 | 0.4530 |
| 5.066 | 0.2005 | 0.6010 |
| 6.080 | 0.2800 | 0.6985 |
| 7.093 | 0.3627 | 0.7610 |
| 8.106 | 0.4480 | 0.8083 |
| 9.119 | 0.5408 | 0.8483 |
| 10.13 | 0.6430 | 0.8838 |
| 11.15 | 0.7427 | 0.9150 |
| 12.16 | 0.8330 | 0.9450 |
| 13.17 | 0.9186 | 0.9736 |

Kehlen, H. - Schneider, F.-U. - Haufe, S. - Barnitzke, W., Auswertung von Taudruckmessungen binärer Systeme im Mitteldruckbereich, Zeitschrift für Physikalische Chemie 1 (1983) doi:10.1515/zpch-1983-26497

**T / K = 130.60**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.100 | 0.2660 | 0.5770 |
| 9.500 | 0.3270 | 0.6860 |
| 11.10 | 0.4240 | 0.7590 |
| 14.50 | 0.6410 | 0.8600 |
| 15.90 | 0.7350 | 0.9090 |

Christiansen, L.J. - Fredenslund, Aa., Vapour-liquid equilibria of the CH4-Ar-CO system, Cryogenics 1 (1974) 10-14. doi:10.1016/0011-2275(74)90037-X

**T / K = 164.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.27 | 0.0380 | 0.1000 |
| 35.43 | 0.3690 | 0.5390 |

Christiansen, L.J. - Fredenslund, Aa. - Mollerup, J., Vapour-liquid equilibrium of the CH4-Ar, CH4-CO, and Ar-CO systems at elevated pressures, Cryogenics 7 (1973) 405-413. doi:10.1016/0011-2275(73)90076-3

**T / K = 164.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.43 | 0.0410 | 0.1130 |
| 22.88 | 0.0980 | 0.2220 |
| 26.18 | 0.1750 | 0.3330 |
| 27.36 | 0.1960 | 0.3620 |
| 30.69 | 0.2680 | 0.4450 |
| 35.14 | 0.3680 | 0.5350 |
| 35.64 | 0.3740 | 0.5420 |
| 38.97 | 0.4410 | 0.5900 |
| 42.09 | 0.5050 | 0.6310 |
| 45.05 | 0.5620 | 0.6680 |
| 48.76 | 0.6300 | 0.7000 |
| 50.99 | 0.6650 | 0.6960 |

Christiansen, L.J. - Fredenslund, Aa. - Mollerup, J., Vapour-liquid equilibrium of the CH4-Ar, CH4-CO, and Ar-CO systems at elevated pressures, Cryogenics 7 (1973) 405-413. doi:10.1016/0011-2275(73)90076-3

**T / K = 178.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 32.10 | 0.0240 | 0.0530 |
| 33.09 | 0.0460 | 0.0900 |
| 36.48 | 0.1090 | 0.1850 |
| 39.85 | 0.1650 | 0.2530 |
| 42.29 | 0.2040 | 0.2920 |

| | | |
|---|---|---|
| 43.66 | 0.2270 | 0.3140 |
| 46.29 | 0.2680 | 0.3550 |
| 49.76 | 0.3220 | 0.3870 |
| 49.95 | 0.3330 | 0.3760 |

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**Enthalpy of mixing**

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Lewis, K.L. - Saville, G. - Staveley, L.A.K., Excess enthalpies of liquid oxygen + argon, oxygen + nitrogen, and argon + methane, The Journal of Chemical Thermodynamics 4 (1975) 389-400. doi:10.1016/0021-9614(75)90178-0

**T / K = 91.50**

**P / bar = UNKNOWN (3.0966)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 77.30 | 0.2800 |
| 93.80 | 0.4030 |
| 101.40 | 0.4880 |
| 101.90 | 0.5150 |
| 85.30 | 0.7260 |
| 69.50 | 0.8070 |

Mosedale, S.E. - Wormald, C.J., The enthalpy of mixing of argon + methane at 123, 130, 140, and 145 K, at pressures up to 9.12 MPa, The Journal of Chemical Thermodynamics 5 (1977) 483-490. doi:10.1016/0021-9614(77)90149-5

**T / K = 123.00**

**P / bar = 60.80**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 41.00 | 0.1560 |
| 54.00 | 0.1860 |
| 72.00 | 0.3540 |
| 89.00 | 0.4300 |
| 91.00 | 0.5060 |
| 84.00 | 0.6150 |
| 63.00 | 0.7930 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 123.00**

**P / bar = 10.10**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -848.00 | 0.1600 |
| -1561.0 | 0.2120 |
| -1302.0 | 0.7120 |
| 401.00 | 0.8600 |

Mosedale, S.E. - Wormald, C.J., The enthalpy of mixing of argon + methane at 123, 130, 140, and 145 K, at pressures up to 9.12 MPa, The Journal of Chemical Thermodynamics 5 (1977) 483-490. doi:10.1016/0021-9614(77)90149-5

**T / K = 130.00**

**P / bar = 40.50**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 28.00 | 0.1340 |
| 49.00 | 0.2420 |
| 48.00 | 0.2700 |
| 63.00 | 0.4490 |
| 68.00 | 0.5550 |
| 45.00 | 0.7650 |

Mosedale, S.E. - Wormald, C.J., The enthalpy of mixing of argon + methane at 123, 130, 140, and 145 K, at pressures up to 9.12 MPa, The Journal of Chemical Thermodynamics 5 (1977) 483-490. doi:10.1016/0021-9614(77)90149-5

**T / K = 130.00**

**P / bar = 80.90**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 40.00 | 0.1500 |
| 64.00 | 0.2820 |
| 84.00 | 0.5080 |
| 85.00 | 0.5950 |
| 23.00 | 0.9340 |

Mosedale, S.E. - Wormald, C.J., The enthalpy of mixing of argon + methane at 123, 130, 140, and 145 K, at pressures up to 9.12 MPa, The Journal of Chemical Thermodynamics 5 (1977) 483-490. doi:10.1016/0021-9614(77)90149-5

**T / K = 140.00**

**P / bar = 40.60**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 16.00 | 0.2670 |
| 15.00 | 0.3780 |
| 9.000 | 0.5250 |
| -2.000 | 0.7070 |
| -7.000 | 0.7970 |
| -6.000 | 0.8990 |

Mosedale, S.E. - Wormald, C.J., The enthalpy of mixing of argon + methane at 123, 130, 140, and 145 K, at pressures up to 9.12 MPa, The Journal of Chemical Thermodynamics 5 (1977) 483-490. doi:10.1016/0021-9614(77)90149-5

**T / K = 140.00**

**P / bar = 61.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 23.00 | 0.1460 |
| 33.00 | 0.3370 |
| 40.00 | 0.4680 |
| 34.00 | 0.6070 |
| 28.00 | 0.7740 |
| 14.00 | 0.8350 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 140.00**

**P / bar = 10.20**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -130.00 | 0.0520 |
| 741.00 | 0.2260 |
| 888.00 | 0.2350 |
| 1909.0 | 0.2920 |
| 3376.0 | 0.4120 |
| 3106.0 | 0.4970 |
| 2631.0 | 0.6160 |
| 1380.0 | 0.8150 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 140.00**

**P / bar = 20.60**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -439.00 | 0.1040 |
| -696.00 | 0.1550 |
| -794.00 | 0.1670 |
| -1605.0 | 0.6280 |
| -601.00 | 0.7000 |
| 1070.0 | 0.7970 |
| 753.00 | 0.8710 |
| 443.00 | 0.9310 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 140.00**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 4.800 | 0.1230 |
| 10.40 | 0.5010 |
| 10.00 | 0.6260 |
| 4.300 | 0.8580 |
| 3.100 | 0.8950 |

Mosedale, S.E. - Wormald, C.J., The enthalpy of mixing of argon + methane at 123, 130, 140, and 145 K, at pressures up to 9.12 MPa, The Journal of Chemical Thermodynamics 5 (1977) 483-490. doi:10.1016/0021-9614(77)90149-5

**T / K = 145.00**

**P / bar = 47.50**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -10.00 | 0.1880 |
| -16.00 | 0.3020 |
| -22.00 | 0.4220 |
| -35.00 | 0.5730 |
| -42.00 | 0.6950 |
| -51.00 | 0.8100 |
| -48.00 | 0.8990 |
| -27.00 | 0.9490 |

Mosedale, S.E. - Wormald, C.J., The enthalpy of mixing of argon + methane at 123, 130, 140, and 145 K, at pressures up to 9.12 MPa, The Journal of Chemical Thermodynamics 5 (1977) 483-490. doi:10.1016/0021-9614(77)90149-5

**T / K = 145.00**

**P / bar = 61.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 12.00 | 0.1930 |
| 15.00 | 0.3250 |
| 7.000 | 0.5180 |
| -10.00 | 0.6780 |
| -17.00 | 0.7980 |
| -13.00 | 0.8570 |

Mosedale, S.E. - Wormald, C.J., The enthalpy of mixing of argon + methane at 123, 130, 140, and 145 K, at pressures up to 9.12 MPa, The Journal of Chemical Thermodynamics 5 (1977) 483-490. doi:10.1016/0021-9614(77)90149-5

**T / K = 145.00**

**P / bar = 81.40**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 28.00 | 0.2720 |
| 37.00 | 0.3960 |
| 39.00 | 0.5380 |

| | |
|---|---|
| 29.00 | 0.7130 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 160.00**

**P / bar = 20.40**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -22.00 | 0.0170 |
| 43.00 | 0.0770 |
| 802.00 | 0.1260 |
| 1668.0 | 0.1630 |
| 2956.0 | 0.1830 |
| 4729.0 | 0.2670 |
| 3998.0 | 0.3150 |
| 3290.0 | 0.4260 |
| 2782.0 | 0.5950 |
| 165.00 | 0.9720 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 160.00**

**P / bar = 40.70**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -488.00 | 0.1680 |
| -285.00 | 0.6030 |
| -187.00 | 0.6340 |
| 922.00 | 0.6870 |
| 804.00 | 0.7750 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 160.00**

**P / bar = 51.60**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -449.00 | 0.1560 |
| -920.00 | 0.7170 |
| -232.00 | 0.7980 |
| 117.00 | 0.8230 |
| 141.00 | 0.8910 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 183.00**

**P / bar = 35.60**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 228.00 | 0.1420 |
| 266.00 | 0.2420 |
| 302.00 | 0.4480 |
| 174.00 | 0.7690 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 183.00**

**P / bar = 45.70**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 2214.0 | 0.2390 |
| 2302.0 | 0.2900 |
| 2172.0 | 0.3810 |
| 1903.0 | 0.4810 |
| 1579.0 | 0.5690 |
| 1186.0 | 0.6920 |
| 580.00 | 0.8540 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 183.00**

**P / bar = 71.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -106.00 | 0.1790 |
| -45.00 | 0.3330 |
| 216.00 | 0.4560 |
| 583.00 | 0.6660 |

Wormald, Christopher J. - Lewis, Keith L. - Mosedale, Stephen, The excess enthalpies of hydrogen + methane, hydrogen + nitrogen, methane + nitrogen, methane + argon, and nitrogen + argon at 298 and 201 K at pressures up to 10.2 MPa, The Journal of Chemical Thermodynamics 1 (1977) 27-42. doi:10.1016/0021-9614(77)90194-X

**T / K = 201.00**

**P / bar =** **51.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 252.00 | 0.1200 |
| 293.00 | 0.2410 |
| 319.00 | 0.3780 |
| 291.00 | 0.5340 |
| 174.00 | 0.7630 |

Wormald, Christopher J. - Lewis, Keith L. - Mosedale, Stephen, The excess enthalpies of hydrogen + methane, hydrogen + nitrogen, methane + nitrogen, methane + argon, and nitrogen + argon at 298 and 201 K at pressures up to 10.2 MPa, The Journal of Chemical Thermodynamics 1 (1977) 27-42. doi:10.1016/0021-9614(77)90194-X

**T / K =** **201.00**

**P / bar =** **66.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 858.00 | 0.1910 |
| 933.00 | 0.2410 |
| 965.00 | 0.3200 |
| 871.00 | 0.5530 |

Wormald, Christopher J. - Lewis, Keith L. - Mosedale, Stephen, The excess enthalpies of hydrogen + methane, hydrogen + nitrogen, methane + nitrogen, methane + argon, and nitrogen + argon at 298 and 201 K at pressures up to 10.2 MPa, The Journal of Chemical Thermodynamics 1 (1977) 27-42. doi:10.1016/0021-9614(77)90194-X

**T / K =** **201.00**

**P / bar =** **86.20**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 454.00 | 0.2680 |
| 517.00 | 0.3790 |
| 598.00 | 0.5160 |
| 523.00 | 0.6490 |

Wormald, Christopher J. - Lewis, Keith L. - Mosedale, Stephen, The excess enthalpies of hydrogen + methane, hydrogen + nitrogen, methane + nitrogen, methane + argon, and nitrogen + argon at 298 and 201 K at pressures up to 10.2 MPa, The Journal of Chemical Thermodynamics 1 (1977) 27-42. doi:10.1016/0021-9614(77)90194-X

**T / K =** **298.00**

**P / bar =** **40.80**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 20.00 | 0.2270 |
| 27.00 | 0.3530 |
| 29.00 | 0.5750 |
| 15.00 | 0.8290 |

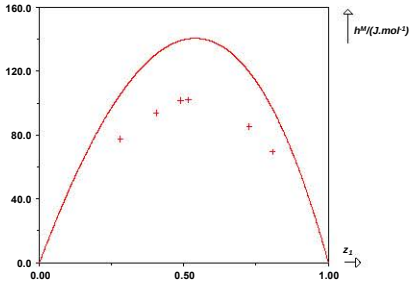
Wormald, Christopher J. - Lewis, Keith L. - Mosedale, Stephen, The excess enthalpies of hydrogen + methane, hydrogen + nitrogen, methane + nitrogen, methane + argon, and nitrogen + argon at 298 and 201 K at pressures up to 10.2 MPa, The Journal of Chemical Thermodynamics 1 (1977) 27-42. doi:10.1016/0021-9614(77)90194-X

**T / K =** **298.00**

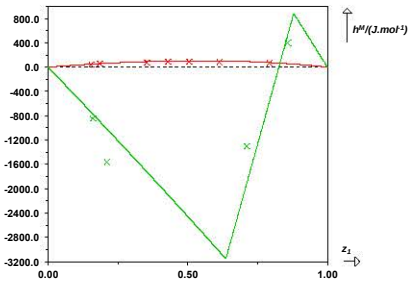
**P / bar =** **81.10**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 59.00 | 0.2570 |
| 73.00 | 0.3640 |
| 73.00 | 0.5080 |
| 66.00 | 0.6390 |
| 36.00 | 0.8300 |

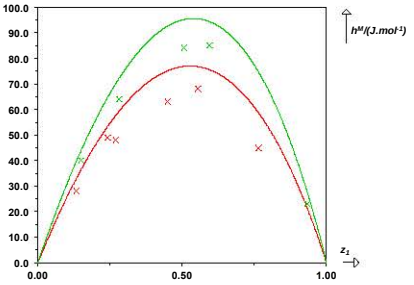
T/K = 91.50 - P/bar = 3.0966



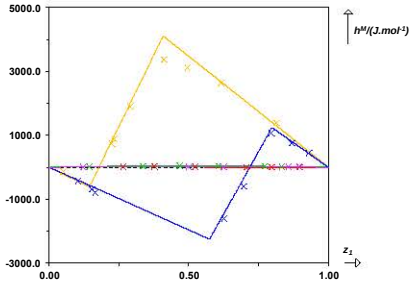

T/K = 123.00 - P/bar = 60.800 10.100



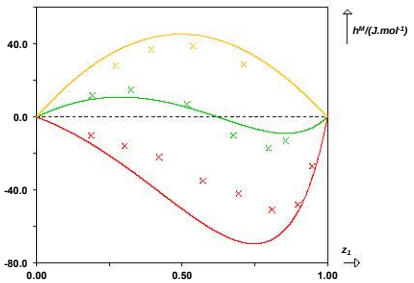

T/K = 130.00 - P/bar = 40.500 80.900



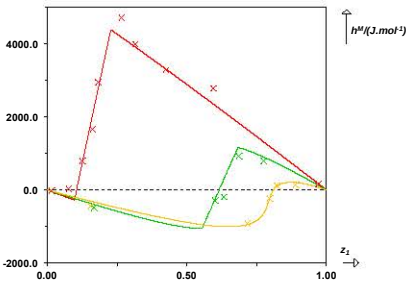

T/K = 140.00 - P/bar = 40.600 61.00 10.200 20.600 4.00



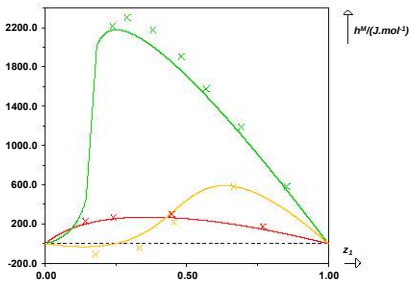

T/K = 145.00 - P/bar = 47.500 61.00 81.400



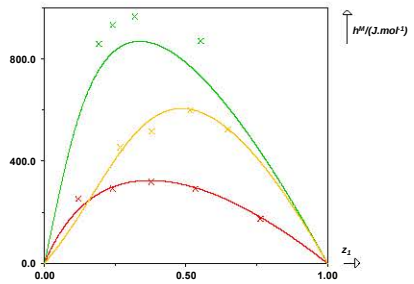

T/K = 160.00 - P/bar = 20.400 40.700 51.600



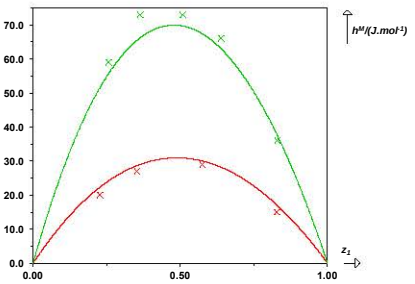

T/K = 183.00 - P/bar = 35.600 45.700 71.00



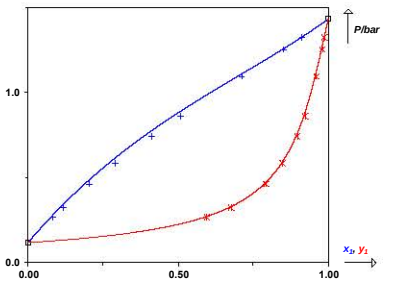

T/K = 201.00 - P/bar = 51.00 66.00 86.200



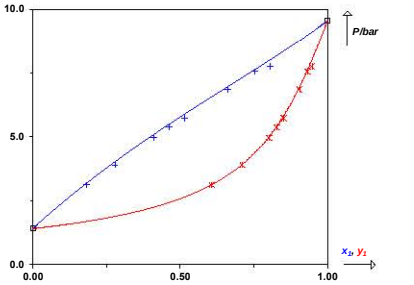

T/K = 298.00 - P/bar = 40.800 81.100



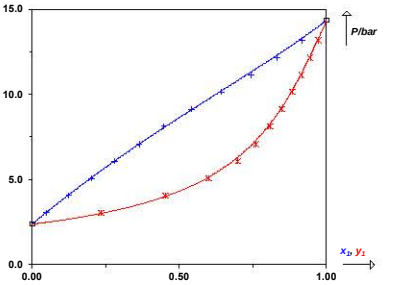

T/K = 90.67



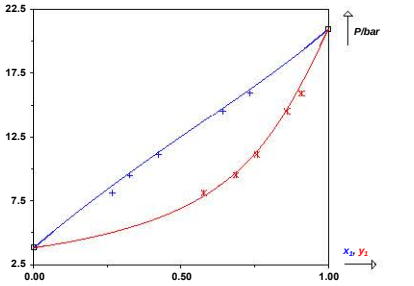

T/K = 115.77



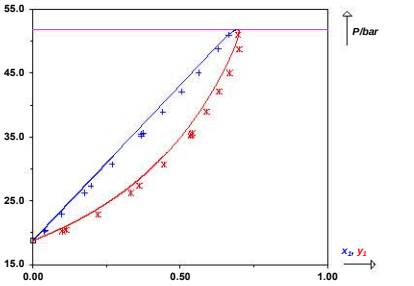

T/K = 123.05



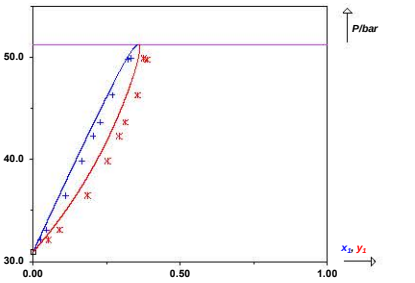

T/K = 130.60




T/K = 164.00




T/K = 178.00



## n-HEPTANE (1) + MONOCHLOROBENZENE (2)

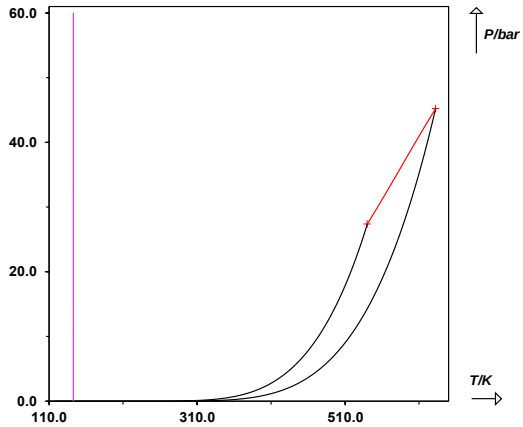
| | | |
|---|---|---|
| **CAS** | 142-82-5 | 108-90-7 |
| **InChiKey** | IMNFDUFMRHMDMM-UHFFFAOYSA-N | MVPPADPHJFYWMZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 540.20 | 632.35 |
| **$P_c$ / bar** | 27.40 | 45.19 |
| **ω** | 0.349 | 0.250 |

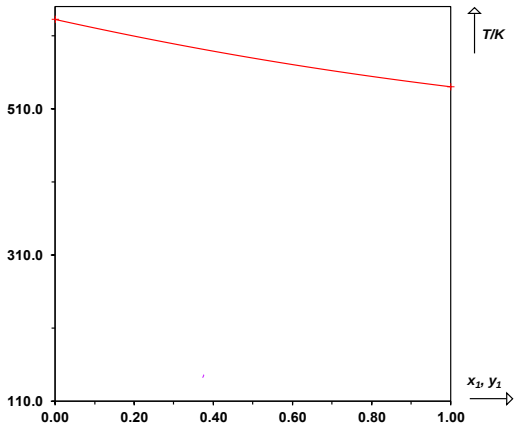
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 86.4
B/MPa = 112

*Deviations*
MAPE on x = 4.2 %
MAPE on y = 3.3 %
MAPE on $h^M$ = 7.7 %
MAPE on $c_P^M$ = 22 %



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**Isothermal phase equilibrium data**

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Owa, M. - Nakaiwa, M. - Akiya, T. - Kawasaki, S. - Hakuta, T. - Namiki, H., Measurement and correlation of vapor-liquid equilibrium of trifluoroethanol/water binary system, Kagaku Gijutsu Kenkyusho Hokoku 9 (1990) 303-307.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0629 | 0.0200 | 0.1142 |
| 0.0760 | 0.0680 | 0.2972 |
| 0.0891 | 0.1236 | 0.4324 |
| 0.0951 | 0.1568 | 0.4832 |
| 0.0986 | 0.1724 | 0.5108 |
| 0.0997 | 0.1815 | 0.5190 |
| 0.1058 | 0.2183 | 0.5518 |
| 0.1167 | 0.2871 | 0.6226 |
| 0.1166 | 0.2880 | 0.6243 |
| 0.1236 | 0.3393 | 0.6630 |
| 0.1303 | 0.3913 | 0.6918 |
| 0.1426 | 0.5044 | 0.7619 |
| 0.1533 | 0.6154 | 0.8084 |
| 0.1640 | 0.7250 | 0.8662 |
| 0.1746 | 0.8422 | 0.9203 |
| 0.1823 | 0.9321 | 0.9645 |

Owa, M. - Nakaiwa, M. - Akiya, T. - Kawasaki, S. - Hakuta, T. - Namiki, H., Measurement and correlation of vapor-liquid equilibrium of trifluoroethanol/water binary system, Kagaku Gijutsu Kenkyusho Hokoku 9 (1990) 303-307.

**T / K = 338.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1205 | 0.0229 | 0.1136 |
| 0.1373 | 0.0607 | 0.2466 |
| 0.1575 | 0.1103 | 0.3727 |
| 0.1770 | 0.1646 | 0.4690 |
| 0.1904 | 0.2107 | 0.5298 |
| 0.2033 | 0.2549 | 0.5698 |
| 0.2082 | 0.2747 | 0.5962 |
| 0.2146 | 0.2990 | 0.6105 |
| 0.2338 | 0.3860 | 0.6809 |
| 0.2354 | 0.3880 | 0.6763 |
| 0.2497 | 0.4602 | 0.7214 |
| 0.2614 | 0.5222 | 0.7547 |
| 0.2847 | 0.6571 | 0.8263 |
| 0.2961 | 0.7215 | 0.8555 |
| 0.3078 | 0.7966 | 0.8932 |
| 0.3180 | 0.8559 | 0.9209 |
| 0.3308 | 0.9460 | 0.9712 |

Owa, M. - Nakaiwa, M. - Akiya, T. - Kawasaki, S. - Hakuta, T. - Namiki, H., Measurement and correlation of vapor-liquid equilibrium of trifluoroethanol/water binary system, Kagaku Gijutsu Kenkyusho Hokoku 9 (1990) 303-307.

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1465 | 0.0211 | 0.1019 |
| 0.2180 | 0.1786 | 0.4761 |
| 0.2411 | 0.2481 | 0.5627 |
| 0.2617 | 0.3173 | 0.6252 |
| 0.3061 | 0.4830 | 0.7326 |
| 0.3262 | 0.5781 | 0.7818 |
| 0.3457 | 0.6723 | 0.8395 |
| 0.3652 | 0.7742 | 0.8837 |
| 0.3821 | 0.8700 | 0.9298 |
| 0.3947 | 0.9419 | 0.9680 |

Bayles, John W. - Letcher, Trevor M., Thermodynamics of some binary liquid mixtures containing aliphatic amines, Journal of Chemical & Engineering Data 3 (1971) 266-271. doi:10.1021/je60050a026

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2516 | 0.0730 | 0.2660 |
| 0.2665 | 0.0960 | 0.3200 |
| 0.2756 | 0.1140 | 0.3500 |
| 0.3054 | 0.1690 | 0.4400 |
| 0.3334 | 0.2300 | 0.5150 |
| 0.3444 | 0.2480 | 0.5450 |
| 0.3893 | 0.3580 | 0.6430 |
| 0.4060 | 0.4100 | 0.6760 |
| 0.4132 | 0.4290 | 0.6910 |
| 0.4228 | 0.4590 | 0.7100 |
| 0.4334 | 0.4970 | 0.7330 |
| 0.4466 | 0.5380 | 0.7580 |
| 0.4653 | 0.6060 | 0.7960 |
| 0.4801 | 0.6530 | 0.8220 |
| 0.4934 | 0.7020 | 0.8460 |
| 0.5017 | 0.7360 | 0.8620 |
| 0.5186 | 0.7940 | 0.8920 |
| 0.5389 | 0.8700 | 0.9300 |
| 0.5465 | 0.9040 | 0.9500 |

Bayles, John W. - Letcher, Trevor M., Thermodynamics of some binary liquid mixtures containing aliphatic amines, Journal of Chemical & Engineering Data 3 (1971) 266-271. doi:10.1021/je60050a026

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4653 | 0.0510 | 0.1850 |
| 0.5394 | 0.1200 | 0.3360 |
| 0.5602 | 0.1410 | 0.3750 |
| 0.5814 | 0.1620 | 0.4100 |
| 0.6134 | 0.1970 | 0.4590 |
| 0.6426 | 0.2330 | 0.5050 |
| 0.6694 | 0.2660 | 0.5400 |
| 0.6857 | 0.2910 | 0.5700 |
| 0.7463 | 0.3830 | 0.6390 |
| 0.7786 | 0.4370 | 0.6780 |
| 0.7819 | 0.4420 | 0.6820 |
| 0.8133 | 0.4990 | 0.7170 |
| 0.8274 | 0.5240 | 0.7330 |
| 0.8535 | 0.5730 | 0.7630 |
| 0.8711 | 0.6050 | 0.7825 |
| 0.9222 | 0.7060 | 0.8370 |
| 0.9435 | 0.7480 | 0.8610 |
| 0.9750 | 0.8155 | 0.8980 |
| 1.000 | 0.8660 | 0.9260 |
| 1.016 | 0.9000 | 0.9440 |

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**Isobaric phase equilibrium data**

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Othmer, Donald F. - Shlechter, Nathan - Koszalka, Walter A., Composition of Vapors From Boiling Binary Solutions, Industrial & Engineering Chemistry 9 (1945) 895-900. doi:10.1021/ie50429a027

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 402.20 | 0.0314 | 0.1103 |
| 397.30 | 0.0880 | 0.2637 |
| 392.70 | 0.1579 | 0.3991 |
| 389.10 | 0.2277 | 0.5020 |
| 386.30 | 0.2962 | 0.5766 |
| 383.70 | 0.3709 | 0.6421 |
| 380.90 | 0.4700 | 0.7138 |
| 378.20 | 0.5865 | 0.7808 |
| 375.40 | 0.7294 | 0.8541 |
| 372.90 | 0.8922 | 0.9387 |

Raviprasad, A. - Venkateswara Rao, K. - Chiranjivi, C., Isobaric vapor-liquid equilibrium data for the systems n-heptane-chlorobenzene and trichloroethylene-methyl isobutyl ketone (MIBK), Indian Chem. Eng. 4 (1976) 47-49.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 401.85 | 0.0280 | 0.1160 |
| 400.75 | 0.0420 | 0.1580 |
| 397.65 | 0.0730 | 0.2380 |
| 390.65 | 0.2060 | 0.4750 |
| 382.45 | 0.3850 | 0.6380 |
| 380.75 | 0.4710 | 0.7000 |
| 379.55 | 0.5160 | 0.7260 |
| 377.85 | 0.6080 | 0.7800 |
| 376.05 | 0.6900 | 0.8280 |
| 374.45 | 0.7740 | 0.8700 |
| 372.05 | 0.9240 | 0.9550 |

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**Enthalpy of mixing**

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Paul, H.I. - Krug, J. - Knapp, H., Measurements of VLE, vE and hE for binary mixtures of n-alkanes with chloro-alkylbenzenes, Fluid Phase Equilibria 3 (1988) 307-324. doi:10.1016/0378-3812(88)85010-6

**T / K = 288.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 302.90 | 0.1282 |
| 356.80 | 0.1576 |
| 397.00 | 0.1877 |
| 438.40 | 0.2185 |
| 476.30 | 0.2502 |
| 511.10 | 0.2827 |
| 541.20 | 0.3160 |
| 568.60 | 0.3503 |
| 589.20 | 0.3854 |
| 608.30 | 0.4215 |
| 620.90 | 0.4586 |
| 628.40 | 0.4968 |
| 627.10 | 0.5360 |
| 619.80 | 0.5764 |
| 603.40 | 0.6179 |
| 574.80 | 0.6607 |
| 541.10 | 0.7048 |
| 493.40 | 0.7502 |
| 431.80 | 0.7971 |
| 352.90 | 0.8454 |

Ruiz, B - Royo, F.M - Gracia, M - Gutiérrez Losa, C, HmE of (1,2-dibromopropane + cyclohexane or benzene or tetrachloromethane) at several temperatures, The Journal of Chemical Thermodynamics 3 (1987) 261-264. doi:10.1016/0021-9614(87)90133-9

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|

| | |
|---|---|
| 258.50 | 0.1108 |
| 339.10 | 0.1464 |
| 455.20 | 0.2181 |
| 552.70 | 0.2942 |
| 624.70 | 0.3781 |
| 669.50 | 0.4679 |
| 663.50 | 0.5571 |
| 612.20 | 0.6627 |
| 481.30 | 0.7757 |
| 267.80 | 0.8920 |

Grolier, J.P.E. - Sosnkowska-Kehiaian, K. - Kehiaian, H.V., Enthalpies de mélange des chlorures organiques avec des hydrocarbures, J. Chim. Phys. Phys. Chim. Biol. 2 (1973) 367-373. doi:10.1051/jcp/1973700367

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 450.00 | 0.1960 |
| 620.00 | 0.3360 |
| 690.00 | 0.4870 |
| 700.00 | 0.5470 |
| 650.00 | 0.6440 |
| 615.00 | 0.6770 |
| 355.00 | 0.8470 |
| 135.00 | 0.9390 |

Paul, H.I. - Krug, J. - Knapp, H., Measurements of VLE, vE and hE for binary mixtures of n-alkanes with chloro-alkylbenzenes, Fluid Phase Equilibria 3 (1988) 307-324. doi:10.1016/0378-3812(88)85010-6

**T / K =** **308.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 289.80 | 0.1282 |
| 341.40 | 0.1576 |
| 385.00 | 0.1877 |
| 427.60 | 0.2185 |
| 465.10 | 0.2502 |
| 496.80 | 0.2827 |
| 526.80 | 0.3160 |
| 552.60 | 0.3503 |
| 578.40 | 0.3854 |
| 596.20 | 0.4215 |
| 606.90 | 0.4586 |
| 610.20 | 0.4968 |
| 604.50 | 0.5360 |
| 590.30 | 0.5764 |
| 574.30 | 0.6179 |
| 547.90 | 0.6607 |
| 512.20 | 0.7048 |
| 458.30 | 0.7502 |
| 400.00 | 0.7971 |
| 323.40 | 0.8454 |

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**Heat capacity of mixing**

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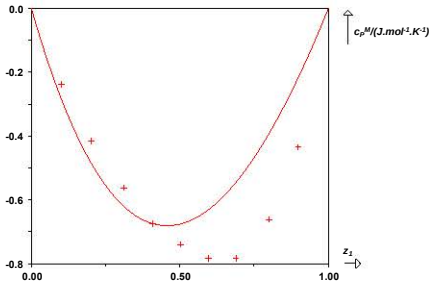
Bendiab, H. - Roux-Desgranges, G. - Roux, A. H. - Grolier, J. -P. E. - Patterson, D., Excess heat capacities of ternary systems containing chlorobenzene or chloronaphthalene, Journal of Solution Chemistry 2 (1994) 307-323. doi:10.1007/BF00973552

**T / K =** **298.15**

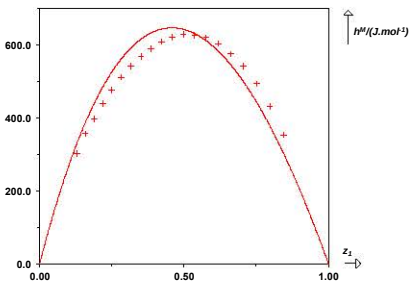
**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.2380 | 0.1010 |
| -0.4160 | 0.1997 |
| -0.5620 | 0.3107 |
| -0.6750 | 0.4083 |
| -0.7400 | 0.5014 |
| -0.7820 | 0.5961 |
| -0.7840 | 0.6894 |
| -0.6620 | 0.7994 |
| -0.4350 | 0.8985 |

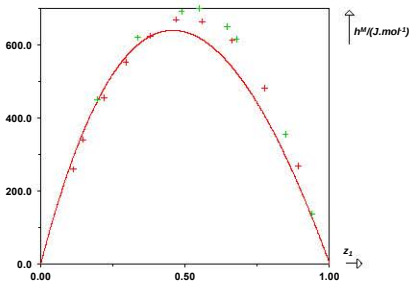
T/K = 298.15 - P/bar = 1.0132



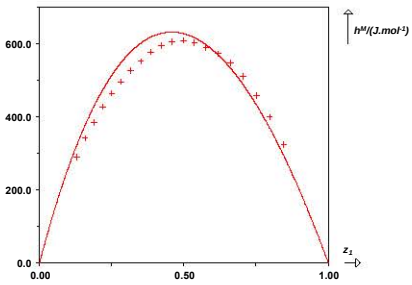

T/K = 288.15 - P/bar = 1.0132



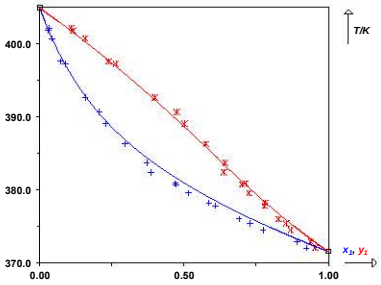

T/K = 298.15 - P/bar = 1.0132 1.0132



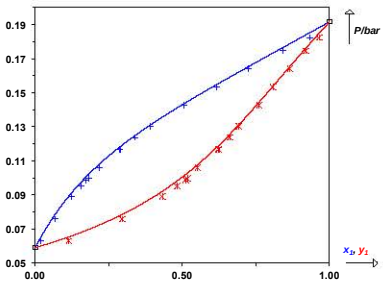

T/K = 308.15 - P/bar = 1.0132



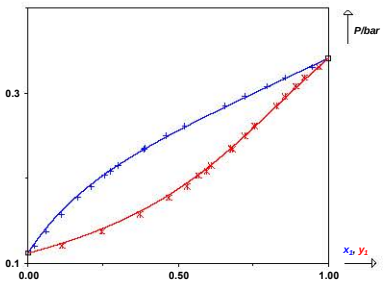

P/bar = 1.01330



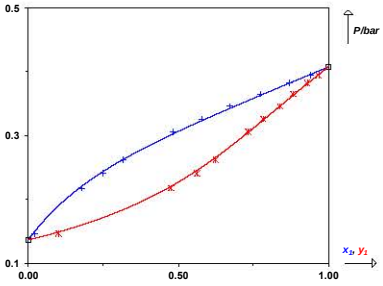

T/K = 323.15



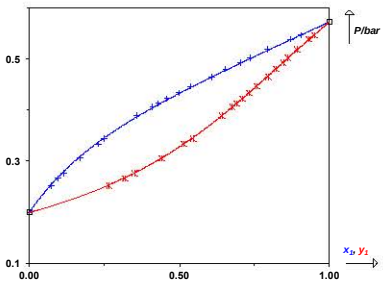

T/K = 338.15



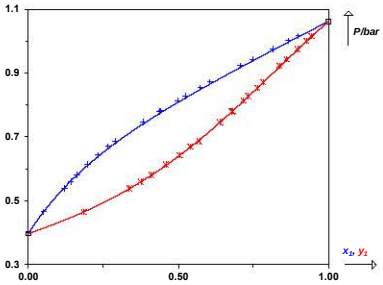

T/K = 343.15




T/K = 353.15




T/K = 373.15



## CYCLOHEXANE (1) + MONOCHLOROBENZENE (2)

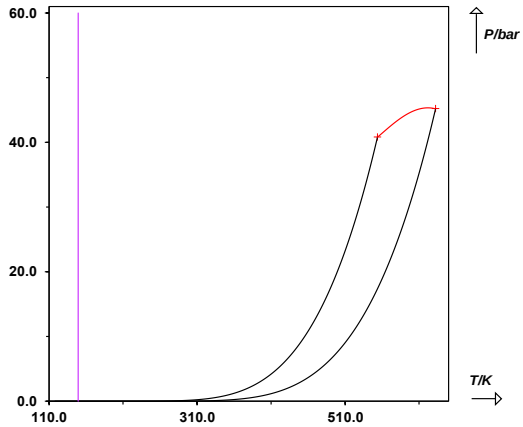
| | | |
|---|---|---|
| **CAS** | 110-82-7 | 108-90-7 |
| **InChiKey** | XDTMQSROBMDMFD-UHFFFAOYSA-N | MVPPADPHJFYWMZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 553.80 | 632.35 |
| **$P_c$ / bar** | 40.80 | 45.19 |
| **ω** | 0.208 | 0.250 |

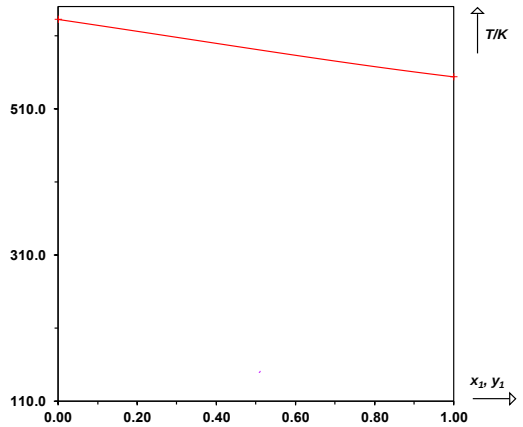
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 92.2
B/MPa = 142

*Deviations*
MAPE on x = 6.6 %
MAPE on y = 5.1 %
MAPE on $h^M$ = 7.8 %
MAPE on $c_P^M$ = 7.3 %



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**Isothermal phase equilibrium data**

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Díaz Peña, M. - Compostizo, A. - Crespo Colín, A. - Escudero, I., Activity coefficients and excess Gibbs free energies at 348.15 K in cyclohexane+chlorobenzene, +fluorobenzene, and +thiophene, The Journal of Chemical Thermodynamics 11 (1980) 1051-1055. doi:10.1016/0021-9614(80)90160-3

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2266 | 0.0566 | 0.3170 |
| 0.2300 | 0.0597 | 0.3285 |
| 0.2414 | 0.0709 | 0.3669 |
| 0.2731 | 0.1048 | 0.4578 |
| 0.2931 | 0.1267 | 0.5046 |
| 0.3169 | 0.1544 | 0.5538 |
| 0.3400 | 0.1829 | 0.5956 |
| 0.3732 | 0.2247 | 0.6469 |
| 0.3939 | 0.2517 | 0.6750 |
| 0.4358 | 0.3089 | 0.7242 |
| 0.4601 | 0.3430 | 0.7492 |
| 0.4883 | 0.3838 | 0.7755 |
| 0.5189 | 0.4292 | 0.8013 |
| 0.5359 | 0.4555 | 0.8146 |
| 0.5607 | 0.4945 | 0.8330 |
| 0.5785 | 0.5237 | 0.8455 |
| 0.5964 | 0.5533 | 0.8575 |
| 0.6267 | 0.6061 | 0.8767 |
| 0.6435 | 0.6354 | 0.8867 |
| 0.6699 | 0.6831 | 0.9025 |
| 0.6901 | 0.7199 | 0.9138 |
| 0.7187 | 0.7718 | 0.9305 |
| 0.7303 | 0.7925 | 0.9364 |
| 0.7553 | 0.8379 | 0.9502 |
| 0.7767 | 0.8758 | 0.9620 |
| 0.8186 | 0.9487 | 0.9836 |

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**Isobaric phase equilibrium data**

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Rolemberg, Marlus P. - Krähenbühl, Maria Alvina, Vapor−Liquid Equilibria of Binary and Ternary Mixtures of Benzene, Cyclohexane, and Chlorobenzene at 40.0 kPa and 101.3 kPa, Journal of Chemical & Engineering Data 2 (2001) 256-260. doi:10.1021/je000059l

**P / bar = 0.4000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 369.25 | 0.0210 | 0.1600 |
| 362.45 | 0.0600 | 0.3510 |
| 348.25 | 0.2280 | 0.6400 |
| 344.95 | 0.2770 | 0.6900 |
| 340.55 | 0.3760 | 0.7730 |
| 337.25 | 0.4570 | 0.8260 |
| 334.35 | 0.5600 | 0.8690 |
| 330.35 | 0.6660 | 0.9230 |
| 328.70 | 0.7800 | 0.9440 |
| 328.10 | 0.8260 | 0.9530 |
| 326.65 | 0.9190 | 0.9790 |

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**Enthalpy of mixing**

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Howell, P.J. - Skillerne de Bristowe, B.J. - Stubley, D., Enthalpies of mixing of pentafluorobenzene with some hydrocarbons, The Journal of Chemical Thermodynamics 2 (1972) 225-231. doi:10.1016/0021-9614(72)90060-2

**T / K = 293.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 183.50 | 0.0825 |
| 179.30 | 0.0826 |
| 381.80 | 0.1843 |
| 694.50 | 0.4862 |
| 697.20 | 0.4978 |
| 504.90 | 0.7939 |
| 292.30 | 0.8994 |

Tanaka, Reiji - Murakami, Sachio - Fujishiro, Ryoichi, Excess enthalpies of mixing of a polar liquid + a non-polar liquid at 298.15 K, The Journal of Chemical Thermodynamics 3 (1974) 209-218. doi:10.1016/0021-9614(74)90172-4

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 84.75 | 0.0339 |
| 191.76 | 0.0803 |
| 298.35 | 0.1326 |
| 395.11 | 0.1869 |
| 475.00 | 0.2368 |
| 557.66 | 0.2982 |
| 618.26 | 0.3550 |
| 662.83 | 0.4099 |
| 689.69 | 0.4706 |
| 696.73 | 0.4890 |
| 699.64 | 0.4933 |
| 702.03 | 0.5363 |
| 692.97 | 0.5886 |

| | |
|---|---|
| 668.07 | 0.6424 |
| 623.43 | 0.6988 |
| 599.73 | 0.7539 |
| 477.91 | 0.8079 |
| 382.82 | 0.8579 |
| 292.84 | 0.8976 |
| 177.13 | 0.9419 |

Amaya, Kazuo, Thermodynamical Studies on Binary Systems Consisting of Polar and Non-polar Liquids. II. The Measurement of the Heats of Mixing for Binary Systems of Polar and Non-polar Liquids, Bulletin of the Chemical Society of Japan 9 (1961) 1278-1285. doi:10.1246/bcsj.34.1278

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 274.10 | 0.1270 |
| 538.90 | 0.2920 |
| 679.60 | 0.4940 |
| 584.30 | 0.7120 |
| 292.30 | 0.8890 |

Anantaraman, A. V. - Bhattacharyya, S. N. - Palit, S. R., Weak dipolar interaction in solutions. Systems: cyclohexane+chlorobenzene and carbon tetrachloride+chlorobenzene, Transactions of the Faraday Society (1961) doi:10.1039/tf9615700040

**T / K =** **308.65**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 185.00 | 0.0969 |
| 361.00 | 0.1945 |
| 482.00 | 0.2928 |
| 609.00 | 0.3917 |
| 670.00 | 0.4913 |
| 667.00 | 0.5916 |
| 572.00 | 0.6924 |
| 434.00 | 0.7944 |
| 253.00 | 0.8968 |

Anantaraman, A. V. - Bhattacharyya, S. N. - Palit, S. R., Weak dipolar interaction in solutions. Systems: cyclohexane+chlorobenzene and carbon tetrachloride+chlorobenzene, Transactions of the Faraday Society (1961) doi:10.1039/tf9615700040

**T / K =** **318.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 213.00 | 0.1209 |
| 348.00 | 0.2068 |
| 446.00 | 0.2785 |
| 591.00 | 0.3876 |
| 649.00 | 0.5071 |
| 632.00 | 0.6173 |
| 528.00 | 0.7155 |
| 385.00 | 0.8170 |
| 196.00 | 0.9192 |

Anantaraman, A. V. - Bhattacharyya, S. N. - Palit, S. R., Weak dipolar interaction in solutions. Systems: cyclohexane+chlorobenzene and carbon tetrachloride+chlorobenzene, Transactions of the Faraday Society (1961) doi:10.1039/tf9615700040

**T / K =** **328.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 125.00 | 0.0827 |
| 289.00 | 0.1866 |
| 460.00 | 0.3083 |
| 552.00 | 0.3744 |
| 607.00 | 0.4755 |
| 624.00 | 0.5837 |
| 549.00 | 0.6998 |
| 442.00 | 0.7735 |
| 272.00 | 0.8768 |

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**Heat capacity of mixing**

---

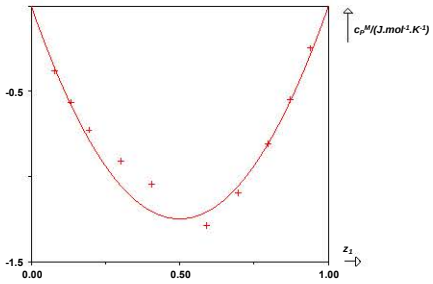
Bendiab, H. - Roux-Desgranges, G. - Roux, A. H. - Grolier, J. -P. E. - Patterson, D., Excess heat capacities of ternary systems containing chlorobenzene or chloronaphthalene, Journal of Solution Chemistry 2 (1994) 307-323. doi:10.1007/BF00973552

**T / K =** **298.15**

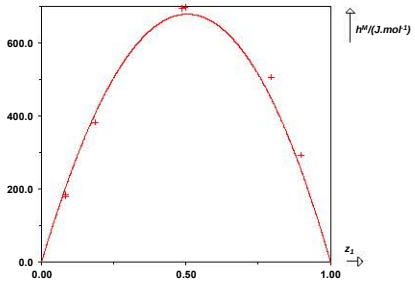
**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.3800 | 0.0785 |
| -0.5640 | 0.1333 |
| -0.7270 | 0.1925 |
| -0.9100 | 0.3008 |
| -1.043 | 0.4044 |
| -1.290 | 0.5893 |
| -1.094 | 0.6960 |
| -0.8090 | 0.7963 |
| -0.5490 | 0.8708 |
| -0.2470 | 0.9384 |

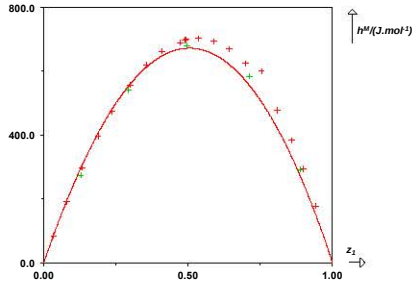
T/K = 298.15 - P/bar = 1.0132



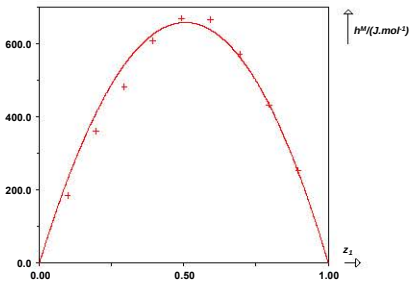

T/K = 293.15 - P/bar = 1.0132



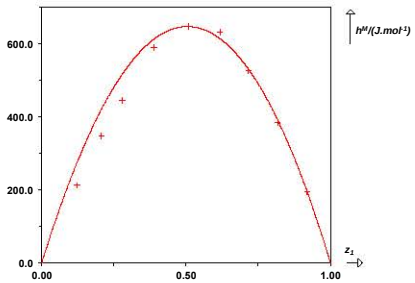

T/K = 298.15 - P/bar = 1.0132 1.0132



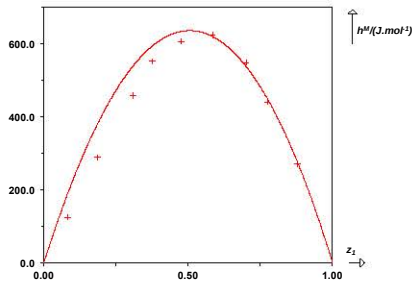

T/K = 308.65 - P/bar = 1.0132



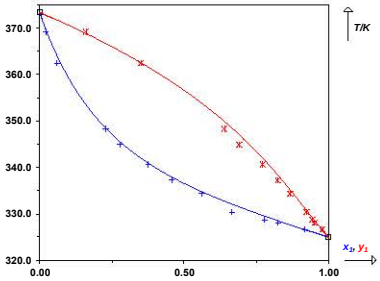

T/K = 318.15 - P/bar = 1.0132



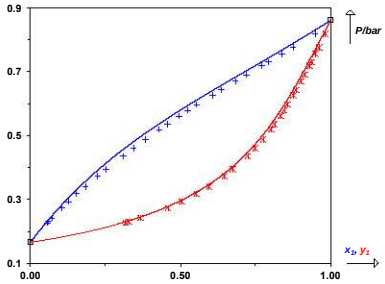

T/K = 328.15 - P/bar = 1.0132




P/bar = 0.39999




T/K = 348.15



## 1,2-DICHLOROETHANE (1) + CARBON TETRACHLORIDE (2)

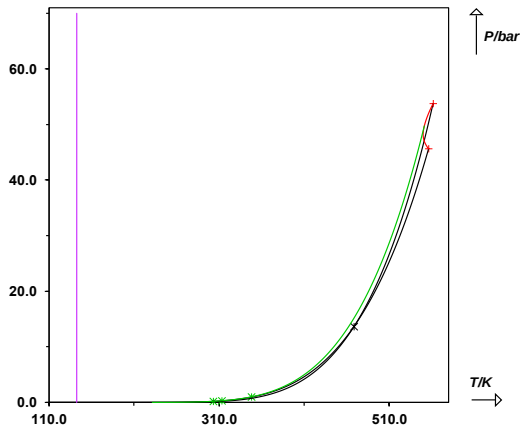
| | | |
|---|---|---|
| **CAS** | 107-06-2 | 56-23-5 |
| **InChiKey** | WSLDOOZREJYCGB-UHFFFAOYSA-N | VZGDMQKNWNREIO-UHFFFAOYSA-N |
| **$T_c$ / K** | 561.60 | 556.35 |
| **$P_c$ / bar** | 53.70 | 45.60 |
| **ω** | 0.287 | 0.193 |

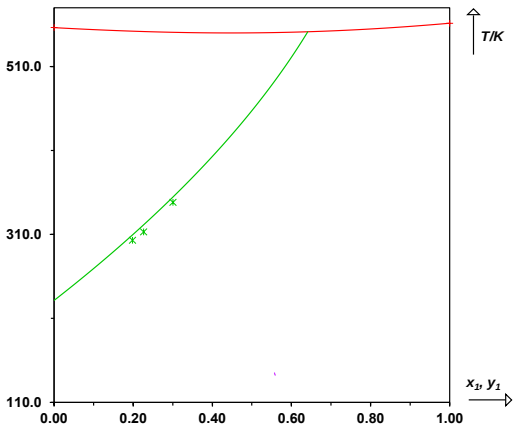
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 137
B/MPa = 163

*Deviations*
MAPE on x = 15 %
MAPE on y = 15 %
MAPE on $x_{az}$ = 4.4 %
MAPE on $P_{az}$ = 1.3 %
MAPE on $h^M$ = 3.2 %
MAPE on $c_P^M$ = 84 %



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**Isothermal phase equilibrium data**

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Azpiazu, Y. - Royo, F. - Gutiérrez Losa, C., Vapour pressures of (tetrachloromethane + α,ω-dichloroalkane), The Journal of Chemical Thermodynamics 6 (1984) 561-565. doi:10.1016/0021-9614(84)90007-7

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1576 | 0.9000 | 0.7780 | |
| 0.1691 | 0.7980 | 0.6710 | |
| 0.1724 | 0.7520 | 0.6300 | |
| 0.1751 | 0.7370 | 0.6170 | |
| 0.1796 | 0.6580 | 0.5510 | |
| 0.1862 | 0.5850 | 0.4610 | |
| 0.1916 | 0.4460 | 0.3760 | |
| 0.1954 | 0.3500 | 0.3030 | |
| 0.1981 | 0.2010 | 0.1990 | |
| 0.1981 | 0.1980 | 0.1980 | AZEO |
| 0.1965 | 0.0990 | 0.1240 | |

Munoz Embid, Jose - Berro, Charles - Otin, Santos - Kehiaian, Henry V., Isothermal vapor-liquid equilibria, excess enthalpies, and excess volumes of 1-chlorobutane + tetrachloromethane, 1,2-dichloroethane + tetrachloromethane, and 1,2-dichloroethane + 1-chlorobutane mixtures, Journal of Chemical & Engineering Data 3 (1990) 266-271. doi:10.1021/je00061a012

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2213 | 0.9505 | 0.8916 | |
| 0.2314 | 0.9085 | 0.8186 | |
| 0.2360 | 0.8886 | 0.7861 | |
| 0.2431 | 0.8529 | 0.7364 | |
| 0.2462 | 0.8357 | 0.7152 | |
| 0.2535 | 0.7935 | 0.6676 | |
| 0.2631 | 0.7240 | 0.5988 | |
| 0.2672 | 0.6904 | 0.5689 | |
| 0.2722 | 0.6436 | 0.5302 | |
| 0.2769 | 0.5928 | 0.4915 | |
| 0.2802 | 0.5496 | 0.4604 | |
| 0.2838 | 0.4968 | 0.4230 | |
| 0.2864 | 0.4499 | 0.3906 | |
| 0.2889 | 0.3925 | 0.3507 | |
| 0.2905 | 0.3415 | 0.3146 | |
| 0.2913 | 0.3001 | 0.2843 | |
| 0.2919 | 0.2505 | 0.2465 | |
| 0.2920 | 0.2261 | 0.2261 | AZEO |
| 0.2920 | 0.2241 | 0.2254 | |
| 0.2919 | 0.1995 | 0.2048 | |
| 0.2911 | 0.1482 | 0.1600 | |
| 0.2907 | 0.1331 | 0.1460 | |
| 0.2878 | 0.0612 | 0.0731 | |

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**Isobaric phase equilibrium data**

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Sagnes, Michele. - Sanchez, Victor., Vapor-liquid equilibriums for fourteen systems consisting of chlorinated hydrocarbons and alcohols, Journal of Chemical & Engineering Data 3 (1971) 351-354. doi:10.1021/je60050a038

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 354.15 | 0.9470 | 0.9000 |
| 353.15 | 0.9000 | 0.8400 |
| 352.45 | 0.8600 | 0.7870 |
| 351.75 | 0.8200 | 0.7400 |
| 351.25 | 0.7870 | 0.7000 |
| 350.55 | 0.7220 | 0.6430 |
| 350.05 | 0.6850 | 0.6020 |
| 349.45 | 0.6120 | 0.5320 |
| 348.95 | 0.5070 | 0.4570 |
| 348.55 | 0.4320 | 0.4020 |
| 348.45 | 0.4050 | 0.3820 |
| 348.45 | 0.2050 | 0.2170 |
| 348.65 | 0.1400 | 0.1570 |
| 349.15 | 0.0620 | 0.0720 |

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**Enthalpy of mixing**

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Baños, Irene - Valero, Jose - Gracia, Mariano - Losa, Celso Gutierrez, Conformational Equilibrium and Calorimetric Behaviour of Systems Containing 1,2-Dichloroethane, Berichte der Bunsengesellschaft für physikalische Chemie 10 (1983) 866-871. doi:10.1002/bbpc.19830871007

**T / K = 288.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 146.00 | 0.9403 |
| 298.00 | 0.8665 |
| 376.00 | 0.8245 |
| 471.00 | 0.7653 |
| 530.00 | 0.7123 |
| 604.00 | 0.6492 |
| 625.00 | 0.6008 |
| 658.00 | 0.4997 |

| | |
|---|---|
| 641.00 | 0.4011 |
| 597.00 | 0.3643 |
| 580.00 | 0.3396 |
| 557.00 | 0.3052 |
| 474.00 | 0.2373 |
| 367.00 | 0.1635 |
| 246.00 | 0.1010 |
| 190.00 | 0.0772 |

Ortega, Juan, Measurements and Analysis of Excess Enthalpies of Alkyl Acetates + 1-Chloroalkanes Using the Unifac Model, Berichte der Bunsengesellschaft für physikalische Chemie 10 (1988) 1146-1149. doi:10.1002/bbpc.198800288

**T / K =** **298.15**

**P / bar =** **1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 229.00 | 0.9200 |
| 441.00 | 0.8122 |
| 577.00 | 0.7033 |
| 656.00 | 0.5787 |
| 667.00 | 0.5046 |
| 636.00 | 0.4000 |
| 558.00 | 0.3036 |
| 420.00 | 0.1995 |
| 242.00 | 0.1021 |

Baños, Irene - Valero, Jose - Gracia, Mariano - Losa, Celso Gutierrez, Conformational Equilibrium and Calorimetric Behaviour of Systems Containing 1,2-Dichloroethane, Berichte der Bunsengesellschaft für physikalische Chemie 10 (1983) 866-871. doi:10.1002/bbpc.19830871007

**T / K =** **308.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 232.00 | 0.9057 |
| 388.00 | 0.8181 |
| 484.00 | 0.7593 |
| 576.00 | 0.6766 |
| 605.00 | 0.6480 |
| 641.00 | 0.5974 |
| 644.00 | 0.5947 |
| 675.00 | 0.5277 |
| 653.00 | 0.4489 |
| 611.00 | 0.3650 |
| 578.00 | 0.3202 |
| 523.00 | 0.2820 |
| 405.00 | 0.1944 |
| 260.00 | 0.1121 |
| 126.00 | 0.0540 |

Munoz Embid, Jose - Berro, Charles - Otin, Santos - Kehiaian, Henry V., Isothermal vapor-liquid equilibria, excess enthalpies, and excess volumes of 1-chlorobutane + tetrachloromethane, 1,2-dichloroethane + tetrachloromethane, and 1,2-dichloroethane + 1-chlorobutane mixtures, Journal of Chemical & Engineering Data 3 (1990) 266-271. doi:10.1021/je00061a012

**T / K =** **313.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 212.00 | 0.0873 |
| 304.00 | 0.1361 |
| 422.00 | 0.2005 |
| 575.00 | 0.3173 |
| 637.00 | 0.4015 |
| 655.00 | 0.4852 |
| 664.00 | 0.5311 |
| 634.00 | 0.6047 |
| 550.00 | 0.7198 |
| 431.00 | 0.8050 |
| 274.00 | 0.8873 |

Baños, Irene - Valero, Jose - Gracia, Mariano - Losa, Celso Gutierrez, Conformational Equilibrium and Calorimetric Behaviour of Systems Containing 1,2-Dichloroethane, Berichte der Bunsengesellschaft für physikalische Chemie 10 (1983) 866-871. doi:10.1002/bbpc.19830871007

**T / K =** **318.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 115.00 | 0.9616 |
| 297.00 | 0.8822 |
| 410.00 | 0.8179 |
| 513.00 | 0.7438 |
| 591.00 | 0.6745 |
| 636.00 | 0.5913 |
| 657.00 | 0.5348 |
| 645.00 | 0.4512 |
| 623.00 | 0.3846 |
| 589.00 | 0.3417 |
| 549.00 | 0.2955 |
| 502.00 | 0.2529 |
| 386.00 | 0.1698 |
| 178.00 | 0.0731 |

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**Heat capacity of mixing**

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Wilhelm, E. - Faradjzadeh, A. - Grolier, J.-P.E., Molar excess heat capacities and excess volumes of 1,2-dichloroethane + cyclooctane, + mesitylene, and + tetrachloromethane, The Journal of Chemical Thermodynamics 10 (1979) 979-984. doi:10.1016/0021-9614(79)90047-8

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.0830 | 0.8671 |
| -0.0160 | 0.7261 |
| -0.1140 | 0.6333 |
| -0.2840 | 0.5036 |
| -0.3430 | 0.3871 |
| -0.3810 | 0.2565 |
| -0.3060 | 0.1241 |

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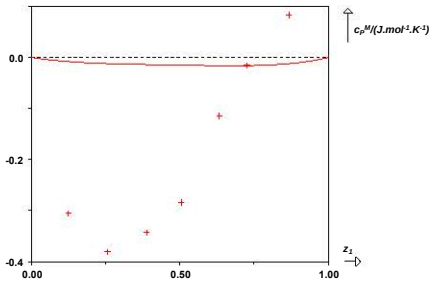
**Azeotropic point**

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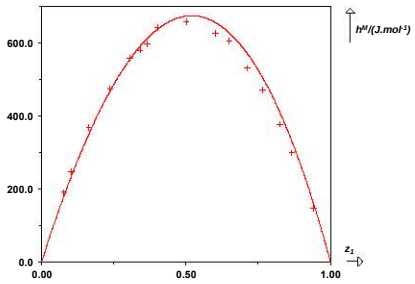
Sagnes, Michele. - Sanchez, Victor., Vapor-liquid equilibriums for fourteen systems consisting of chlorinated hydrocarbons and alcohols, Journal of Chemical & Engineering Data 3 (1971) 351-354. doi:10.1021/je60050a038

| T / K | P / bar | $x_1$ |
|---|---|---|
| 348.35 | 1.013 | 0.3000 |

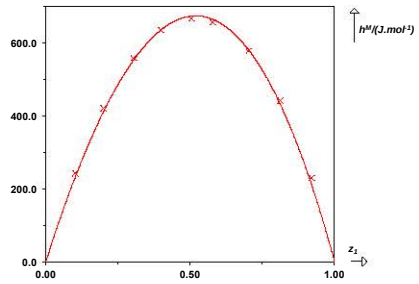
T/K = 298.15 - P/bar = 1.0132



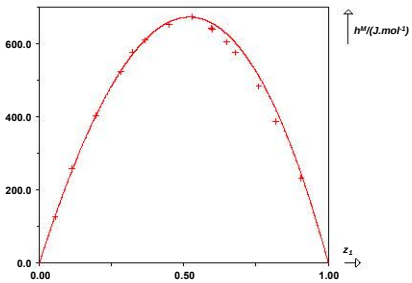

T/K = 288.15 - P/bar = 1.0132



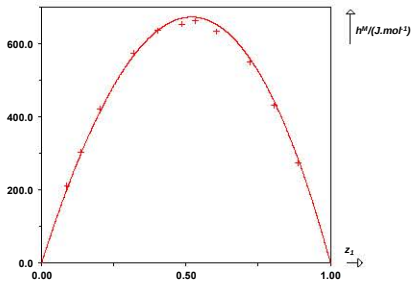

T/K = 298.15 - P/bar = 1.0100



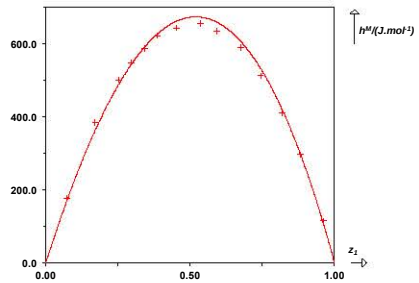

T/K = 308.15 - P/bar = 1.0132



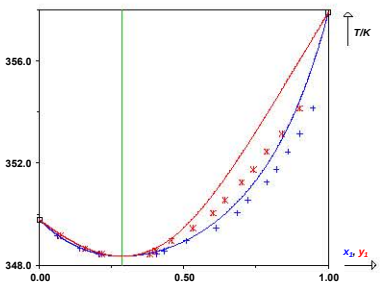

T/K = 313.15 - P/bar = 1.0132



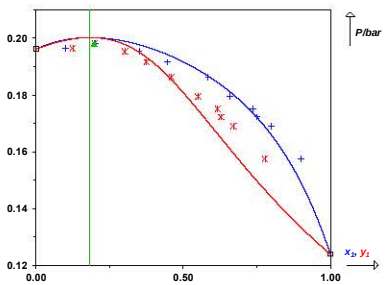

T/K = 318.15 - P/bar = 1.0132



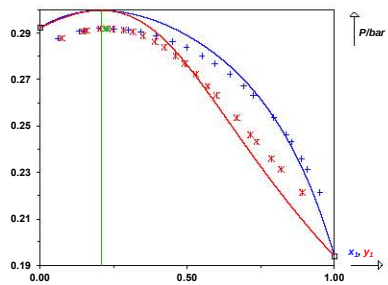

P/bar = 1.01330



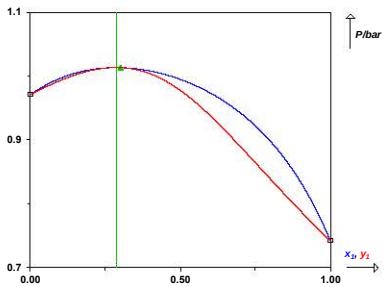

T/K = 303.15




T/K = 313.15




T/K = 348.35



## NITROGEN (1) + METHANE (2)

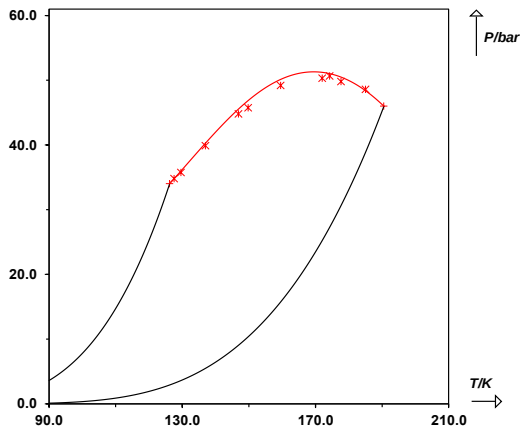
| | | |
|---|---|---|
| **CAS** | 7727-37-9 | 74-82-8 |
| **InChiKey** | MDFFNEOEWAXZRQ-UHFFFAOYSA-N | VNWKTOKETHGBQD-UHFFFAOYSA-N |
| **$T_c$ / K** | 126.20 | 190.56 |
| **$P_c$ / bar** | 34.00 | 45.99 |
| **ω** | 0.038 | 0.012 |

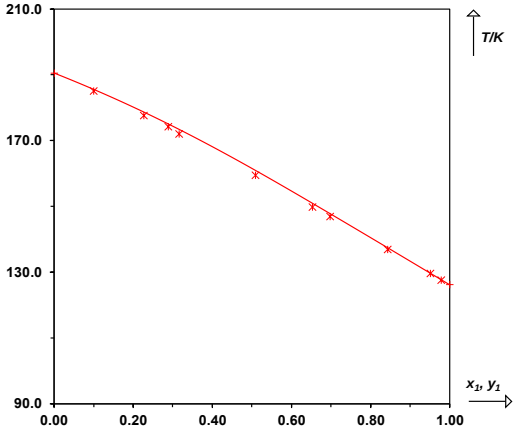
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 82.5
B/MPa = 105

*Deviations*
MAPE on x = 5.7 %
MAPE on y = 2.4 %
MAPE on $x_c$ = 4.2 %
MAPE on $P_c$ = 1.2 %
MAPE on $h^M$ = 8.4 %



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**Isothermal phase equilibrium data**

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Sprow, F. B. - Prausnitz, J. M., Vapor-Liquid equilibria for five cryogenic mixtures, AIChE Journal 4 (1966) 780-784. doi:10.1002/aic.690120427

**T / K = 90.67**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.9583 | 0.1330 | 0.8890 |
| 1.265 | 0.2000 | 0.9200 |
| 1.417 | 0.2380 | 0.9280 |
| 1.783 | 0.3410 | 0.9470 |
| 2.060 | 0.4290 | 0.9590 |
| 2.359 | 0.5310 | 0.9680 |
| 2.641 | 0.6280 | 0.9750 |
| 3.178 | 0.8110 | 0.9850 |
| 3.648 | 0.9520 | 0.9950 |

Parrish, W. R. - Hiza, M. J., Liquid-Vapor Equilibria in the Nitrogen-Methane System between 95 and 120 K, Advances in Cryogenic Engineering (1995) 300-308.

**T / K = 95.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.254 | 0.2679 | 0.9216 |
| 2.737 | 0.3562 | 0.9374 |
| 3.018 | 0.4249 | 0.9460 |
| 3.431 | 0.5271 | 0.9573 |
| 3.646 | 0.5889 | 0.9618 |
| 4.247 | 0.7495 | 0.9756 |
| 4.580 | 0.8271 | 0.9823 |

Parrish, W. R. - Hiza, M. J., Liquid-Vapor Equilibria in the Nitrogen-Methane System between 95 and 120 K, Advances in Cryogenic Engineering (1995) 300-308.

**T / K = 100.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.988 | 0.1329 | 0.8336 |
| 2.960 | 0.2397 | 0.8907 |
| 3.621 | 0.3301 | 0.9168 |
| 3.989 | 0.3831 | 0.9277 |
| 4.396 | 0.4463 | 0.9372 |
| 4.706 | 0.5069 | 0.9448 |
| 5.032 | 0.5638 | 0.9508 |
| 5.598 | 0.6671 | 0.9618 |
| 6.451 | 0.8133 | 0.9764 |

Han, Xiao Hong - Zhang, Yu Jia - Gao, Zan Jun - Xu, Ying Jie - Wang, Qin - Chen, Guang Ming, Vapor−Liquid Equilibrium for the Mixture Nitrogen (N2) + Methane (CH4) in the Temperature Range of (110 to 125) K, Journal of Chemical & Engineering Data 5 (2012) 1621-1626. doi:10.1021/je201299u

**T / K = 100.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3893 | 0.0041 | 0.1345 |
| 3.001 | 0.2675 | 0.9000 |
| 3.973 | 0.4052 | 0.9312 |
| 4.860 | 0.5333 | 0.9522 |
| 6.098 | 0.7489 | 0.9752 |
| 6.789 | 0.8588 | 0.9881 |

Han, Xiao Hong - Zhang, Yu Jia - Gao, Zan Jun - Xu, Ying Jie - Wang, Qin - Chen, Guang Ming, Vapor−Liquid Equilibrium for the Mixture Nitrogen (N2) + Methane (CH4) in the Temperature Range of (110 to 125) K, Journal of Chemical & Engineering Data 5 (2012) 1621-1626. doi:10.1021/je201299u

**T / K = 114.99**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.051 | 0.0296 | 0.3571 |
| 2.303 | 0.0395 | 0.4424 |
| 3.906 | 0.1102 | 0.6796 |
| 4.727 | 0.1532 | 0.7456 |
| 5.537 | 0.1932 | 0.7882 |
| 7.119 | 0.2838 | 0.8405 |
| 8.532 | 0.3619 | 0.8740 |
| 9.042 | 0.3932 | 0.8836 |
| 12.05 | 0.5900 | 0.9262 |

Stryjek, Roman - Chappelear, Patsy S. - Kobayashi, Riki, Low-temperature vapor-liquid equilibriums of nitrogen-methane system, Journal of Chemical & Engineering Data 4 (1974) 334-339. doi:10.1021/je60063a023

**T / K = 122.04**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.792 | 0.0165 | 0.1963 |
| 3.447 | 0.0351 | 0.3466 |
| 5.171 | 0.0850 | 0.5588 |
| 6.881 | 0.1411 | 0.6655 |
| 13.79 | 0.4283 | 0.8411 |
| 19.63 | 0.7093 | 0.9109 |
| 20.70 | 0.7524 | 0.9225 |
| 21.44 | 0.7837 | 0.9308 |
| 24.41 | 0.8962 | 0.9589 |
| 26.20 | 0.9514 | 0.9785 |
| 27.46 | 0.9880 | 0.9946 |

Stryjek, Roman - Chappelear, Patsy S. - Kobayashi, Riki, Low-temperature vapor-liquid equilibriums of nitrogen-methane system, Journal of Chemical &

Engineering Data 4 (1974) 334-339. doi:10.1021/je60063a023

**T / K = 127.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.530 | 0.0097 | 0.1144 | |
| 5.171 | 0.0471 | 0.3786 | |
| 6.881 | 0.0912 | 0.5318 | |
| 13.79 | 0.3040 | 0.7662 | |
| 20.55 | 0.5475 | 0.8564 | |
| 27.03 | 0.7825 | 0.9129 | |
| 28.75 | 0.8353 | 0.9263 | |
| 30.54 | 0.8822 | 0.9410 | |
| 31.72 | 0.9122 | 0.9521 | |
| 32.41 | 0.9308 | 0.9604 | |
| 33.10 | 0.9412 | 0.9644 | |
| 33.72 | 0.9540 | 0.9709 | |
| 34.41 | 0.9674 | 0.9761 | |
| 34.61 | 0.9724 | 0.9781 | |
| 34.68 | 0.9741 | 0.9779 | |
| 34.78 | 0.9777 | 0.9777 | CRIT |

Cines, M.R. - Roach, J.T. - Hogan, R.J. - Roland, C.H., Nitrogen-methane vapor-liquid equilibria, Chem. Eng. Progr. Symp. Ser. 6 (1953) 1-10.

**T / K = 133.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.826 | 0.0080 | 0.0790 |
| 5.516 | 0.0210 | 0.1780 |
| 6.205 | 0.0360 | 0.2600 |
| 6.895 | 0.0500 | 0.3300 |
| 8.618 | 0.0860 | 0.4600 |
| 10.34 | 0.1250 | 0.5500 |
| 12.07 | 0.1640 | 0.6180 |
| 13.79 | 0.2050 | 0.6680 |
| 17.24 | 0.3010 | 0.7390 |
| 20.68 | 0.4060 | 0.7890 |
| 24.13 | 0.5130 | 0.8290 |
| 27.58 | 0.6210 | 0.8600 |
| 31.03 | 0.7250 | 0.8880 |
| 34.47 | 0.8220 | 0.9120 |

Bloomer, O.T. - Parent, J.D., Liquid-vapor phase behavior of the methane-nitrogen system, Chem. Eng. Progr. Symp. Ser. 6 (1953) 11-24.

**T / K = 133.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0513 | 0.3379 |
| 10.34 | 0.1209 | 0.5467 |
| 13.79 | 0.2102 | 0.6647 |
| 17.24 | 0.3055 | 0.7313 |
| 20.68 | 0.4058 | 0.7797 |
| 24.13 | 0.5072 | 0.8176 |
| 27.58 | 0.6152 | 0.8475 |
| 31.03 | 0.7166 | 0.8734 |
| 34.47 | 0.8036 | 0.8945 |

Kidnay, A.J. - Miller, R.C. - Parrish, W.R. - Hiza, M.J., Liquid-vapour phase equilibria in the N2-CH4 system from 130 to 180 K, Cryogenics 9 (1975) 531-540. doi:10.1016/0011-2275(75)90149-6

**T / K = 140.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.221 | 0.0132 | 0.1051 |
| 8.298 | 0.0316 | 0.2166 |
| 9.258 | 0.0485 | 0.2952 |
| 10.11 | 0.0637 | 0.3498 |
| 14.06 | 0.1372 | 0.5228 |
| 18.05 | 0.2165 | 0.6214 |
| 21.94 | 0.3008 | 0.6850 |
| 26.59 | 0.4063 | 0.7383 |
| 30.76 | 0.5026 | 0.7726 |
| 32.69 | 0.5512 | 0.7849 |
| 36.33 | 0.6304 | 0.8038 |
| 37.86 | 0.6662 | 0.8107 |
| 40.39 | 0.7267 | 0.8128 |
| 42.00 | 0.7788 | 0.8032 |

Cines, M.R. - Roach, J.T. - Hogan, R.J. - Roland, C.H., Nitrogen-methane vapor-liquid equilibria, Chem. Eng. Progr. Symp. Ser. 6 (1953) 1-10.

**T / K = 144.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.618 | 0.0090 | 0.0700 |
| 10.34 | 0.0360 | 0.2100 |
| 12.07 | 0.0630 | 0.3170 |
| 13.79 | 0.0890 | 0.3950 |
| 17.24 | 0.1450 | 0.5120 |
| 20.68 | 0.2060 | 0.5920 |
| 24.13 | 0.2770 | 0.6510 |
| 27.58 | 0.3520 | 0.6920 |
| 31.03 | 0.4310 | 0.7260 |
| 34.47 | 0.5090 | 0.7520 |
| 37.92 | 0.5880 | 0.7700 |
| 41.37 | 0.6680 | 0.7830 |

Bloomer, O.T. - Parent, J.D., Liquid-vapor phase behavior of the methane-nitrogen system, Chem. Eng. Progr. Symp. Ser. 6 (1953) 11-24.

**T / K = 144.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|

| | | |
|---|---|---|
| 10.34 | 0.0394 | 0.2185 |
| 13.79 | 0.0908 | 0.3977 |
| 17.24 | 0.1497 | 0.5023 |
| 20.68 | 0.2152 | 0.5804 |
| 24.13 | 0.2820 | 0.6358 |
| 27.58 | 0.3476 | 0.6801 |
| 31.03 | 0.4181 | 0.7120 |
| 34.47 | 0.4970 | 0.7363 |
| 37.92 | 0.5737 | 0.7523 |

Stryjek, Roman - Chappelear, Patsy S. - Kobayashi, Riki, Low-temperature vapor-liquid equilibriums of nitrogen-methane system, Journal of Chemical & Engineering Data 4 (1974) 334-339. doi:10.1021/je60063a023

**T / K = 149.82**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 12.34 | 0.0284 | 0.1529 | |
| 13.96 | 0.0514 | 0.2404 | |
| 17.20 | 0.0985 | 0.3683 | |
| 20.62 | 0.1503 | 0.4579 | |
| 27.34 | 0.2579 | 0.5779 | |
| 34.13 | 0.3778 | 0.6480 | |
| 40.96 | 0.5034 | 0.6867 | |
| 44.75 | 0.5866 | 0.6878 | |
| 45.78 | 0.6528 | 0.6528 | CRIT |

Cines, M.R. - Roach, J.T. - Hogan, R.J. - Roland, C.H., Nitrogen-methane vapor-liquid equilibria, Chem. Eng. Progr. Symp. Ser. 6 (1953) 1-10.

**T / K = 155.37**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.79 | 0.0060 | 0.0400 |
| 17.24 | 0.0460 | 0.2130 |
| 20.68 | 0.0890 | 0.3340 |
| 24.13 | 0.1360 | 0.4160 |
| 27.58 | 0.1850 | 0.4790 |
| 31.03 | 0.2380 | 0.5260 |
| 34.47 | 0.2950 | 0.5650 |
| 37.92 | 0.3540 | 0.5970 |
| 41.37 | 0.4150 | 0.6200 |
| 44.82 | 0.4790 | 0.6340 |

Bloomer, O.T. - Parent, J.D., Liquid-vapor phase behavior of the methane-nitrogen system, Chem. Eng. Progr. Symp. Ser. 6 (1953) 11-24.

**T / K = 155.37**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.79 | 0.0075 | 0.0448 |
| 17.24 | 0.0497 | 0.2021 |
| 20.68 | 0.0934 | 0.3235 |
| 24.13 | 0.1406 | 0.4076 |
| 27.58 | 0.1881 | 0.4679 |
| 31.03 | 0.2391 | 0.5153 |
| 34.47 | 0.2921 | 0.5515 |
| 37.92 | 0.3479 | 0.5799 |
| 41.37 | 0.4043 | 0.5992 |
| 44.82 | 0.4626 | 0.6084 |

Kidnay, A.J. - Miller, R.C. - Parrish, W.R. - Hiza, M.J., Liquid-vapour phase equilibria in the N2-CH4 system from 130 to 180 K, Cryogenics 9 (1975) 531-540. doi:10.1016/0011-2275(75)90149-6

**T / K = 160.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 16.81 | 0.0095 | 0.0438 |
| 17.97 | 0.0223 | 0.0979 |
| 18.99 | 0.0334 | 0.1394 |
| 19.91 | 0.0448 | 0.1742 |
| 21.94 | 0.0684 | 0.2406 |
| 22.10 | 0.0714 | 0.2458 |
| 26.19 | 0.1205 | 0.3442 |
| 30.38 | 0.1756 | 0.4184 |
| 33.95 | 0.2243 | 0.4657 |
| 38.46 | 0.2820 | 0.5051 |
| 42.29 | 0.3333 | 0.5289 |
| 46.15 | 0.3937 | 0.5422 |
| 47.86 | 0.4246 | 0.5360 |
| 48.38 | 0.4310 | 0.5315 |

Bloomer, O.T. - Parent, J.D., Liquid-vapor phase behavior of the methane-nitrogen system, Chem. Eng. Progr. Symp. Ser. 6 (1953) 11-24.

**T / K = 166.48**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.68 | 0.0017 | 0.0068 |
| 24.13 | 0.0369 | 0.1287 |
| 27.58 | 0.0728 | 0.2211 |
| 31.03 | 0.1104 | 0.2876 |
| 34.47 | 0.1489 | 0.3385 |
| 37.92 | 0.1901 | 0.3789 |
| 41.37 | 0.2370 | 0.4098 |
| 44.82 | 0.2873 | 0.4316 |
| 48.26 | 0.3435 | 0.4379 |

Kidnay, A.J. - Miller, R.C. - Parrish, W.R. - Hiza, M.J., Liquid-vapour phase equilibria in the N2-CH4 system from 130 to 180 K, Cryogenics 9 (1975) 531-540. doi:10.1016/0011-2275(75)90149-6

**T / K = 170.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 24.27 | 0.0082 | 0.0291 |
| 25.39 | 0.0189 | 0.0652 |
| 26.20 | 0.0276 | 0.0889 |
| 27.47 | 0.0399 | 0.1219 |
| 28.43 | 0.0495 | 0.1458 |
| 30.36 | 0.0688 | 0.1875 |
| 34.43 | 0.1115 | 0.2593 |
| 38.58 | 0.1562 | 0.3135 |
| 42.52 | 0.2001 | 0.3519 |
| 46.31 | 0.2466 | 0.3743 |
| 48.33 | 0.2729 | 0.3784 |
| 48.95 | 0.2915 | 0.3798 |
| 49.39 | 0.3066 | 0.3801 |

Stryjek, Roman - Chappelear, Patsy S. - Kobayashi, Riki, Low-temperature vapor-liquid equilibriums of nitrogen-methane system, Journal of Chemical & Engineering Data 4 (1974) 334-339. doi:10.1021/je60063a023

**T / K = 172.04**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 25.55 | 0.0060 | 0.0194 | |
| 26.89 | 0.0169 | 0.0525 | |
| 27.65 | 0.0245 | 0.0740 | |
| 31.23 | 0.0576 | 0.1532 | |
| 34.48 | 0.0925 | 0.2157 | |
| 37.92 | 0.1287 | 0.2646 | |
| 41.23 | 0.1657 | 0.3009 | |
| 48.47 | 0.2599 | 0.3445 | |
| 50.33 | 0.3156 | 0.3156 | CRIT |

Stryjek, Roman - Chappelear, Patsy S. - Kobayashi, Riki, Low-temperature vapor-liquid equilibriums of nitrogen-methane system, Journal of Chemical & Engineering Data 4 (1974) 334-339. doi:10.1021/je60063a023

**T / K = 177.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 31.03 | 0.0041 | 0.0120 | |
| 34.51 | 0.0326 | 0.0794 | |
| 36.82 | 0.0555 | 0.1266 | |
| 39.58 | 0.0828 | 0.1693 | |
| 41.99 | 0.1097 | 0.2023 | |
| 44.82 | 0.1391 | 0.2286 | |
| 46.61 | 0.1631 | 0.2459 | |
| 48.26 | 0.1816 | 0.2495 | |
| 48.88 | 0.1929 | 0.2488 | |
| 49.64 | 0.2026 | 0.2458 | |
| 49.78 | 0.2272 | 0.2272 | CRIT |

Kidnay, A.J. - Miller, R.C. - Parrish, W.R. - Hiza, M.J., Liquid-vapour phase equilibria in the N2-CH4 system from 130 to 180 K, Cryogenics 9 (1975) 531-540. doi:10.1016/0011-2275(75)90149-6

**T / K = 180.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.11 | 0.0089 | 0.0230 |
| 35.40 | 0.0202 | 0.0494 |
| 36.72 | 0.0327 | 0.0738 |
| 37.87 | 0.0434 | 0.0936 |
| 39.45 | 0.0588 | 0.1192 |
| 40.24 | 0.0632 | 0.1260 |
| 42.72 | 0.0863 | 0.1572 |
| 44.75 | 0.1083 | 0.1786 |
| 46.56 | 0.1254 | 0.1919 |
| 48.70 | 0.1567 | 0.1992 |

Stryjek, Roman - Chappelear, Patsy S. - Kobayashi, Riki, Low-temperature vapor-liquid equilibriums of nitrogen-methane system, Journal of Chemical & Engineering Data 4 (1974) 334-339. doi:10.1021/je60063a023

**T / K = 183.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 39.71 | 0.0254 | 0.0493 |
| 41.23 | 0.0416 | 0.0774 |
| 42.96 | 0.0568 | 0.0964 |
| 45.09 | 0.0785 | 0.1251 |
| 46.47 | 0.0911 | 0.1357 |
| 47.51 | 0.1060 | 0.1425 |
| 48.26 | 0.1165 | 0.1449 |
| 48.47 | 0.1175 | 0.1425 |

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**Isobaric phase equilibrium data**

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Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 34.47**

| T / K | $x_1$ |
|---|---|
| 174.87 | 0.0611 |
| 170.98 | 0.1002 |
| 155.59 | 0.2888 |
| 143.76 | 0.5088 |
| 136.76 | 0.6970 |
| 131.93 | 0.8422 |

| | |
|---|---|
| 128.48 | 0.9515 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 34.47**

| T / K | $x_1$ |
|---|---|
| 178.82 | 0.0611 |
| 177.21 | 0.1002 |
| 168.87 | 0.2888 |
| 157.71 | 0.5088 |
| 146.82 | 0.6970 |
| 136.87 | 0.8422 |
| 129.43 | 0.9515 |

Brandt, L. W. - Stroud, Lowell., Phase Equilibria in Natural Gas Systems. Apparatus with Windowed Cell for 800 P.S.I.G. and Temperatures to −320° F., Industrial & Engineering Chemistry 5 (1958) 849-852. doi:10.1021/ie50581a046

**P / bar = 34.47**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 174.82 | 0.0540 | 0.1320 |
| 173.71 | 0.0660 | 0.1640 |
| 172.59 | 0.0850 | 0.2010 |
| 163.15 | 0.1860 | 0.4070 |
| 160.93 | 0.2020 | 0.4300 |
| 158.15 | 0.2430 | 0.4900 |
| 154.82 | 0.3070 | 0.5780 |
| 150.37 | 0.3660 | 0.6360 |
| 137.04 | 0.7080 | 0.8390 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 37.92**

| T / K | $x_1$ |
|---|---|
| 178.09 | 0.0611 |
| 174.21 | 0.1002 |
| 159.26 | 0.2888 |
| 146.93 | 0.5088 |
| 139.71 | 0.6970 |
| 134.65 | 0.8422 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 37.92**

| T / K | $x_1$ |
|---|---|
| 181.48 | 0.0611 |
| 179.71 | 0.1002 |
| 170.98 | 0.2888 |
| 159.48 | 0.5088 |
| 148.04 | 0.6970 |
| 137.82 | 0.8422 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 41.37**

| T / K | $x_1$ |
|---|---|
| 181.15 | 0.0611 |
| 177.37 | 0.1002 |
| 162.82 | 0.2888 |
| 150.09 | 0.5088 |
| 142.71 | 0.6970 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 41.37**

| T / K | $x_1$ |
|---|---|
| 183.87 | 0.0611 |
| 182.04 | 0.1002 |
| 172.82 | 0.2888 |
| 160.93 | 0.5088 |
| 148.98 | 0.6970 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 44.82**

| T / K | $x_1$ |
|---|---|
| 184.15 | 0.0611 |
| 180.48 | 0.1002 |
| 166.37 | 0.2888 |

| | |
|---|---|
| 153.37 | 0.5088 |
| 146.93 | 0.6970 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 44.82**

| T / K | $x_1$ |
|---|---|
| 186.09 | 0.0611 |
| 184.21 | 0.1002 |
| 174.37 | 0.2888 |
| 161.93 | 0.5088 |
| 149.04 | 0.6970 |

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**Enthalpy of mixing**

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McClure, D.W - Lewis, K.L - Miller, R.C - Staveley, L.A.K, Excess enthalpies and Gibbs free energies for nitrogen + methane at temperatures below the critical point of nitrogen, The Journal of Chemical Thermodynamics 8 (1976) 785-792. doi:10.1016/0021-9614(76)90057-4

**T / K = 91.50**

**P / bar = UNKNOWN (8.2035)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 60.80 | 0.1170 |
| 109.90 | 0.2470 |
| 136.90 | 0.4110 |
| 139.80 | 0.4790 |
| 136.70 | 0.5140 |
| 106.80 | 0.7140 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 183.00**

**P / bar = 21.40**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 53.00 | 0.2200 |
| 67.00 | 0.3320 |
| 70.00 | 0.4430 |
| 69.00 | 0.5670 |
| 53.00 | 0.7210 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 183.00**

**P / bar = 40.80**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 2006.0 | 0.1060 |
| 3059.0 | 0.1770 |
| 2823.0 | 0.2980 |
| 2747.0 | 0.3240 |
| 2688.0 | 0.3610 |
| 2425.0 | 0.4180 |
| 2337.0 | 0.4550 |
| 1422.0 | 0.6660 |

Lewis, K.L. - Mosedale, S.E. - Wormald, C.J., The enthalpies of mixing of methane + argon, methane + nitrogen, and methane + hydrogen in the gaseous and two-phase regions, The Journal of Chemical Thermodynamics 2 (1977) 121-131. doi:10.1016/0021-9614(77)90077-5

**T / K = 183.00**

**P / bar = 71.60**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 131.00 | 0.1510 |
| 330.00 | 0.2360 |
| 850.00 | 0.3460 |
| 1068.0 | 0.4450 |
| 1053.0 | 0.5330 |
| 725.00 | 0.7200 |
| 379.00 | 0.8530 |

Klein, R. R. - Bennett, C. O. - Dodgge, B. F., Experimental heats of mixing for gaseous nitrogen and methane, AIChE Journal 4 (1971) 958-965. doi:10.1002/aic.690170432

**T / K = 195.15**

**P / bar = 20.27**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 45.00 | 0.6000 |
| 48.00 | 0.5000 |
| 47.00 | 0.4000 |
| 43.00 | 0.3000 |

Klein, R. R. - Bennett, C. O. - Dodgge, B. F., Experimental heats of mixing for gaseous nitrogen and methane, AIChE Journal 4 (1971) 958-965. doi:10.1002/aic.690170432

**T / K = 195.15**

**P / bar = 81.06**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 910.00 | 0.6000 |
| 1040.0 | 0.5000 |
| 1090.0 | 0.4000 |
| 972.00 | 0.3000 |

Wormald, Christopher J. - Lewis, Keith L. - Mosedale, Stephen, The excess enthalpies of hydrogen + methane, hydrogen + nitrogen, methane + nitrogen, methane + argon, and nitrogen + argon at 298 and 201 K at pressures up to 10.2 MPa, The Journal of Chemical Thermodynamics 1 (1977) 27-42. doi:10.1016/0021-9614(77)90194-X

**T / K = 201.00**

**P / bar = 30.50**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 65.00 | 0.2590 |
| 77.00 | 0.3520 |
| 81.00 | 0.4500 |
| 82.00 | 0.5310 |
| 71.00 | 0.6510 |
| 56.00 | 0.7390 |

Wormald, Christopher J. - Lewis, Keith L. - Mosedale, Stephen, The excess enthalpies of hydrogen + methane, hydrogen + nitrogen, methane + nitrogen, methane + argon, and nitrogen + argon at 298 and 201 K at pressures up to 10.2 MPa, The Journal of Chemical Thermodynamics 1 (1977) 27-42. doi:10.1016/0021-9614(77)90194-X

**T / K = 201.00**

**P / bar = 51.50**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 337.00 | 0.2410 |
| 396.00 | 0.3490 |
| 394.00 | 0.4820 |

Wormald, Christopher J. - Lewis, Keith L. - Mosedale, Stephen, The excess enthalpies of hydrogen + methane, hydrogen + nitrogen, methane + nitrogen, methane + argon, and nitrogen + argon at 298 and 201 K at pressures up to 10.2 MPa, The Journal of Chemical Thermodynamics 1 (1977) 27-42. doi:10.1016/0021-9614(77)90194-X

**T / K = 201.00**

**P / bar = 65.80**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 874.00 | 0.0700 |
| 1107.0 | 0.1600 |
| 1195.0 | 0.2490 |
| 1140.0 | 0.3480 |
| 1071.0 | 0.4410 |
| 906.00 | 0.5530 |
| 486.00 | 0.7640 |

Klein, R. R. - Bennett, C. O. - Dodgge, B. F., Experimental heats of mixing for gaseous nitrogen and methane, AIChE Journal 4 (1971) 958-965. doi:10.1002/aic.690170432

**T / K = 233.15**

**P / bar = 40.53**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 70.60 | 0.6000 |
| 76.00 | 0.5000 |
| 74.10 | 0.4000 |
| 65.70 | 0.3000 |

Klein, R. R. - Bennett, C. O. - Dodgge, B. F., Experimental heats of mixing for gaseous nitrogen and methane, AIChE Journal 4 (1971) 958-965. doi:10.1002/aic.690170432

**T / K = 233.15**

**P / bar = 81.06**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 261.50 | 0.6000 |
| 293.50 | 0.5000 |
| 301.90 | 0.4000 |
| 282.70 | 0.3000 |

Klein, R. R. - Bennett, C. O. - Dodgge, B. F., Experimental heats of mixing for gaseous nitrogen and methane, AIChE Journal 4 (1971) 958-965. doi:10.1002/aic.690170432

**T / K = 253.15**

**P / bar = 20.27**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 19.70 | 0.6000 |
| 21.10 | 0.5000 |
| 20.70 | 0.4000 |
| 18.50 | 0.3000 |

Klein, R. R. - Bennett, C. O. - Dodgge, B. F., Experimental heats of mixing for gaseous nitrogen and methane, AIChE Journal 4 (1971) 958-965. doi:10.1002/aic.690170432

**T / K = 253.15**

**P / bar = 60.80**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 98.20 | 0.6000 |
| 107.10 | 0.5000 |
| 106.90 | 0.4000 |
| 96.60 | 0.3000 |

Klein, R. R. - Bennett, C. O. - Dodgge, B. F., Experimental heats of mixing for gaseous nitrogen and methane, AIChE Journal 4 (1971) 958-965. doi:10.1002/aic.690170432

**T / K = 253.15**

**P / bar = 101.33**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 228.80 | 0.6000 |
| 251.60 | 0.5000 |
| 252.80 | 0.4000 |
| 229.60 | 0.3000 |

Klein, R. R. - Bennett, C. O. - Dodgge, B. F., Experimental heats of mixing for gaseous nitrogen and methane, AIChE Journal 4 (1971) 958-965. doi:10.1002/aic.690170432

**T / K = 273.15**

**P / bar = 40.53**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 40.40 | 0.6000 |
| 43.20 | 0.5000 |
| 42.40 | 0.4000 |
| 37.70 | 0.3000 |

Klein, R. R. - Bennett, C. O. - Dodgge, B. F., Experimental heats of mixing for gaseous nitrogen and methane, AIChE Journal 4 (1971) 958-965. doi:10.1002/aic.690170432

**T / K = 273.15**

**P / bar = 81.06**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 108.30 | 0.6000 |
| 117.30 | 0.5000 |
| 116.00 | 0.4000 |
| 103.90 | 0.3000 |

Wormald, Christopher J. - Lewis, Keith L. - Mosedale, Stephen, The excess enthalpies of hydrogen + methane, hydrogen + nitrogen, methane + nitrogen, methane + argon, and nitrogen + argon at 298 and 201 K at pressures up to 10.2 MPa, The Journal of Chemical Thermodynamics 1 (1977) 27-42. doi:10.1016/0021-9614(77)90194-X

**T / K = 298.00**

**P / bar = 61.80**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 54.00 | 0.2810 |
| 64.00 | 0.3770 |
| 63.00 | 0.4350 |
| 58.00 | 0.5700 |
| 46.00 | 0.7110 |

Wormald, Christopher J. - Lewis, Keith L. - Mosedale, Stephen, The excess enthalpies of hydrogen + methane, hydrogen + nitrogen, methane + nitrogen, methane + argon, and nitrogen + argon at 298 and 201 K at pressures up to 10.2 MPa, The Journal of Chemical Thermodynamics 1 (1977) 27-42. doi:10.1016/0021-9614(77)90194-X

**T / K = 298.00**

**P / bar = 102.30**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 109.00 | 0.2790 |
| 122.00 | 0.4010 |
| 120.00 | 0.5260 |
| 107.00 | 0.6420 |
| 81.00 | 0.7570 |

Klein, R. R. - Bennett, C. O. - Dodgge, B. F., Experimental heats of mixing for gaseous nitrogen and methane, AIChE Journal 4 (1971) 958-965. doi:10.1002/aic.690170432

**T / K = 313.15**

**P / bar = 40.53**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 27.90 | 0.6000 |
| 29.60 | 0.5000 |
| 28.70 | 0.4000 |
| 24.90 | 0.3000 |

Klein, R. R. - Bennett, C. O. - Dodgge, B. F., Experimental heats of mixing for gaseous nitrogen and methane, AIChE Journal 4 (1971) 958-965. doi:10.1002/aic.690170432

**T / K = 313.15**

**P / bar = 81.06**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 64.30 | 0.6000 |
| 69.40 | 0.5000 |
| 67.50 | 0.4000 |
| 58.60 | 0.3000 |

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**Critical point**

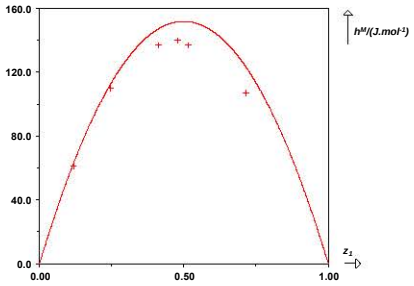
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Bloomer, O.T. - Parent, J.D., Liquid-vapor phase behavior of the methane-nitrogen system, Chem. Eng. Progr. Symp. Ser. 6 (1953) 11-24.

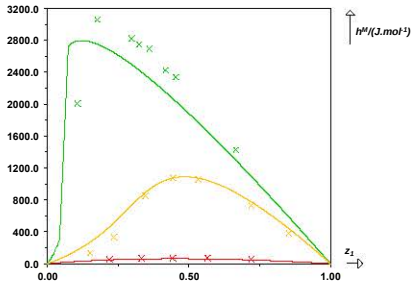
| T / K | P / bar | $x_1$ |
|---|---|---|
| 185.09 | 48.61 | 0.1002 |
| 174.21 | 50.68 | 0.2879 |
| 159.54 | 49.23 | 0.5088 |
| 146.93 | 44.82 | 0.6970 |

| | | |
|---|---|---|
| 136.87 | 39.85 | 0.8423 |
| 129.59 | 35.78 | 0.9515 |

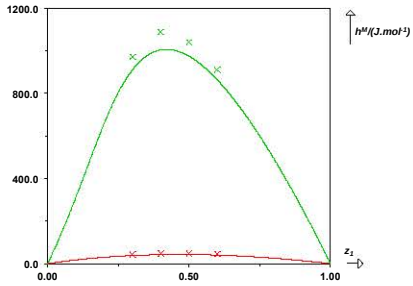
T/K = 91.50 - P/bar = 8.2035



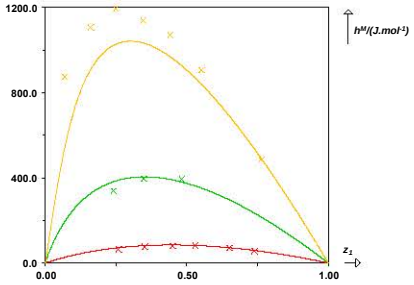

T/K = 183.00 - P/bar = 21.400 40.800 71.600



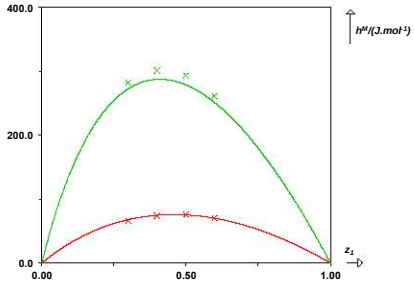

T/K = 195.15 - P/bar = 20.2650 81.0600



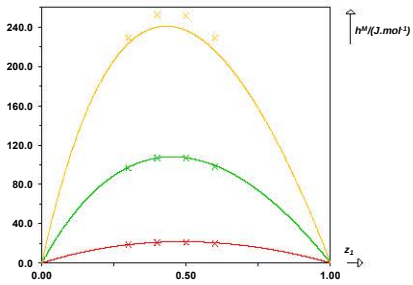

T/K = 201.00 - P/bar = 30.500 51.500 65.800



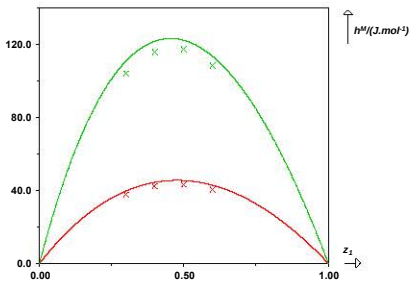

T/K = 233.15 - P/bar = 40.5300 81.0600



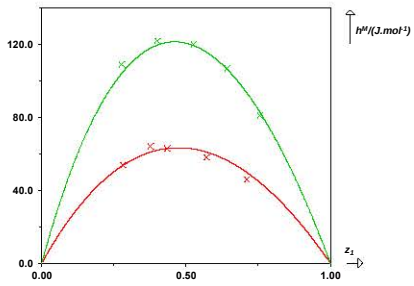

T/K = 253.15 - P/bar = 20.2650 60.7950 101.3300



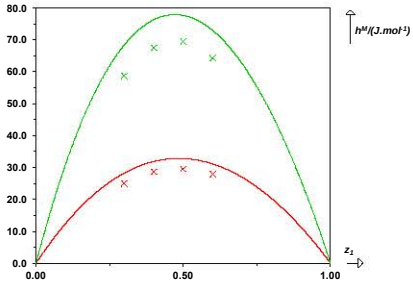

T/K = 273.15 - P/bar = 40.5300 81.0600



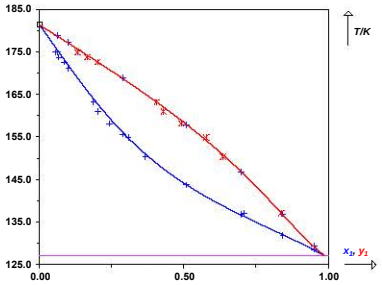

T/K = 298.00 - P/bar = 61.800 102.300



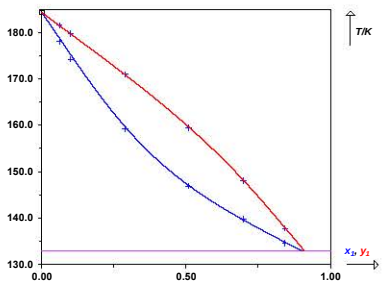

T/K = 313.15 - P/bar = 40.5300 81.0600



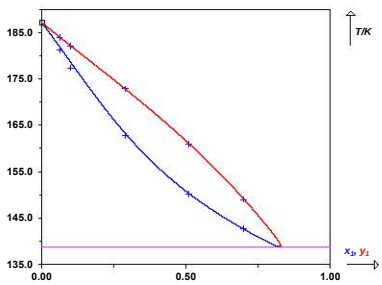

P/bar = 34.47400



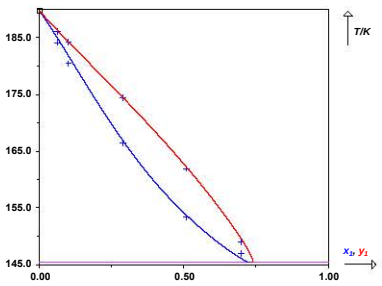

P/bar = 37.92100



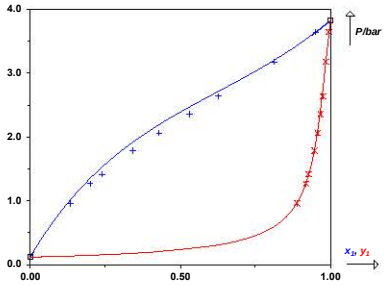

P/bar = 41.36900



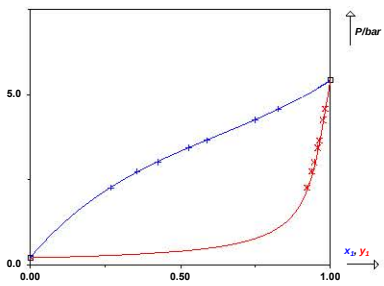

P/bar = 44.81600



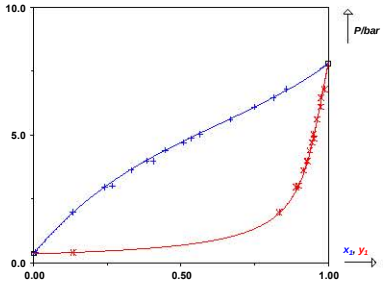

T/K = 90.67



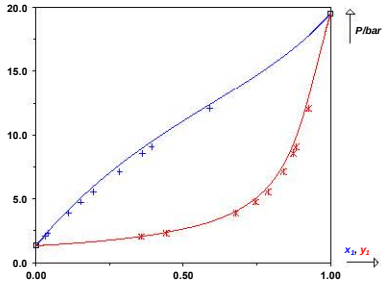

T/K = 95.00



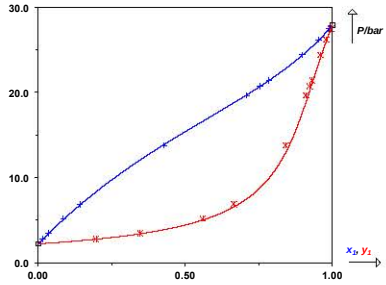
T/K = 100.00



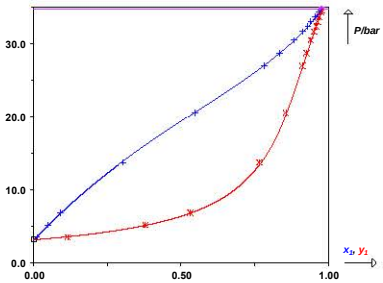

T/K = 114.99



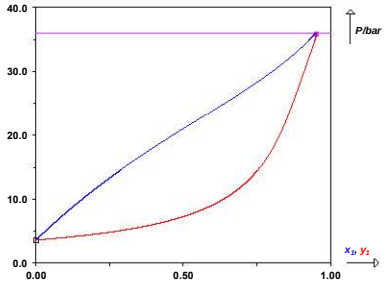

T/K = 122.04



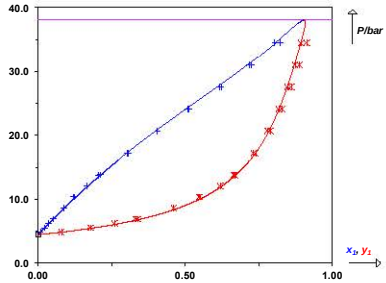

T/K = 127.59



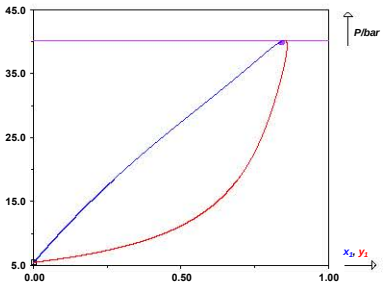

T/K = 129.59



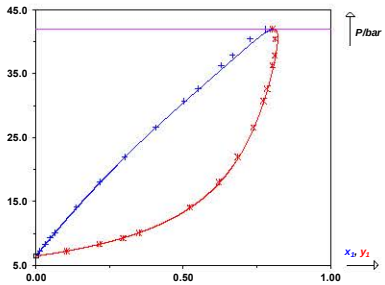

T/K = 133.15



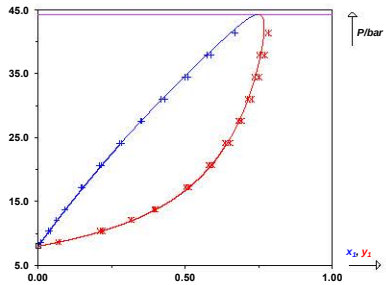

T/K = 136.87



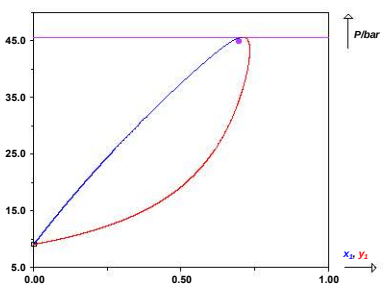

T/K = 140.00



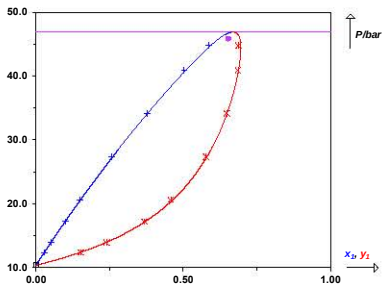

T/K = 144.26



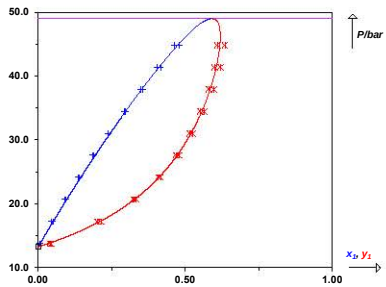

T/K = 146.93



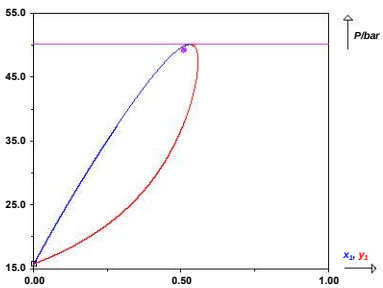

T/K = 149.82



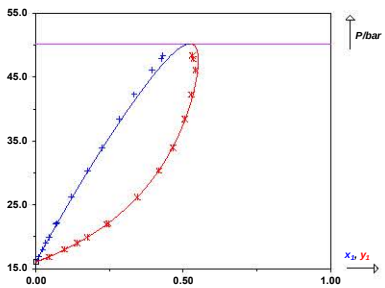

T/K = 155.37



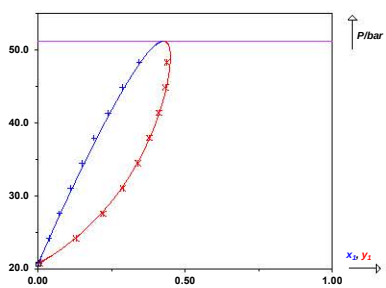

T/K = 159.54



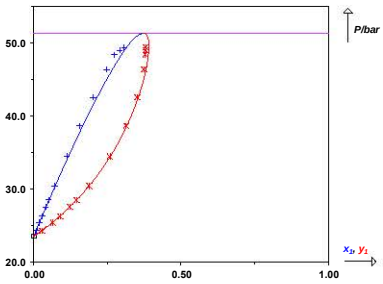

T/K = 160.00



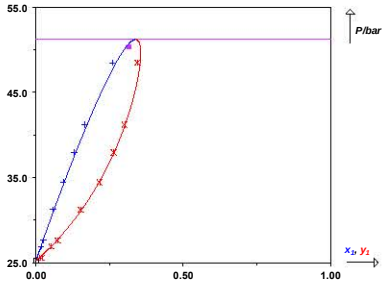

T/K = 166.48



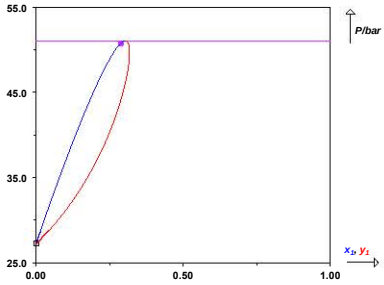
T/K = 170.00



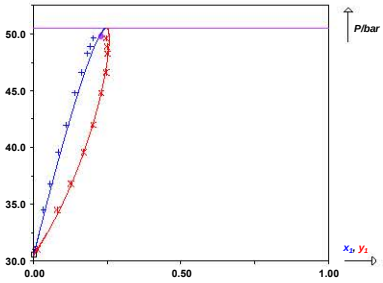

T/K = 172.04



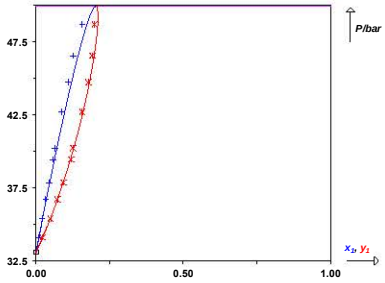

T/K = 174.21



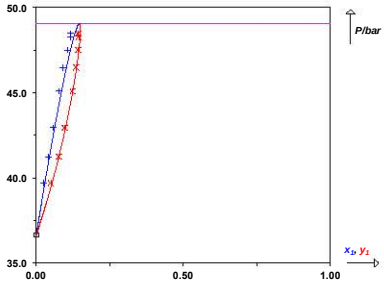

T/K = 177.59



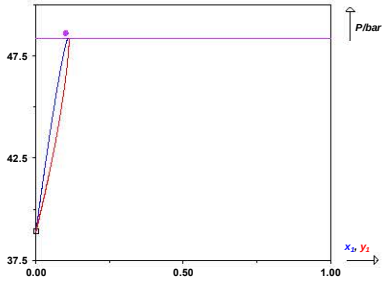

T/K = 180.00




T/K = 183.15




T/K = 185.09



## METHANE (1) + ETHANE (2)

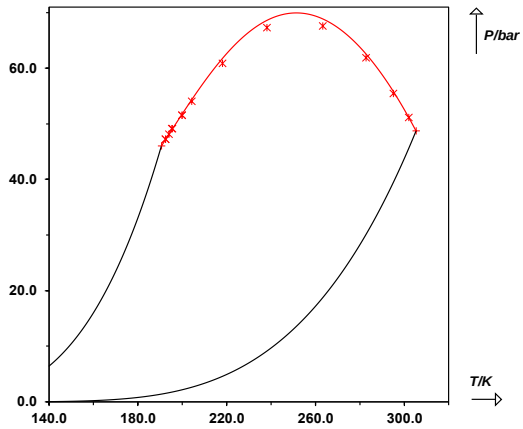
| | | |
|---|---|---|
| **CAS** | 74-82-8 | 74-84-0 |
| **InChiKey** | VNWKTOKETHGBQD-UHFFFAOYSA-N | OTMSDBZUPAUEDD-UHFFFAOYSA-N |
| **$T_c$ / K** | 190.56 | 305.32 |
| **$P_c$ / bar** | 45.99 | 48.72 |
| **ω** | 0.012 | 0.099 |

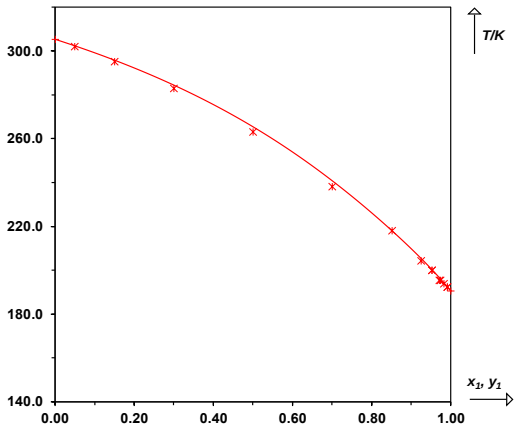
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 26.3
B/MPa = 37.7

*Deviations*
MAPE on x = 24 %
MAPE on y = 2.6 %
MAPE on $x_c$ = 4.4 %
MAPE on $P_c$ = 0.69 %
MAPE on $h^M$ = 11 %



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**Isothermal phase equilibrium data**

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Gomes de Azevedo, E.J.S. - Calado, J.C.G., Thermodynamics of liquid methane+ethane, Fluid Phase Equilibria (1989) 21-34. doi:10.1016/0378-3812(89)80003-2

**T / K = 90.69**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0359 | 0.2144 | 0.9997 |
| 0.0499 | 0.3194 | 0.9998 |
| 0.0582 | 0.3901 | 0.9999 |
| 0.0649 | 0.4466 | 0.9999 |
| 0.0709 | 0.5106 | 0.9999 |
| 0.0795 | 0.6006 | 0.9999 |
| 0.0900 | 0.7132 | 1.0000 |
| 0.0992 | 0.8226 | 1.0000 |

Miller, R.C. - Kidnay, A.J. - Hiza, M.J., Liquid + vapor equilibria in methane + ethene and in methane + ethane from 150.00 to 190.00 K, The Journal of Chemical Thermodynamics 2 (1977) 167-178. doi:10.1016/0021-9614(77)90082-9

**T / K = 160.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.233 | 0.0602 | 0.8270 |
| 2.026 | 0.1118 | 0.8970 |
| 2.037 | 0.1127 | 0.8986 |
| 3.050 | 0.1720 | 0.9344 |
| 3.995 | 0.2225 | 0.9511 |
| 4.116 | 0.2292 | 0.9534 |
| 5.294 | 0.3035 | 0.9652 |
| 5.984 | 0.3504 | 0.9704 |
| 7.930 | 0.4795 | 0.9794 |
| 9.930 | 0.6203 | 0.9854 |
| 11.95 | 0.7596 | 0.9909 |

Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-ethane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 9-12. doi:10.1021/je60052a022

**T / K = 190.87**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.724 | 0.0340 | 0.4724 |
| 4.171 | 0.0714 | 0.6513 |
| 6.895 | 0.1386 | 0.7907 |
| 11.03 | 0.2384 | 0.8709 |
| 17.24 | 0.3955 | 0.9181 |
| 24.13 | 0.5687 | 0.9425 |
| 34.48 | 0.8150 | 0.9647 |
| 38.82 | 0.9007 | 0.9750 |
| 42.20 | 0.9474 | 0.9832 |
| 43.44 | 0.9646 | 0.9869 |
| 44.26 | 0.9749 | 0.9898 |
| 44.89 | 0.9819 | 0.9919 |
| 45.51 | 0.9882 | 0.9944 |
| 45.78 | 0.9916 | 0.9958 |
| 46.06 | 0.9938 | 0.9969 |
| 46.20 | 0.9956 | 0.9977 |

Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-ethane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 9-12. doi:10.1021/je60052a022

**T / K = 192.37**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 2.689 | 0.0308 | 0.4339 | |
| 4.240 | 0.0681 | 0.6358 | |
| 6.895 | 0.1364 | 0.7755 | |
| 11.03 | 0.2299 | 0.8605 | |
| 17.24 | 0.3854 | 0.9087 | |
| 24.13 | 0.5512 | 0.9372 | |
| 34.48 | 0.7885 | 0.9607 | |
| 41.37 | 0.9154 | 0.9755 | |
| 44.13 | 0.9529 | 0.9822 | |
| 45.64 | 0.9715 | 0.9862 | |
| 46.54 | 0.9813 | 0.9897 | |
| 47.02 | 0.9858 | 0.9910 | |
| 47.23 | 0.9912 | 0.9912 | CRIT |

Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-ethane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 9-12. doi:10.1021/je60052a022

**T / K = 199.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.103 | 0.0214 | 0.3005 |
| 4.482 | 0.0512 | 0.5098 |
| 6.895 | 0.1039 | 0.6800 |
| 11.03 | 0.1875 | 0.7957 |
| 17.24 | 0.3100 | 0.8679 |
| 24.13 | 0.4526 | 0.9052 |
| 34.48 | 0.6601 | 0.9337 |
| 41.37 | 0.7852 | 0.9461 |
| 48.26 | 0.8942 | 0.9562 |
| 49.57 | 0.9126 | 0.9584 |
| 50.06 | 0.9175 | 0.9578 |
| 50.47 | 0.9222 | 0.9575 |

| | | | |
|---|---|---|---|
| 51.02 | 0.9319 | 0.9577 | |
| 51.57 | 0.9520 | 0.9520 | CRIT |

Wei, Michael S.-W. - Brown, Trent S. - Kidnay, Arthur J. - Sloan, E. Dendy, Vapor + Liquid Equilibria for the Ternary System Methane + Ethane + Carbon Dioxide at 230 K and Its Constituent Binaries at Temperatures from 207 to 270 K, Journal of Chemical & Engineering Data 4 (1995) 726-731. doi:10.1021/je00020a002

**T / K = 210.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.660 | 0.1100 | 0.6411 |
| 10.91 | 0.1304 | 0.6807 |
| 16.10 | 0.2263 | 0.7782 |
| 20.55 | 0.2947 | 0.8244 |
| 26.51 | 0.3938 | 0.8574 |
| 38.26 | 0.5885 | 0.8990 |
| 43.82 | 0.6700 | 0.9101 |
| 46.56 | 0.7137 | 0.9134 |
| 48.41 | 0.7477 | 0.9162 |
| 51.82 | 0.7944 | 0.9170 |
| 53.30 | 0.8149 | 0.9177 |
| 53.78 | 0.8218 | 0.9179 |
| 55.82 | 0.8552 | 0.9151 |

Wei, Michael S.-W. - Brown, Trent S. - Kidnay, Arthur J. - Sloan, E. Dendy, Vapor + Liquid Equilibria for the Ternary System Methane + Ethane + Carbon Dioxide at 230 K and Its Constituent Binaries at Temperatures from 207 to 270 K, Journal of Chemical & Engineering Data 4 (1995) 726-731. doi:10.1021/je00020a002

**T / K = 230.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.450 | 0.0186 | 0.1957 |
| 9.380 | 0.0315 | 0.2420 |
| 10.27 | 0.0417 | 0.2968 |
| 11.58 | 0.0585 | 0.3737 |
| 13.20 | 0.0787 | 0.4445 |
| 15.80 | 0.1110 | 0.5276 |
| 21.18 | 0.1785 | 0.6319 |
| 27.56 | 0.2573 | 0.7100 |
| 33.39 | 0.3294 | 0.7538 |
| 39.16 | 0.4002 | 0.7806 |
| 43.09 | 0.4480 | 0.7948 |
| 50.93 | 0.5392 | 0.8133 |
| 55.58 | 0.5962 | 0.8163 |
| 60.33 | 0.6543 | 0.8146 |
| 62.22 | 0.6813 | 0.8113 |
| 63.61 | 0.7017 | 0.8056 |
| 64.87 | 0.7341 | 0.7915 |
| 11.50 | 0.0571 | 0.3679 |
| 15.20 | 0.1045 | 0.5113 |
| 25.30 | 0.2324 | 0.6831 |
| 35.50 | 0.3574 | 0.7637 |
| 45.60 | 0.4790 | 0.8003 |
| 55.70 | 0.5994 | 0.8158 |
| 64.90 | 0.7231 | 0.8037 |

Wei, Michael S.-W. - Brown, Trent S. - Kidnay, Arthur J. - Sloan, E. Dendy, Vapor + Liquid Equilibria for the Ternary System Methane + Ethane + Carbon Dioxide at 230 K and Its Constituent Binaries at Temperatures from 207 to 270 K, Journal of Chemical & Engineering Data 4 (1995) 726-731. doi:10.1021/je00020a002

**T / K = 250.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.63 | 0.0247 | 0.1489 |
| 18.81 | 0.0561 | 0.2734 |
| 28.49 | 0.1497 | 0.4911 |
| 40.83 | 0.2733 | 0.6125 |
| 48.98 | 0.3521 | 0.6550 |
| 59.51 | 0.4638 | 0.6795 |

Davalos, Juan - Anderson, Wayne R. - Phelps, Robert E. - Kidnay, Arthur J., Liquid-Vapor Equilibria at 250.00K for Systems Containing Methane, Ethane, and Carbon Dioxide, Journal of Chemical & Engineering Data 1 (1976) 81-84. doi:10.1021/je60068a030

**T / K = 250.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.30 | 0.0240 | 0.1340 |
| 22.29 | 0.0890 | 0.3650 |
| 22.80 | 0.0970 | 0.3830 |
| 32.93 | 0.1960 | 0.5400 |
| 45.60 | 0.3200 | 0.6430 |
| 55.93 | 0.4260 | 0.6730 |
| 66.57 | 0.5460 | 0.6730 |

Gupta, Mukesh K. - Gardner, Glenn C. - Hegarty, Michael J. - Kidnay, Arthur J., Liquid-vapor equilibriums for the N2 + CH4 + C2H6 system from 260 to 280 K, Journal of Chemical & Engineering Data 4 (1980) 313-318. doi:10.1021/je60087a016

**T / K = 260.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 18.04 | 0.0088 | 0.0467 |
| 19.68 | 0.0239 | 0.1150 |
| 21.89 | 0.0445 | 0.1922 |
| 23.53 | 0.0592 | 0.2387 |
| 25.60 | 0.0788 | 0.2924 |
| 30.38 | 0.1220 | 0.3810 |

| | | |
|---|---|---|
| 35.15 | 0.1652 | 0.4483 |
| 41.13 | 0.2189 | 0.5052 |
| 50.97 | 0.3087 | 0.5664 |
| 55.91 | 0.3545 | 0.5823 |
| 60.19 | 0.3952 | 0.5896 |
| 63.48 | 0.4297 | 0.5897 |
| 66.04 | 0.4615 | 0.5823 |

Gupta, Mukesh K. - Gardner, Glenn C. - Hegarty, Michael J. - Kidnay, Arthur J., Liquid-vapor equilibriums for the N2 + CH4 + C2H6 system from 260 to 280 K, Journal of Chemical & Engineering Data 4 (1980) 313-318. doi:10.1021/je60087a016

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 22.83 | 0.0070 | 0.0298 |
| 24.21 | 0.0188 | 0.0762 |
| 26.45 | 0.0357 | 0.1332 |
| 31.10 | 0.0739 | 0.2361 |
| 35.54 | 0.1127 | 0.3140 |
| 40.53 | 0.1550 | 0.3768 |
| 45.90 | 0.1984 | 0.4237 |
| 49.71 | 0.2315 | 0.4484 |
| 50.93 | 0.2419 | 0.4558 |
| 61.02 | 0.3321 | 0.4889 |

Wei, Michael S.-W. - Brown, Trent S. - Kidnay, Arthur J. - Sloan, E. Dendy, Vapor + Liquid Equilibria for the Ternary System Methane + Ethane + Carbon Dioxide at 230 K and Its Constituent Binaries at Temperatures from 207 to 270 K, Journal of Chemical & Engineering Data 4 (1995) 726-731. doi:10.1021/je00020a002

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 23.07 | 0.0080 | 0.0347 |
| 24.86 | 0.0235 | 0.0926 |
| 26.06 | 0.0330 | 0.1247 |
| 28.19 | 0.0498 | 0.1728 |
| 30.30 | 0.0682 | 0.2211 |
| 34.40 | 0.1031 | 0.2852 |
| 39.16 | 0.1443 | 0.3591 |
| 48.82 | 0.2256 | 0.4430 |
| 54.63 | 0.2763 | 0.4722 |
| 58.09 | 0.3088 | 0.4831 |
| 61.39 | 0.3516 | 0.4874 |
| 62.82 | 0.3684 | 0.4869 |
| 63.40 | 0.3751 | 0.4855 |
| 64.74 | 0.3922 | 0.4811 |

Gupta, Mukesh K. - Gardner, Glenn C. - Hegarty, Michael J. - Kidnay, Arthur J., Liquid-vapor equilibriums for the N2 + CH4 + C2H6 system from 260 to 280 K, Journal of Chemical & Engineering Data 4 (1980) 313-318. doi:10.1021/je60087a016

**T / K = 280.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 28.88 | 0.0081 | 0.0279 |
| 30.75 | 0.0231 | 0.0744 |
| 32.04 | 0.0335 | 0.1036 |
| 36.56 | 0.0693 | 0.1864 |
| 40.38 | 0.0996 | 0.2404 |
| 44.16 | 0.1292 | 0.2818 |
| 47.12 | 0.1528 | 0.3091 |
| 50.41 | 0.1798 | 0.3336 |
| 53.30 | 0.2044 | 0.3512 |
| 56.46 | 0.2333 | 0.3654 |
| 59.84 | 0.2668 | 0.3719 |
| 60.87 | 0.2774 | 0.3711 |
| 61.91 | 0.2913 | 0.3675 |
| 62.66 | 0.3046 | 0.3609 |
| 62.92 | 0.3109 | 0.3557 |

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**Isobaric phase equilibrium data**

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Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 6.895**

| T / K | $x_1$ |
|---|---|
| 184.26 | 0.8516 |
| 173.04 | 0.9250 |
| 158.59 | 0.9750 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 6.895**

| T / K | $x_1$ |
|---|---|
| 188.26 | 0.1498 |
| 168.32 | 0.3002 |
| 154.71 | 0.5002 |
| 148.26 | 0.7000 |
| 144.54 | 0.8516 |
| 142.93 | 0.9250 |
| 141.82 | 0.9750 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 10.34**

| T / K | $y_1$ |
|---|---|
| 240.59 | 0.0500 |
| 236.54 | 0.1498 |
| 230.43 | 0.3002 |
| 220.82 | 0.5002 |
| 207.04 | 0.7000 |
| 192.09 | 0.8516 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 10.34**

| T / K | $x_1$ |
|---|---|
| 179.48 | 0.9250 |
| 164.98 | 0.9750 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 10.34**

| T / K | $x_1$ |
|---|---|
| 228.15 | 0.0500 |
| 203.87 | 0.1498 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 10.34**

| T / K | $x_1$ |
|---|---|
| 182.48 | 0.3002 |
| 166.04 | 0.5002 |
| 157.98 | 0.7000 |
| 153.71 | 0.8516 |
| 151.87 | 0.9250 |
| 150.32 | 0.9750 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 17.24**

| T / K | $y_1$ |
|---|---|
| 258.21 | 0.0500 |
| 253.65 | 0.1498 |
| 246.37 | 0.3002 |
| 234.76 | 0.5002 |
| 219.21 | 0.7000 |
| 202.43 | 0.8516 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 17.24**

| T / K | $x_1$ |
|---|---|
| 188.87 | 0.9250 |
| 174.09 | 0.9750 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 17.24**

| T / K | $x_1$ |
|---|---|
| 248.32 | 0.0500 |
| 226.37 | 0.1498 |
| 202.37 | 0.3002 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 17.24**

| T / K | $x_1$ |
|---|---|
| 183.09 | 0.5002 |
| 172.54 | 0.7000 |
| 167.09 | 0.8516 |
| 164.48 | 0.9250 |
| 162.76 | 0.9750 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 44.82**

| T / K | $y_1$ |
|---|---|
| 297.32 | 0.0500 |
| 289.82 | 0.1498 |
| 279.21 | 0.3002 |
| 263.04 | 0.5002 |
| 242.26 | 0.7000 |
| 221.48 | 0.8516 |
| 206.37 | 0.9250 |
| 194.93 | 0.9750 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 44.82**

| T / K | $x_1$ |
|---|---|
| 293.87 | 0.0500 |
| 277.54 | 0.1498 |
| 253.71 | 0.3002 |
| 226.82 | 0.5002 |
| 209.21 | 0.7000 |
| 200.09 | 0.8516 |
| 195.09 | 0.9250 |
| 191.65 | 0.9750 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 51.71**

| T / K | $x_1$ |
|---|---|
| 294.93 | 0.1498 |
| 283.54 | 0.3002 |
| 266.48 | 0.5002 |
| 244.98 | 0.7000 |
| 223.26 | 0.8516 |
| 207.59 | 0.9250 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 51.71**

| T / K | $x_1$ |
|---|---|
| 286.98 | 0.1498 |
| 263.71 | 0.3002 |
| 235.76 | 0.5002 |
| 216.48 | 0.7000 |
| 206.54 | 0.8516 |
| 201.37 | 0.9250 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 58.61**

| T / K | $x_1$ |
|---|---|
| 285.54 | 0.3002 |
| 268.76 | 0.5002 |
| 246.43 | 0.7000 |
| 223.32 | 0.8516 |

Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

**P / bar = 58.61**

| T / K | $x_1$ |
|---|---|
| 273.54 | 0.3002 |
| 244.71 | 0.5002 |
| 223.76 | 0.7000 |
| 213.71 | 0.8516 |

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**Enthalpy of mixing**

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Miller, R. C. - Staveley, L. A. K., Excess Enthalpies for Some Binary Liquid Mixtures of Low-Molecular-Weight Alkanes, Advances in Cryogenic Engineering (1960) 493-500.

**T / K = 91.50**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 67.00 | 0.2825 |
| 80.00 | 0.4008 |
| 82.70 | 0.5105 |
| 84.90 | 0.6039 |

| | |
|---|---|
| 77.60 | 0.7044 |
| 65.80 | 0.7879 |

Miller, R. C. - Staveley, L. A. K., Excess Enthalpies for Some Binary Liquid Mixtures of Low-Molecular-Weight Alkanes, Advances in Cryogenic Engineering (1960) 493-500.

**T / K =** **112.00**

**P / bar =** **UNKNOWN (2.0923)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 56.20 | 0.3020 |
| 64.10 | 0.3912 |
| 68.10 | 0.5136 |
| 66.30 | 0.6200 |
| 61.10 | 0.6841 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K =** **266.70**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 2.820 | 0.1750 |
| 3.710 | 0.2810 |
| 4.180 | 0.3770 |
| 4.500 | 0.4680 |
| 4.340 | 0.5490 |
| 3.730 | 0.6510 |
| 2.800 | 0.7860 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K =** **282.20**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 2.310 | 0.2110 |
| 3.210 | 0.3380 |
| 3.480 | 0.4360 |
| 3.590 | 0.4940 |
| 3.610 | 0.6420 |
| 2.430 | 0.7640 |
| 2.080 | 0.8410 |
| 1.150 | 0.8660 |

Hutchings, D.J. - Lewis, E.J. - Wormald, C.J., Excess enthalpies of mixtures of methane + each of the n-alkanes from ethane to n-octane, The Journal of Chemical Thermodynamics 6 (1978) 559-566. doi:10.1016/0021-9614(78)90044-7

**T / K =** **298.20**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 1.750 | 0.1680 |
| 2.290 | 0.2450 |
| 2.760 | 0.3590 |
| 2.990 | 0.4340 |
| 3.230 | 0.5930 |
| 3.070 | 0.6420 |
| 2.710 | 0.7160 |
| 2.420 | 0.7320 |
| 1.540 | 0.8240 |

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**Critical point**

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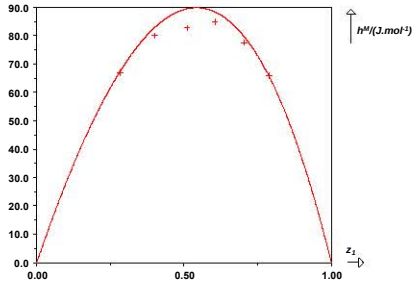
Ellington, R.T. - Eakin, B.E. - Parent, J.D. - Gami, D.C. - Bloomer, O.T., Vapor-liquid phase equilibriums in the binary systems of CH4, C2H6, and N2, Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties (1959) 180-194.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 195.37 | 49.16 | 0.9746 |
| 204.26 | 54.02 | 0.9250 |
| 217.98 | 60.88 | 0.8516 |
| 237.98 | 67.29 | 0.7000 |
| 263.15 | 67.64 | 0.5002 |
| 282.87 | 61.85 | 0.3002 |
| 294.98 | 55.50 | 0.1498 |
| 302.04 | 51.09 | 0.0500 |

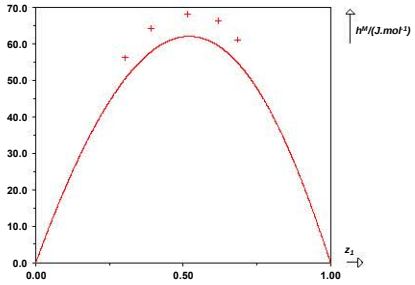
Wichterle, Ivan - Kobayashi, Riki, Vapor-liquid equilibrium of methane-ethane system at low temperatures and high pressures, Journal of Chemical & Engineering Data 1 (1972) 9-12. doi:10.1021/je60052a022

| T / K | P / bar | $x_1$ |
|---|---|---|
| 199.92 | 51.57 | 0.9520 |
| 195.44 | 49.14 | 0.9706 |
| 193.92 | 48.13 | 0.9821 |
| 192.39 | 47.22 | 0.9912 |

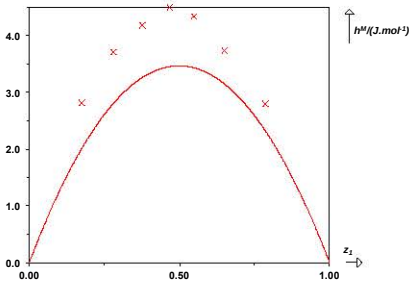
T/K = 91.50 - P/bar = 1.0132



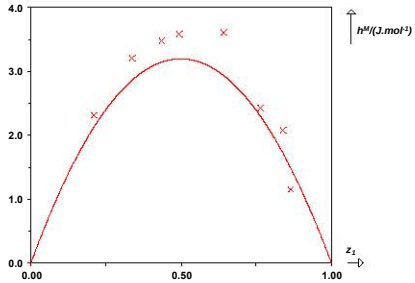

T/K = 112.00 - P/bar = 2.0923



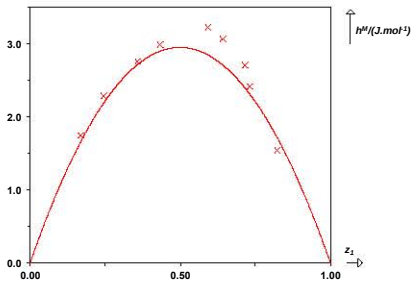

T/K = 266.70 - P/bar = 1.0132



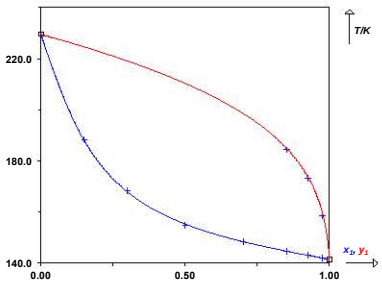

T/K = 282.20 - P/bar = 1.0132



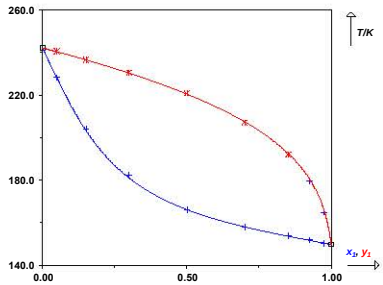

T/K = 298.20 - P/bar = 1.0132



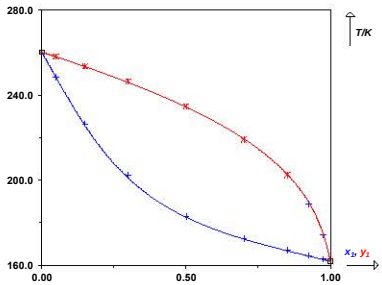

P/bar = 6.89480



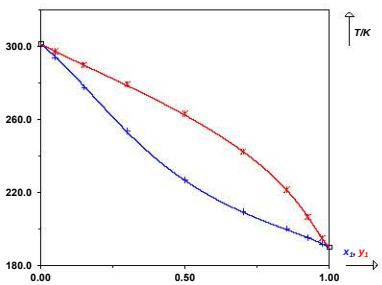

P/bar = 10.34200



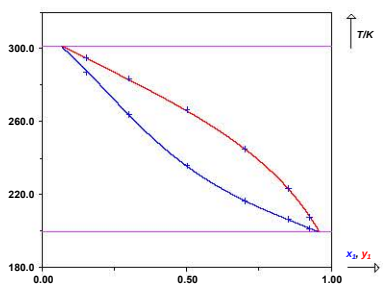

P/bar = 17.23700



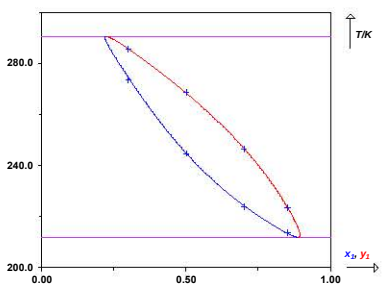

P/bar = 44.81600



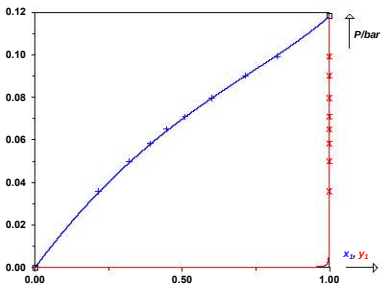

P/bar = 51.71100



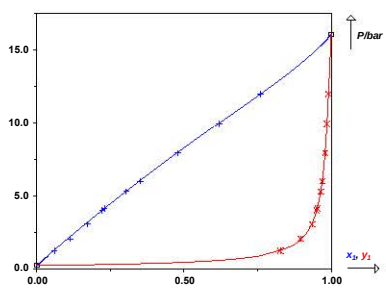

P/bar = 58.60500



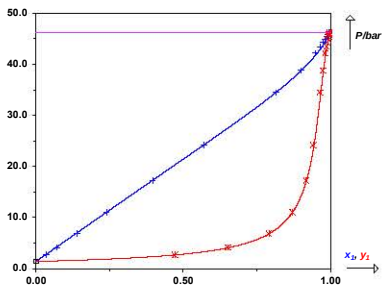

T/K = 90.69



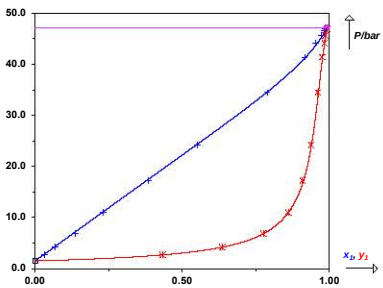

T/K = 160.00



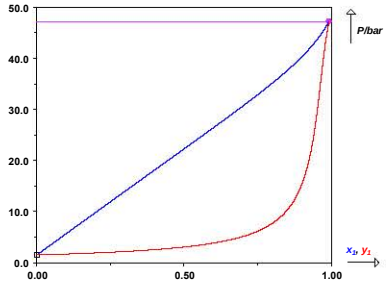

T/K = 190.87



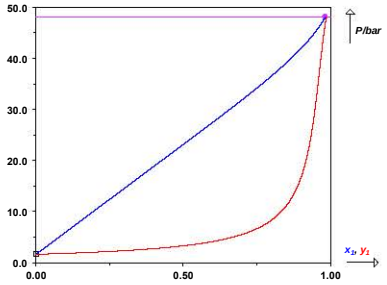

T/K = 192.37



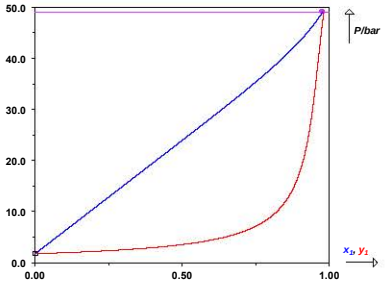
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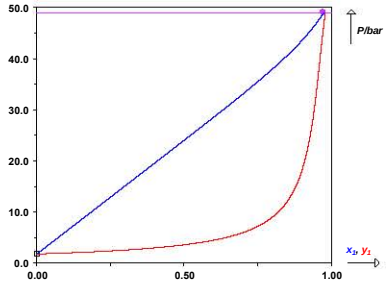

T/K = 193.92



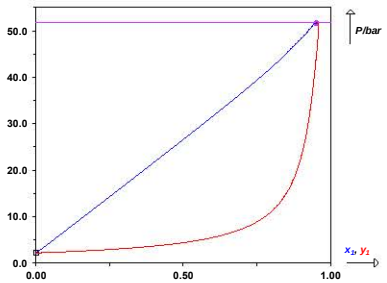

T/K = 195.37



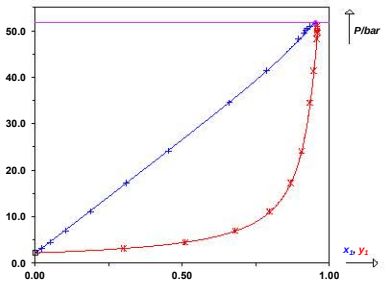

T/K = 195.44



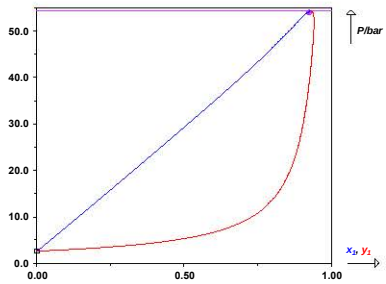

T/K = 199.92



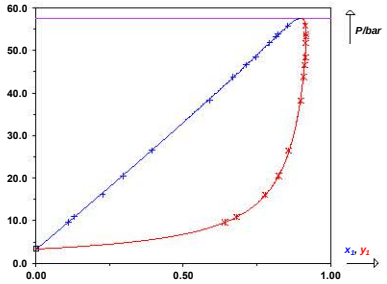

T/K = 199.93



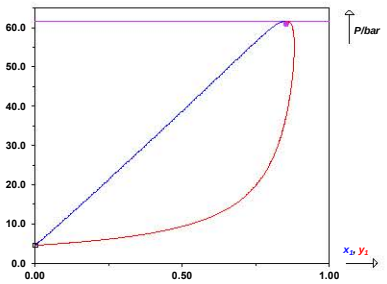

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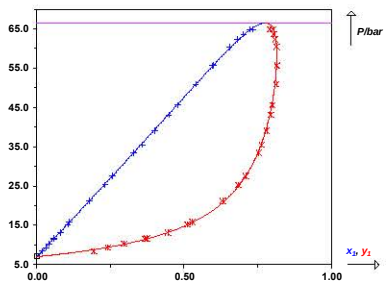

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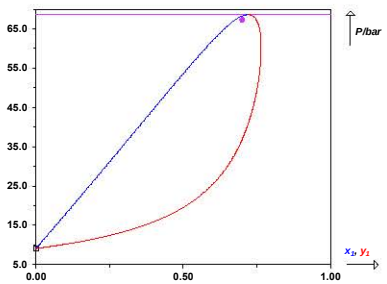

T/K = 217.98



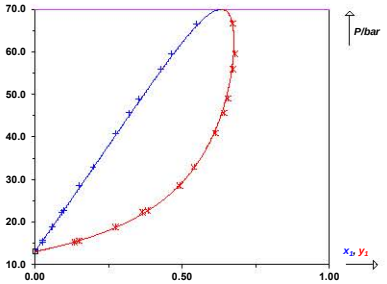

T/K = 230.00



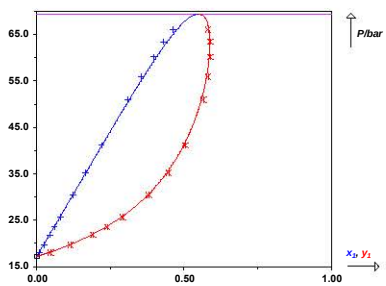

T/K = 237.98



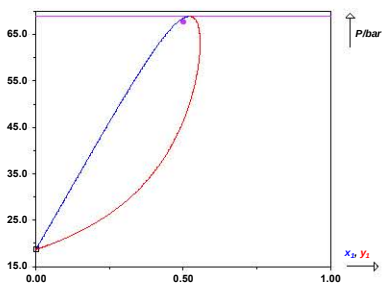

T/K = 250.00



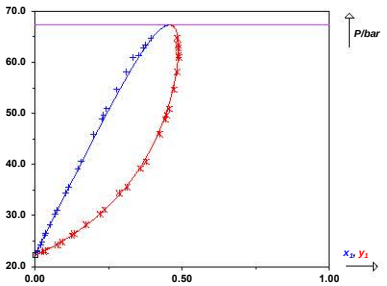

T/K = 260.00



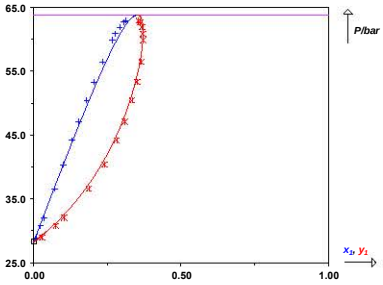

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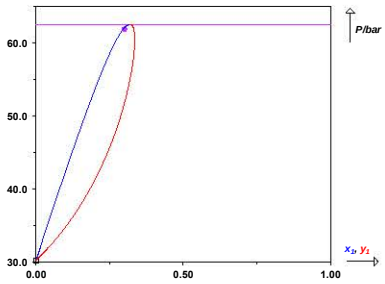

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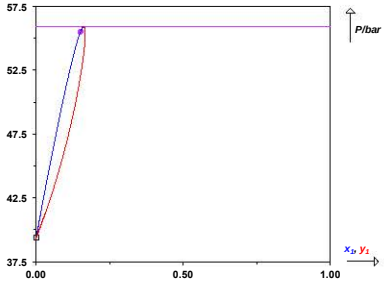
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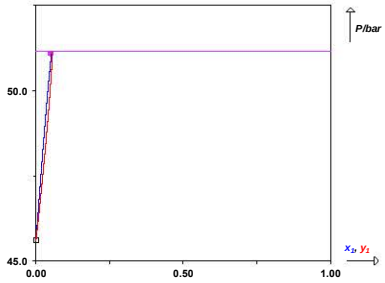

T/K = 282.87




T/K = 294.98




T/K = 302.04



## BENZENE (1) + n-HEPTANE (2)

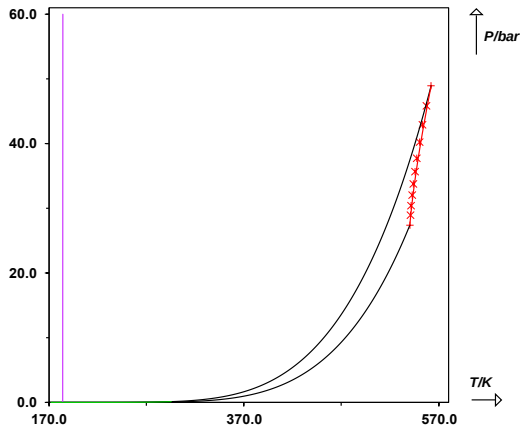
| | | |
|---|---|---|
| **CAS** | 71-43-2 | 142-82-5 |
| **InChiKey** | UHOVQNZJYSORNB-UHFFFAOYSA-N | IMNFDUFMRHMDMM-UHFFFAOYSA-N |
| **$T_c$ / K** | 562.05 | 540.20 |
| **$P_c$ / bar** | 48.95 | 27.40 |
| **ω** | 0.210 | 0.349 |

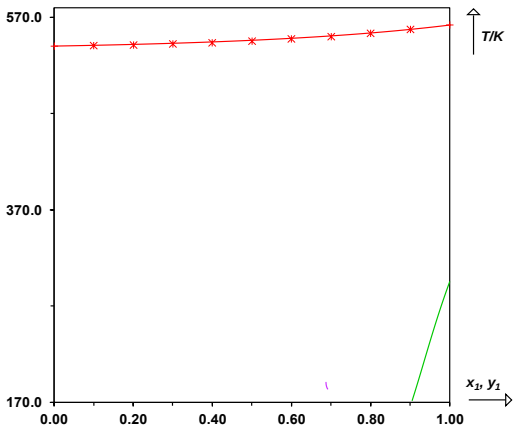
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 96.4
B/MPa = 196

*Deviations*
MAPE on x = 5.6 %
MAPE on y = 5 %
MAPE on $x_c$ = 8.1 %
MAPE on $P_c$ = 2.8 %
MAPE on $h^M$ = 9 %
MAPE on $c_P^M$ = 8.7 %



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**Isothermal phase equilibrium data**

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Werner, Günter - Schuberth, Horst, Das Phasengleichgewicht flüssig-flüssig des Systems Benzol/n-Heptan/Acetonitril sowie die Phasengleichgewichte dampfförmig-flüssig der entsprechenden binären Systeme bei 20,0 °C, Journal für Praktische Chemie 5-6 (1966) 225-239. doi:10.1002/prac.19660310501

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0507 | 0.0280 | 0.0900 |
| 0.0557 | 0.0700 | 0.2050 |
| 0.0615 | 0.1320 | 0.3280 |
| 0.0668 | 0.1840 | 0.4100 |
| 0.0700 | 0.2260 | 0.4660 |
| 0.0740 | 0.2790 | 0.5250 |
| 0.0773 | 0.3300 | 0.5750 |
| 0.0836 | 0.4410 | 0.6570 |
| 0.0871 | 0.5060 | 0.7010 |
| 0.0889 | 0.5520 | 0.7210 |
| 0.0929 | 0.6530 | 0.7780 |
| 0.0965 | 0.7540 | 0.8340 |
| 0.0979 | 0.8010 | 0.8590 |
| 0.0995 | 0.8690 | 0.8990 |
| 0.0999 | 0.8880 | 0.9100 |

Harris, Kenneth R. - Dunlop, Peter J., Vapour pressures and excess Gibbs energies of mixtures of benzene with chlorobenzene, n-hexane, and n-heptane at 25°C, The Journal of Chemical Thermodynamics 6 (1970) 805-811. doi:10.1016/0021-9614(70)90023-6

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0736 | 0.0965 | 0.2477 |
| 0.0815 | 0.1665 | 0.3692 |
| 0.0944 | 0.2942 | 0.5283 |
| 0.1019 | 0.3854 | 0.6092 |
| 0.1025 | 0.3914 | 0.6144 |
| 0.1091 | 0.4899 | 0.6831 |
| 0.1092 | 0.4903 | 0.6836 |
| 0.1093 | 0.4905 | 0.6841 |
| 0.1157 | 0.6027 | 0.7501 |
| 0.1199 | 0.6936 | 0.7985 |
| 0.1236 | 0.8017 | 0.8558 |
| 0.1260 | 0.8892 | 0.9087 |

Sun, Y. - Yen, W.H., Vapor Pressures and Excess Gibbs Free Energies of Benzene-Cyclohexane, Benzene-n-Heptane and Gyclohexane-n-Heptane, Gaodeng Xuexiao Huaxue Xuebao 1 (1986) 54-58.

**T / K = 308.19**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1242 | 0.1438 | 0.3208 |
| 0.1401 | 0.2411 | 0.4567 |
| 0.1438 | 0.2574 | 0.4756 |
| 0.1536 | 0.3278 | 0.5482 |
| 0.1648 | 0.4252 | 0.6299 |
| 0.1685 | 0.4679 | 0.6607 |
| 0.1699 | 0.4773 | 0.6671 |
| 0.1787 | 0.5722 | 0.7272 |
| 0.1803 | 0.6033 | 0.7453 |
| 0.1864 | 0.6941 | 0.7957 |
| 0.1944 | 0.8226 | 0.8668 |
| 0.1977 | 0.9001 | 0.9158 |

Messow, U. - Schuetze, D. - Pfestorf, R. - Kuchenbecker, D. - Suehnel, K., Thermodynamische Untersuchungen an Lösungsmittel/n-Paraffin-Systemen, Z. Phys. Chem. Leipzig 1 (1977) 24-32.

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1488 | 0.1180 | 0.2750 |
| 0.1725 | 0.2440 | 0.4520 |
| 0.1815 | 0.3030 | 0.5190 |
| 0.2107 | 0.5120 | 0.6830 |
| 0.2221 | 0.6330 | 0.7550 |
| 0.2287 | 0.6990 | 0.7970 |
| 0.2333 | 0.7710 | 0.8400 |
| 0.2395 | 0.8440 | 0.8830 |

Palmer, David A. - Smith, Buford D., Thermodynamic excess property measurements for acetonitrile-benzene-n-heptane system at 45°C, Journal of Chemical & Engineering Data 1 (1972) 71-76. doi:10.1021/je60052a037

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1687 | 0.0604 | 0.1551 |
| 0.1836 | 0.1180 | 0.2645 |
| 0.1907 | 0.1432 | 0.3082 |
| 0.2108 | 0.2370 | 0.4396 |
| 0.2211 | 0.2841 | 0.4906 |
| 0.2271 | 0.3105 | 0.5237 |
| 0.2389 | 0.3777 | 0.5783 |
| 0.2443 | 0.4195 | 0.6157 |
| 0.2561 | 0.4798 | 0.6672 |
| 0.2680 | 0.5856 | 0.7288 |
| 0.2749 | 0.6412 | 0.7639 |

| | | |
|---|---|---|
| 0.2798 | 0.6913 | 0.7893 |
| 0.2890 | 0.7738 | 0.8415 |
| 0.2968 | 0.9183 | 0.9288 |
| 0.3001 | 0.9779 | 0.9759 |

Kudryavtseva, L.S. - Viit, H. - Eisen, O.G., Vapor-liquid equilibrium in 1-heptene-heptane, 1-heptene-octane, heptane-octane, benzene-thiophene, benzene-heptane, and thiophene-heptane binary systems at 55.deg., Eesti NSV Tead. Akad. Toim. Keem. Geol. 4 (1971) 292-296.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2367 | 0.0100 | 0.0340 |
| 0.2421 | 0.0200 | 0.0650 |
| 0.2580 | 0.0500 | 0.1480 |
| 0.2725 | 0.0830 | 0.2180 |
| 0.3000 | 0.1590 | 0.3390 |
| 0.3153 | 0.2100 | 0.4010 |
| 0.3286 | 0.2570 | 0.4530 |
| 0.3489 | 0.3360 | 0.5300 |
| 0.3629 | 0.4000 | 0.5820 |
| 0.3780 | 0.4730 | 0.6380 |
| 0.3913 | 0.5400 | 0.6870 |
| 0.4018 | 0.6000 | 0.7270 |
| 0.4114 | 0.6600 | 0.7660 |
| 0.4204 | 0.7200 | 0.8040 |
| 0.4274 | 0.7770 | 0.8380 |
| 0.4312 | 0.8110 | 0.8590 |
| 0.4353 | 0.8600 | 0.8860 |
| 0.4390 | 0.9120 | 0.9250 |

Hanson, Donald O. - Van Winkle, Matthew, Alteration of the relative volatility of hexane-1-hexene by oxygenated and chlorinated solvents, Journal of Chemical & Engineering Data 3 (1967) 319-325. doi:10.1021/je60034a009

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3165 | 0.0870 | 0.1870 |
| 0.3172 | 0.0880 | 0.1880 |
| 0.3537 | 0.1800 | 0.3400 |
| 0.3875 | 0.2800 | 0.4630 |
| 0.4233 | 0.4040 | 0.5780 |
| 0.4744 | 0.6180 | 0.7380 |
| 0.4916 | 0.7130 | 0.7960 |
| 0.5040 | 0.7950 | 0.8470 |
| 0.5164 | 0.9070 | 0.9220 |
| 0.5178 | 0.9080 | 0.9230 |

Bayles, John W. - Letcher, Trevor M., Thermodynamics of some binary liquid mixtures containing aliphatic amines, Journal of Chemical & Engineering Data 3 (1971) 266-271. doi:10.1021/je60050a026

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5876 | 0.0240 | 0.0490 |
| 0.6765 | 0.1500 | 0.2680 |
| 0.6867 | 0.1650 | 0.2880 |
| 0.7110 | 0.2010 | 0.3430 |
| 0.7317 | 0.2320 | 0.3800 |
| 0.7638 | 0.2880 | 0.4440 |
| 0.8935 | 0.5500 | 0.6780 |
| 0.9198 | 0.6210 | 0.7250 |
| 0.9503 | 0.7110 | 0.7880 |

Messow, U. - Schuetze, D. - Pfestorf, R. - Kuchenbecker, D. - Suehnel, K., Thermodynamische Untersuchungen an Lösungsmittel/n-Paraffin-Systemen, Z. Phys. Chem. Leipzig 1 (1977) 24-32.

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.7182 | 0.2130 | 0.3650 |
| 0.7398 | 0.2460 | 0.4070 |
| 0.7571 | 0.2780 | 0.4450 |
| 0.7729 | 0.2980 | 0.4680 |
| 0.7969 | 0.3490 | 0.5190 |
| 0.8762 | 0.5100 | 0.6570 |
| 0.9049 | 0.5830 | 0.7080 |
| 0.9295 | 0.6260 | 0.7390 |
| 0.9427 | 0.6910 | 0.7860 |
| 0.9747 | 0.7830 | 0.8500 |
| 0.9798 | 0.8040 | 0.8620 |

Brown, I, Liquid-Vapour Equilibria. III. The Systems Benzene- n-heptane, n-Hexane-chlorobenzene, and cyclohexane-nitrobenzene, Australian Journal of Chemistry 3 (1952) doi:10.1071/CH9520530

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.6061 | 0.0464 | 0.0988 |
| 0.6350 | 0.0861 | 0.1729 |
| 0.7125 | 0.2004 | 0.3473 |
| 0.7593 | 0.2792 | 0.4412 |
| 0.8180 | 0.3842 | 0.5464 |
| 0.8668 | 0.4857 | 0.6304 |
| 0.9063 | 0.5824 | 0.7009 |
| 0.9450 | 0.6904 | 0.7759 |
| 0.9730 | 0.7842 | 0.8384 |
| 0.9979 | 0.8972 | 0.9149 |

Brown, I - Ewald, Ah, Liquid-Vapour Equilibria II. The System Benzene-Heptane, Australian Journal of Chemistry 2 (1951) doi:10.1071/CH9510198

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5868 | 0.0211 | 0.0429 |
| 0.6040 | 0.0458 | 0.0901 |
| 0.6383 | 0.0929 | 0.1723 |
| 0.7029 | 0.1895 | 0.3224 |
| 0.7635 | 0.2883 | 0.4399 |
| 0.8194 | 0.3909 | 0.5446 |
| 0.8691 | 0.4951 | 0.6315 |
| 0.9046 | 0.5819 | 0.6930 |
| 0.9420 | 0.6848 | 0.7668 |
| 0.9955 | 0.8832 | 0.9038 |
| 1.010 | 0.9793 | 0.9810 |

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**Isobaric phase equilibrium data**

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Nielsen, R. L. - Weber, J. H., Vapor-Liquid Equilibria at Subatmospheric Pressures. Binary and Ternary Systems Containing Ethyl Alcohol, Benzene, and n-Heptane., Journal of Chemical & Engineering Data 2 (1959) 145-151. doi:10.1021/je60002a011

**P / bar = 0.5333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 347.05 | 0.1000 | 0.2180 |
| 343.65 | 0.2000 | 0.3730 |
| 341.15 | 0.3000 | 0.4900 |
| 339.15 | 0.4000 | 0.5830 |
| 337.55 | 0.5000 | 0.6600 |
| 336.45 | 0.6000 | 0.7270 |
| 335.25 | 0.7000 | 0.7880 |
| 334.55 | 0.8000 | 0.8490 |
| 333.95 | 0.9000 | 0.9160 |

Sieg, L., Flüssigkeit-Dampf-Gleichgewichte in binären Systemen von Kohlenwasserstoffen verschiedenen Typs: Flüssigkeit-Dampf-Gleichgewichte in binären Systemen von Kohlenwasserstoffen verschiedenen Typs, Chemie Ingenieur Technik 15 (1950) 322-326. doi:10.1002/cite.330221503

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 368.58 | 0.0880 | 0.1680 |
| 366.67 | 0.1440 | 0.2540 |
| 366.50 | 0.1520 | 0.2680 |
| 364.75 | 0.2030 | 0.3420 |
| 362.97 | 0.2770 | 0.4270 |
| 362.25 | 0.2990 | 0.4550 |
| 361.83 | 0.3180 | 0.4740 |
| 361.03 | 0.3530 | 0.5120 |
| 360.05 | 0.4030 | 0.5540 |
| 358.88 | 0.4570 | 0.6040 |
| 357.90 | 0.5240 | 0.6570 |
| 357.07 | 0.5760 | 0.6980 |
| 356.61 | 0.6080 | 0.7190 |
| 355.44 | 0.6980 | 0.7790 |
| 354.75 | 0.7710 | 0.8300 |
| 353.90 | 0.8310 | 0.8700 |
| 353.40 | 0.9350 | 0.9470 |

Sieg, L., Flüssigkeit-Dampf-Gleichgewichte in binären Systemen von Kohlenwasserstoffen verschiedenen Typs: Flüssigkeit-Dampf-Gleichgewichte in binären Systemen von Kohlenwasserstoffen verschiedenen Typs, Chemie Ingenieur Technik 15 (1950) 322-326. doi:10.1002/cite.330221503

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 368.73 | 0.0770 | 0.1520 |
| 366.86 | 0.1340 | 0.2490 |
| 364.75 | 0.2020 | 0.3460 |
| 364.11 | 0.2300 | 0.3820 |
| 359.82 | 0.4090 | 0.5660 |
| 357.86 | 0.5190 | 0.6560 |
| 356.84 | 0.5860 | 0.7060 |
| 355.85 | 0.6590 | 0.7560 |
| 354.97 | 0.7240 | 0.8000 |
| 353.90 | 0.8300 | 0.8700 |
| 353.60 | 0.8940 | 0.9150 |
| 353.42 | 0.9340 | 0.9460 |
| 353.30 | 0.9850 | 0.9860 |

Michishita, T. - Arai, Y. - Saito, S., Vapor-liquid equilibriums of hydrocarbons at atmospheric pressure, Kagaku Kogaku 1 (1971) 111-0. doi:10.1252/kakoronbunshu1953.35.111

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 370.55 | 0.0230 | 0.0480 |
| 367.15 | 0.1160 | 0.2170 |
| 366.05 | 0.1510 | 0.2690 |
| 364.85 | 0.1920 | 0.3250 |
| 363.45 | 0.2440 | 0.3900 |
| 361.45 | 0.3230 | 0.4830 |
| 361.25 | 0.3320 | 0.4870 |
| 361.15 | 0.3340 | 0.4940 |
| 360.95 | 0.3420 | 0.5020 |

| | | |
|---|---|---|
| 359.75 | 0.4060 | 0.5610 |
| 358.85 | 0.4480 | 0.5990 |
| 357.25 | 0.5490 | 0.6790 |
| 356.35 | 0.6100 | 0.7230 |
| 355.55 | 0.6750 | 0.7680 |
| 355.25 | 0.6990 | 0.7820 |
| 354.95 | 0.7290 | 0.8020 |
| 354.75 | 0.7450 | 0.8130 |
| 354.45 | 0.7680 | 0.8270 |
| 354.05 | 0.8250 | 0.8640 |
| 353.75 | 0.8810 | 0.9010 |
| 353.55 | 0.9030 | 0.9220 |
| 353.35 | 0.9400 | 0.9490 |

Kao, Chien-Ping Chai - Miller, Ralph N. - Sturgis, James F., Double Azeotropy in Binary Mixtures 1,1,1,2,3,4,4,5,5,5-Decafluoropentane + Tetrahydrofuran, Journal of Chemical & Engineering Data 2 (2001) 229-233. doi:10.1021/je000212b

**P / bar = 3.025**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 410.34 | 0.0956 | 0.1593 |
| 407.14 | 0.1927 | 0.2929 |
| 404.07 | 0.3052 | 0.4208 |
| 401.58 | 0.4008 | 0.5249 |
| 398.74 | 0.5503 | 0.6467 |
| 397.22 | 0.6459 | 0.7304 |
| 396.68 | 0.6735 | 0.7542 |
| 395.26 | 0.7740 | 0.8309 |
| 394.38 | 0.8569 | 0.8858 |
| 393.73 | 0.9656 | 0.9706 |

Kao, Chien-Ping Chai - Miller, Ralph N. - Sturgis, James F., Double Azeotropy in Binary Mixtures 1,1,1,2,3,4,4,5,5,5-Decafluoropentane + Tetrahydrofuran, Journal of Chemical & Engineering Data 2 (2001) 229-233. doi:10.1021/je000212b

**P / bar = 8.106**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 461.49 | 0.0030 | 0.0042 |
| 459.56 | 0.0748 | 0.1028 |
| 458.10 | 0.1248 | 0.1690 |
| 456.09 | 0.1988 | 0.2636 |
| 453.84 | 0.2751 | 0.3547 |
| 451.14 | 0.3744 | 0.4651 |
| 449.20 | 0.4510 | 0.5436 |
| 446.75 | 0.5513 | 0.6383 |
| 444.70 | 0.6491 | 0.7212 |
| 442.17 | 0.7795 | 0.8204 |
| 440.99 | 0.8704 | 0.8875 |

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**Enthalpy of mixing**

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Vilcu, R. - Stanciu, F., Excess thermodynamic functions from calorimetric data, Rev. Roum. Chim. 2 (1966) 175-182.

**T / K = 288.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 219.81 | 0.0811 |
| 385.39 | 0.1536 |
| 568.19 | 0.2188 |
| 709.12 | 0.2776 |
| 834.55 | 0.3309 |
| 915.28 | 0.3793 |
| 970.50 | 0.4234 |
| 1008.4 | 0.4636 |
| 1005.0 | 0.5005 |
| 979.38 | 0.7041 |
| 912.97 | 0.7339 |
| 831.75 | 0.7645 |
| 741.15 | 0.7960 |
| 602.90 | 0.8282 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 293.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 265.43 | 0.0990 |
| 494.57 | 0.1906 |
| 696.83 | 0.2756 |
| 848.66 | 0.3547 |
| 913.60 | 0.4284 |
| 981.31 | 0.4973 |
| 996.37 | 0.5619 |
| 996.93 | 0.6225 |
| 954.01 | 0.6795 |
| 878.41 | 0.7332 |
| 776.91 | 0.7839 |
| 654.81 | 0.8318 |
| 500.71 | 0.8772 |
| 323.53 | 0.9203 |
| 123.03 | 0.9611 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K =** **298.15**

**P / bar =** **1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 233.01 | 0.0990 |
| 410.01 | 0.1906 |
| 596.14 | 0.2756 |
| 760.89 | 0.3547 |
| 864.75 | 0.4284 |
| 911.31 | 0.4973 |
| 957.34 | 0.5619 |
| 958.92 | 0.6225 |
| 925.41 | 0.6795 |
| 859.45 | 0.7332 |
| 771.27 | 0.7839 |
| 635.37 | 0.8318 |
| 491.73 | 0.8772 |
| 313.03 | 0.9203 |
| 126.18 | 0.9611 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K =** **303.15**

**P / bar =** **1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 204.79 | 0.0990 |
| 414.18 | 0.1906 |
| 574.10 | 0.2756 |
| 709.49 | 0.3547 |
| 812.70 | 0.4284 |
| 873.10 | 0.4973 |
| 894.88 | 0.5619 |
| 881.90 | 0.6225 |
| 830.61 | 0.6795 |
| 766.57 | 0.7332 |
| 703.39 | 0.7839 |
| 585.05 | 0.8318 |
| 445.40 | 0.8772 |
| 300.37 | 0.9203 |
| 130.17 | 0.9611 |

Hammerl, I. - Raetzsch, M.T., Enthalpies of mixing of normal paraffins with aromatics, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg 3 (1973) 175-178.

**T / K =** **313.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 228.00 | 0.1000 |
| 445.00 | 0.2000 |
| 632.00 | 0.3000 |
| 773.00 | 0.4000 |
| 856.00 | 0.5000 |
| 866.00 | 0.6000 |
| 794.00 | 0.7000 |
| 630.00 | 0.8000 |
| 368.00 | 0.9000 |

Palmer, David A. - Smith, Buford D., Thermodynamic excess property measurements for acetonitrile-benzene-n-heptane system at 45°C, Journal of Chemical & Engineering Data 1 (1972) 71-76. doi:10.1021/je60052a037

**T / K =** **318.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 201.39 | 0.0779 |
| 364.67 | 0.1446 |
| 491.11 | 0.2022 |
| 642.26 | 0.2828 |
| 741.90 | 0.3487 |
| 806.80 | 0.4034 |
| 869.18 | 0.4819 |
| 892.63 | 0.5646 |
| 888.02 | 0.5991 |
| 874.62 | 0.6226 |
| 878.81 | 0.6245 |
| 828.57 | 0.6875 |
| 742.74 | 0.7557 |
| 608.76 | 0.8250 |
| 428.31 | 0.8919 |
| 215.20 | 0.9519 |

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**Heat capacity of mixing**

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Tanaka, Reiji, Excess heat capacities for mixture of benzene with n-heptane at 293.15, 298.15, and 303.15 K, Journal of Chemical & Engineering Data 2 (1987) 176-177. doi:10.1021/je00048a014

**T / K =** **293.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -1.008 | 0.0919 |

| | |
|---|---|
| -1.992 | 0.1968 |
| -2.721 | 0.2947 |
| -3.220 | 0.3855 |
| -3.543 | 0.4861 |
| -3.633 | 0.5840 |
| -3.443 | 0.6908 |
| -3.021 | 0.7773 |
| -2.078 | 0.8814 |

Karbalai Ghassemi, M.H. - Grolier, J.P.E., Excess heat capacity. Cyclohexane-n-hexane system, Int. Data Ser. Sel. Data Mixtures Ser. A 2 (1976) 95-96.

**T / K = 298.20**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.5830 | 0.0487 |
| -1.857 | 0.1928 |
| -2.530 | 0.2880 |
| -3.030 | 0.3886 |
| -3.065 | 0.4007 |
| -3.315 | 0.4929 |
| -3.456 | 0.5841 |
| -3.407 | 0.6310 |
| -3.336 | 0.6558 |
| -3.130 | 0.7294 |
| -2.792 | 0.7924 |
| -2.751 | 0.7940 |
| -2.260 | 0.8591 |
| -1.900 | 0.8873 |
| -1.637 | 0.9123 |
| -1.284 | 0.9317 |

Tanaka, Reiji, Excess heat capacities for mixture of benzene with n-heptane at 293.15, 298.15, and 303.15 K, Journal of Chemical & Engineering Data 2 (1987) 176-177. doi:10.1021/je00048a014

**T / K = 303.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.9010 | 0.0880 |
| -1.864 | 0.1972 |
| -2.547 | 0.2953 |
| -3.012 | 0.3857 |
| -3.340 | 0.4905 |
| -3.428 | 0.5845 |
| -3.232 | 0.6968 |
| -2.846 | 0.7784 |
| -1.971 | 0.8801 |

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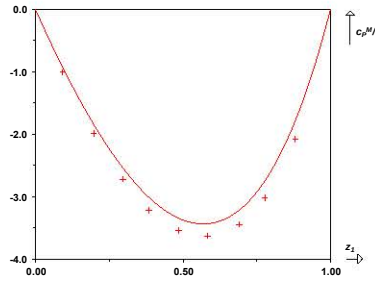
**Critical point**

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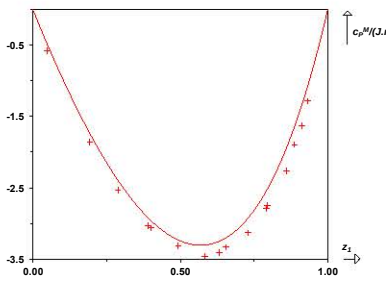
Kay, W.B. - Hissong, D., The critical properties of hydrocarbons. I. Simple mixtures, Proc. Am. Pet. Inst. Refin. Dep. (1967) 653-722.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 540.75 | 28.94 | 0.1000 |
| 541.45 | 30.44 | 0.2000 |
| 542.45 | 32.08 | 0.3000 |
| 543.75 | 33.78 | 0.4000 |
| 545.45 | 35.66 | 0.5000 |
| 547.45 | 37.76 | 0.6000 |
| 550.05 | 40.21 | 0.7000 |
| 553.15 | 42.92 | 0.8000 |
| 557.25 | 45.85 | 0.9000 |

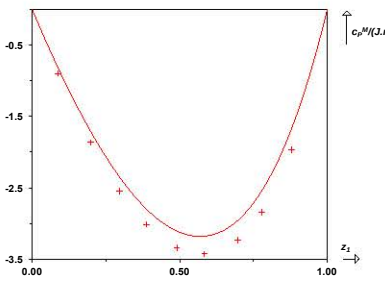
T/K = 293.15 - P/bar = 1.0132



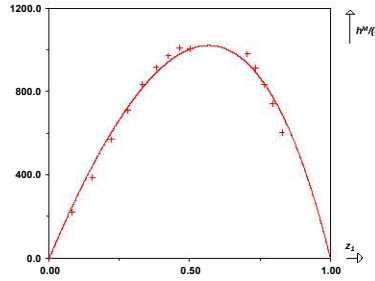

T/K = 298.20 - P/bar = 1.0132



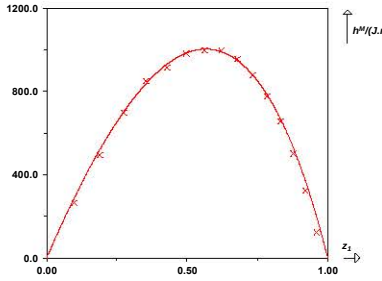

T/K = 303.15 - P/bar = 1.0132



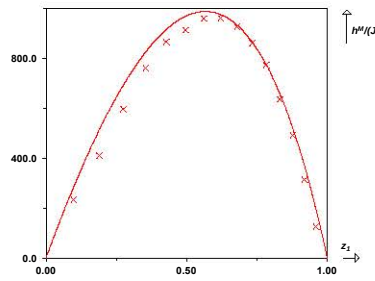

T/K = 288.15 - P/bar = 1.0132



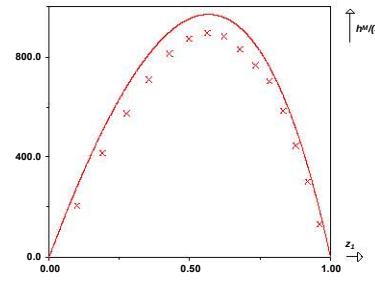

T/K = 293.15 - P/bar = 1.0100



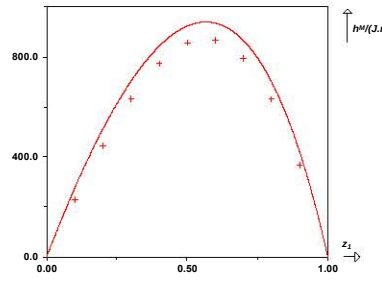

T/K = 298.15 - P/bar = 1.0100



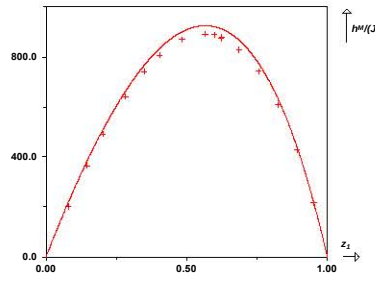

T/K = 303.15 - P/bar = 1.0100



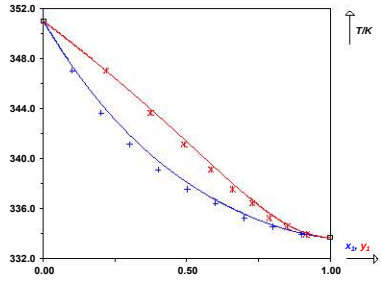

T/K = 313.15 - P/bar = 1.0132



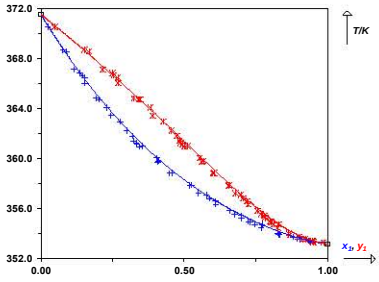

T/K = 318.15 - P/bar = 1.0132



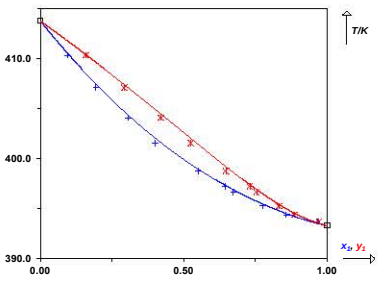

P/bar = 0.53329



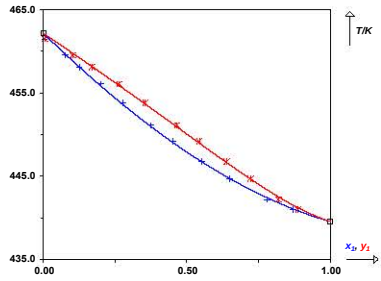

P/bar = 1.01330



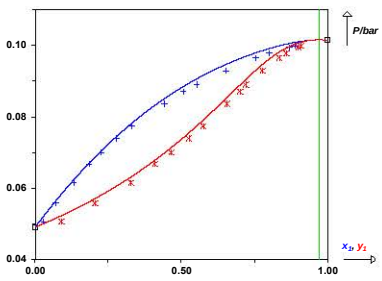

P/bar = 3.02500



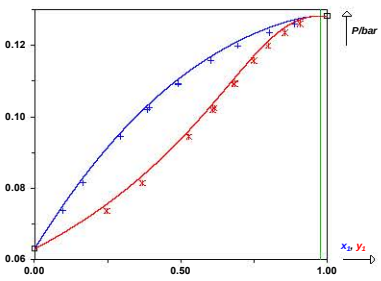

P/bar = 8.10600



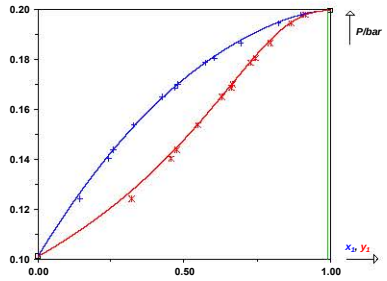

T/K = 293.15



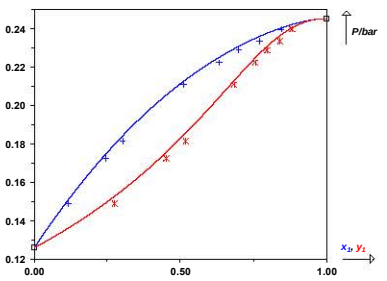

T/K = 298.15



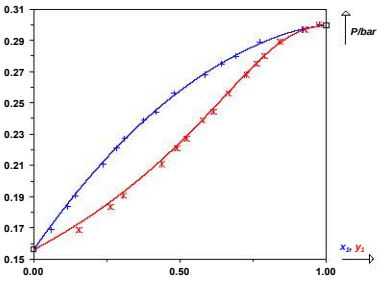
T/K = 308.19



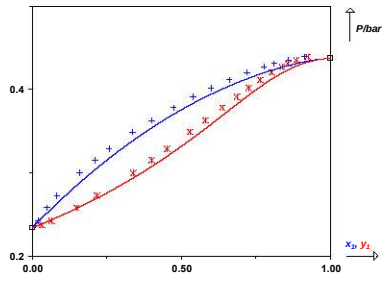

T/K = 313.15



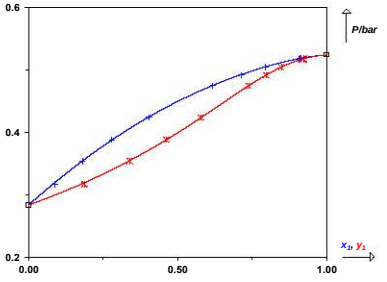

T/K = 318.15



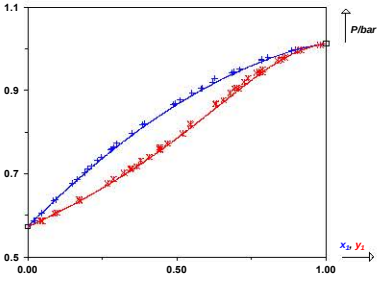

T/K = 328.15



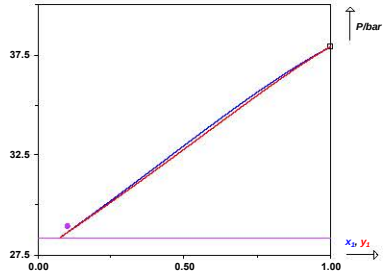

T/K = 333.15



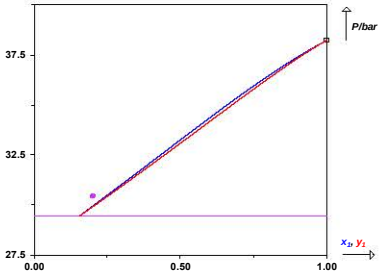

T/K = 353.15



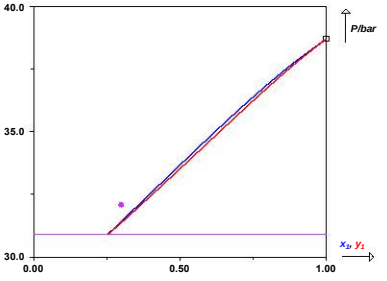

T/K = 540.75



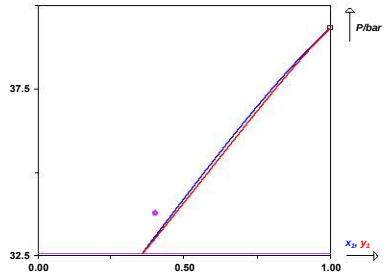

T/K = 541.45



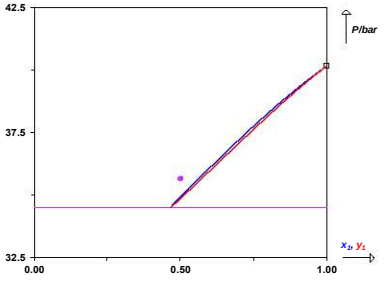

T/K = 542.45



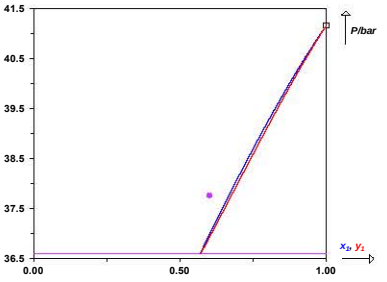

T/K = 543.75



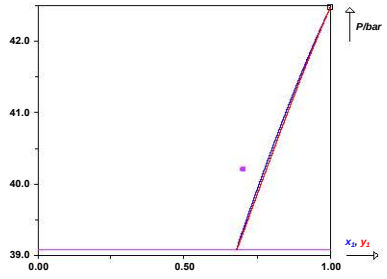

T/K = 545.45



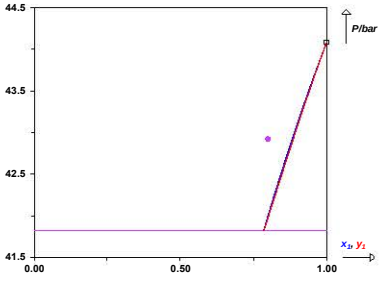

T/K = 547.45



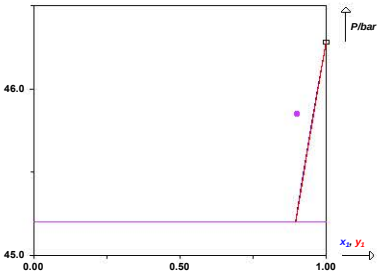

T/K = 550.05




T/K = 553.15




T/K = 557.25



## BENZENE (1) + CYCLOHEXANE (2)

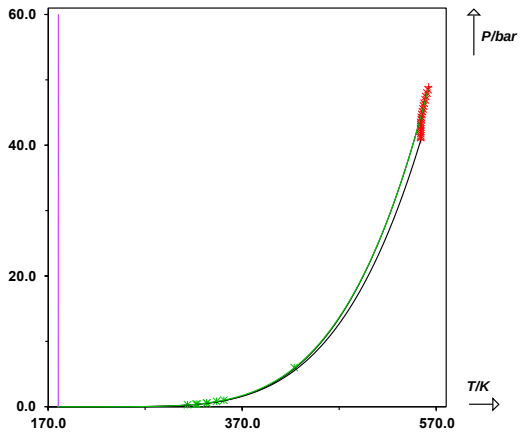
| | | |
|---|---|---|
| **CAS** | 71-43-2 | 110-82-7 |
| **InChiKey** | UHOVQNZJYSORNB-UHFFFAOYSA-N | XDTMQSROBMDMFD-UHFFFAOYSA-N |
| **$T_c$ / K** | 562.05 | 553.80 |
| **$P_c$ / bar** | 48.95 | 40.80 |
| **ω** | 0.210 | 0.208 |

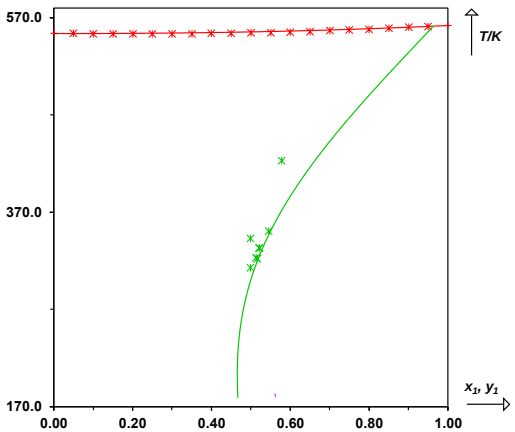
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 81.5
B/MPa = 214

*Deviations*
MAPE on x = 15 %
MAPE on y = 15 %
MAPE on $x_c$ = 230 %
MAPE on $P_c$ = 91 %
MAPE on $x_{az}$ = 7.6 %
MAPE on $P_{az}$ = 0.61 %
MAPE on $h^M$ = 6.6 %
MAPE on $c_P^M$ = 65 %



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**Isothermal phase equilibrium data**

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Tasić, Aleksandar - Djordjević, Bojan - Grozdanić, Dušan - Afgan, Naim - Malić, Dragomir, Vapour—liquid equilibria of the systems acetone—benzene, benzene—cyclohexane and acetone—cyclohexane at 25°C, Chemical Engineering Science 2 (1978) 189-197. doi:10.1016/0009-2509(78)85053-2

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1361 | 0.1035 | 0.1375 | |
| 0.1393 | 0.1750 | 0.2170 | |
| 0.1423 | 0.2760 | 0.3130 | |
| 0.1441 | 0.3770 | 0.4015 | |
| 0.1446 | 0.4330 | 0.4460 | |
| 0.1449 | 0.5090 | 0.5050 | |
| 0.1444 | 0.5830 | 0.5620 | |
| 0.1425 | 0.6940 | 0.6505 | |
| 0.1393 | 0.7945 | 0.7410 | |
| 0.1341 | 0.9005 | 0.8565 | |
| 0.1309 | 0.9500 | 0.9220 | |

Mentzer, R.A. - Greenkorn, R.A. - Chao, K.C., Bubble pressures and vapor-liquid equilibria for four binary hydrocarbon mixtures, The Journal of Chemical Thermodynamics 9 (1982) 817-830. doi:10.1016/0021-9614(82)90155-0

**T / K = 313.10**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2592 | 0.1193 | 0.1589 | |
| 0.2683 | 0.2498 | 0.2929 | |
| 0.2707 | 0.2963 | 0.3348 | |
| 0.2722 | 0.3369 | 0.3697 | |
| 0.2723 | 0.3465 | 0.3777 | |
| 0.2733 | 0.3849 | 0.4093 | |
| 0.2743 | 0.4366 | 0.4507 | |
| 0.2743 | 0.4403 | 0.4537 | |
| 0.2747 | 0.4968 | 0.4979 | |
| 0.2747 | 0.4985 | 0.4985 | AZEO |
| 0.2746 | 0.5304 | 0.5239 | |
| 0.2744 | 0.5563 | 0.5441 | |
| 0.2742 | 0.5775 | 0.5607 | |
| 0.2733 | 0.6228 | 0.5964 | |
| 0.2731 | 0.6284 | 0.6009 | |
| 0.2706 | 0.7040 | 0.6634 | |
| 0.2652 | 0.8006 | 0.7508 | |
| 0.2564 | 0.9013 | 0.8604 | |

Kurihara, Kiyofumi - Uchiyama, Masanori - Kojima, Kazuo, Isothermal Vapor−Liquid Equilibria for Benzene + Cyclohexane + 1-Propanol and for Three Constituent Binary Systems, Journal of Chemical & Engineering Data 1 (1997) 149-154. doi:10.1021/je9602475

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.3688 | 0.0340 | 0.0480 | |
| 0.3748 | 0.0740 | 0.1010 | |
| 0.3794 | 0.1070 | 0.1420 | |
| 0.3831 | 0.1380 | 0.1770 | |
| 0.3842 | 0.1470 | 0.1870 | |
| 0.3905 | 0.2010 | 0.2450 | |
| 0.3936 | 0.2390 | 0.2820 | |
| 0.3957 | 0.2740 | 0.3140 | |
| 0.3967 | 0.2870 | 0.3260 | |
| 0.3999 | 0.3350 | 0.3660 | |
| 0.4009 | 0.3650 | 0.3930 | |
| 0.4021 | 0.4040 | 0.4260 | |
| 0.4031 | 0.4480 | 0.4630 | |
| 0.4032 | 0.4770 | 0.4860 | |
| 0.4036 | 0.5130 | 0.5130 | AZEO |
| 0.4033 | 0.5310 | 0.5270 | |
| 0.4031 | 0.5600 | 0.5500 | |
| 0.4027 | 0.5910 | 0.5740 | |
| 0.4007 | 0.6570 | 0.6260 | |
| 0.3995 | 0.6900 | 0.6530 | |
| 0.3955 | 0.7550 | 0.7140 | |
| 0.3922 | 0.7950 | 0.7510 | |
| 0.3902 | 0.8120 | 0.7680 | |
| 0.3868 | 0.8440 | 0.8010 | |
| 0.3805 | 0.8970 | 0.8580 | |
| 0.3781 | 0.9140 | 0.8790 | |
| 0.3747 | 0.9340 | 0.9040 | |

Boublík, T., An estimate of limiting values of relative volatility with help of the theorem of corresponding states. II. Binary systems of tetrachloromethane, benzene, and cyclohexane, Collection of Czechoslovak Chemical Communications 7 (1963) 1771-1779. doi:10.1135/cccc19631771

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.5342 | 0.0672 | 0.0912 | |
| 0.5593 | 0.2261 | 0.2670 | |
| 0.5673 | 0.3201 | 0.3526 | |
| 0.5751 | 0.4320 | 0.4480 | |
| 0.5762 | 0.5203 | 0.5203 | AZEO |
| 0.5742 | 0.6029 | 0.5895 | |
| 0.5698 | 0.7095 | 0.6770 | |
| 0.5608 | 0.7952 | 0.7563 | |
| 0.5492 | 0.8752 | 0.8386 | |

| | | | |
|---|---|---|---|
| 0.5462 | 0.8932 | 0.8600 | |

Kurihara, Kiyofumi - Uchiyama, Masanori - Kojima, Kazuo, Isothermal Vapor−Liquid Equilibria for Benzene + Cyclohexane + 1-Propanol and for Three Constituent Binary Systems, Journal of Chemical & Engineering Data 1 (1997) 149-154. doi:10.1021/je9602475

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.5356 | 0.0700 | 0.0950 | |
| 0.5358 | 0.0760 | 0.1020 | |
| 0.5410 | 0.1020 | 0.1340 | |
| 0.5448 | 0.1260 | 0.1640 | |
| 0.5548 | 0.1780 | 0.2210 | |
| 0.5561 | 0.2020 | 0.2430 | |
| 0.5619 | 0.2340 | 0.2750 | |
| 0.5628 | 0.2700 | 0.3090 | |
| 0.5693 | 0.3360 | 0.3670 | |
| 0.5702 | 0.3510 | 0.3800 | |
| 0.5703 | 0.3740 | 0.4010 | |
| 0.5744 | 0.4400 | 0.4560 | |
| 0.5746 | 0.4500 | 0.4650 | |
| 0.5749 | 0.4610 | 0.4730 | |
| 0.5752 | 0.4710 | 0.4810 | |
| 0.5756 | 0.4780 | 0.4870 | |
| 0.5759 | 0.4880 | 0.4950 | |
| 0.5760 | 0.4990 | 0.5030 | |
| 0.5761 | 0.5090 | 0.5110 | |
| 0.5762 | 0.5220 | 0.5220 | AZEO |
| 0.5761 | 0.5330 | 0.5310 | |
| 0.5760 | 0.5380 | 0.5350 | |
| 0.5759 | 0.5470 | 0.5420 | |
| 0.5757 | 0.5560 | 0.5490 | |
| 0.5743 | 0.6020 | 0.5870 | |
| 0.5713 | 0.6730 | 0.6440 | |
| 0.5689 | 0.7090 | 0.6770 | |
| 0.5642 | 0.7640 | 0.7270 | |
| 0.5613 | 0.7880 | 0.7490 | |
| 0.5569 | 0.8280 | 0.7900 | |
| 0.5496 | 0.8700 | 0.8360 | |
| 0.5443 | 0.8950 | 0.8650 | |
| 0.5430 | 0.9030 | 0.8730 | |
| 0.5410 | 0.9170 | 0.8890 | |
| 0.5358 | 0.9440 | 0.9220 | |

Scatchard, George. - Wood, S. E. - Mochel, J. M., Vapor–Liquid Equilibrium. III. Benzene–Cyclohexane Mixtures., The Journal of Physical Chemistry 1 (1939) 119-130. doi:10.1021/j150388a009

**T / K = 343.13**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.7567 | 0.1186 | 0.1486 | |
| 0.7798 | 0.2409 | 0.2805 | |
| 0.7948 | 0.3759 | 0.3982 | |
| 0.8003 | 0.4945 | 0.4975 | |
| 0.8003 | 0.4990 | 0.4990 | AZEO |
| 0.7990 | 0.6180 | 0.6027 | |
| 0.7912 | 0.7248 | 0.6962 | |
| 0.7703 | 0.8659 | 0.8311 | |

Dong, Jilian - Feng, Chuanzhuang - Li, Yonghong, Isothermal Vapor−Liquid Equilibrium for Methanol and 2,3-Dimethyl-1-butene at 343.06 K, 353.27 K, 363.19 K, and 372.90 K, Journal of Chemical & Engineering Data 5 (2011) 2386-2392. doi:10.1021/je101304x

**T / K = 403.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.728 | 0.1107 | 0.1301 |
| 3.776 | 0.1676 | 0.1943 |
| 3.812 | 0.2184 | 0.2426 |
| 3.851 | 0.2715 | 0.3005 |
| 3.890 | 0.3402 | 0.3645 |
| 3.919 | 0.3948 | 0.4213 |
| 3.935 | 0.4408 | 0.4560 |
| 3.950 | 0.4986 | 0.5083 |
| 3.961 | 0.5552 | 0.5619 |
| 3.965 | 0.6048 | 0.6017 |
| 3.945 | 0.7382 | 0.7276 |
| 3.888 | 0.8537 | 0.8441 |

Wiśniewska, Barbara - Gregorowicz, Jacek - Malanowski, Stanisław, Development of a vapour-liquid equilibrium apparatus to work at pressures up to 3 MPa, Fluid Phase Equilibria (1993) 173-186. doi:10.1016/0378-3812(93)87174-Y

**T / K = 413.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.620 | 0.0996 | 0.1164 |
| 4.741 | 0.2226 | 0.2503 |
| 4.802 | 0.3086 | 0.3343 |
| 4.849 | 0.3761 | 0.3981 |
| 4.884 | 0.4506 | 0.4683 |
| 4.909 | 0.5307 | 0.5407 |
| 4.920 | 0.6335 | 0.6295 |
| 4.906 | 0.7308 | 0.7169 |
| 4.817 | 0.8827 | 0.8685 |

Wiśniewska, Barbara - Gregorowicz, Jacek - Malanowski, Stanisław, Development of a vapour-liquid equilibrium apparatus to work at pressures up to

3 MPa, Fluid Phase Equilibria (1993) 173-186. doi:10.1016/0378-3812(93)87174-Y

**T / K = 423.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.673 | 0.0984 | 0.1156 | |
| 5.814 | 0.2198 | 0.2461 | |
| 5.886 | 0.3063 | 0.3316 | |
| 5.947 | 0.3727 | 0.3948 | |
| 5.994 | 0.4521 | 0.4685 | |
| 6.023 | 0.5326 | 0.5420 | |
| 6.034 | 0.5769 | 0.5775 | |
| 6.034 | 0.5778 | 0.5778 | AZEO |
| 6.035 | 0.5920 | 0.5862 | |
| 6.043 | 0.6381 | 0.6304 | |
| 6.029 | 0.7256 | 0.7201 | |
| 5.942 | 0.8785 | 0.8698 | |

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**Isobaric phase equilibrium data**

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Lafuente, C. - Pardo, J. - Santate, J. - Royo, F. - Urieta, J., Use of a Fischer-Labodest apparatus to study the liquid-vapor equilibrium of the benzene-cyclohexane system at different pressures, Rev. Acad. Cienc. Exact. Fis. Quim. Nat. Zaragoza (1992) 183-190.

**P / bar = 0.4000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 324.35 | 0.0979 | 0.1300 |
| 323.95 | 0.1487 | 0.1920 |
| 323.55 | 0.2014 | 0.2464 |
| 323.25 | 0.2578 | 0.3039 |
| 322.95 | 0.3032 | 0.3426 |
| 322.85 | 0.3382 | 0.3713 |
| 322.75 | 0.3614 | 0.3919 |
| 322.65 | 0.3999 | 0.4235 |
| 322.45 | 0.4380 | 0.4542 |
| 322.45 | 0.5777 | 0.5668 |
| 322.55 | 0.6410 | 0.6169 |
| 322.75 | 0.6953 | 0.6618 |
| 323.05 | 0.7675 | 0.7244 |
| 323.45 | 0.8219 | 0.7797 |
| 323.85 | 0.8802 | 0.8410 |

Sieg, L., Flüssigkeit-Dampf-Gleichgewichte in binären Systemen von Kohlenwasserstoffen verschiedenen Typs: Flüssigkeit-Dampf-Gleichgewichte in binären Systemen von Kohlenwasserstoffen verschiedenen Typs, Chemie Ingenieur Technik 15 (1950) 322-326. doi:10.1002/cite.330221503

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 353.18 | 0.0680 | 0.0910 |
| 352.90 | 0.1000 | 0.1300 |
| 352.10 | 0.1880 | 0.2240 |
| 352.05 | 0.2050 | 0.2400 |
| 351.50 | 0.2830 | 0.3180 |
| 351.51 | 0.2880 | 0.3220 |
| 351.05 | 0.3850 | 0.4070 |
| 351.00 | 0.3880 | 0.4120 |
| 350.83 | 0.5890 | 0.5830 |
| 350.91 | 0.6800 | 0.6590 |
| 350.97 | 0.6980 | 0.6700 |
| 351.40 | 0.7900 | 0.7580 |
| 351.50 | 0.7980 | 0.7660 |
| 352.10 | 0.8940 | 0.8630 |
| 352.17 | 0.8990 | 0.8720 |

Ridgway, Kenneth - Butler, Paul Alexander, Physical properties of the ternary system benzene-cyclohexane-hexane, Journal of Chemical & Engineering Data 4 (1967) 509-515. doi:10.1021/je60035a012

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 352.95 | 0.0770 | 0.0960 |
| 352.65 | 0.0960 | 0.1180 |
| 352.40 | 0.1180 | 0.1450 |
| 352.20 | 0.1450 | 0.1760 |
| 352.00 | 0.1760 | 0.2080 |
| 351.85 | 0.2080 | 0.2430 |
| 351.65 | 0.2450 | 0.2800 |
| 351.40 | 0.2800 | 0.3140 |
| 351.25 | 0.3140 | 0.3460 |
| 351.10 | 0.3460 | 0.3750 |
| 351.00 | 0.3750 | 0.4020 |
| 350.90 | 0.4020 | 0.4260 |
| 350.80 | 0.6280 | 0.6120 |
| 350.85 | 0.6450 | 0.6280 |
| 350.90 | 0.6630 | 0.6450 |
| 350.95 | 0.6850 | 0.6630 |
| 351.05 | 0.7120 | 0.6850 |
| 351.15 | 0.7420 | 0.7120 |
| 351.20 | 0.7750 | 0.7440 |
| 351.45 | 0.8060 | 0.7750 |
| 351.70 | 0.8360 | 0.8060 |
| 351.95 | 0.8650 | 0.8360 |
| 352.20 | 0.8920 | 0.8650 |
| 352.40 | 0.9160 | 0.8920 |

Rao, V. N. Kumarkrishna - Swami, D. R. - Rao, M. Narasinga, Vapor-liquid equilibria of Benzene–n-hexane and benzene-cyclohexane systems, AIChE Journal 2 (1957) 191-197. doi:10.1002/aic.690030213

**P / bar = 11.44**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 462.35 | 0.0241 | 0.0260 |
| 461.25 | 0.1550 | 0.1700 |
| 460.45 | 0.2385 | 0.2613 |
| 459.75 | 0.3390 | 0.3618 |
| 458.95 | 0.8855 | 0.8777 |
| 459.35 | 0.9551 | 0.9497 |

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**Enthalpy of mixing**

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Elliott, Keith - Wormald, Christopher J., A precision differential flow calorimeter the excess enthalpy of benzene + cyclohexane between 280.15 K and 393.15 K, The Journal of Chemical Thermodynamics 9 (1976) 881-893. doi:10.1016/0021-9614(76)90166-X

**T / K = 280.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 422.20 | 0.1483 |
| 524.70 | 0.1963 |
| 687.40 | 0.2880 |
| 791.10 | 0.3776 |
| 837.70 | 0.4478 |
| 849.40 | 0.5482 |
| 794.10 | 0.6475 |
| 726.50 | 0.7095 |
| 600.10 | 0.7853 |
| 509.60 | 0.8296 |
| 438.60 | 0.8597 |
| 343.60 | 0.8954 |

Yan, Wei-Dong - Lin, Rui-Sen - Yen, Wen-Hsing, Excess enthalpies of seven binary liquid systems, Thermochimica Acta (1990) 171-184. doi:10.1016/0040-6031(90)80143-M

**T / K = 293.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 43.44 | 0.0126 |
| 116.39 | 0.0352 |
| 218.67 | 0.0686 |
| 292.40 | 0.0953 |
| 389.06 | 0.1347 |
| 479.73 | 0.1791 |
| 557.84 | 0.2201 |
| 619.23 | 0.2577 |
| 699.67 | 0.2921 |
| 708.52 | 0.3221 |
| 739.54 | 0.3508 |
| 762.99 | 0.3747 |
| 793.67 | 0.4168 |
| 809.07 | 0.4383 |
| 821.40 | 0.4521 |
| 823.19 | 0.4545 |
| 828.21 | 0.4977 |
| 828.53 | 0.5497 |
| 801.48 | 0.6206 |
| 794.01 | 0.6313 |
| 790.35 | 0.6365 |
| 779.15 | 0.6560 |
| 749.08 | 0.6841 |
| 720.29 | 0.7064 |
| 689.44 | 0.7270 |
| 646.96 | 0.7531 |
| 596.48 | 0.7824 |
| 538.25 | 0.8116 |
| 466.55 | 0.8438 |
| 374.12 | 0.8783 |
| 322.09 | 0.8983 |
| 272.00 | 0.9165 |
| 203.66 | 0.9388 |
| 94.55 | 0.9722 |
| 31.67 | 0.9908 |

Didaoui-Nemouchi, S. - Ait-Kaci, A. - Rogalski, M., Enthalpies of mixing of binary and ternary mixtures containing diisopropylether, benzene and cyclohexane at 303.15 K, Journal of Thermal Analysis and Calorimetry 1 (2005) 85-88. doi:10.1007/s10973-004-0566-5

**T / K = 303.15**

**P / bar = 1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 313.90 | 0.8880 |
| 511.40 | 0.8010 |
| 677.80 | 0.7010 |
| 778.50 | 0.5890 |
| 777.00 | 0.5520 |
| 772.10 | 0.4790 |
| 761.80 | 0.4560 |
| 736.10 | 0.4190 |
| 698.90 | 0.3690 |
| 684.70 | 0.3570 |

| | |
|---|---|
| 643.00 | 0.3240 |
| 491.10 | 0.2140 |
| 377.00 | 0.1580 |
| 347.10 | 0.1400 |
| 303.00 | 0.1230 |
| 266.80 | 0.1000 |

van Ness, H.C. - Abbott, M.M., Excess enthalpy. Benzene-cyclohexane system, Int. Data Ser. Sel. Data Mixtures Ser. A 3 (1974) 160-161.

**T / K = 323.15**

**P / bar = 2.100**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 69.70 | 0.0253 |
| 204.90 | 0.0783 |
| 333.80 | 0.1355 |
| 472.80 | 0.2096 |
| 573.50 | 0.2771 |
| 645.60 | 0.3410 |
| 697.20 | 0.4081 |
| 719.60 | 0.4592 |
| 713.40 | 0.5788 |
| 696.30 | 0.6141 |
| 672.40 | 0.6485 |
| 647.80 | 0.6765 |
| 596.50 | 0.7236 |
| 523.50 | 0.7758 |
| 437.20 | 0.8257 |
| 329.10 | 0.8778 |
| 197.70 | 0.9318 |
| 75.70 | 0.9752 |

Elliott, Keith - Wormald, Christopher J., A precision differential flow calorimeter the excess enthalpy of benzene + cyclohexane between 280.15 K and 393.15 K, The Journal of Chemical Thermodynamics 9 (1976) 881-893. doi:10.1016/0021-9614(76)90166-X

**T / K = 348.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 328.10 | 0.1493 |
| 411.40 | 0.1955 |
| 464.30 | 0.2336 |
| 536.90 | 0.2880 |
| 615.60 | 0.3781 |
| 651.60 | 0.4474 |
| 658.40 | 0.5483 |
| 614.00 | 0.6471 |
| 558.20 | 0.7096 |
| 461.50 | 0.7854 |
| 390.50 | 0.8301 |
| 337.60 | 0.8588 |
| 261.40 | 0.8943 |

Elliott, Keith - Wormald, Christopher J., A precision differential flow calorimeter the excess enthalpy of benzene + cyclohexane between 280.15 K and 393.15 K, The Journal of Chemical Thermodynamics 9 (1976) 881-893. doi:10.1016/0021-9614(76)90166-X

**T / K = 373.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 305.00 | 0.1493 |
| 373.20 | 0.1960 |
| 427.40 | 0.2333 |
| 492.20 | 0.2814 |
| 569.20 | 0.3773 |
| 600.20 | 0.4474 |
| 606.30 | 0.5489 |
| 570.10 | 0.6472 |
| 518.70 | 0.7098 |
| 426.00 | 0.7863 |
| 360.50 | 0.8300 |
| 309.60 | 0.8588 |
| 236.90 | 0.8967 |

Lohmann, Jürgen - Bölts, Rainer - Gmehling, Jürgen, Excess Enthalpy Data for Seven Binary Systems at Temperatures between 50 and 140 °C, Journal of Chemical & Engineering Data 2 (2001) 208-211. doi:10.1021/je000297g

**T / K = 413.15**

**P / bar = 14.10**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 111.80 | 0.0604 |
| 217.00 | 0.1196 |
| 342.20 | 0.2059 |
| 431.00 | 0.2895 |
| 493.00 | 0.3704 |
| 527.10 | 0.4490 |
| 538.30 | 0.5500 |
| 504.10 | 0.6470 |
| 449.10 | 0.7174 |
| 378.70 | 0.7857 |
| 288.20 | 0.8521 |
| 174.40 | 0.9167 |
| 92.60 | 0.9587 |

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**Heat capacity of mixing**

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Tanaka, Reiji, Determination of excess heat capacities of (benzene + tetrachloromethane and + cyclohexane) between 293.15 and 303.15 K by use of a Picker flow calorimeter, The Journal of Chemical Thermodynamics 3 (1982) 259-268. doi:10.1016/0021-9614(82)90016-7

**T / K =** **293.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -1.012 | 0.0955 |
| -1.796 | 0.1944 |
| -2.424 | 0.2972 |
| -2.795 | 0.3916 |
| -2.981 | 0.4980 |
| -2.936 | 0.5953 |
| -2.654 | 0.6966 |
| -2.120 | 0.7957 |
| -1.302 | 0.8931 |

Páramo, R. - Zouine, M. - Casanova, C., New Batch Cells Adapted To Measure Saturated Heat Capacities of Liquids, Journal of Chemical & Engineering Data 3 (2002) 441-448. doi:10.1021/je0155103

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -1.010 | 0.1044 |
| -1.840 | 0.1997 |
| -2.370 | 0.2934 |
| -2.720 | 0.3995 |
| -2.910 | 0.5004 |
| -2.820 | 0.5969 |
| -2.600 | 0.7034 |
| -2.090 | 0.8022 |
| -1.180 | 0.8979 |

D'arcy, Patrick J. - Hazlett, John D. - Kiyohara, Osamu - Benson, George C., Excess heat capacities of mixtures of benzene with cyclohexane at 298.15 K, Thermochimica Acta 2 (1977) 297-300. doi:10.1016/0040-6031(77)85030-2

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.9900 | 0.0981 |
| -1.061 | 0.1076 |
| -1.724 | 0.1965 |
| -1.770 | 0.1974 |
| -1.807 | 0.1999 |
| -2.301 | 0.2873 |
| -2.337 | 0.2883 |
| -2.717 | 0.3956 |
| -2.751 | 0.3966 |
| -2.906 | 0.5009 |
| -2.872 | 0.5041 |
| -2.885 | 0.5183 |
| -2.835 | 0.5954 |
| -2.857 | 0.5959 |
| -2.588 | 0.6960 |
| -2.504 | 0.7052 |
| -2.052 | 0.7953 |
| -2.032 | 0.7994 |
| -1.979 | 0.8017 |
| -1.283 | 0.8911 |
| -1.152 | 0.9020 |

Tanaka, Reiji, Determination of excess heat capacities of (benzene + tetrachloromethane and + cyclohexane) between 293.15 and 303.15 K by use of a Picker flow calorimeter, The Journal of Chemical Thermodynamics 3 (1982) 259-268. doi:10.1016/0021-9614(82)90016-7

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -1.084 | 0.1096 |
| -1.824 | 0.2029 |
| -2.410 | 0.3033 |
| -2.776 | 0.4023 |
| -2.930 | 0.5030 |
| -2.831 | 0.6200 |
| -2.568 | 0.7029 |
| -2.043 | 0.7988 |
| -1.335 | 0.8866 |
| -1.068 | 0.1079 |
| -1.842 | 0.2053 |
| -2.406 | 0.3023 |
| -2.764 | 0.3969 |
| -2.924 | 0.4968 |
| -2.872 | 0.6044 |
| -2.564 | 0.7060 |
| -2.047 | 0.7994 |
| -1.243 | 0.8955 |

Grolier, J.-P. E. - Wilhelm, Emmerich - Hamedi, M. H., Molar Heat Capacity and Isothermal Compressibility of Binary Liquid Mixtures: Carbon Tetrachloride +

Benzene, Carbon Tetrachloride + Cylohexane and Benzene + Cylohexane, Berichte der Bunsengesellschaft für physikalische Chemie 12 (1978) 1282-1290. doi:10.1002/bbpc.19780821204

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -1.215 | 0.1231 |
| -1.788 | 0.1994 |
| -2.419 | 0.3124 |
| -2.661 | 0.3768 |
| -2.807 | 0.4252 |
| -2.911 | 0.5035 |
| -2.769 | 0.6285 |
| -2.388 | 0.7356 |
| -1.686 | 0.8433 |
| -1.309 | 0.8848 |
| -1.099 | 0.9148 |

Tanaka, Reiji, Determination of excess heat capacities of (benzene + tetrachloromethane and + cyclohexane) between 293.15 and 303.15 K by use of a Picker flow calorimeter, The Journal of Chemical Thermodynamics 3 (1982) 259-268. doi:10.1016/0021-9614(82)90016-7

**T / K = 303.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -1.168 | 0.1208 |
| -1.813 | 0.2046 |
| -2.408 | 0.3093 |
| -2.728 | 0.3993 |
| -2.888 | 0.5073 |
| -2.820 | 0.6055 |
| -2.501 | 0.7090 |
| -1.965 | 0.8058 |
| -1.213 | 0.8966 |

Páramo, R. - Zouine, M. - Casanova, C., New Batch Cells Adapted To Measure Saturated Heat Capacities of Liquids, Journal of Chemical & Engineering Data 3 (2002) 441-448. doi:10.1021/je0155103

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.8800 | 0.1040 |
| -1.630 | 0.1995 |
| -2.300 | 0.2984 |
| -2.700 | 0.3968 |
| -2.840 | 0.4979 |
| -2.800 | 0.5982 |
| -2.430 | 0.7017 |
| -1.810 | 0.8063 |
| -1.150 | 0.8979 |

Páramo, R. - Zouine, M. - Casanova, C., New Batch Cells Adapted To Measure Saturated Heat Capacities of Liquids, Journal of Chemical & Engineering Data 3 (2002) 441-448. doi:10.1021/je0155103

**T / K = 318.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.8300 | 0.1040 |
| -1.570 | 0.1995 |
| -2.210 | 0.2984 |
| -2.570 | 0.3968 |
| -2.710 | 0.4979 |
| -2.660 | 0.5982 |
| -2.290 | 0.7017 |
| -1.690 | 0.8063 |
| -1.050 | 0.8979 |

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**Critical point**

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Hissong, D.W. - Kay, W.B., Critical properties of hydrocarbons. II. Correlational studies, Proc. Am. Pet. Inst. Refin. Dep. (1968) 397-463.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 553.81 | 41.18 | 0.0500 |
| 553.63 | 41.45 | 0.1000 |
| 553.52 | 41.76 | 0.1500 |
| 553.45 | 42.09 | 0.2000 |
| 553.41 | 42.46 | 0.2500 |
| 553.47 | 42.82 | 0.3000 |
| 553.62 | 43.18 | 0.3500 |
| 553.84 | 43.55 | 0.4000 |
| 554.10 | 43.93 | 0.4500 |
| 554.41 | 44.32 | 0.5000 |
| 554.78 | 44.71 | 0.5500 |
| 555.28 | 45.12 | 0.6000 |
| 555.88 | 45.53 | 0.6500 |
| 556.58 | 45.97 | 0.7000 |
| 557.34 | 46.43 | 0.7500 |
| 558.21 | 46.93 | 0.8000 |
| 559.13 | 47.44 | 0.8500 |
| 560.13 | 47.97 | 0.9000 |
| 561.21 | 48.53 | 0.9500 |

---

**Azeotropic point**

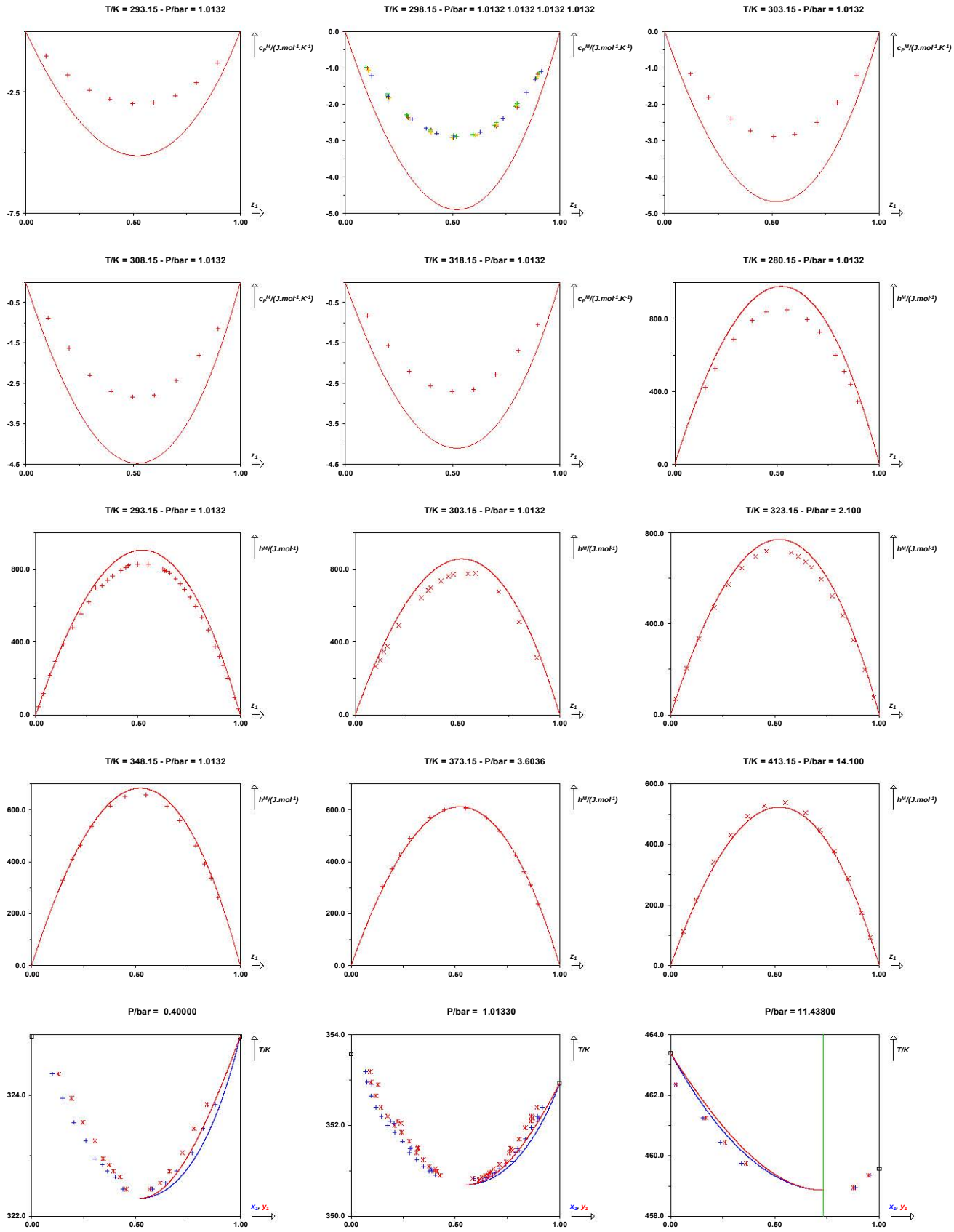
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Sieg, L., Flüssigkeit-Dampf-Gleichgewichte in binären Systemen von Kohlenwasserstoffen verschiedenen Typs: Flüssigkeit-Dampf-Gleichgewichte in binären Systemen von Kohlenwasserstoffen verschiedenen Typs, Chemie Ingenieur Technik 15 (1950) 322-326. doi:10.1002/cite.330221503

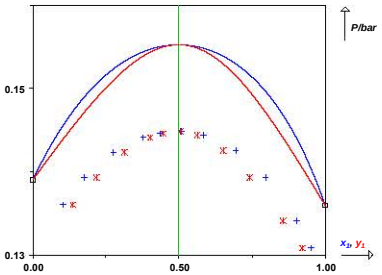
| T / K | P / bar | $x_1$ |
|---|---|---|
| 350.77 | 1.013 | 0.5450 |

Lafuente, C. - Pardo, J. - Santate, J. - Royo, F. - Urieta, J., Use of a Fischer-Labodest apparatus to study the liquid-vapor equilibrium of the benzene-cyclohexane system at different pressures, Rev. Acad. Cienc. Exact. Fis. Quim. Nat. Zaragoza (1992) 183-190.

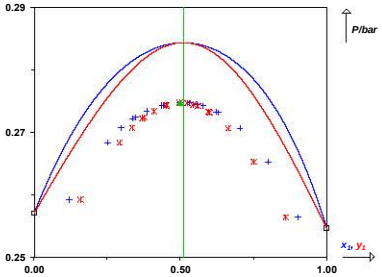
| T / K | P / bar | $x_1$ |
|---|---|---|
| 322.35 | 0.4000 | 0.5160 |


T/K = 293.15 - P/bar = 1.0132
T/K = 298.15 - P/bar = 1.0132 1.0132 1.0132 1.0132
T/K = 303.15 - P/bar = 1.0132
T/K = 308.15 - P/bar = 1.0132
T/K = 318.15 - P/bar = 1.0132
T/K = 280.15 - P/bar = 1.0132
T/K = 293.15 - P/bar = 1.0132
T/K = 303.15 - P/bar = 1.0132
T/K = 323.15 - P/bar = 2.100
T/K = 348.15 - P/bar = 1.0132
T/K = 373.15 - P/bar = 3.6036
T/K = 413.15 - P/bar = 14.100
P/bar = 0.40000
P/bar = 1.01330
P/bar = 11.43800
$c_p^M/(J.mol^{-1}.K^{-1})$
$h^M/(J.mol^{-1})$
T/K
$z_1$
$x_1, y_1$

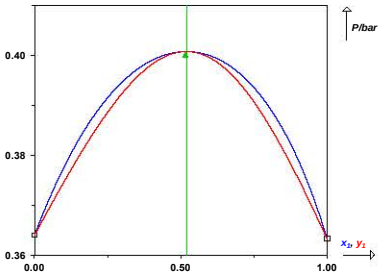
T/K = 298.15



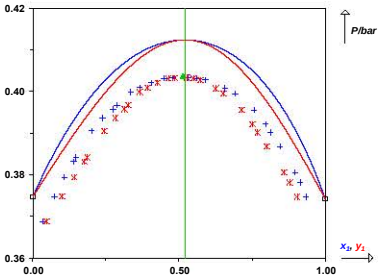

T/K = 313.10



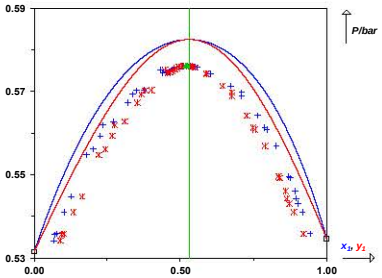

T/K = 322.35



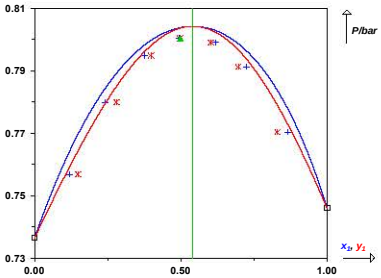

T/K = 323.15



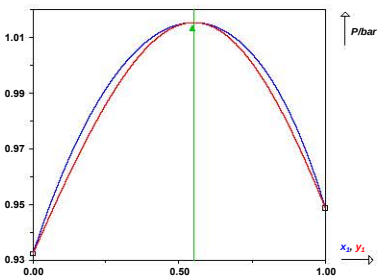

T/K = 333.15



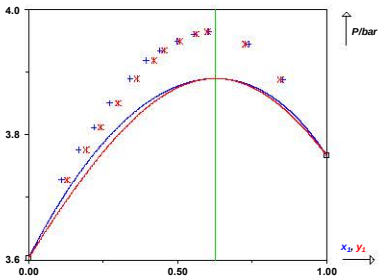

T/K = 343.13



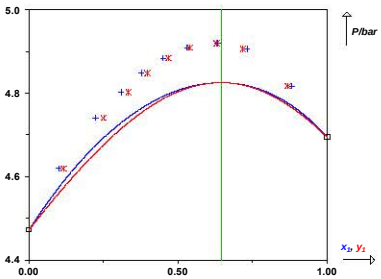

T/K = 350.77



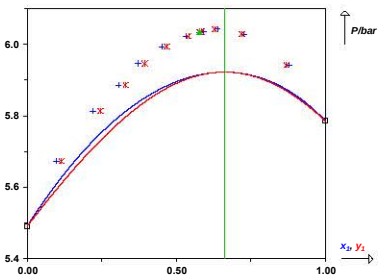

T/K = 403.15



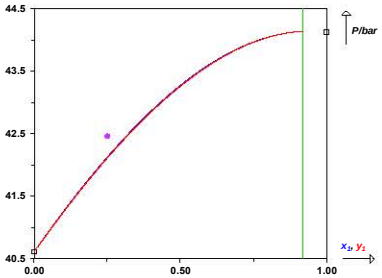

T/K = 413.15



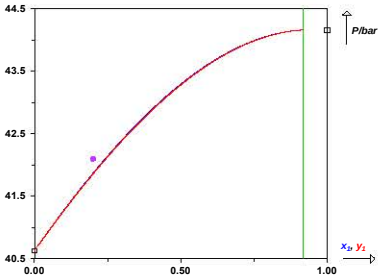

T/K = 423.15



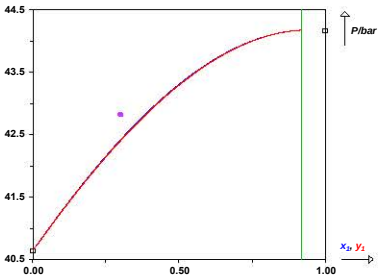

T/K = 553.41



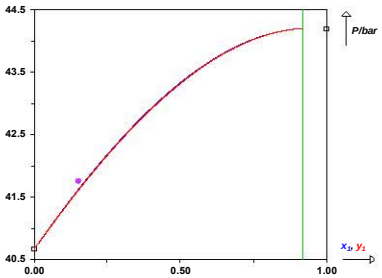

T/K = 553.45



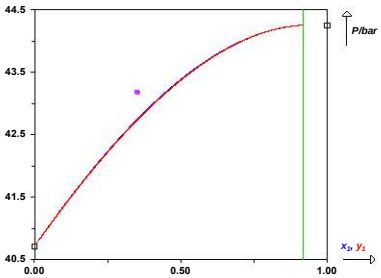

T/K = 553.47



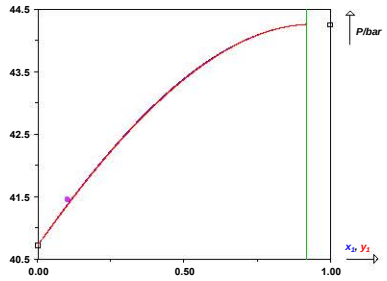

T/K = 553.52



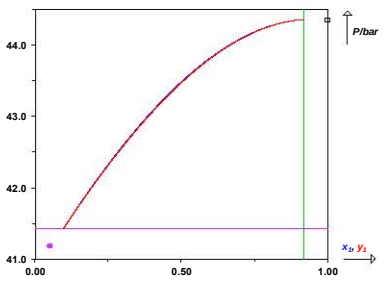

T/K = 553.62



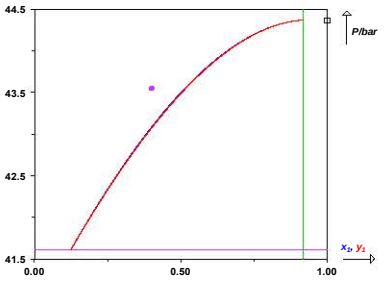
T/K = 553.63



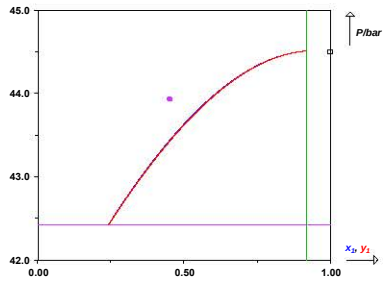

T/K = 553.81



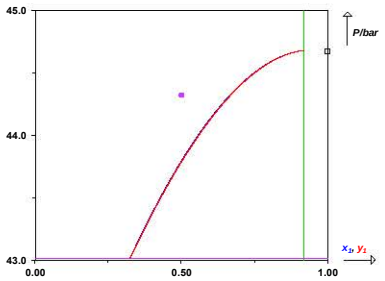

T/K = 553.84



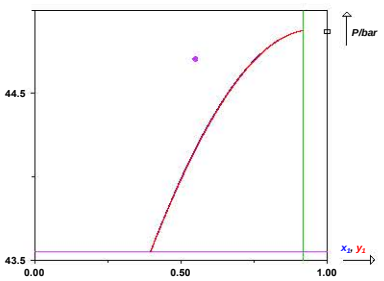

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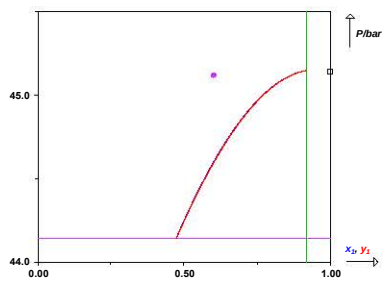

T/K = 554.41



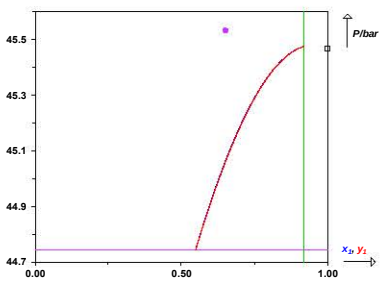

T/K = 554.78



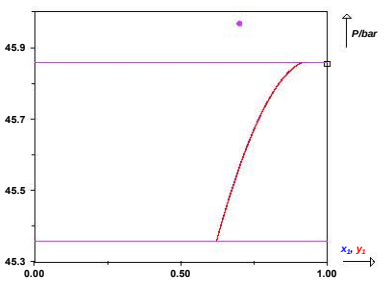

T/K = 555.28



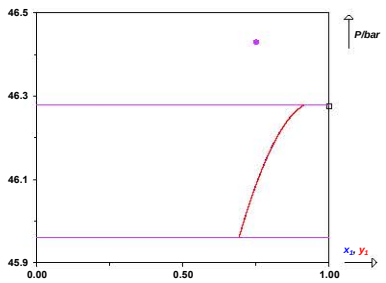

T/K = 555.88



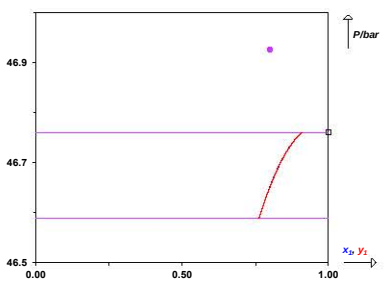

T/K = 556.58




T/K = 557.34




T/K = 558.21



## ETHYLENE (1) + XENON (2)

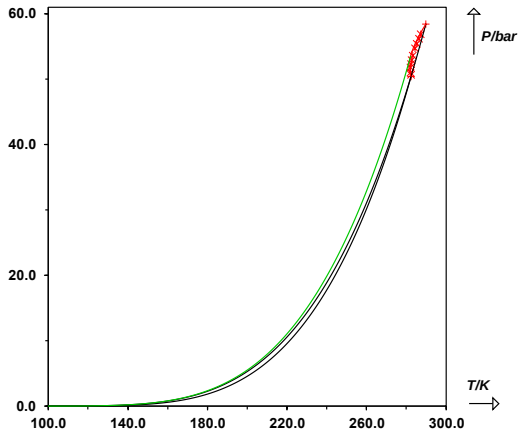
| | | |
|---|---|---|
| **CAS** | 74-85-1 | 7440-63-3 |
| **InChiKey** | VGGSQFUCUMXWEO-UHFFFAOYSA-N | FHNFHKCVQCLJFQ-UHFFFAOYSA-N |
| **$T_c$ / K** | 282.34 | 289.74 |
| **$P_c$ / bar** | 50.41 | 58.40 |
| **ω** | 0.086 | 0.000 |

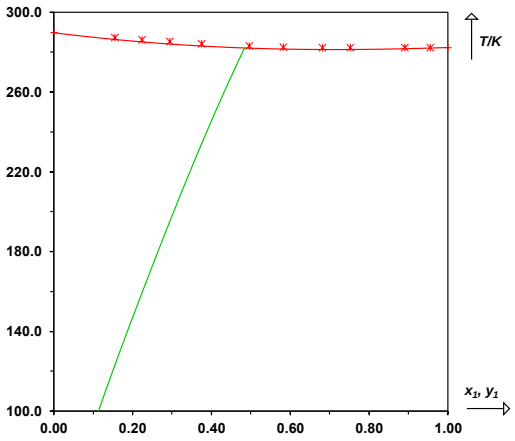
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 91.9
B/MPa = 129

*Deviations*
MAPE on x = 36 %
MAPE on y = 34 %
MAPE on $h^M$ = 7.3 %



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**Isothermal phase equilibrium data**

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Calado, J.C.G. - Soares, V.A.M., Thermodynamics of liquid ethylene + xenon at 161.38 K, The Journal of Chemical Thermodynamics 9 (1977) 911-913. doi:10.1016/0021-9614(77)90176-8

**T / K = 161.38**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.6896 | 0.1317 | 0.2140 |
| 0.7418 | 0.2629 | 0.3644 |
| 0.7891 | 0.4432 | 0.5222 |
| 0.8103 | 0.5381 | 0.5978 |
| 0.8275 | 0.6698 | 0.6982 |
| 0.8337 | 0.7691 | 0.7770 |
| 0.8298 | 0.9095 | 0.9028 |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 203.03**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.709 | 0.2527 | 0.2906 |
| 5.916 | 0.4301 | 0.4632 |
| 5.992 | 0.5134 | 0.5355 |
| 6.033 | 0.5727 | 0.5841 |
| 6.047 | 0.7987 | 0.7983 |
| 5.964 | 0.9034 | 0.8892 |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 224.03**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.91 | 0.3277 | 0.3638 |
| 12.19 | 0.5802 | 0.5838 |
| 12.20 | 0.7694 | 0.7654 |
| 12.14 | 0.8242 | 0.8221 |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 250.16**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 23.88 | 0.0883 | 0.0919 |
| 25.38 | 0.4478 | 0.4543 |
| 25.48 | 0.5085 | 0.5097 |
| 25.56 | 0.5413 | 0.5415 |
| 25.57 | 0.5834 | 0.5833 |
| 25.55 | 0.6416 | 0.6423 |
| 25.33 | 0.7424 | 0.7341 |
| 24.83 | 0.9011 | 0.8916 |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 262.18**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 32.03 | 0.0482 | 0.0525 |
| 32.80 | 0.1822 | 0.1932 |
| 33.45 | 0.3534 | 0.3618 |
| 33.51 | 0.3725 | 0.3807 |
| 33.53 | 0.3830 | 0.3914 |
| 33.64 | 0.4661 | 0.4710 |
| 33.68 | 0.5007 | 0.5043 |
| 33.42 | 0.7726 | 0.7645 |
| 33.22 | 0.8408 | 0.8397 |
| 32.83 | 0.9343 | 0.9336 |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 269.54**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 38.44 | 0.1166 | 0.1229 |
| 38.68 | 0.1545 | 0.1631 |
| 39.03 | 0.2214 | 0.2318 |
| 39.27 | 0.2770 | 0.2862 |
| 39.52 | 0.3483 | 0.3580 |
| 39.59 | 0.3702 | 0.3776 |
| 39.78 | 0.4653 | 0.4698 |
| 39.81 | 0.4993 | 0.5015 |
| 39.83 | 0.5482 | 0.5485 |
| 39.76 | 0.6511 | 0.6495 |
| 39.73 | 0.6763 | 0.6721 |
| 39.59 | 0.7343 | 0.7290 |
| 39.36 | 0.8081 | 0.7936 |
| 38.85 | 0.9070 | 0.9022 |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 274.67**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 43.57 | 0.1612 | 0.1679 |

| | | |
|---|---|---|
| 44.13 | 0.2771 | 0.2822 |
| 44.51 | 0.4426 | 0.4467 |
| 44.60 | 0.4702 | 0.4720 |
| 44.62 | 0.5305 | 0.5300 |
| 44.49 | 0.6608 | 0.6577 |
| 44.40 | 0.6985 | 0.6856 |
| 44.08 | 0.7845 | 0.7752 |
| 43.79 | 0.8461 | 0.8366 |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 282.08**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 50.47 | 0.0388 | 0.0451 | |
| 50.97 | 0.1036 | 0.1048 | |
| 51.01 | 0.1100 | 0.1100 | CRIT |
| 51.79 | 0.2544 | 0.2563 | |
| 51.93 | 0.2753 | 0.2781 | |
| 52.06 | 0.3118 | 0.3141 | |
| 52.10 | 0.3253 | 0.3276 | |
| 52.24 | 0.3766 | 0.3805 | |
| 52.30 | 0.4207 | 0.4220 | |
| 52.37 | 0.5169 | 0.5166 | |
| 52.31 | 0.5959 | 0.5880 | |
| 51.90 | 0.7181 | 0.7096 | |
| 51.30 | 0.8370 | 0.8321 | |
| 50.62 | 0.9324 | 0.9250 | |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 282.61**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 52.95 | 0.4258 | 0.4265 | |
| 52.70 | 0.6820 | 0.6794 | |
| 52.27 | 0.7778 | 0.7738 | |
| 51.22 | 0.9302 | 0.9269 | |
| 52.93 | 0.4180 | 0.4180 | CRIT |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 283.17**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 53.59 | 0.5302 | 0.5305 |
| 53.55 | 0.5739 | 0.5746 |
| 53.47 | 0.6211 | 0.6205 |
| 53.15 | 0.7077 | 0.7046 |
| 52.57 | 0.8206 | 0.8124 |
| 51.95 | 0.9061 | 0.9022 |
| 53.61 | 0.5040 | 0.5040 CRIT |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 284.20**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 54.50 | 0.6904 | 0.6882 | |
| 54.23 | 0.7421 | 0.7394 | |
| 53.88 | 0.8036 | 0.8004 | |
| 53.21 | 0.8963 | 0.8925 | |
| 54.70 | 0.6250 | 0.6250 | CRIT |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 285.19**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 55.39 | 0.7175 | 0.7161 | |
| 55.02 | 0.7816 | 0.7789 | |
| 54.52 | 0.8603 | 0.8524 | |
| 54.17 | 0.9051 | 0.8987 | |
| 55.44 | 0.7050 | 0.7050 | CRIT |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 286.19**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 56.12 | 0.7892 | 0.7848 | |
| 55.99 | 0.8086 | 0.8059 | |
| 55.56 | 0.8663 | 0.8636 | |
| 55.00 | 0.9319 | 0.9299 | |
| 56.17 | 0.7760 | 0.7760 | CRIT |

Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

**T / K = 287.18**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 56.77 | 0.8592 | 0.8578 |
| 56.68 | 0.8699 | 0.8681 |
| 56.20 | 0.9261 | 0.9241 |

| | | | |
|---|---|---|---|
| 55.61 | 0.9852 | 0.9847 | |
| 56.85 | 0.8450 | 0.8450 | CRIT |

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**Enthalpy of mixing**

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Lainez, A - Rebelo, L.P.N - Calado, J.C.G - Streett, W.B - Zollweg, J.A, Excess enthalpies of liquid (ethene + xenon) at 162.9 K, The Journal of Chemical Thermodynamics 1 (1987) 35-38. doi:10.1016/0021-9614(87)90159-5

**T / K =** **162.90**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 217.10 | 0.2543 |
| 261.66 | 0.3721 |
| 274.85 | 0.4419 |
| 285.24 | 0.4950 |
| 286.86 | 0.5557 |
| 275.14 | 0.6285 |
| 230.81 | 0.7394 |

---

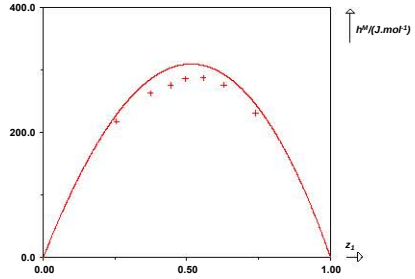
**Critical point**

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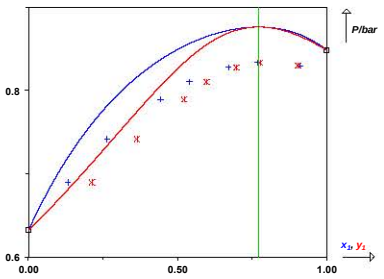
Nunes da Ponte, M. - Chokappa, D. - Calado, J.C.G. - Zollweg, J. - Streett, W.B., Vapor-liquid equilibrium in the xenon + ethene system, J. Phys. Chem. 6 (1986) 1147-1152. doi:10.1021/j100278a037

| T / K | P / bar | $x_1$ |
|---|---|---|
| 282.08 | 51.77 | 0.2480 |
| 282.25 | 50.66 | 0.0440 |
| 282.25 | 52.26 | 0.3190 |

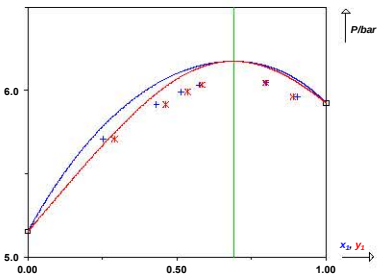
T/K = 162.90 - P/bar = 1.0132



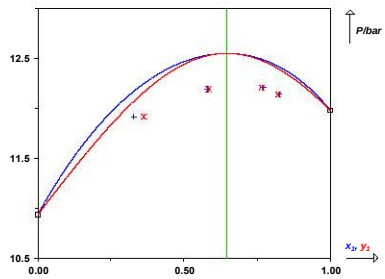

T/K = 161.38



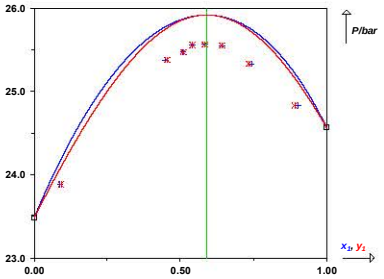

T/K = 203.03



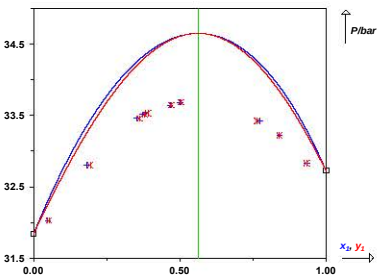

T/K = 224.03



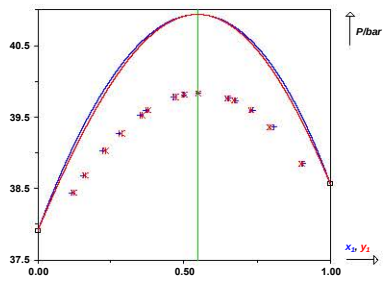

T/K = 250.16



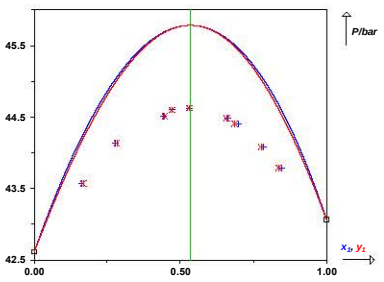

T/K = 262.18



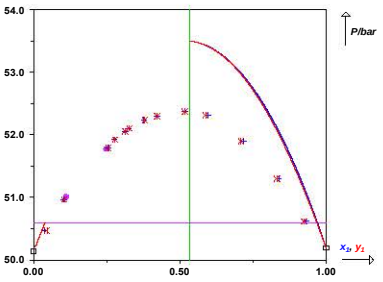

T/K = 269.54



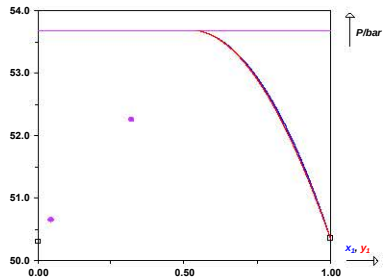

T/K = 274.67



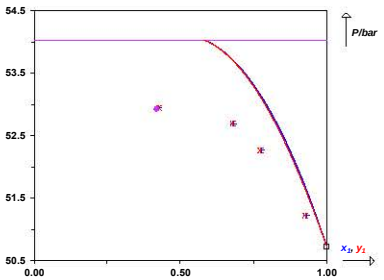

T/K = 282.08



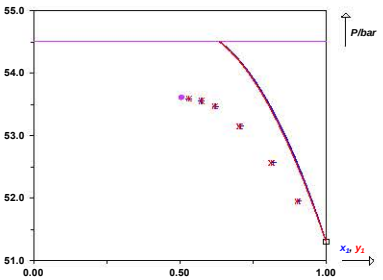

T/K = 282.25

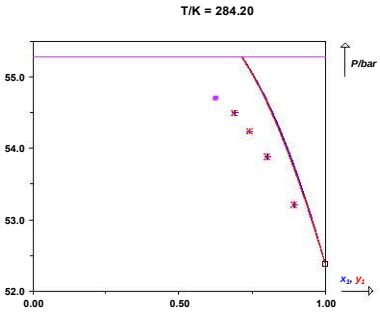


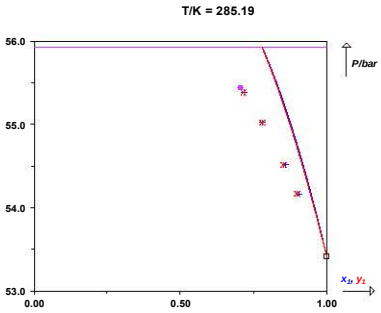

T/K = 282.61

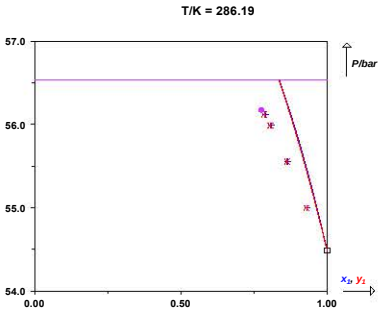


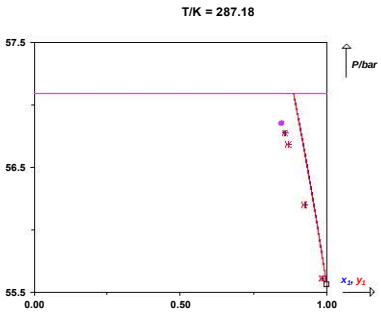

T/K = 283.17




T/K = 284.20
P/bar
55.0
54.0
53.0
52.0
0.00
0.50
1.00
x1, y1


T/K = 285.19
P/bar
56.0
55.0
54.0
53.0
0.00
0.50
1.00
x1, y1


T/K = 286.19
P/bar
57.0
56.0
55.0
54.0
0.00
0.50
1.00
x1, y1


T/K = 287.18
P/bar
57.5
56.5
55.5
0.00
0.50
1.00
x1, y1

## 1,2-DICHLOROETHANE (1) + TOLUENE (2)

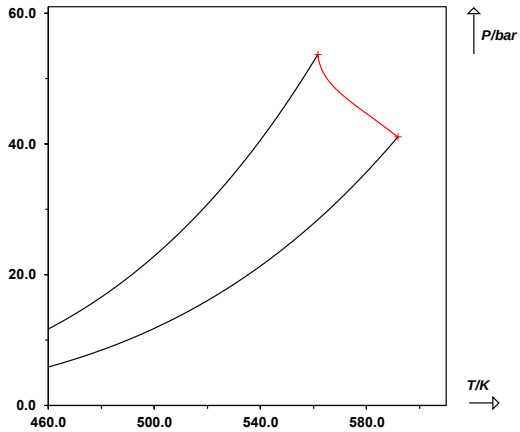
| | | |
|---|---|---|
| **CAS** | 107-06-2 | 108-88-3 |
| **InChiKey** | WSLDOOZREJYCGB-UHFFFAOYSA-N | YXFVVABEGXRONW-UHFFFAOYSA-N |
| **$T_c$ / K** | 561.60 | 591.75 |
| **$P_c$ / bar** | 53.70 | 41.08 |
| **ω** | 0.287 | 0.264 |

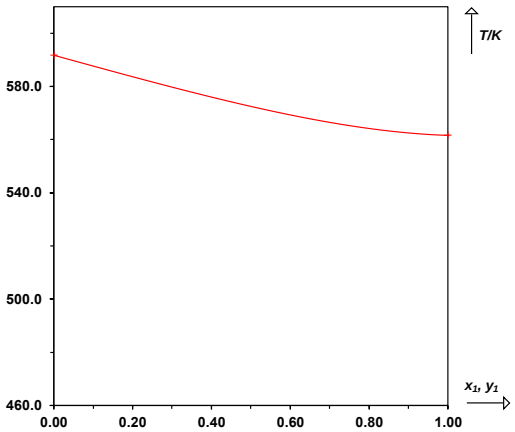
Non ideal with entropic causes

**PPR78 results**

*Parameters*
A/MPa = 35.3
B/MPa = -7.18

*Deviations*
MAPE on x = 9.8 %
MAPE on y = 7.8 %
MAPE on $h^M$ = 95 %
MAPE on $c_P^M$ = 88 %



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**Isobaric phase equilibrium data**

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Ellis, S.R.M. - Contractor, R.M., Vapor-liquid equilibriums at reduced pressure, Chem. Eng. London 1 (1964) 10-13.

**P / bar = 0.2666**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 338.85 | 0.1100 | 0.2250 |
| 335.55 | 0.2150 | 0.3930 |
| 332.65 | 0.3250 | 0.5330 |
| 330.55 | 0.4040 | 0.6210 |
| 330.30 | 0.4165 | 0.6375 |
| 326.95 | 0.5630 | 0.7600 |
| 323.55 | 0.7270 | 0.8700 |
| 321.55 | 0.8440 | 0.9315 |

Rollet, A.P. - Toledano, P. - Elkaim, G. - Sonez, M., Ebulliometry of volatile solutes. II, Publ. Sci. Univ. Alger Ser. B (1956) 403-425.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 381.67 | 0.0500 | 0.1046 |
| 379.66 | 0.1000 | 0.1999 |
| 375.89 | 0.2000 | 0.3645 |
| 372.47 | 0.3000 | 0.4991 |
| 369.40 | 0.4000 | 0.6092 |
| 366.67 | 0.5000 | 0.7000 |
| 364.24 | 0.6000 | 0.7762 |
| 362.06 | 0.7000 | 0.8414 |
| 360.08 | 0.8000 | 0.8988 |
| 358.28 | 0.9000 | 0.9509 |
| 357.43 | 0.9500 | 0.9757 |

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**Enthalpy of mixing**

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Baud, E., Thermal analysis of binary mixtures, Bull. Soc. Chim. Fr. (1915) 329-345.

**T / K = 290.65**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -42.71 | 0.0790 |
| -78.29 | 0.2620 |
| -66.15 | 0.3850 |
| -25.12 | 0.5370 |
| -2.554 | 0.6180 |
| 31.40 | 0.8030 |
| 18.42 | 0.9440 |

Tschamler, H., Über binäre flüssige Mischungen VI: Mischungswärmen, Molwärmen, Volumeffekte und Zustands-diagramme von 1,2-Dichloräthan mit Benzol und n-Alkylbenzolen, Monatshefte für Chemie 6 (1948) 499-507. doi:10.1007/BF00898687

**T / K = 295.40**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -54.43 | 0.1000 |
| -83.74 | 0.2000 |
| -87.92 | 0.3000 |
| -66.99 | 0.4000 |
| -39.78 | 0.5000 |
| -10.47 | 0.6000 |
| 20.93 | 0.7000 |
| 37.68 | 0.8000 |
| 35.59 | 0.9000 |

Ortega, J. - Placido, J., Excess enthalpies of 12 binary liquid mixtures of α,ω-dichloroalkanes (C2, C4, C6) + benzene, toluene, ethylbenzene, or butylbenzene at 298.15 K, ELDATA Int. Electron. J. Phys. Chem. Data 3 (1996) 111-120.

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -39.40 | 0.0698 |
| -69.20 | 0.1469 |
| -94.90 | 0.2230 |
| -113.20 | 0.2973 |
| -122.90 | 0.3664 |
| -123.20 | 0.4284 |
| -102.10 | 0.5260 |
| -84.80 | 0.5677 |
| -66.40 | 0.6117 |
| -48.10 | 0.6593 |
| -31.50 | 0.7060 |
| -16.60 | 0.7554 |
| -3.600 | 0.8091 |
| 4.200 | 0.8583 |
| 6.300 | 0.9108 |
| 3.300 | 0.9585 |

---

**Heat capacity of mixing**

---

Tschamler, H., Über binäre flüssige Mischungen VI: Mischungswärmen, Molwärmen, Volumeffekte und Zustands-diagramme von 1,2-Dichloräthan mit Benzol und n-Alkylbenzolen, Monatshefte für Chemie 6 (1948) 499-507. doi:10.1007/BF00898687

**T / K =** **295.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -2.256 | 0.1000 |
| -2.652 | 0.2000 |
| -1.934 | 0.3000 |
| -1.664 | 0.4000 |
| -1.051 | 0.5000 |
| 0.3167 | 0.6000 |
| 1.644 | 0.7000 |
| 2.523 | 0.8000 |
| 2.122 | 0.9000 |

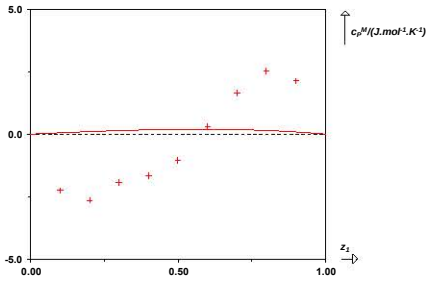
Wilhelm, Emmerich - Grolier, J.-P. E. - Ghassemi, M. H. Karbalai, Molar Heat Capacities of Binary Liquid Mixtures: 1,2-Dichlorethane + Benzene, + Toluene, and + p-Xylene, Berichte der Bunsengesellschaft für physikalische Chemie 10 (1977) 925-930. doi:10.1002/bbpc.19770811009

**T / K =** **298.15**

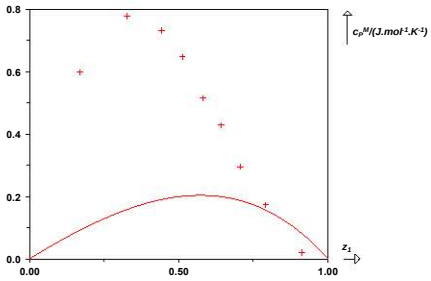
**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.5980 | 0.1687 |
| 0.7780 | 0.3275 |
| 0.7320 | 0.4417 |
| 0.6470 | 0.5130 |
| 0.5150 | 0.5816 |
| 0.4290 | 0.6433 |
| 0.2960 | 0.7079 |
| 0.1740 | 0.7915 |
| 0.0220 | 0.9144 |

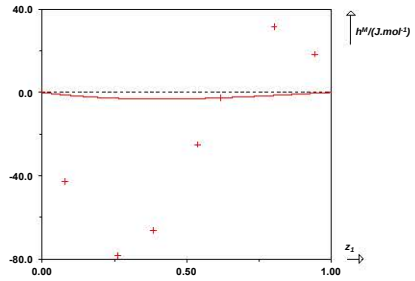
T/K = 295.15 - P/bar = 1.0132



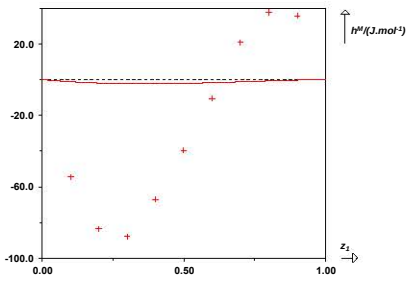

T/K = 298.15 - P/bar = 1.0132



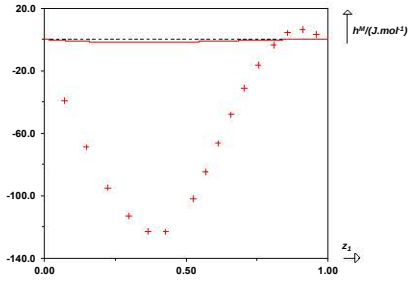

T/K = 290.65 - P/bar = 1.0132



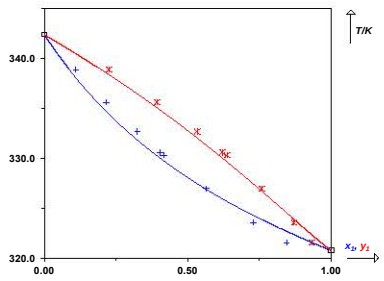

T/K = 295.40 - P/bar = 1.0132



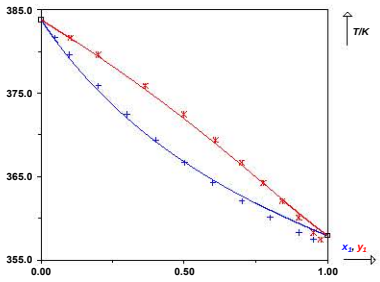

T/K = 298.15 - P/bar = 1.0132




P/bar = 0.26664




P/bar = 1.01330



# E-NA systems (AC = 2)

## CARBON DIOXIDE (1) + TOLUENE (2)

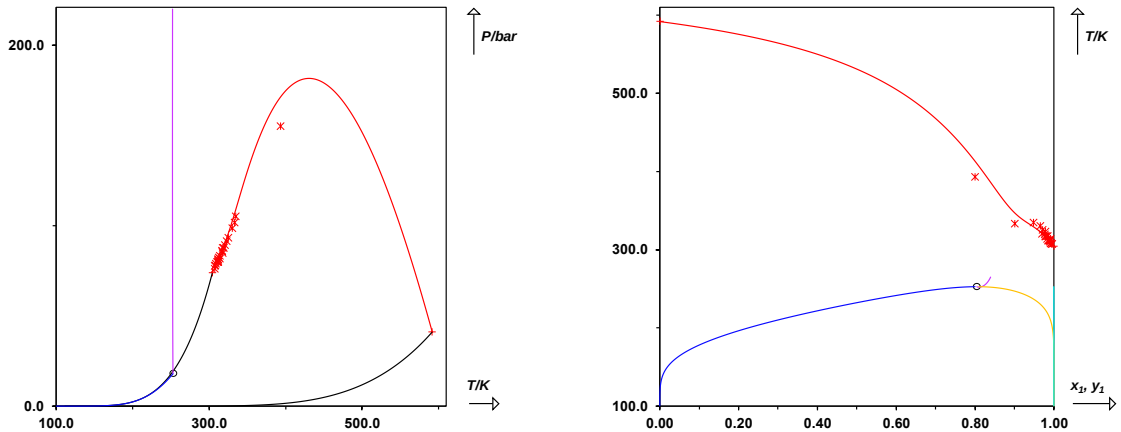
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 108-88-3 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | YXFVVABEGXRONW-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 591.75 |
| **$P_c$ / bar** | 73.83 | 41.08 |
| **ω** | 0.2240 | 0.2640 |

Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 298
B/MPa = 800

*Deviations*
MAPE on x = 8.9 %
MAPE on y = 9.8 %
MAPE on $x_c$ = 11 %
MAPE on $P_c$ = 1.8 %
MAPE on $h^M$ = 26 %



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**Isothermal phase equilibrium data**

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Hong, J.H. - Kobayashi, R., Multicomponent vapor-liquid equilibria measurements for the development of an extractive distillation process for the processing of gas issuing from a carbon dioxide/EOR project, Ind. Eng. Chem. Process Design Develop. (1986) 584-589. doi:10.1021/i200033a041

**T / K = 263.14**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.890 | 0.1494 | 0.9992 |
| 10.34 | 0.2373 | 0.9994 |
| 13.79 | 0.3201 | 0.9994 |
| 17.24 | 0.4425 | 0.9995 |
| 20.62 | 0.6133 | 0.9994 |
| 22.20 | 0.7456 | 0.9994 |

Naidoo, Paramespri - Ramjugernath, Deresh - Raal, Johan David, A new high-pressure vapour–liquid equilibrium apparatus, Fluid Phase Equilibria 1-2 (2008) 104-112. doi:10.1016/j.fluid.2008.05.002

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.050 | 0.0578 | 0.9947 |
| 8.780 | 0.1274 | 0.9948 |
| 12.77 | 0.1928 | 0.9951 |
| 16.24 | 0.2511 | 0.9964 |
| 22.23 | 0.3709 | 0.9968 |
| 29.40 | 0.5249 | 0.9981 |
| 35.32 | 0.6988 | 0.9989 |
| 37.83 | 0.7980 | 0.9990 |

Fink, Samuel D. - Hershey, Harry C., Modeling the vapor-liquid equilibria of 1,1,1-trichloroethane + carbon dioxide and toluene + carbon dioxide at 308, 323, and 353 K, Industrial & Engineering Chemistry Research 2 (1990) 295-306. doi:10.1021/ie00098a022

**T / K = 308.16**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.040 | 0.0627 | 0.9889 |
| 14.75 | 0.1229 | 0.9918 |
| 22.01 | 0.1886 | 0.9892 |
| 23.67 | 0.2110 | 0.9949 |
| 29.93 | 0.2745 | 0.9923 |
| 32.00 | 0.2990 | 0.9956 |
| 38.43 | 0.3732 | 0.9944 |
| 48.43 | 0.4923 | 0.9925 |
| 48.95 | 0.5118 | 0.9947 |
| 53.15 | 0.5724 | 0.9919 |
| 55.91 | 0.6288 | 0.9950 |
| 59.17 | 0.6896 | 0.9936 |
| 63.21 | 0.7962 | 0.9945 |
| 66.38 | 0.8502 | 0.9951 |
| 69.21 | 0.9082 | 0.9948 |

Fink, Samuel D. - Hershey, Harry C., Modeling the vapor-liquid equilibria of 1,1,1-trichloroethane + carbon dioxide and toluene + carbon dioxide at 308, 323, and 353 K, Industrial & Engineering Chemistry Research 2 (1990) 295-306. doi:10.1021/ie00098a022

**T / K = 323.17**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.400 | 0.0426 | 0.9522 |
| 11.05 | 0.0786 | 0.9680 |
| 12.67 | 0.0857 | 0.9747 |
| 16.40 | 0.1211 | 0.9801 |
| 29.65 | 0.2197 | 0.9890 |
| 38.19 | 0.2846 | 0.9917 |
| 41.76 | 0.3200 | 0.9903 |
| 55.49 | 0.4466 | 0.9905 |
| 63.58 | 0.5341 | 0.9903 |
| 70.06 | 0.6113 | 0.9909 |
| 71.17 | 0.6162 | 0.9901 |
| 76.73 | 0.7076 | 0.9896 |
| 81.62 | 0.7920 | 0.9877 |
| 87.73 | 0.8913 | 0.9841 |

Park, S.D. - Kim, C.H. - Choi, C.S., Phase equilibria and mixture densities measurements of carbon dioxide-toluene system under high pressure, Hwahak Konghak 4 (1990) 438-443.

**T / K = 333.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 44.50 | 0.3482 | 0.9888 |
| 64.40 | 0.4944 | 0.9889 |
| 81.60 | 0.6441 | 0.9861 |
| 98.00 | 0.8169 | 0.9568 |

Fink, Samuel D. - Hershey, Harry C., Modeling the vapor-liquid equilibria of 1,1,1-trichloroethane + carbon dioxide and toluene + carbon dioxide at 308, 323, and 353 K, Industrial & Engineering Chemistry Research 2 (1990) 295-306. doi:10.1021/ie00098a022

**T / K = 353.18**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.180 | 0.0232 | 0.8810 |
| 7.650 | 0.0375 | 0.9237 |
| 7.770 | 0.0376 | 0.9197 |

| | | |
|---|---|---|
| 10.88 | 0.0567 | 0.9424 |
| 14.82 | 0.0784 | 0.9534 |
| 22.80 | 0.1235 | 0.9711 |
| 29.54 | 0.1631 | 0.9753 |
| 37.31 | 0.2093 | 0.9790 |
| 47.65 | 0.2683 | 0.9826 |
| 55.87 | 0.3137 | 0.9824 |
| 64.39 | 0.3645 | 0.9811 |
| 74.63 | 0.4191 | 0.9815 |
| 83.55 | 0.4769 | 0.9804 |
| 92.95 | 0.5352 | 0.9768 |
| 98.85 | 0.5885 | 0.9744 |
| 110.89 | 0.6750 | 0.9626 |
| 115.16 | 0.7194 | 0.9592 |
| 116.81 | 0.7385 | 0.9546 |
| 123.50 | 0.8301 | 0.9324 |

Park, S.D. - Kim, C.H. - Choi, C.S., Phase equilibria and mixture densities measurements of carbon dioxide-toluene system under high pressure, Hwahak Konghak 4 (1990) 438-443.

**T / K = 363.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 39.80 | 0.2332 | 0.9753 |
| 60.80 | 0.3439 | 0.9776 |
| 83.50 | 0.4564 | 0.9761 |
| 103.00 | 0.5673 | 0.9727 |
| 123.80 | 0.6910 | 0.9612 |
| 133.00 | 0.7790 | 0.9432 |

Kim, Choon-Ho - Vimalchand, P. - Donohue, Marc D., Vapor-liquid equilibria for binary mixtures of carbon dioxide with benzene, toluene and p-xylene, Fluid Phase Equilibria 3 (1986) 299-311. doi:10.1016/0378-3812(86)87014-5

**T / K = 373.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.150 | 0.0190 | 0.7540 |
| 12.56 | 0.0570 | 0.8820 |
| 20.16 | 0.0960 | 0.9360 |
| 29.31 | 0.1430 | 0.9530 |
| 37.47 | 0.1810 | 0.9620 |
| 45.77 | 0.2260 | 0.9670 |
| 54.89 | 0.2690 | 0.9690 |

Morris, William O. - Donohue, Marc D., Vapor-liquid equilibria in mixtures containing carbon dioxide, toluene, and 1-methylnaphthalene, Journal of Chemical & Engineering Data 3 (1985) 259-263. doi:10.1021/je00041a007

**T / K = 383.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.930 | 0.0217 | 0.7710 |
| 9.720 | 0.0385 | 0.8470 |
| 19.05 | 0.0807 | 0.9080 |
| 31.80 | 0.1400 | 0.9380 |
| 48.15 | 0.2100 | 0.9510 |
| 64.05 | 0.2840 | 0.9550 |
| 113.00 | 0.5220 | 0.9530 |
| 128.00 | 0.6070 | 0.9360 |

Kim, Choon-Ho - Vimalchand, P. - Donohue, Marc D., Vapor-liquid equilibria for binary mixtures of carbon dioxide with benzene, toluene and p-xylene, Fluid Phase Equilibria 3 (1986) 299-311. doi:10.1016/0378-3812(86)87014-5

**T / K = 393.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.13 | 0.0460 | 0.8390 |
| 18.09 | 0.0690 | 0.8770 |
| 26.77 | 0.1100 | 0.9220 |
| 34.92 | 0.1480 | 0.9360 |
| 43.41 | 0.1800 | 0.9450 |
| 52.72 | 0.2270 | 0.9490 |
| 64.50 | 0.2760 | 0.9520 |

Park, S.D. - Kim, C.H. - Choi, C.S., Phase equilibria and mixture densities measurements of carbon dioxide-toluene system under high pressure, Hwahak Konghak 4 (1990) 438-443.

**T / K = 393.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 64.40 | 0.2922 | 0.9548 |
| 89.40 | 0.3955 | 0.9543 |
| 111.10 | 0.4898 | 0.9481 |
| 135.80 | 0.5950 | 0.9320 |
| 153.50 | 0.7016 | 0.8879 |

Morris, William O. - Donohue, Marc D., Vapor-liquid equilibria in mixtures containing carbon dioxide, toluene, and 1-methylnaphthalene, Journal of Chemical & Engineering Data 3 (1985) 259-263. doi:10.1021/je00041a007

**T / K = 413.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.100 | 0.0176 | 0.6230 |
| 13.40 | 0.0409 | 0.7660 |
| 24.65 | 0.0835 | 0.8470 |
| 35.90 | 0.1300 | 0.8720 |
| 47.90 | 0.1770 | 0.9080 |
| 73.15 | 0.2860 | 0.9280 |
| 98.65 | 0.3830 | 0.9260 |

| | | |
|---|---|---|
| 113.15 | 0.4370 | 0.9210 |
| 131.70 | 0.5460 | 0.9040 |

Ng, Heng-Joo - Robinson, Donald B., Equilibrium-phase properties of the toluene-carbon dioxide system, Journal of Chemical & Engineering Data 4 (1978) 325-327. doi:10.1021/je60079a020

**T / K = 477.04**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.79 | 0.0127 | 0.2660 |
| 29.37 | 0.0722 | 0.6380 |
| 49.78 | 0.1400 | 0.7490 |
| 70.40 | 0.2090 | 0.7850 |
| 91.70 | 0.2760 | 0.7930 |
| 119.07 | 0.3780 | 0.7870 |
| 136.24 | 0.4450 | 0.7700 |
| 152.24 | 0.5690 | 0.7160 |

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**Enthalpy of mixing**

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Wormald, C.J - Eyears, J.M, Excess molar enthalpies and excess molar volumes of {xCO2 + (1−x)C6H5CH3} at 298.15, 304.10, and 308.15 K from 7.5 to 12.6 MPa, The Journal of Chemical Thermodynamics 8 (1987) 845-856. doi:10.1016/0021-9614(87)90031-0

**T / K = 304.10**

**P / bar = 76.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -24.00 | 0.1450 |
| -42.00 | 0.2540 |
| -116.00 | 0.3980 |
| -250.00 | 0.4880 |
| -395.00 | 0.5570 |
| -450.00 | 0.6000 |
| -725.00 | 0.7150 |
| -798.00 | 0.7530 |
| -866.00 | 0.7950 |
| -990.00 | 0.8670 |
| -941.00 | 0.8670 |
| -960.00 | 0.8840 |
| -938.00 | 0.8960 |
| -962.00 | 0.8960 |
| -923.00 | 0.9060 |
| -964.00 | 0.9150 |
| -916.00 | 0.9390 |
| -765.00 | 0.9540 |
| -665.00 | 0.9690 |
| -629.00 | 0.9710 |
| -492.00 | 0.9870 |

Cordray, D.R - Christensen, J.J - Izatt, R.M, The excess enthalpies of (carbon dioxide + toluene) at 308.15, 358.15, and 573.15 K from 6.98 to 16.63 MPa, The Journal of Chemical Thermodynamics 7 (1986) 647-656. doi:10.1016/0021-9614(86)90066-2

**T / K = 358.15**

**P / bar = 138.80**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -172.00 | 0.0796 |
| -299.00 | 0.1169 |
| -493.00 | 0.1873 |
| -649.00 | 0.2525 |
| -832.00 | 0.3129 |
| -1020.0 | 0.3691 |
| -1150.0 | 0.4216 |
| -1320.0 | 0.4706 |
| -1440.0 | 0.5166 |
| -1590.0 | 0.5598 |
| -1700.0 | 0.6004 |
| -1810.0 | 0.6386 |
| -1910.0 | 0.6747 |
| -1880.0 | 0.6747 |
| -1960.0 | 0.7089 |
| -1970.0 | 0.7413 |
| -1980.0 | 0.7719 |
| -1940.0 | 0.8011 |
| -1900.0 | 0.8288 |
| -1760.0 | 0.8552 |
| -1540.0 | 0.8803 |
| -1330.0 | 0.9043 |
| -962.00 | 0.9272 |
| -644.00 | 0.9492 |

Pando, C - Renuncio, J.A.R - Schofield, R.S - Izatt, R.M - Christensen, J.J, The excess enthalpies of (carbon dioxide + toluene) at 308.15, 385.15, and 413.15 K from 7.60 to 12.67 MPa, The Journal of Chemical Thermodynamics 8 (1983) 747-755. doi:10.1016/0021-9614(83)90141-6

**T / K = 413.15**

**P / bar = 106.40**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -118.00 | 0.0389 |
| -298.00 | 0.0946 |
| -478.00 | 0.1472 |
| -624.00 | 0.1970 |
| -791.00 | 0.2443 |
| -923.00 | 0.2891 |
| -1066.0 | 0.3317 |

| | |
|---|---|
| -1178.0 | 0.3723 |
| -1255.0 | 0.4109 |
| -1236.0 | 0.4234 |
| -1192.0 | 0.4357 |
| -1153.0 | 0.4478 |
| -844.00 | 0.5167 |
| -686.00 | 0.5489 |
| -433.00 | 0.6094 |
| -171.00 | 0.6650 |
| 47.00 | 0.7165 |
| 160.00 | 0.7407 |
| 258.00 | 0.7641 |
| 457.00 | 0.8084 |
| 549.00 | 0.8294 |
| 651.00 | 0.8496 |
| 806.00 | 0.8882 |
| 889.00 | 0.9065 |
| 978.00 | 0.9242 |
| 807.00 | 0.9414 |
| 608.00 | 0.9580 |
| 374.00 | 0.9742 |
| 134.00 | 0.9898 |

Christensen, J.J - Zebolsky, D.M - Izatt, R.M, The excess enthalpies of (carbon dioxide + toluene) at 470.15 and 573.15 K from 7.60 to 12.67 MPa, The Journal of Chemical Thermodynamics 1 (1985) 1-10. doi:10.1016/0021-9614(85)90025-4

| **T / K =** | **470.15** |
|---|---|
| **P / bar =** | **126.70** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 285.00 | 0.4653 |
| 540.00 | 0.5113 |
| 756.00 | 0.5545 |
| 1030.0 | 0.5952 |
| 1240.0 | 0.6337 |
| 1440.0 | 0.6701 |
| 1630.0 | 0.7045 |
| 1820.0 | 0.7371 |
| 1980.0 | 0.7682 |
| 2190.0 | 0.7977 |
| 2260.0 | 0.8119 |

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**Critical point**

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Reaves, J. Todd - Griffith, Aron T. - Roberts, Christopher B., Critical Properties of Dilute Carbon Dioxide + Entrainer and Ethane + Entrainer Mixtures, Journal of Chemical & Engineering Data 4 (1998) 683-686. doi:10.1021/je9702753

| T / K | P / bar | $x_1$ |
|---|---|---|
| 307.20 | 76.10 | 0.9950 |
| 313.70 | 81.70 | 0.9910 |
| 311.40 | 79.80 | 0.9900 |
| 311.40 | 79.70 | 0.9890 |
| 311.90 | 80.60 | 0.9860 |
| 317.30 | 84.80 | 0.9840 |
| 317.10 | 86.00 | 0.9790 |
| 319.40 | 87.60 | 0.9770 |
| 325.10 | 93.20 | 0.9710 |
| 330.20 | 98.50 | 0.9660 |

Zhang, J.C. - Wu, X.Y. - Cao, W.L., Phase Equilibrium Properties of Supercritical Carbon Dioxide in Binary System, Gaodeng Xuexiao Huaxue Xuebao 1 (2002) 10-13.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 307.25 | 77.60 | 0.9947 |
| 308.95 | 78.80 | 0.9929 |
| 311.55 | 81.20 | 0.9900 |
| 312.15 | 82.50 | 0.9863 |
| 317.75 | 87.70 | 0.9816 |
| 322.85 | 91.40 | 0.9785 |

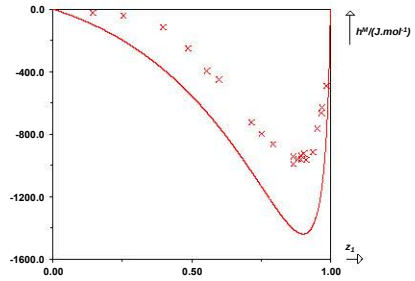
Wu, Weize - Ke, Jie - Poliakoff, Martyn, Phase Boundaries of CO2 + Toluene, CO2 + Acetone, and CO2 + Ethanol at High Temperatures and High Pressures, Journal of Chemical & Engineering Data 4 (2006) 1398-1403. doi:10.1021/je060099a

| T / K | P / bar | $x_1$ |
|---|---|---|
| 333.20 | 101.60 | 0.9000 |
| 393.20 | 155.10 | 0.8000 |

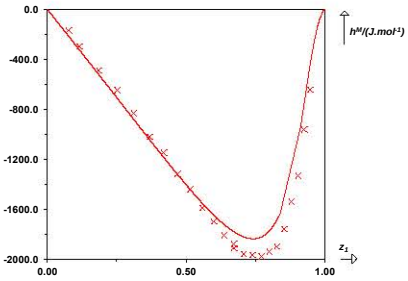
Zhang, Haifei - Liu, Zhimin - Han, Buxing, Critical points and phase behavior of toluene-CO2 and toluene-H2-CO2 mixture in CO2-rich region, The Journal of Supercritical Fluids 3 (2000) 185-192. doi:10.1016/S0896-8446(00)00081-4

| T / K | P / bar | $x_1$ |
|---|---|---|
| 308.05 | 77.82 | 0.9915 |
| 310.15 | 79.76 | 0.9893 |
| 311.95 | 81.27 | 0.9851 |
| 314.15 | 83.21 | 0.9823 |
| 316.65 | 85.64 | 0.9787 |
| 320.55 | 89.09 | 0.9694 |
| 335.05 | 105.00 | 0.9478 |

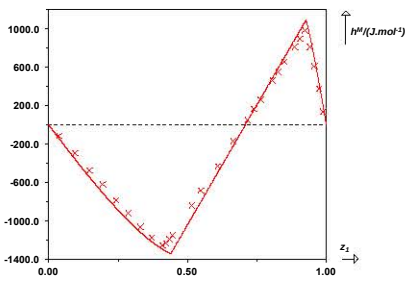
T/K = 304.10 - P/bar = 76.00



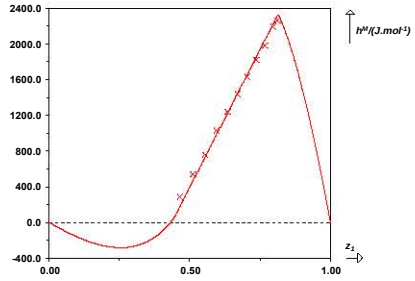

T/K = 358.15 - P/bar = 138.800



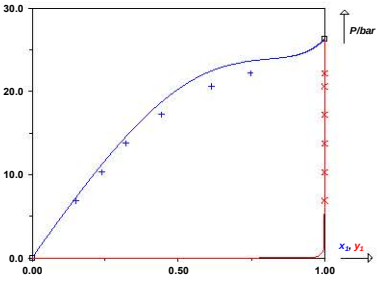

T/K = 413.15 - P/bar = 106.400



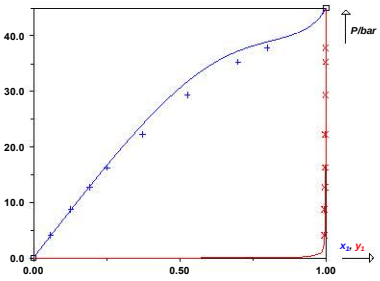

T/K = 470.15 - P/bar = 126.700



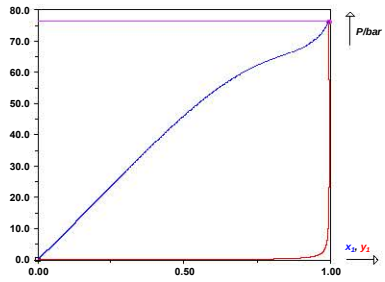

T/K = 263.14



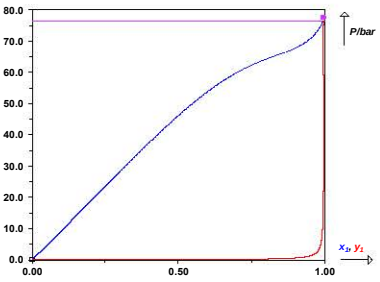

T/K = 283.15



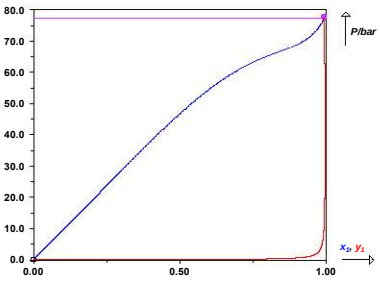

T/K = 307.20



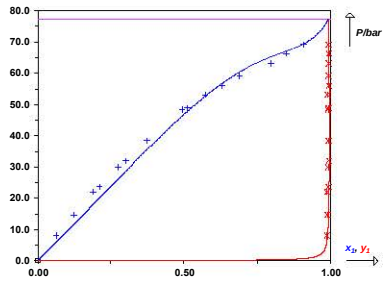

T/K = 307.25



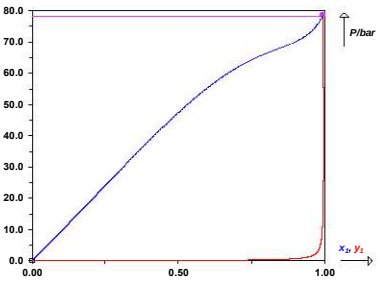

T/K = 308.05



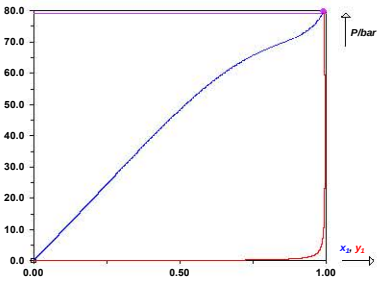

T/K = 308.16



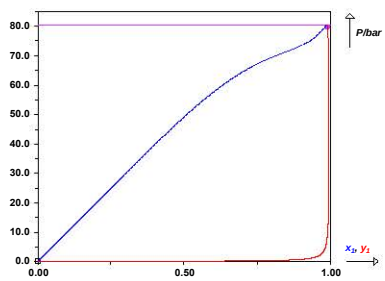

T/K = 308.95



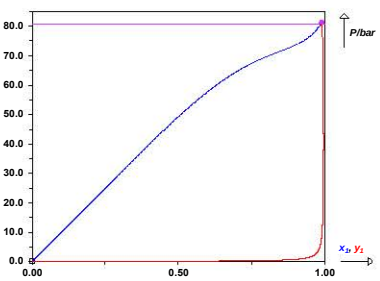

T/K = 310.15



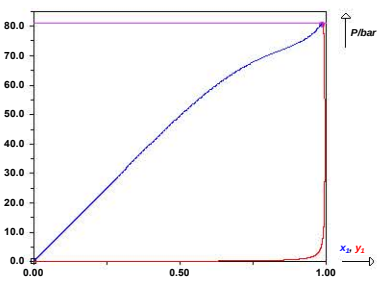

T/K = 311.40



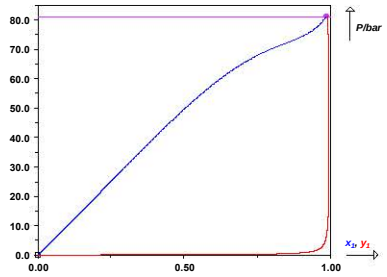

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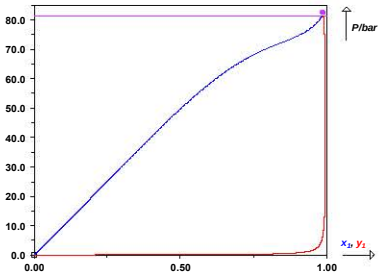

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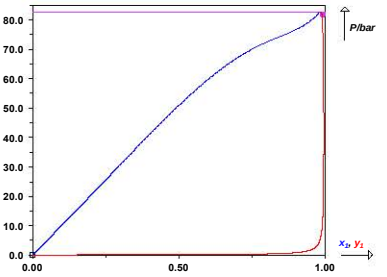
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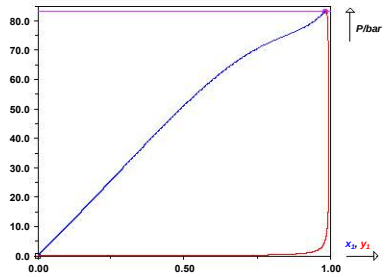

T/K = 312.15



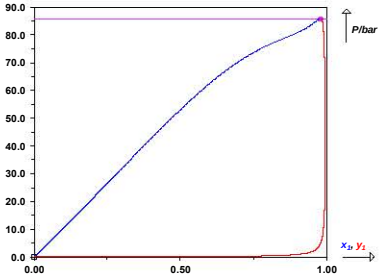

T/K = 313.70



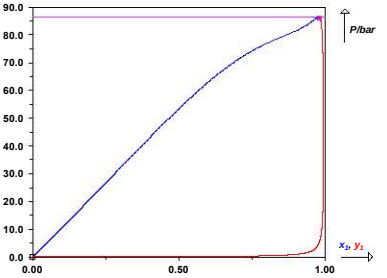

T/K = 314.15



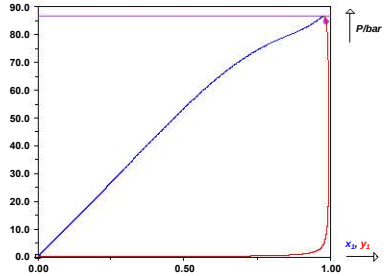

T/K = 316.65



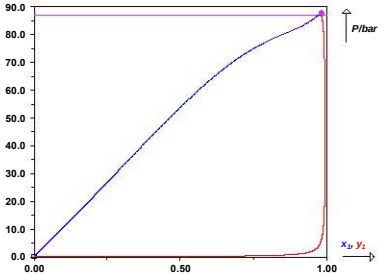

T/K = 317.10



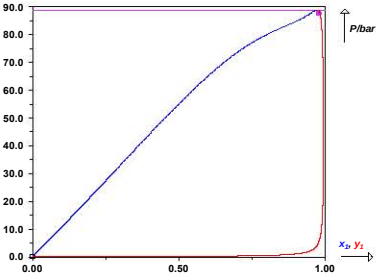

T/K = 317.30



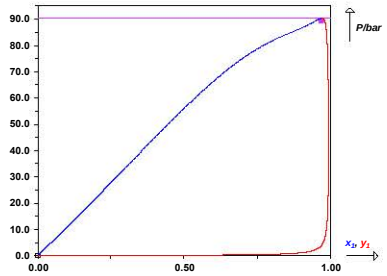

T/K = 317.75



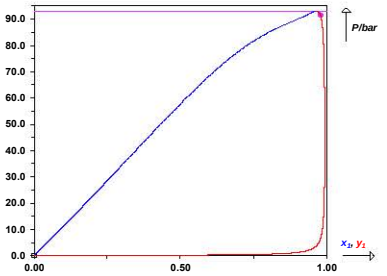

T/K = 319.40



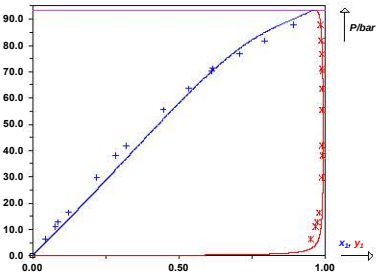

T/K = 320.55



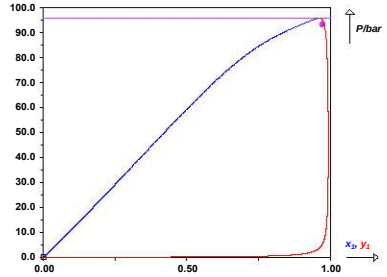

T/K = 322.85



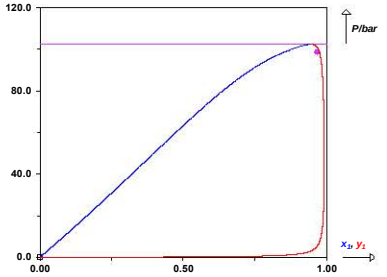

T/K = 323.17



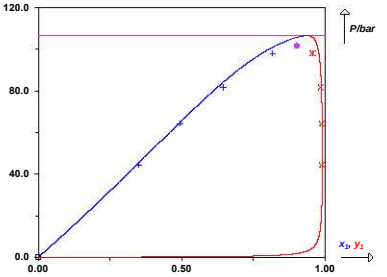

T/K = 325.10



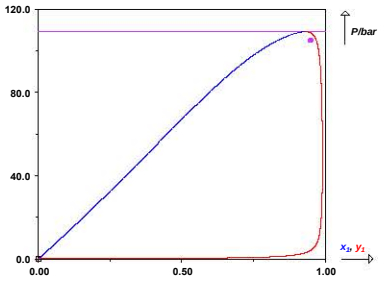

T/K = 330.20



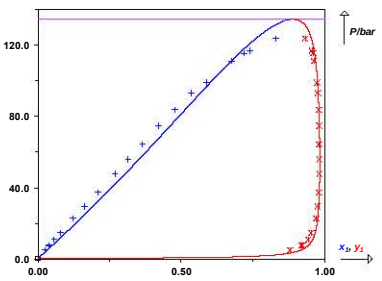

T/K = 333.20



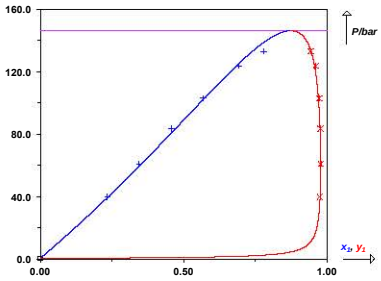
T/K = 335.05



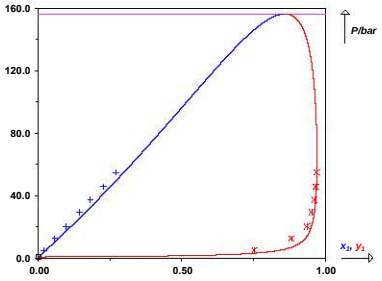

T/K = 353.18



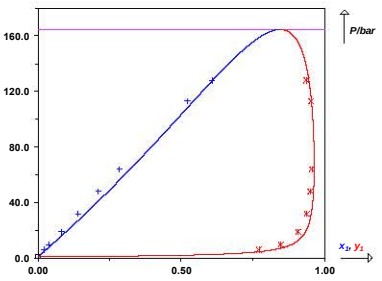

T/K = 363.20



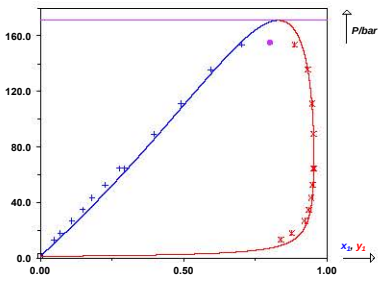

T/K = 373.20



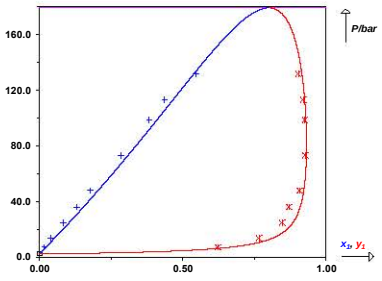

T/K = 383.15



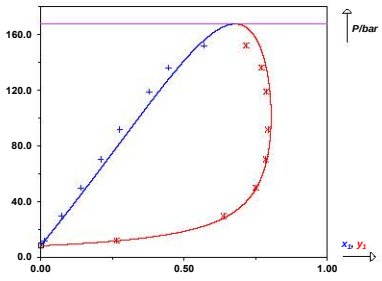

T/K = 393.20




T/K = 413.15




T/K = 477.04



## CARBON DIOXIDE (1) + n-DECANE (2)

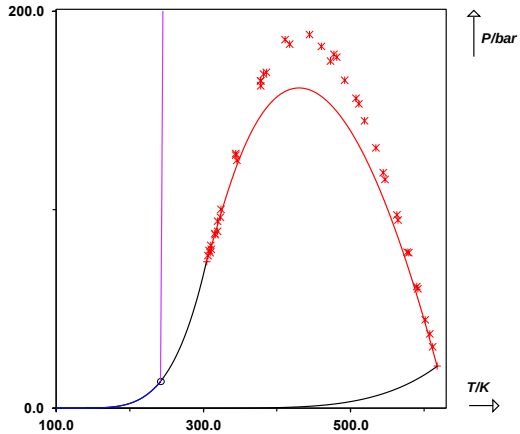
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 124-18-5 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | DIOQZVSQGTUSAI-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 617.70 |
| **$P_c$ / bar** | 73.83 | 21.10 |
| **ω** | 0.2240 | 0.4920 |

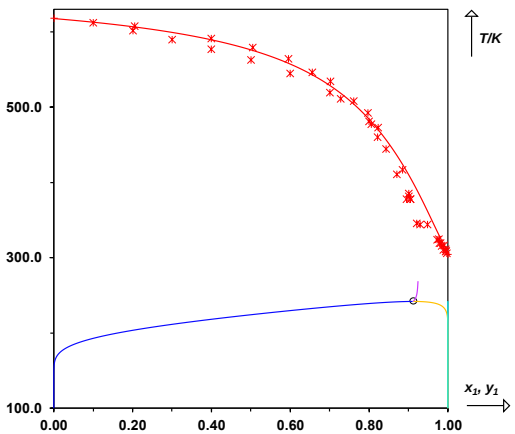
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 165
B/MPa = 782

*Deviations*
MAPE on x = 26 %
MAPE on y = 15 %
MAPE on $x_c$ = 13 %
MAPE on $P_c$ = 8 %
MAPE on $h^M$ = 250 %



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**Isothermal phase equilibrium data**

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Jiménez-Gallegos, R. - Galicia-Luna, L. A. - Elizalde-Solis, O., Experimental Vapor−Liquid Equilibria for the Carbon Dioxide + Octane and Carbon Dioxide + Decane Systems, Journal of Chemical & Engineering Data 5 (2006) 1624-1628. doi:10.1021/je060111z

**T / K = 319.11**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.85 | 0.3395 | 0.9991 |
| 45.49 | 0.4243 | 0.9990 |
| 56.78 | 0.5262 | 0.9988 |
| 68.74 | 0.6338 | 0.9980 |
| 78.80 | 0.7336 | 0.9961 |
| 85.09 | 0.8847 | 0.9926 |
| 86.78 | 0.9240 | 0.9889 |
| 89.02 | 0.9731 | 0.9868 |

Iwai, Yoshio - Hosotani, Noriaki - Morotomi, Tatsuo - Koga, Yoshio - Arai, Yasuhiko, High-Pressure Vapor-Liquid Equilibria for Carbon Dioxide + Linalool, Journal of Chemical & Engineering Data 4 (1994) 900-902. doi:10.1021/je00016a059

**T / K = 344.30**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 55.10 | 0.3834 | 0.9975 |
| 85.50 | 0.5936 | 0.9968 |
| 118.50 | 0.8058 | 0.9877 |

Nagarajan, N. - Robinson, R. L., Equilibrium phase compositions, phase densities, and interfacial tensions for carbon dioxide + hydrocarbon systems. 2. Carbon dioxide + n-decane, Journal of Chemical & Engineering Data 2 (1986) 168-171. doi:10.1021/je00044a012

**T / K = 344.30**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 89.60 | 0.6150 | 0.9940 |
| 96.50 | 0.6570 | 0.9930 |
| 103.40 | 0.7020 | 0.9900 |
| 110.20 | 0.7530 | 0.9870 |
| 113.80 | 0.7750 | 0.9860 |
| 117.30 | 0.8040 | 0.9830 |
| 119.00 | 0.8150 | 0.9810 |
| 120.70 | 0.8340 | 0.9790 |
| 122.20 | 0.8470 | 0.9760 |
| 124.00 | 0.8660 | 0.9710 |
| 124.90 | 0.8770 | 0.9680 |
| 125.50 | 0.8830 | 0.9650 |
| 126.20 | 0.8860 | 0.9600 |
| 126.70 | 0.8930 | 0.9550 |
| 127.00 | 0.8970 | 0.9530 |
| 127.30 | 0.9180 | 0.9350 |

Iwai, Yoshio - Hosotani, Noriaki - Morotomi, Tatsuo - Koga, Yoshio - Arai, Yasuhiko, High-Pressure Vapor-Liquid Equilibria for Carbon Dioxide + Linalool, Journal of Chemical & Engineering Data 4 (1994) 900-902. doi:10.1021/je00016a059

**T / K = 377.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.79 | 0.0931 | 0.9892 |
| 27.58 | 0.1774 | 0.9926 |
| 41.37 | 0.2549 | 0.9933 |
| 86.19 | 0.4798 | 0.9931 |
| 103.42 | 0.5602 | 0.9912 |
| 120.66 | 0.6394 | 0.9877 |
| 137.90 | 0.7173 | 0.9789 |
| 155.13 | 0.7968 | 0.9640 |

Iwai, Yoshio - Hosotani, Noriaki - Morotomi, Tatsuo - Koga, Yoshio - Arai, Yasuhiko, High-Pressure Vapor-Liquid Equilibria for Carbon Dioxide + Linalool, Journal of Chemical & Engineering Data 4 (1994) 900-902. doi:10.1021/je00016a059

**T / K = 410.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.79 | 0.0796 | 0.9677 |
| 27.58 | 0.1548 | 0.9797 |
| 41.37 | 0.2240 | 0.9830 |
| 55.16 | 0.2879 | 0.9848 |
| 68.95 | 0.3476 | 0.9850 |
| 86.19 | 0.4183 | 0.9849 |
| 103.42 | 0.4878 | 0.9831 |
| 120.66 | 0.5576 | 0.9804 |
| 137.90 | 0.6277 | 0.9748 |
| 155.13 | 0.6954 | 0.9633 |
| 172.37 | 0.7635 | 0.9436 |

Iwai, Yoshio - Hosotani, Noriaki - Morotomi, Tatsuo - Koga, Yoshio - Arai, Yasuhiko, High-Pressure Vapor-Liquid Equilibria for Carbon Dioxide + Linalool, Journal of Chemical & Engineering Data 4 (1994) 900-902. doi:10.1021/je00016a059

**T / K = 444.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.79 | 0.0683 | 0.9182 |
| 27.58 | 0.1372 | 0.9517 |
| 41.37 | 0.2018 | 0.9617 |
| 55.16 | 0.2623 | 0.9657 |
| 68.95 | 0.3195 | 0.9672 |
| 86.19 | 0.3865 | 0.9674 |

| | | |
|---|---|---|
| 103.42 | 0.4510 | 0.9652 |
| 120.66 | 0.5156 | 0.9614 |
| 137.90 | 0.5795 | 0.9548 |
| 155.13 | 0.6461 | 0.9427 |
| 172.37 | 0.7170 | 0.9220 |

Iwai, Yoshio - Hosotani, Noriaki - Morotomi, Tatsuo - Koga, Yoshio - Arai, Yasuhiko, High-Pressure Vapor-Liquid Equilibria for Carbon Dioxide + Linalool, Journal of Chemical & Engineering Data 4 (1994) 900-902. doi:10.1021/je00016a059

**T / K = 477.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.79 | 0.0578 | 0.8231 |
| 27.58 | 0.1238 | 0.9017 |
| 41.37 | 0.1861 | 0.9255 |
| 55.16 | 0.2445 | 0.9346 |
| 68.95 | 0.2993 | 0.9377 |
| 86.19 | 0.3650 | 0.9379 |
| 103.42 | 0.4304 | 0.9353 |
| 120.66 | 0.4952 | 0.9292 |
| 137.90 | 0.5605 | 0.9177 |
| 155.13 | 0.6287 | 0.8978 |
| 172.37 | 0.7178 | 0.8545 |

Iwai, Yoshio - Hosotani, Noriaki - Morotomi, Tatsuo - Koga, Yoshio - Arai, Yasuhiko, High-Pressure Vapor-Liquid Equilibria for Carbon Dioxide + Linalool, Journal of Chemical & Engineering Data 4 (1994) 900-902. doi:10.1021/je00016a059

**T / K = 510.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.79 | 0.0450 | 0.6548 |
| 27.58 | 0.1104 | 0.8116 |
| 41.37 | 0.1730 | 0.8578 |
| 55.16 | 0.2308 | 0.8684 |
| 68.95 | 0.2868 | 0.8724 |
| 86.19 | 0.3550 | 0.8739 |
| 103.42 | 0.4206 | 0.8706 |
| 120.66 | 0.4880 | 0.8608 |
| 137.90 | 0.5717 | 0.8347 |

Inomata, Hiroshi - Tuchiya, Kazuhiro - Arai, Kunio - Saito, Shozaburo, Measurement of vapor-liquid equilibria at elevated temperatures and pressures using a flow type apparatus., Journal of Chemical Engineering of Japan 5 (1986) 386-391. doi:10.1252/jcej.19.386

**T / K = 520.40**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 30.90 | 0.1110 | 0.7990 |
| 46.10 | 0.1870 | 0.8320 |
| 60.80 | 0.2470 | 0.8510 |
| 90.50 | 0.3760 | 0.8650 |
| 119.10 | 0.4930 | 0.8400 |
| 139.70 | 0.6060 | 0.7830 |

Sebastian, Herbert M. - Simnick, James J. - Lin, Ho-Mu - Chao, Kwang-Chu, Vapor-liquid equilibrium in binary mixtures of carbon dioxide + n-decane and carbon dioxide + n-hexadecane, Journal of Chemical & Engineering Data 2 (1980) 138-140. doi:10.1021/je60085a012

**T / K = 542.95**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 19.64 | 0.0656 | 0.5700 |
| 30.02 | 0.1147 | 0.6818 |
| 40.02 | 0.1628 | 0.7357 |
| 51.68 | 0.2145 | 0.7655 |

Sebastian, Herbert M. - Simnick, James J. - Lin, Ho-Mu - Chao, Kwang-Chu, Vapor-liquid equilibrium in binary mixtures of carbon dioxide + n-decane and carbon dioxide + n-hexadecane, Journal of Chemical & Engineering Data 2 (1980) 138-140. doi:10.1021/je60085a012

**T / K = 583.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.02 | 0.0427 | 0.2489 |
| 30.40 | 0.0974 | 0.4115 |
| 41.04 | 0.1558 | 0.5015 |
| 51.07 | 0.2125 | 0.5419 |

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**Enthalpy of mixing**

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Pando, C. - Renuncio, J.A.R. - McFall, T.A. - Izatt, R.M. - Christensen, J.J., The excess enthalpies of (carbon dioxide + decane) from 283.15 to 323.15 K at 7.58 MPa, The Journal of Chemical Thermodynamics 2 (1983) 173-180. doi:10.1016/0021-9614(83)90157-X

**T / K = 283.15**

**P / bar = 75.80**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 293.00 | 0.0631 |
| 411.00 | 0.0631 |
| 627.00 | 0.1480 |
| 890.00 | 0.1480 |
| 974.00 | 0.2230 |
| 977.00 | 0.2230 |
| 1155.0 | 0.2897 |
| 1321.0 | 0.3495 |
| 1336.0 | 0.3495 |

| | |
|---|---|
| 1424.0 | 0.4033 |
| 1441.0 | 0.4521 |
| 1476.0 | 0.4964 |
| 1446.0 | 0.5369 |
| 1412.0 | 0.6083 |
| 1375.0 | 0.6692 |
| 1329.0 | 0.6692 |
| 1241.0 | 0.7217 |
| 1274.0 | 0.7217 |
| 1146.0 | 0.7674 |
| 1002.0 | 0.8077 |
| 1002.0 | 0.8077 |
| 901.00 | 0.8434 |
| 749.00 | 0.8752 |
| 762.00 | 0.8752 |
| 619.00 | 0.9038 |
| 461.00 | 0.9296 |
| 471.00 | 0.9296 |
| 333.00 | 0.9530 |
| 166.00 | 0.9743 |
| 175.00 | 0.9743 |

Pando, C. - Renuncio, J.A.R. - McFall, T.A. - Izatt, R.M. - Christensen, J.J., The excess enthalpies of (carbon dioxide + decane) from 283.15 to 323.15 K at 7.58 MPa, The Journal of Chemical Thermodynamics 2 (1983) 173-180. doi:10.1016/0021-9614(83)90157-X

| **T / K =** | **308.15** |
|---|---|
| **P / bar =** | **75.80** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| -246.00 | 0.0631 |
| -182.00 | 0.0631 |
| -457.00 | 0.1209 |
| -354.00 | 0.1209 |
| -563.00 | 0.1480 |
| -442.00 | 0.1480 |
| -723.00 | 0.2230 |
| -1097.0 | 0.2897 |
| -1205.0 | 0.3495 |
| -1442.0 | 0.4033 |
| -1612.0 | 0.4522 |
| -1870.0 | 0.4996 |
| -2117.0 | 0.5371 |
| -2572.0 | 0.6083 |
| -2920.0 | 0.6693 |
| -3228.0 | 0.7218 |
| -3516.0 | 0.7676 |
| -3839.0 | 0.8078 |
| -4064.0 | 0.8435 |
| -4291.0 | 0.8753 |
| -4434.0 | 0.9038 |
| -4750.0 | 0.9296 |
| -4490.0 | 0.9530 |
| -3761.0 | 0.9603 |
| -3010.0 | 0.9675 |
| -1276.0 | 0.9843 |
| -5.100 | 0.9939 |

Pando, C. - Renuncio, J.A.R. - McFall, T.A. - Izatt, R.M. - Christensen, J.J., The excess enthalpies of (carbon dioxide + decane) from 283.15 to 323.15 K at 7.58 MPa, The Journal of Chemical Thermodynamics 2 (1983) 173-180. doi:10.1016/0021-9614(83)90157-X

| **T / K =** | **323.15** |
|---|---|
| **P / bar =** | **75.80** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| -464.00 | 0.0631 |
| -428.00 | 0.0631 |
| -453.00 | 0.0631 |
| -778.00 | 0.1480 |
| -1053.0 | 0.2230 |
| -1422.0 | 0.2897 |
| -1697.0 | 0.3495 |
| -2226.0 | 0.4521 |
| -2214.0 | 0.4521 |
| -2458.0 | 0.4964 |
| -2644.0 | 0.5369 |
| -2617.0 | 0.5369 |
| -3006.0 | 0.6083 |
| -3106.0 | 0.6692 |
| -2660.0 | 0.7217 |
| -2175.0 | 0.7674 |
| -1808.0 | 0.8077 |
| -1146.0 | 0.8752 |
| -851.00 | 0.9038 |
| -612.00 | 0.9296 |
| -412.00 | 0.9530 |
| -168.00 | 0.9743 |
| 4.900 | 0.9939 |

Christensen, J.J. - Cordray, D. - Izatt, R.M., The excess enthalpies of (carbon dioxide + decane) from 293.15 to 573.15 K at 12.50 MPa, The Journal of Chemical Thermodynamics 1 (1986) 53-61. doi:10.1016/0021-9614(86)90043-1

| **T / K =** | **470.15** |
|---|---|
| **P / bar =** | **125.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| -124.00 | 0.0705 |

| | |
|---|---|
| -211.00 | 0.1340 |
| -280.00 | 0.1917 |
| -322.00 | 0.2442 |
| -369.00 | 0.2922 |
| -398.00 | 0.3363 |
| -405.00 | 0.3769 |
| -419.00 | 0.4144 |
| -414.00 | 0.4492 |
| -392.00 | 0.4815 |
| -326.00 | 0.5117 |
| -215.00 | 0.5399 |
| -143.00 | 0.5662 |
| -43.00 | 0.5910 |
| 11.00 | 0.6142 |
| 168.00 | 0.6568 |
| 321.00 | 0.6948 |
| 408.00 | 0.7290 |
| 510.00 | 0.7599 |
| 673.00 | 0.8010 |
| 694.00 | 0.8135 |
| 825.00 | 0.8584 |
| 898.00 | 0.8685 |
| 911.00 | 0.8782 |
| 1000.0 | 0.8876 |
| 1010.0 | 0.8876 |
| 1000.0 | 0.8966 |
| 1010.0 | 0.9052 |
| 1030.0 | 0.9136 |
| 997.00 | 0.9136 |
| 1060.0 | 0.9217 |
| 1120.0 | 0.9294 |
| 1110.0 | 0.9294 |
| 961.00 | 0.9442 |
| 746.00 | 0.9580 |
| 526.00 | 0.9710 |
| 328.00 | 0.9831 |

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**Critical point**

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Gurdial, Gurdev S. - Foster, Neil R. - Yun, S. L. Jimmy - Tilly, Kevin D., Phase Behavior of Supercritical Fluid—Entrainer Systems, Supercritical Fluid Engineering Science (1992) 34-45.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 305.90 | 77.00 | 0.9971 |
| 307.80 | 79.40 | 0.9941 |
| 310.00 | 82.10 | 0.9880 |
| 315.20 | 88.00 | 0.9845 |
| 319.50 | 94.30 | 0.9809 |
| 324.20 | 100.30 | 0.9773 |

Gulari, Es. - Saad, H. - Bae, Y. C., Effect of Critical Phenomena on Transport Properties in the Supercritical Region, Supercritical Fluids (1987) 2-14.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 323.37 | 96.10 | 0.9720 |
| 319.10 | 89.00 | 0.9790 |
| 316.20 | 87.30 | 0.9900 |
| 309.01 | 78.20 | 0.9960 |

Juntarachat, Niramol - Bello, Salma - Privat, Romain - Jaubert, Jean-Noël, Validation of a new apparatus using the dynamic method for determining the critical properties of binary mixtures containing CO2 and a n-alkane, Fluid Phase Equilibria (2012) 66-70. doi:10.1016/j.fluid.2012.04.010

| T / K | P / bar | $x_1$ |
|---|---|---|
| 607.32 | 37.39 | 0.2051 |
| 591.43 | 60.21 | 0.3987 |
| 578.84 | 78.36 | 0.5048 |
| 564.13 | 94.83 | 0.5946 |
| 546.30 | 115.24 | 0.6555 |
| 534.04 | 131.23 | 0.7016 |
| 507.65 | 156.15 | 0.7613 |
| 492.23 | 165.09 | 0.7970 |
| 472.75 | 175.01 | 0.8223 |
| 416.86 | 183.36 | 0.8852 |
| 385.23 | 169.22 | 0.9008 |
| 345.41 | 124.85 | 0.9201 |

Reamer, H. H. - Sage, B. H., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the n-Decane-CO2 System., Journal of Chemical & Engineering Data 4 (1963) 508-513. doi:10.1021/je60019a010

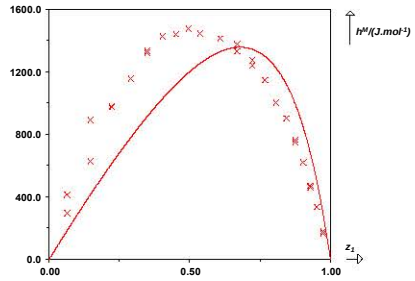
| T / K | P / bar | $x_1$ |
|---|---|---|
| 310.93 | 79.98 | 0.9946 |
| 344.26 | 128.24 | 0.9477 |
| 377.59 | 164.92 | 0.9046 |
| 410.93 | 185.61 | 0.8705 |
| 444.26 | 188.36 | 0.8430 |
| 477.59 | 178.37 | 0.8050 |
| 510.93 | 153.34 | 0.7280 |
| 611.76 | 30.89 | 0.1000 |
| 601.76 | 44.61 | 0.2000 |
| 589.54 | 61.36 | 0.3000 |
| 577.04 | 78.60 | 0.4000 |
| 563.01 | 97.22 | 0.5000 |
| 544.68 | 118.59 | 0.6000 |

| | | |
|---|---|---|
| 519.26 | 144.86 | 0.7000 |
| 480.79 | 176.78 | 0.8000 |
| 381.48 | 168.37 | 0.9000 |

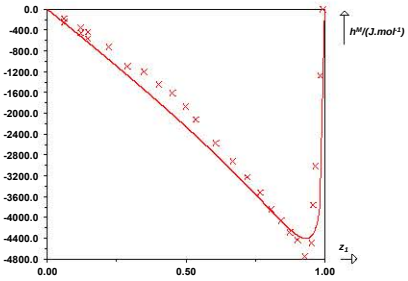
Polikhronidi, N. G. - Batyrova, R. G. - Abdulagatov, I. M. - Stepanov, G. V., Isochoric Heat Capacity of CO2 + n-Decane Mixtures in the Critical Region, International Journal of Thermophysics 3 (2006) 729-759. doi:10.1007/s10765-006-0056-z

| T / K | P / bar | $x_1$ |
|---|---|---|
| 377.50 | 162.50 | 0.9050 |
| 460.15 | 182.30 | 0.8220 |

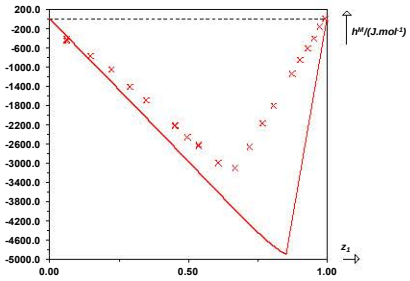
T/K = 283.15 - P/bar = 75.800



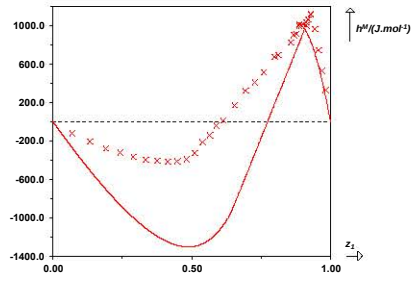

T/K = 308.15 - P/bar = 75.800



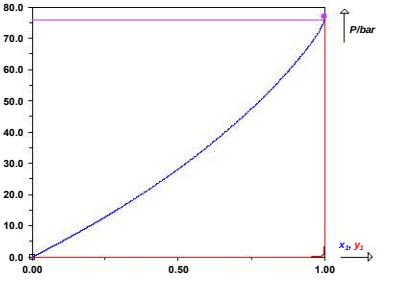

T/K = 323.15 - P/bar = 75.800



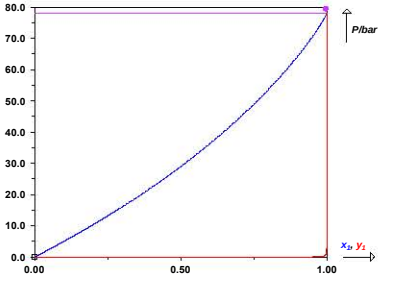

T/K = 470.15 - P/bar = 125.00



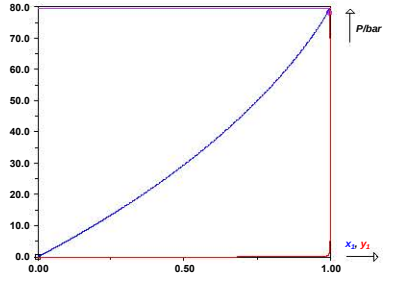

T/K = 305.90



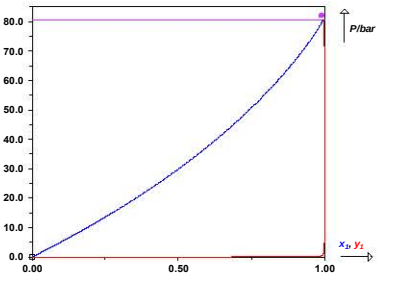

T/K = 307.80



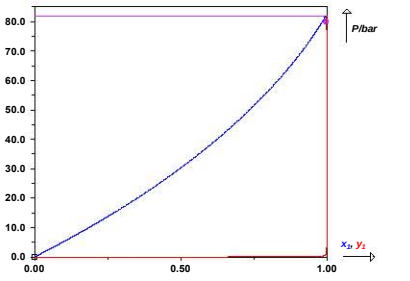

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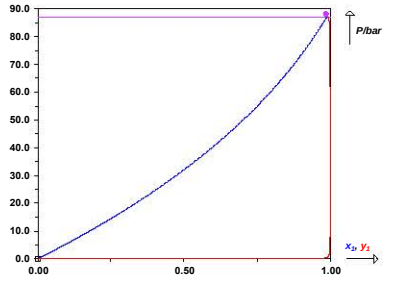

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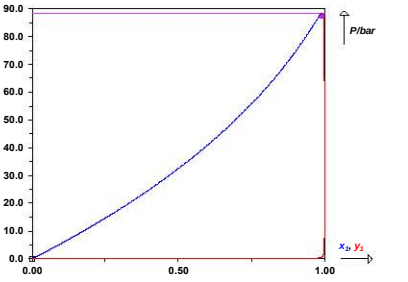

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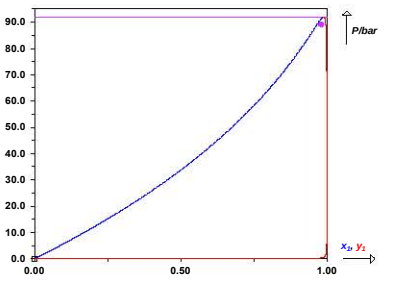

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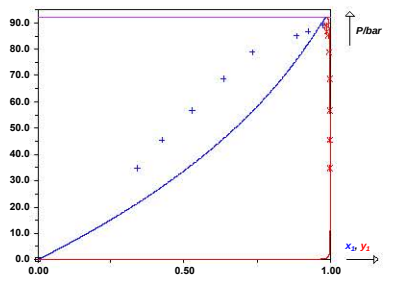

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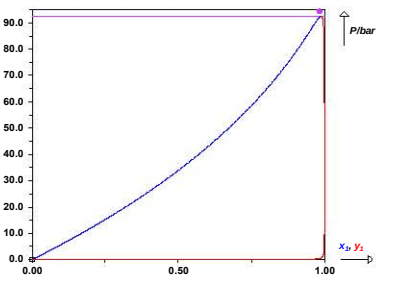

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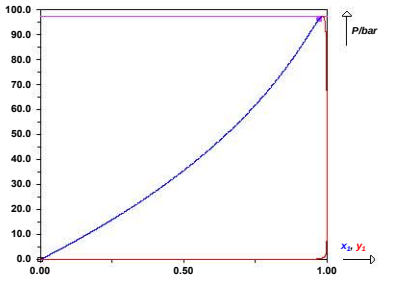

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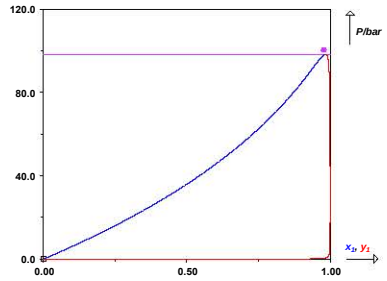

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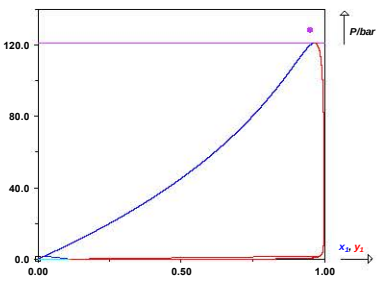

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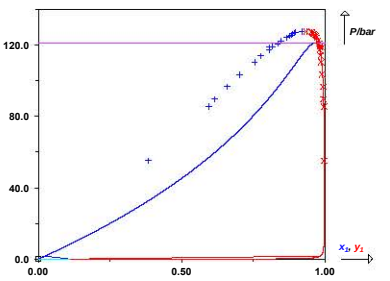
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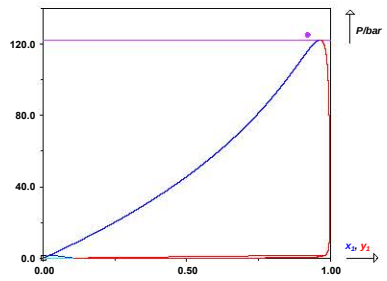

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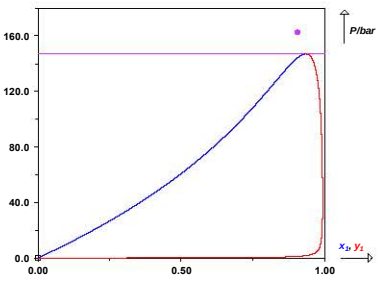

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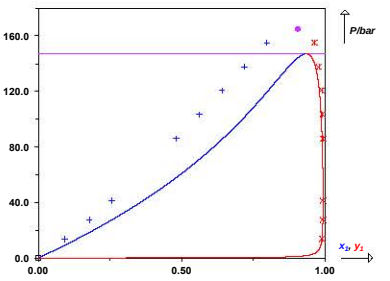

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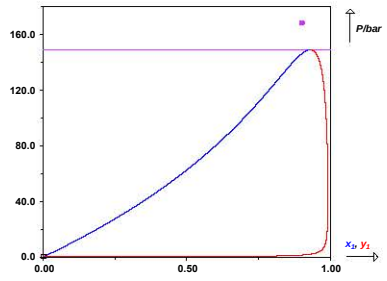

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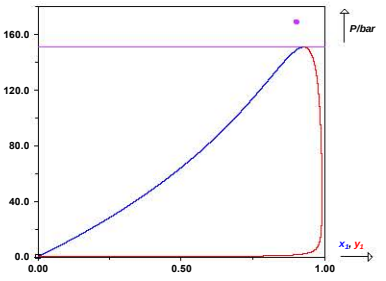

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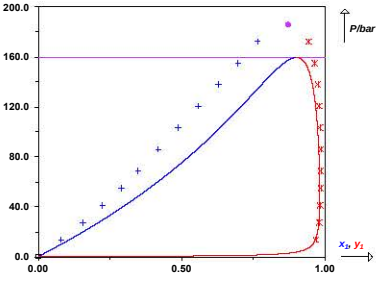

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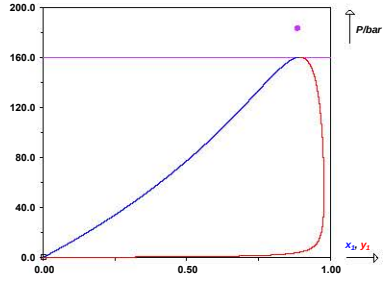

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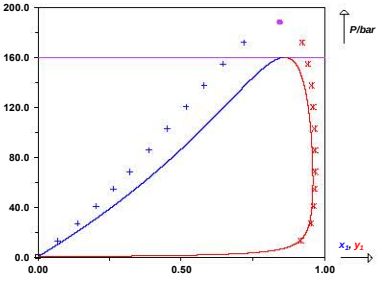

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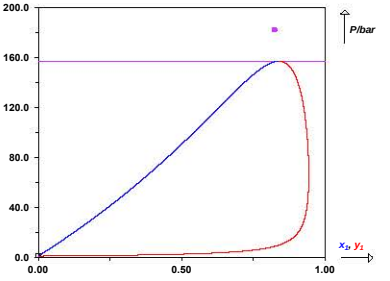

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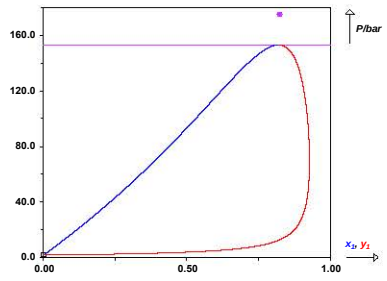

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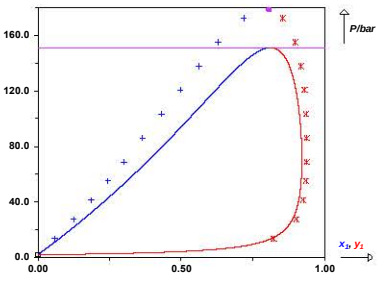

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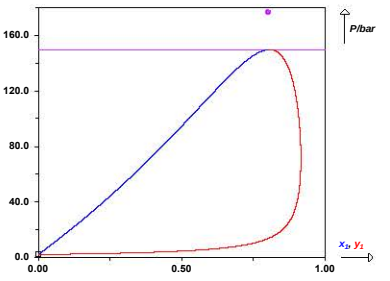

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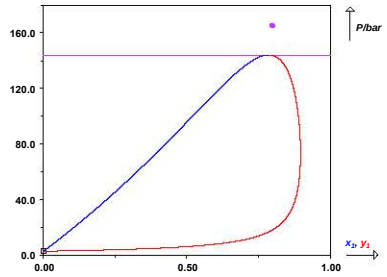

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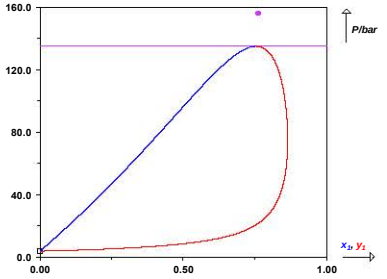

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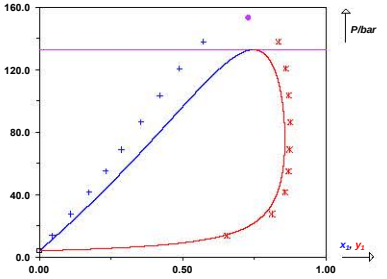
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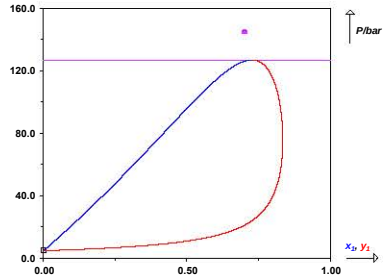

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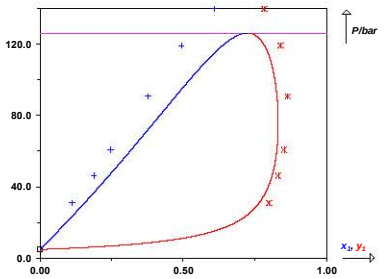

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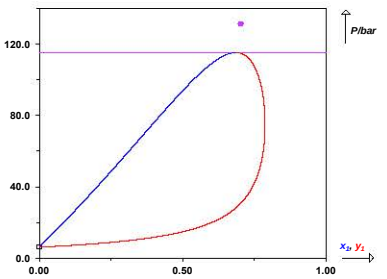

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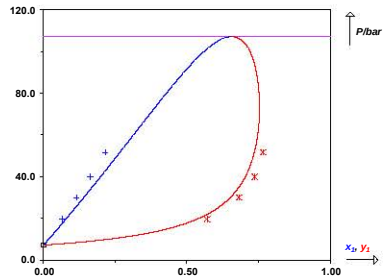

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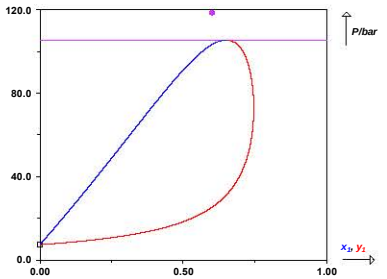

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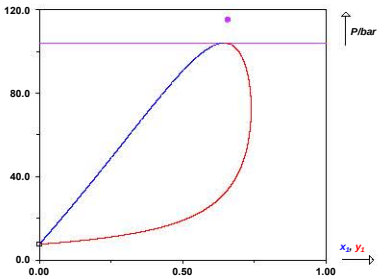

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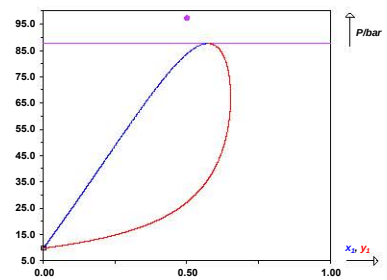

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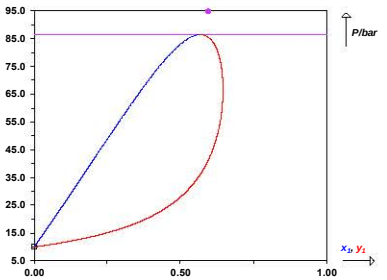

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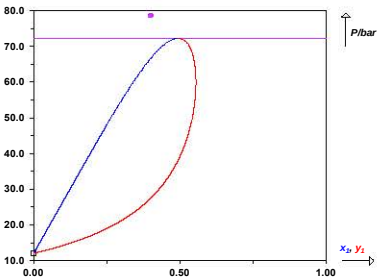

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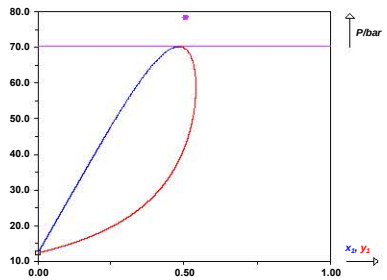

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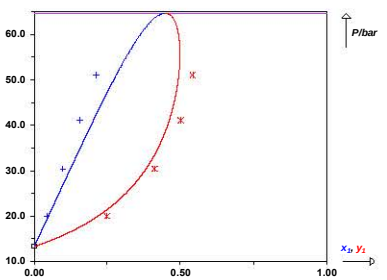

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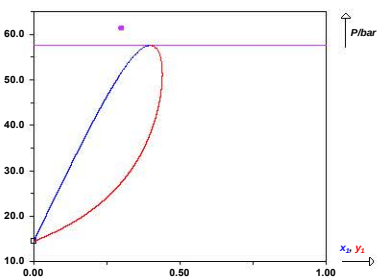

T/K = 578.84

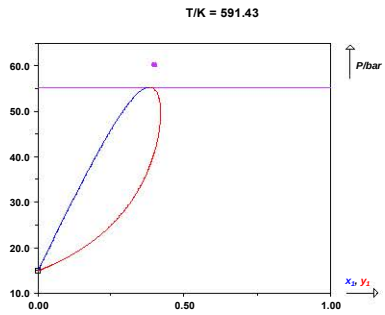


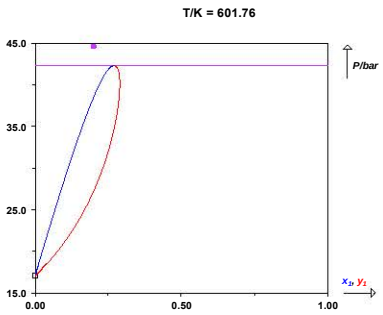

T/K = 583.65

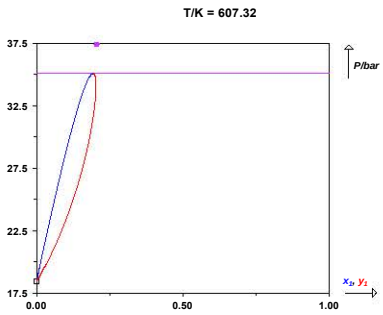


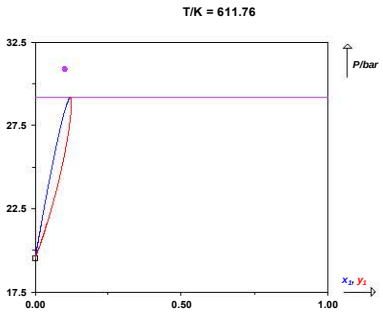

T/K = 589.54




T/K = 591.43
P/bar
60.0
50.0
40.0
30.0
20.0
10.0
0.00
0.50
1.00
x1, y1


T/K = 601.76
P/bar
45.0
35.0
25.0
15.0
0.00
0.50
1.00
x1, y1


T/K = 607.32
P/bar
37.5
32.5
27.5
22.5
17.5
0.00
0.50
1.00
x1, y1


T/K = 611.76
P/bar
32.5
27.5
22.5
17.5
0.00
0.50
1.00
x1, y1

## METHANE (1) + CARBON DIOXIDE (2)

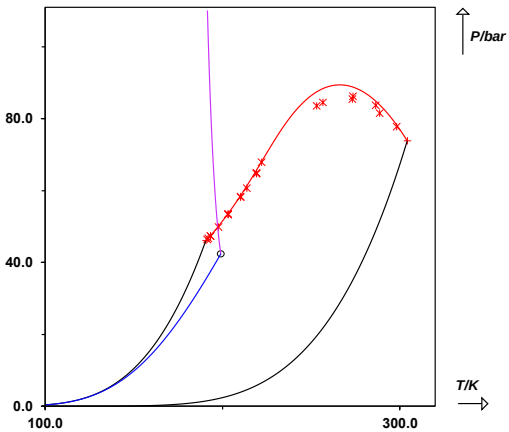
| | | |
|---|---|---|
| **CAS** | 74-82-8 | 124-38-9 |
| **InChiKey** | VNWKTOKETHGBQD-UHFFFAOYSA-N | CURLTUGMZLYLDI-UHFFFAOYSA-N |
| **$T_c$ / K** | 190.56 | 304.21 |
| **$P_c$ / bar** | 45.99 | 73.83 |
| **ω** | 0.0120 | 0.2240 |

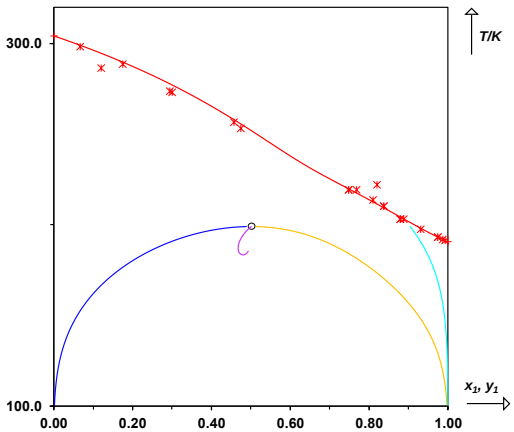
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 380
B/MPa = 699

*Deviations*
MAPE on x = 5.8 %
MAPE on y = 2.6 %
MAPE on $x_c$ = 360 %
MAPE on $P_c$ = 21 %
MAPE on $h^M$ = 8.6 %



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**Isothermal phase equilibrium data**

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Mraw, Stephen C. - Hwang, Shuen-Cheng - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-carbon dioxide system at low temperatures, Journal of Chemical & Engineering Data 2 (1978) 135-139. doi:10.1021/je60077a014

**T / K = 173.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 24.66 | 0.9507 | 0.9896 |
| 24.82 | 0.9563 | 0.9908 |
| 25.17 | 0.9686 | 0.9934 |
| 25.51 | 0.9809 | 0.9960 |

Mraw, Stephen C. - Hwang, Shuen-Cheng - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-carbon dioxide system at low temperatures, Journal of Chemical & Engineering Data 2 (1978) 135-139. doi:10.1021/je60077a014

**T / K = 183.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 33.60 | 0.9350 | 0.9770 |
| 33.78 | 0.9393 | 0.9785 |
| 34.47 | 0.9553 | 0.9842 |
| 35.16 | 0.9712 | 0.9898 |
| 35.85 | 0.9872 | 0.9955 |

Mraw, Stephen C. - Hwang, Shuen-Cheng - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-carbon dioxide system at low temperatures, Journal of Chemical & Engineering Data 2 (1978) 135-139. doi:10.1021/je60077a014

**T / K = 193.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 42.89 | 0.8853 | 0.9473 |
| 43.44 | 0.8992 | 0.9507 |
| 44.13 | 0.9136 | 0.9554 |
| 44.82 | 0.9272 | 0.9591 |
| 45.51 | 0.9385 | 0.9635 |
| 46.20 | 0.9517 | 0.9677 |
| 46.88 | 0.9622 | 0.9718 |

Mraw, Stephen C. - Hwang, Shuen-Cheng - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-carbon dioxide system at low temperatures, Journal of Chemical & Engineering Data 2 (1978) 135-139. doi:10.1021/je60077a014

**T / K = 203.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 48.26 | 0.7307 | 0.8914 | |
| 48.95 | 0.7491 | 0.8952 | |
| 49.64 | 0.7683 | 0.8962 | |
| 50.33 | 0.7879 | 0.8973 | |
| 51.02 | 0.8051 | 0.8976 | |
| 51.71 | 0.8229 | 0.8978 | |
| 52.40 | 0.8388 | 0.8967 | |
| 53.09 | 0.8568 | 0.8933 | |
| 53.37 | 0.8784 | 0.8784 | CRIT |

Mraw, Stephen C. - Hwang, Shuen-Cheng - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-carbon dioxide system at low temperatures, Journal of Chemical & Engineering Data 2 (1978) 135-139. doi:10.1021/je60077a014

**T / K = 210.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 42.20 | 0.3062 | 0.8482 |
| 43.09 | 0.3175 | 0.8568 |
| 44.82 | 0.3604 | 0.8587 |
| 46.54 | 0.4056 | 0.8596 |
| 48.26 | 0.4555 | 0.8602 |
| 49.99 | 0.5205 | 0.8609 |
| 51.71 | 0.5881 | 0.8610 |
| 53.43 | 0.6486 | 0.8608 |
| 55.16 | 0.7018 | 0.8587 |
| 56.88 | 0.7544 | 0.8539 |

Al-Sahhaf, Taher A. - Kidnay, Arthur J. - Sloan, E. Dendy, Liquid + vapor equilibriums in the nitrogen + carbon dioxide + methane system, Industrial & Engineering Chemistry Fundamentals 4 (1983) 372-380. doi:10.1021/i100012a004

**T / K = 219.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.98 | 0.0339 | 0.5457 |
| 19.00 | 0.0579 | 0.6493 |
| 24.32 | 0.0859 | 0.7100 |
| 31.20 | 0.1308 | 0.7590 |
| 38.61 | 0.1923 | 0.7890 |

Mraw, Stephen C. - Hwang, Shuen-Cheng - Kobayashi, Riki, Vapor-liquid equilibrium of the methane-carbon dioxide system at low temperatures, Journal of Chemical & Engineering Data 2 (1978) 135-139. doi:10.1021/je60077a014

**T / K = 219.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0049 | 0.1860 |
| 13.79 | 0.0355 | 0.5461 |
| 20.68 | 0.0681 | 0.6745 |
| 27.58 | 0.1054 | 0.7384 |
| 34.47 | 0.1535 | 0.7740 |

| | | |
|---|---|---|
| 41.37 | 0.2180 | 0.7960 |
| 48.26 | 0.3056 | 0.8078 |
| 55.16 | 0.4368 | 0.8115 |
| 62.05 | 0.6204 | 0.8027 |
| 63.43 | 0.6620 | 0.7948 |

Wei, Michael S.-W. - Brown, Trent S. - Kidnay, Arthur J. - Sloan, E. Dendy, Vapor + Liquid Equilibria for the Ternary System Methane + Ethane + Carbon Dioxide at 230 K and Its Constituent Binaries at Temperatures from 207 to 270 K, Journal of Chemical & Engineering Data 4 (1995) 726-731. doi:10.1021/je00020a002

**T / K = 230.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.78 | 0.0070 | 0.1553 |
| 14.53 | 0.0221 | 0.3480 |
| 17.86 | 0.0365 | 0.4550 |
| 20.92 | 0.0503 | 0.5218 |
| 25.51 | 0.0730 | 0.5929 |
| 29.16 | 0.0920 | 0.6320 |
| 35.03 | 0.1269 | 0.6770 |
| 39.68 | 0.1577 | 0.7005 |
| 45.65 | 0.2042 | 0.7237 |
| 51.16 | 0.2560 | 0.7368 |
| 56.40 | 0.3171 | 0.7449 |
| 58.55 | 0.3416 | 0.7466 |
| 60.86 | 0.3805 | 0.7461 |
| 63.53 | 0.4187 | 0.7448 |
| 65.86 | 0.4523 | 0.7411 |
| 66.63 | 0.4762 | 0.7369 |
| 67.36 | 0.4952 | 0.7338 |
| 69.01 | 0.5407 | 0.7247 |
| 69.91 | 0.5814 | 0.7004 |
| 11.50 | 0.0209 | 0.1941 |
| 15.20 | 0.0282 | 0.3766 |
| 25.30 | 0.0719 | 0.5851 |
| 35.50 | 0.1302 | 0.6792 |
| 45.60 | 0.2037 | 0.7200 |
| 55.70 | 0.3018 | 0.7393 |
| 64.90 | 0.4362 | 0.7381 |
| 65.90 | 0.4511 | 0.7423 |

Webster, Leigh A. - Kidnay, Arthur J., Vapor−Liquid Equilibria for the Methane−Propane−Carbon Dioxide Systems at 230 K and 270 K, Journal of Chemical & Engineering Data 3 (2001) 759-764. doi:10.1021/je000307d

**T / K = 230.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 14.20 | 0.0213 | 0.3385 |
| 16.51 | 0.0307 | 0.4196 |
| 19.31 | 0.0441 | 0.4900 |
| 22.57 | 0.0597 | 0.5512 |
| 24.88 | 0.0714 | 0.5851 |
| 33.75 | 0.1199 | 0.6670 |
| 40.03 | 0.1617 | 0.7012 |
| 44.97 | 0.1994 | 0.7199 |
| 55.73 | 0.3093 | 0.7432 |
| 58.36 | 0.3404 | 0.7454 |
| 62.41 | 0.4010 | 0.7443 |
| 64.17 | 0.4323 | 0.7442 |
| 65.12 | 0.4530 | 0.7422 |
| 66.54 | 0.4815 | 0.7382 |
| 66.49 | 0.4862 | 0.7371 |
| 69.12 | 0.5302 | 0.7286 |
| 69.70 | 0.5393 | 0.7245 |
| 70.00 | 0.5480 | 0.7217 |
| 70.04 | 0.5521 | 0.7222 |
| 70.72 | 0.5682 | 0.7156 |
| 71.12 | 0.5774 | 0.7102 |
| 71.45 | 0.5888 | 0.7066 |

Al-Sahhaf, Taher A. - Kidnay, Arthur J. - Sloan, E. Dendy, Liquid + vapor equilibriums in the nitrogen + carbon dioxide + methane system, Industrial & Engineering Chemistry Fundamentals 4 (1983) 372-380. doi:10.1021/i100012a004

**T / K = 240.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 21.04 | 0.0328 | 0.3480 |
| 30.59 | 0.0761 | 0.5160 |
| 40.89 | 0.1315 | 0.6050 |
| 51.98 | 0.2074 | 0.6550 |
| 61.20 | 0.2873 | 0.6742 |
| 66.57 | 0.3475 | 0.6771 |
| 70.73 | 0.4016 | 0.6728 |
| 72.65 | 0.4315 | 0.6672 |
| 73.97 | 0.4525 | 0.6624 |
| 75.94 | 0.4914 | 0.6473 |
| 76.60 | 0.5048 | 0.6388 |
| 77.72 | 0.5475 | 0.6199 |

Wei, Michael S.-W. - Brown, Trent S. - Kidnay, Arthur J. - Sloan, E. Dendy, Vapor + Liquid Equilibria for the Ternary System Methane + Ethane + Carbon Dioxide at 230 K and Its Constituent Binaries at Temperatures from 207 to 270 K, Journal of Chemical & Engineering Data 4 (1995) 726-731. doi:10.1021/je00020a002

**T / K = 250.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|

| | | |
|---|---|---|
| 19.67 | 0.0065 | 0.0782 |
| 20.71 | 0.0106 | 0.1174 |
| 23.15 | 0.0201 | 0.1952 |
| 24.88 | 0.0269 | 0.2408 |
| 27.59 | 0.0379 | 0.3001 |
| 29.64 | 0.0465 | 0.3381 |
| 31.31 | 0.0536 | 0.3655 |
| 34.46 | 0.0676 | 0.4090 |
| 38.36 | 0.0863 | 0.4533 |
| 42.00 | 0.1041 | 0.4855 |
| 47.92 | 0.1368 | 0.5262 |
| 53.78 | 0.1715 | 0.5559 |
| 61.50 | 0.2246 | 0.5812 |
| 67.15 | 0.2711 | 0.5914 |
| 73.99 | 0.3366 | 0.5856 |
| 76.84 | 0.3718 | 0.5761 |
| 79.83 | 0.4163 | 0.5523 |
| 80.53 | 0.4252 | 0.5408 |

Wei, Michael S.-W. - Brown, Trent S. - Kidnay, Arthur J. - Sloan, E. Dendy, Vapor + Liquid Equilibria for the Ternary System Methane + Ethane + Carbon Dioxide at 230 K and Its Constituent Binaries at Temperatures from 207 to 270 K, Journal of Chemical & Engineering Data 4 (1995) 726-731. doi:10.1021/je00020a002

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 35.58 | 0.0151 | 0.0766 |
| 36.73 | 0.0198 | 0.1047 |
| 38.83 | 0.0305 | 0.1461 |
| 41.46 | 0.0377 | 0.1778 |
| 45.06 | 0.0504 | 0.2203 |
| 49.15 | 0.0724 | 0.2661 |
| 58.51 | 0.1154 | 0.3372 |
| 70.93 | 0.1834 | 0.3942 |
| 78.68 | 0.2407 | 0.4061 |
| 81.97 | 0.2696 | 0.3952 |
| 82.82 | 0.2803 | 0.3887 |
| 83.81 | 0.2995 | 0.3782 |

Webster, Leigh A. - Kidnay, Arthur J., Vapor–Liquid Equilibria for the Methane–Propane–Carbon Dioxide Systems at 230 K and 270 K, Journal of Chemical & Engineering Data 3 (2001) 759-764. doi:10.1021/je000307d

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 38.83 | 0.0264 | 0.1352 |
| 39.13 | 0.0276 | 0.1402 |
| 41.04 | 0.0342 | 0.1680 |
| 44.13 | 0.0477 | 0.2093 |
| 47.87 | 0.0640 | 0.2517 |
| 49.87 | 0.0723 | 0.2706 |
| 54.33 | 0.0919 | 0.3085 |
| 55.03 | 0.0948 | 0.3128 |
| 65.37 | 0.1479 | 0.3702 |
| 69.59 | 0.1739 | 0.3847 |
| 73.05 | 0.1949 | 0.3945 |
| 79.46 | 0.2435 | 0.3977 |
| 80.03 | 0.2490 | 0.3974 |
| 81.31 | 0.2602 | 0.3934 |
| 82.07 | 0.2688 | 0.3894 |
| 83.89 | 0.2901 | 0.3762 |
| 84.19 | 0.2991 | 0.3704 |

Al-Sahhaf, Taher A. - Kidnay, Arthur J. - Sloan, E. Dendy, Liquid + vapor equilibriums in the nitrogen + carbon dioxide + methane system, Industrial & Engineering Chemistry Fundamentals 4 (1983) 372-380. doi:10.1021/i100012a004

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 36.73 | 0.0183 | 0.1048 |
| 38.10 | 0.0235 | 0.1273 |
| 43.87 | 0.0457 | 0.2086 |
| 51.83 | 0.0793 | 0.2885 |
| 59.43 | 0.1167 | 0.3451 |
| 61.56 | 0.1261 | 0.3543 |
| 70.83 | 0.1785 | 0.3901 |
| 79.69 | 0.2463 | 0.3980 |
| 82.23 | 0.2737 | 0.3916 |
| 84.15 | 0.3060 | 0.3742 |

Somait, Fahad A. - Kidnay, Arthur J., Liquid-vapor equilibriums at 270.00 K for systems containing nitrogen, methane, and carbon dioxide, Journal of Chemical & Engineering Data 4 (1978) 301-305. doi:10.1021/je60079a019

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 38.35 | 0.0237 | 0.1269 |
| 43.92 | 0.0455 | 0.2082 |
| 48.79 | 0.0666 | 0.2629 |
| 52.69 | 0.0838 | 0.2962 |
| 60.80 | 0.1226 | 0.3519 |
| 66.27 | 0.1533 | 0.3774 |
| 77.01 | 0.2224 | 0.4006 |
| 82.48 | 0.2740 | 0.3895 |
| 84.32 | 0.3060 | 0.3726 |
| 45.60 | 0.0538 | 0.2300 |

| | | |
|---|---|---|
| 60.80 | 0.1226 | 0.3519 |

Xu, Nanping - Dong, Junhang - Wang, Yanru - Shi, Jun, High pressure vapor liquid equilibria at 293 K for systems containing nitrogen, methane and carbon dioxide, Fluid Phase Equilibria (1992) 175-186. doi:10.1016/0378-3812(92)85150-7

**T / K = 288.50**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 55.90 | 0.0150 | 0.0520 | |
| 62.10 | 0.0420 | 0.1080 | |
| 71.10 | 0.0860 | 0.1670 | |
| 75.10 | 0.1120 | 0.1850 | |
| 78.20 | 0.1280 | 0.1950 | |
| 78.70 | 0.1290 | 0.1940 | |
| 81.50 | 0.1750 | 0.1750 | CRIT |

Xu, N. - Dong, J. - Wang, Y. - Shi, J., Vapor Liquid Equilibria For N2-CH4-CO2 System Near Critical Region, Huagong Xuebao 5 (1992) 640-644.

**T / K = 298.36**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 72.90 | 0.0300 | 0.0560 | |
| 75.00 | 0.0420 | 0.0660 | |
| 76.80 | 0.0520 | 0.0720 | |
| 77.40 | 0.0580 | 0.0710 | |
| 77.80 | 0.0670 | 0.0670 | CRIT |

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**Enthalpy of mixing**

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Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 283.15**

**P / bar = 10.13**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 17.00 | 0.1000 |
| 29.00 | 0.2000 |
| 46.00 | 0.4000 |
| 47.00 | 0.5000 |
| 40.00 | 0.6000 |
| 32.00 | 0.7000 |
| 24.00 | 0.8000 |
| 13.00 | 0.9000 |

Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Direct determination of enthalpy of mixing for the binary gaseous system methane-carbon dioxide by an isothermal flow calorimeter, Journal of Chemical & Engineering Data 3 (1982) 258-264. doi:10.1021/je00029a010

**T / K = 293.15**

**P / bar = 5.070**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 17.90 | 0.2530 |
| 25.63 | 0.4770 |
| 26.39 | 0.5010 |
| 18.45 | 0.8160 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 293.15**

**P / bar = 30.40**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 80.00 | 0.1000 |
| 134.00 | 0.2000 |
| 180.00 | 0.4000 |
| 177.00 | 0.5000 |
| 165.00 | 0.6000 |
| 143.00 | 0.7000 |
| 102.00 | 0.8000 |
| 56.00 | 0.9000 |

Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Direct determination of enthalpy of mixing for the binary gaseous system methane-carbon dioxide by an isothermal flow calorimeter, Journal of Chemical & Engineering Data 3 (1982) 258-264. doi:10.1021/je00029a010

**T / K = 305.15**

**P / bar = 15.20**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 38.85 | 0.1810 |
| 57.82 | 0.4430 |
| 50.23 | 0.6890 |
| 31.01 | 0.8430 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 305.15**

**P / bar = 40.53**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 105.00 | 0.1000 |
| 162.00 | 0.2000 |
| 223.00 | 0.4000 |
| 224.00 | 0.5000 |

| | |
|---|---|
| 208.00 | 0.6000 |
| 175.00 | 0.7000 |
| 130.00 | 0.8000 |
| 71.00 | 0.9000 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 305.15**

**P / bar = 81.06**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 3600.0 | 0.1000 |
| 3990.0 | 0.2000 |
| 3500.0 | 0.4000 |
| 3040.0 | 0.5000 |
| 2540.0 | 0.6000 |
| 1915.0 | 0.7000 |
| 1330.0 | 0.8000 |
| 691.00 | 0.9000 |

Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Direct determination of enthalpy of mixing for the binary gaseous system methane-carbon dioxide by an isothermal flow calorimeter, Journal of Chemical & Engineering Data 3 (1982) 258-264. doi:10.1021/je00029a010

**T / K = 313.15**

**P / bar = 5.070**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 11.17 | 0.2520 |
| 18.51 | 0.4560 |
| 14.60 | 0.6440 |
| 9.881 | 0.7700 |

Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Direct determination of enthalpy of mixing for the binary gaseous system methane-carbon dioxide by an isothermal flow calorimeter, Journal of Chemical & Engineering Data 3 (1982) 258-264. doi:10.1021/je00029a010

**T / K = 313.15**

**P / bar = 46.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 137.50 | 0.1580 |
| 220.00 | 0.3510 |
| 226.88 | 0.5140 |
| 193.13 | 0.6860 |
| 145.05 | 0.7820 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 313.15**

**P / bar = 40.53**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 80.00 | 0.1000 |
| 128.00 | 0.2000 |
| 180.00 | 0.4000 |
| 180.00 | 0.5000 |
| 165.00 | 0.6000 |
| 141.00 | 0.7000 |
| 103.00 | 0.8000 |
| 55.00 | 0.9000 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 313.15**

**P / bar = 81.06**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 878.00 | 0.1000 |
| 1210.0 | 0.2000 |
| 1243.0 | 0.4000 |
| 1168.0 | 0.5000 |
| 998.00 | 0.6000 |
| 800.00 | 0.7000 |
| 577.00 | 0.8000 |
| 298.00 | 0.9000 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 323.15**

**P / bar = 10.13**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 9.000 | 0.1000 |
| 18.00 | 0.2000 |
| 30.00 | 0.4000 |
| 31.00 | 0.5000 |
| 29.00 | 0.6000 |
| 24.00 | 0.7000 |
| 17.00 | 0.8000 |
| 8.000 | 0.9000 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 323.15**

**P / bar = 50.66**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 90.00 | 0.1000 |
| 165.00 | 0.2000 |
| 245.00 | 0.4000 |
| 245.00 | 0.5000 |
| 220.00 | 0.6000 |
| 187.00 | 0.7000 |
| 135.00 | 0.8000 |
| 78.00 | 0.9000 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 323.15**

**P / bar = 91.19**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 570.00 | 0.1000 |
| 850.00 | 0.2000 |
| 1040.0 | 0.4000 |
| 1000.0 | 0.5000 |
| 900.00 | 0.6000 |
| 740.00 | 0.7000 |
| 550.00 | 0.8000 |
| 305.00 | 0.9000 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 333.15**

**P / bar = 30.40**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 32.00 | 0.1000 |
| 55.00 | 0.2000 |
| 90.00 | 0.4000 |
| 97.00 | 0.5000 |
| 90.00 | 0.6000 |
| 77.00 | 0.7000 |
| 55.00 | 0.8000 |
| 30.00 | 0.9000 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 333.15**

**P / bar = 70.93**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 185.00 | 0.1000 |
| 300.00 | 0.2000 |
| 387.00 | 0.4000 |
| 376.00 | 0.5000 |
| 335.00 | 0.6000 |
| 282.00 | 0.7000 |
| 215.00 | 0.8000 |
| 114.00 | 0.9000 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 343.15**

**P / bar = 10.13**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 7.000 | 0.1000 |
| 16.00 | 0.2000 |
| 22.00 | 0.4000 |
| 24.00 | 0.5000 |
| 22.00 | 0.6000 |
| 19.00 | 0.7000 |
| 15.00 | 0.8000 |
| 6.000 | 0.9000 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 343.15**

**P / bar = 50.66**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 70.00 | 0.1000 |
| 120.00 | 0.2000 |
| 163.00 | 0.4000 |
| 165.00 | 0.5000 |
| 153.00 | 0.6000 |
| 130.00 | 0.7000 |
| 96.00 | 0.8000 |
| 53.00 | 0.9000 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

**T / K = 343.15**

**P / bar = 91.19**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 235.00 | 0.1000 |
| 410.00 | 0.2000 |

| | |
|---|---|
| 520.00 | 0.4000 |
| 510.00 | 0.5000 |
| 470.00 | 0.6000 |
| 395.00 | 0.7000 |
| 285.00 | 0.8000 |
| 155.00 | 0.9000 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

| **T / K =** | **353.15** |
|---|---|
| **P / bar =** | **30.40** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 28.00 | 0.1000 |
| 48.00 | 0.2000 |
| 73.00 | 0.4000 |
| 76.00 | 0.5000 |
| 70.00 | 0.6000 |
| 58.00 | 0.7000 |
| 46.00 | 0.8000 |
| 26.00 | 0.9000 |

Lee, J. I. - Mather, A. E., The excess enthalpy of gaseous mixtures of carbon dioxide with methane, The Canadian Journal of Chemical Engineering 1 (1972) 95-100. doi:10.1002/cjce.5450500117

| **T / K =** | **353.15** |
|---|---|
| **P / bar =** | **70.93** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 111.00 | 0.1000 |
| 187.00 | 0.2000 |
| 262.00 | 0.4000 |
| 264.00 | 0.5000 |
| 245.00 | 0.6000 |
| 210.00 | 0.7000 |
| 157.00 | 0.8000 |
| 86.00 | 0.9000 |

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**Critical point**

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Arai, Yasuhiko - Kaminishi, Gen-Ichi - Saito, Shozaburo, The Experimental Determination Of The P-V-T-X Relations For The Carbon Dioxide-Nitrogen And The Carbon Dioxide-Methane Systems, Journal of Chemical Engineering of Japan 2 (1971) 113-122. doi:10.1252/jcej.4.113

| T / K | P / bar | $x_1$ |
|---|---|---|
| 273.15 | 85.52 | 0.3000 |
| 253.15 | 83.49 | 0.4750 |

Mraw, S.C. - Hwang, S.C. - Kobayashi, R., The Vapor-Liquid Equilibrium of the CH4 - CO2 System at Low Temperatures, GPA Research Report (1977) 1-18.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 219.26 | 64.74 | 0.7483 |
| 210.15 | 58.26 | 0.8370 |
| 193.15 | 47.37 | 0.9736 |
| 219.26 | 64.87 | 0.7483 |
| 203.15 | 53.45 | 0.8784 |

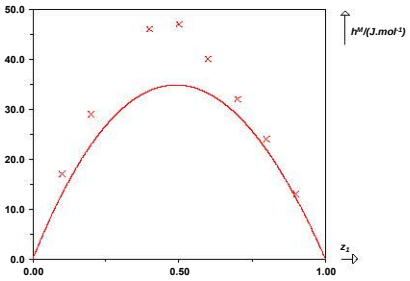
Hwang, S.C. - Lin, H.M. - Chappelear, P.S. - Kobayashi, R., Dew-Point Values for the Methane - Carbon Dioxide System, GPA Research Report (1976) 1-14.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 219.26 | 64.67 | 0.7680 |
| 213.71 | 60.67 | 0.8100 |
| 210.15 | 58.19 | 0.8370 |
| 203.15 | 53.30 | 0.8880 |
| 197.59 | 49.85 | 0.9314 |
| 193.15 | 47.30 | 0.9736 |
| 191.87 | 46.68 | 0.9873 |
| 191.20 | 46.33 | 0.9932 |

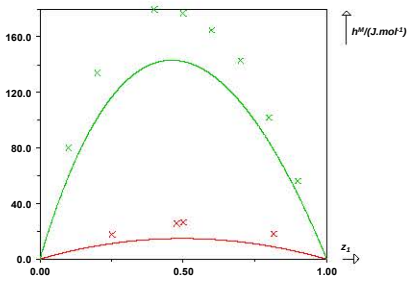
Donnelly, Harold G. - Katz, Donald L., Phase Equilibria in the Carbon Dioxide–Methane System, Industrial & Engineering Chemistry 3 (1954) 511-517. doi:10.1021/ie50531a036

| T / K | P / bar | $x_1$ |
|---|---|---|
| 286.48 | 83.77 | 0.1200 |
| 273.71 | 86.19 | 0.2950 |
| 256.48 | 84.46 | 0.4570 |
| 222.04 | 67.91 | 0.8200 |

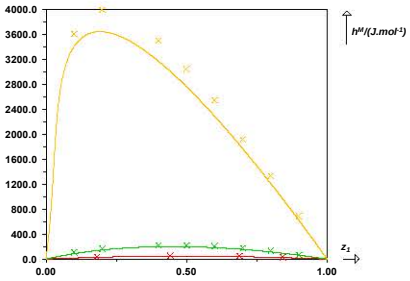
T/K = 283.15 - P/bar = 10.1330



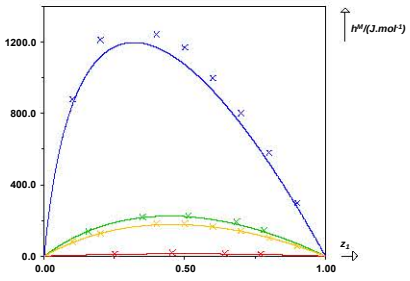

T/K = 293.15 - P/bar = 5.0700 30.3980



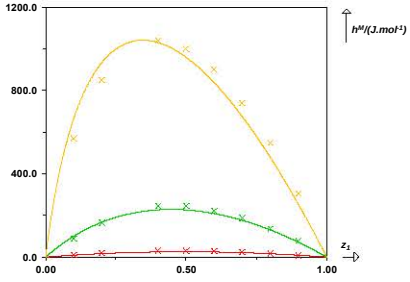

T/K = 305.15 - P/bar = 15.200 40.5300 81.0600



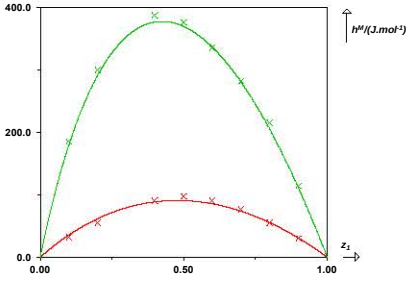

T/K = 313.15 - P/bar = 5.0700 46.00 40.5300 81.0600



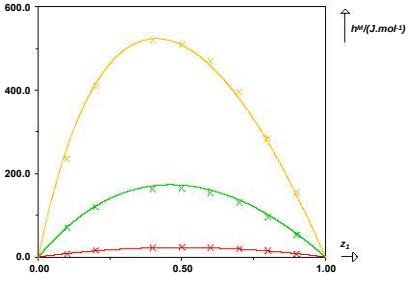

T/K = 323.15 - P/bar = 10.1330 50.6630 91.1920



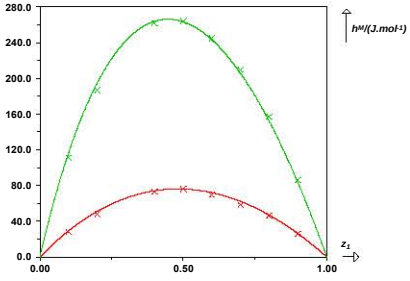

T/K = 333.15 - P/bar = 30.3980 70.9270



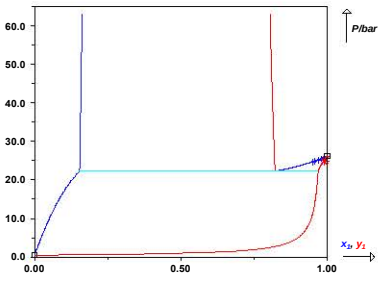

T/K = 343.15 - P/bar = 10.1330 50.6630 91.1920



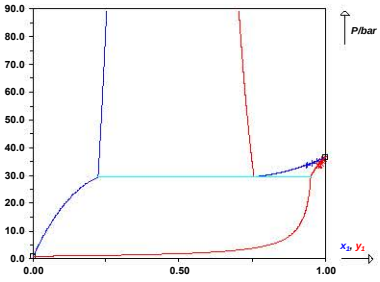

T/K = 353.15 - P/bar = 30.3980 70.9270



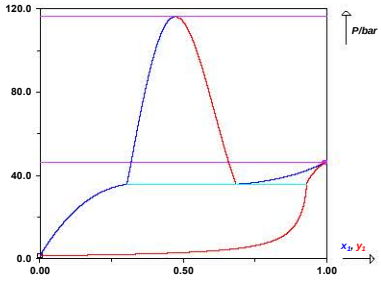

T/K = 173.15



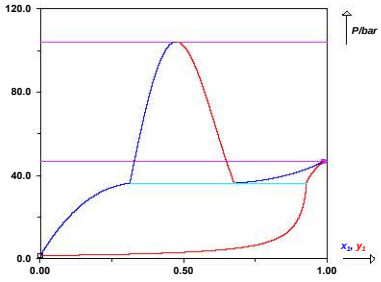

T/K = 183.15



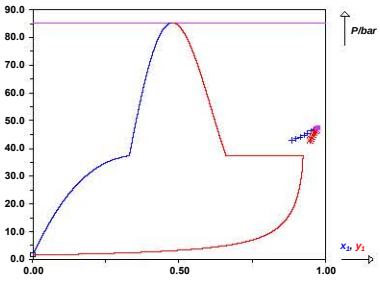

T/K = 191.20



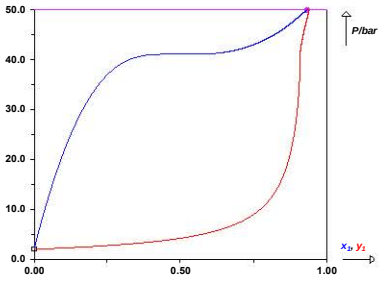

T/K = 191.87



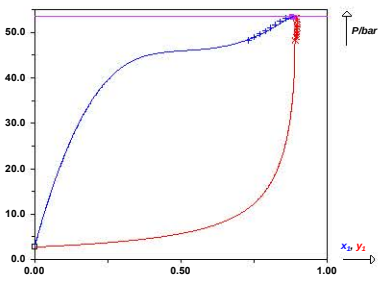

T/K = 193.15



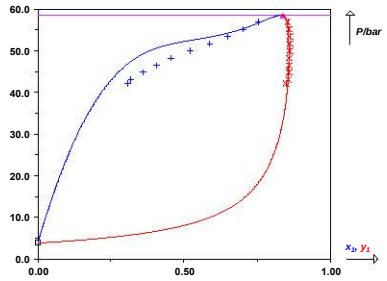

T/K = 197.59



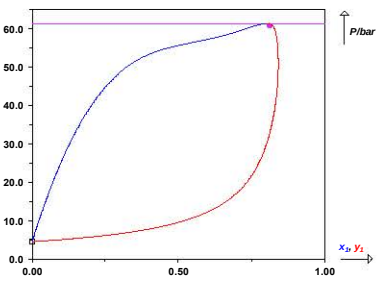

T/K = 203.15



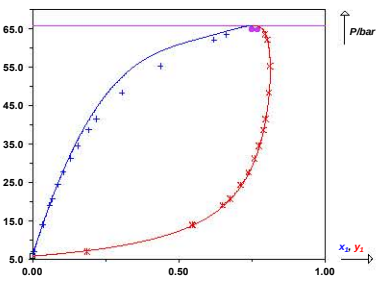
T/K = 210.15



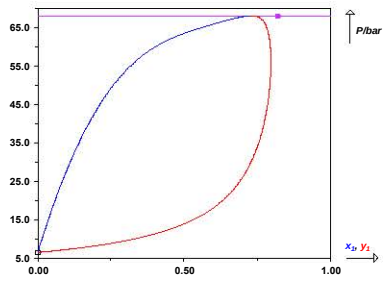

T/K = 213.71



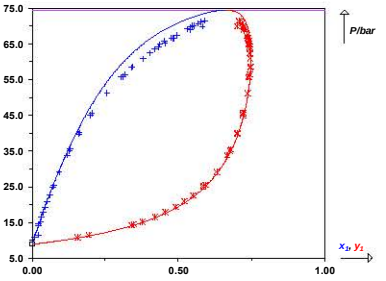

T/K = 219.26



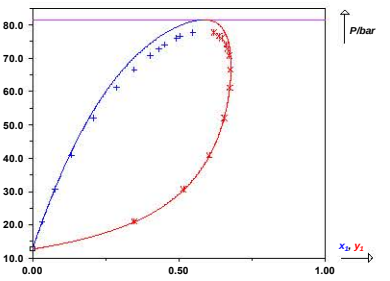

T/K = 222.04



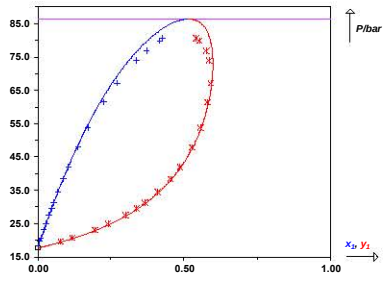

T/K = 230.00



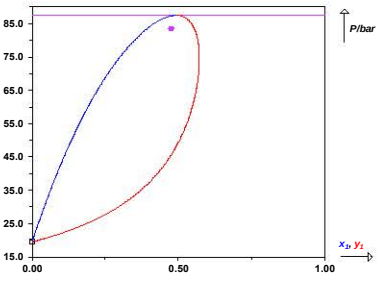

T/K = 240.00



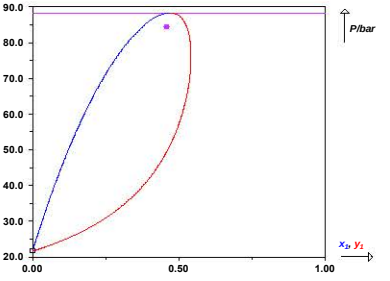

T/K = 250.00



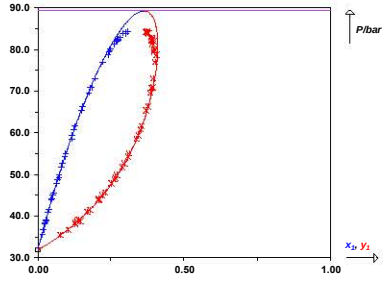

T/K = 253.15



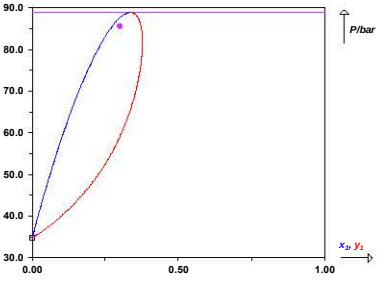

T/K = 256.48



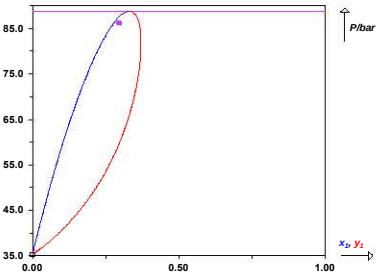

T/K = 270.00



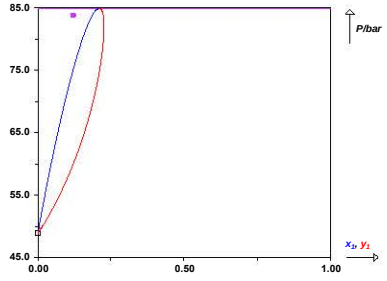

T/K = 273.15



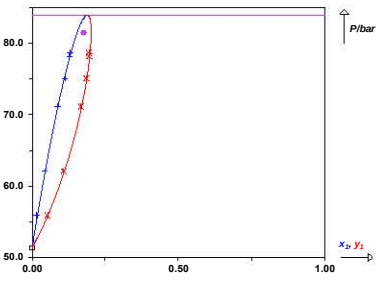

T/K = 273.71



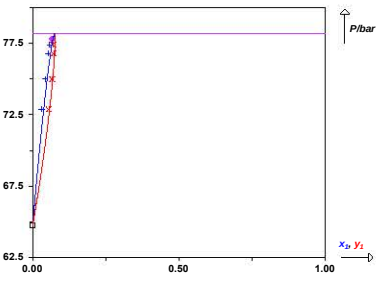

T/K = 286.48




T/K = 288.50




T/K = 298.36



## CARBON DIOXIDE (1) + CYCLOPENTANE (2)

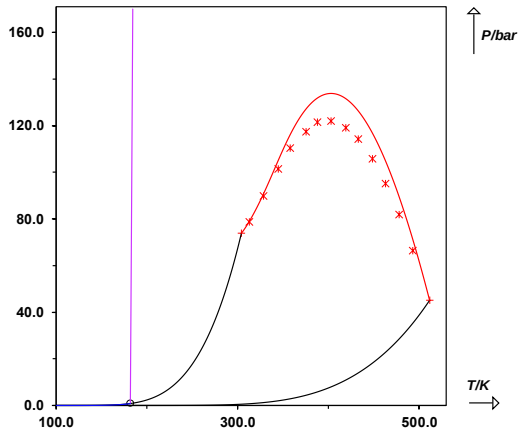
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 287-92-3 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | RGSFGYAAUTVSQA-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 511.70 |
| **$P_c$ / bar** | 73.83 | 45.10 |
| **ω** | 0.2240 | 0.1950 |

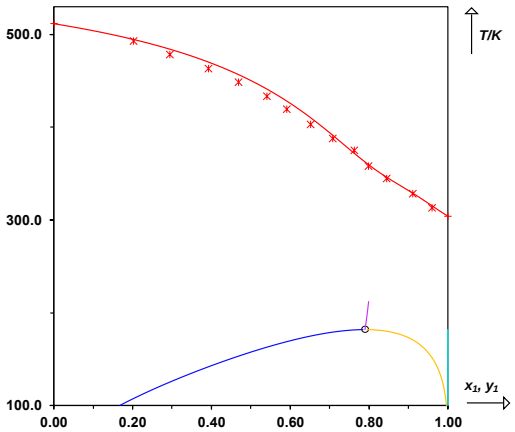
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 357
B/MPa = 341

*Deviations*
MAPE on x = 3.8 %
MAPE on y = 4.3 %
MAPE on $x_c$ = 5.5 %
MAPE on $P_c$ = 7.3 %



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**Isothermal phase equilibrium data**

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Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to 12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

**T / K = 313.08**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.310 | 0.0260 | 0.7580 | |
| 6.830 | 0.0470 | 0.8760 | |
| 12.07 | 0.0900 | 0.9180 | |
| 18.55 | 0.1480 | 0.9420 | |
| 25.79 | 0.2160 | 0.9510 | |
| 32.96 | 0.2880 | 0.9560 | |
| 54.54 | 0.5790 | 0.9640 | |
| 75.36 | 0.9170 | 0.9630 | |
| 78.81 | 0.9520 | 0.9690 | |
| 78.80 | 0.9590 | 0.9590 | CRIT |

Chen, Xiaoting - Hou, Yucui - Wu, Weize - Ren, Shuhang - Zhang, Jianwei - Fan, Jinlong, High pressure phase behavior and density of the carbon dioxide+1-methylimidazole binary system, The Journal of Supercritical Fluids 3 (2009) 310-314. doi:10.1016/j.supflu.2009.04.003

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.452 | 0.0480 | 0.8610 |
| 12.87 | 0.0980 | 0.9260 |
| 18.04 | 0.1360 | 0.9470 |
| 23.56 | 0.1950 | 0.9590 |
| 38.00 | 0.3560 | 0.9730 |
| 42.57 | 0.4080 | 0.9760 |
| 59.64 | 0.6460 | 0.9750 |
| 73.57 | 0.8440 | 0.9720 |

Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to 12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

**T / K = 328.23**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.030 | 0.0290 | 0.7180 | |
| 8.550 | 0.0510 | 0.8270 | |
| 20.62 | 0.1420 | 0.9060 | |
| 27.65 | 0.1960 | 0.9310 | |
| 34.34 | 0.2500 | 0.9360 | |
| 41.51 | 0.3080 | 0.9430 | |
| 48.19 | 0.3670 | 0.9500 | |
| 55.16 | 0.4410 | 0.9550 | |
| 61.85 | 0.5130 | 0.9570 | |
| 68.88 | 0.5970 | 0.9530 | |
| 88.53 | 0.8560 | 0.9480 | |
| 89.70 | 0.9110 | 0.9110 | CRIT |

Chen, Xiaoting - Hou, Yucui - Wu, Weize - Ren, Shuhang - Zhang, Jianwei - Fan, Jinlong, High pressure phase behavior and density of the carbon dioxide+1-methylimidazole binary system, The Journal of Supercritical Fluids 3 (2009) 310-314. doi:10.1016/j.supflu.2009.04.003

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.67 | 0.0580 | 0.8120 |
| 17.15 | 0.0990 | 0.8890 |
| 24.95 | 0.1620 | 0.9290 |
| 29.65 | 0.1870 | 0.9320 |
| 35.45 | 0.2430 | 0.9410 |
| 42.22 | 0.2860 | 0.9510 |
| 48.76 | 0.3490 | 0.9560 |
| 54.51 | 0.4180 | 0.9570 |
| 75.78 | 0.6480 | 0.9490 |
| 82.63 | 0.7260 | 0.9490 |

Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to 12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

**T / K = 344.70**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.720 | 0.0210 | 0.5850 | |
| 9.930 | 0.0460 | 0.7650 | |
| 16.13 | 0.0790 | 0.8390 | |
| 23.30 | 0.1240 | 0.8770 | |
| 29.85 | 0.1650 | 0.8970 | |
| 37.16 | 0.2130 | 0.9100 | |
| 44.62 | 0.2620 | 0.9180 | |
| 52.17 | 0.3190 | 0.9240 | |
| 59.65 | 0.3800 | 0.9270 | |
| 67.27 | 0.4400 | 0.9280 | |
| 74.83 | 0.5080 | 0.9270 | |
| 82.45 | 0.5800 | 0.9250 | |
| 89.93 | 0.6600 | 0.9190 | |
| 97.07 | 0.7420 | 0.9060 | |
| 101.12 | 0.8050 | 0.8840 | |
| 101.30 | 0.8450 | 0.8450 | CRIT |

Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to 12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

**T / K = 358.06**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 6.760 | 0.0200 | 0.4540 | |
| 10.43 | 0.0400 | 0.6820 | |
| 16.96 | 0.0750 | 0.7890 | |
| 23.68 | 0.1130 | 0.8380 | |
| 31.10 | 0.1540 | 0.8660 | |
| 39.27 | 0.2020 | 0.8830 | |
| 45.93 | 0.2410 | 0.8930 | |
| 54.23 | 0.2940 | 0.9010 | |
| 61.92 | 0.3430 | 0.9030 | |
| 82.86 | 0.4930 | 0.9040 | |
| 89.86 | 0.5480 | 0.8990 | |
| 96.86 | 0.6080 | 0.8930 | |
| 103.80 | 0.6730 | 0.8790 | |
| 109.42 | 0.7430 | 0.8480 | |
| 110.30 | 0.7990 | 0.7990 | CRIT |

Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to 12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

**T / K = 375.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 7.720 | 0.0170 | 0.4050 | |
| 11.76 | 0.0360 | 0.5890 | |
| 16.96 | 0.0600 | 0.6950 | |
| 24.71 | 0.0980 | 0.7700 | |
| 31.03 | 0.1290 | 0.8030 | |
| 38.85 | 0.1700 | 0.8330 | |
| 44.96 | 0.2020 | 0.8460 | |
| 52.24 | 0.2410 | 0.8550 | |
| 73.73 | 0.3650 | 0.8650 | |
| 80.32 | 0.4030 | 0.8620 | |
| 88.01 | 0.4540 | 0.8590 | |
| 96.18 | 0.5140 | 0.8480 | |
| 103.66 | 0.5750 | 0.8440 | |
| 110.52 | 0.6330 | 0.8370 | |
| 117.30 | 0.7630 | 0.7630 | CRIT |

Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to 12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

**T / K = 388.11**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 9.100 | 0.0160 | 0.2990 | |
| 13.18 | 0.0340 | 0.5150 | |
| 19.98 | 0.0650 | 0.6570 | |
| 25.95 | 0.0940 | 0.7150 | |
| 33.16 | 0.1280 | 0.7610 | |
| 39.75 | 0.1600 | 0.7880 | |
| 53.16 | 0.2230 | 0.8180 | |
| 60.00 | 0.2590 | 0.8270 | |
| 67.27 | 0.2980 | 0.8330 | |
| 75.03 | 0.3390 | 0.8370 | |
| 82.31 | 0.3730 | 0.8380 | |
| 89.52 | 0.4150 | 0.8370 | |
| 96.45 | 0.4560 | 0.8320 | |
| 103.45 | 0.5000 | 0.8250 | |
| 110.45 | 0.5480 | 0.8130 | |
| 117.32 | 0.6080 | 0.7890 | |
| 120.27 | 0.6430 | 0.7650 | |
| 121.40 | 0.7070 | 0.7070 | CRIT |

Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to 12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

**T / K = 403.07**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 10.02 | 0.0090 | 0.1670 | |
| 14.83 | 0.0280 | 0.4030 | |
| 21.28 | 0.0550 | 0.5520 | |
| 28.49 | 0.0860 | 0.6380 | |
| 35.63 | 0.1180 | 0.6900 | |
| 43.73 | 0.1540 | 0.7250 | |
| 51.97 | 0.1900 | 0.7510 | |
| 59.59 | 0.2250 | 0.7670 | |
| 67.07 | 0.2600 | 0.7760 | |
| 75.79 | 0.3020 | 0.7820 | |
| 83.34 | 0.3400 | 0.7830 | |
| 91.10 | 0.3800 | 0.7860 | |
| 98.65 | 0.4210 | 0.7790 | |
| 105.44 | 0.4630 | 0.7710 | |
| 112.17 | 0.5080 | 0.7560 | |
| 118.76 | 0.5620 | 0.7290 | |
| 122.00 | 0.6520 | 0.6520 | CRIT |

Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to

12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

**T / K = 419.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 12.97 | 0.0090 | 0.1290 | |
| 16.82 | 0.0240 | 0.2940 | |
| 22.24 | 0.0450 | 0.4330 | |
| 29.31 | 0.0740 | 0.5400 | |
| 36.38 | 0.1050 | 0.6020 | |
| 44.69 | 0.1380 | 0.6520 | |
| 51.35 | 0.1680 | 0.6750 | |
| 58.42 | 0.1980 | 0.6950 | |
| 66.52 | 0.2330 | 0.7110 | |
| 73.38 | 0.2640 | 0.7170 | |
| 81.28 | 0.3010 | 0.7210 | |
| 89.24 | 0.3370 | 0.7250 | |
| 97.41 | 0.3820 | 0.7200 | |
| 105.44 | 0.4270 | 0.7110 | |
| 113.61 | 0.4830 | 0.6850 | |
| 117.80 | 0.5260 | 0.6520 | |
| 119.10 | 0.5910 | 0.5910 | CRIT |

Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to 12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

**T / K = 433.21**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 16.82 | 0.0120 | 0.1370 | |
| 20.11 | 0.0240 | 0.2470 | |
| 25.40 | 0.0450 | 0.3680 | |
| 32.26 | 0.0720 | 0.4700 | |
| 39.61 | 0.1010 | 0.5340 | |
| 47.02 | 0.1320 | 0.5800 | |
| 53.82 | 0.1600 | 0.6080 | |
| 61.65 | 0.1930 | 0.6320 | |
| 68.92 | 0.2240 | 0.6480 | |
| 75.58 | 0.2550 | 0.6570 | |
| 82.72 | 0.2880 | 0.6630 | |
| 90.20 | 0.3240 | 0.6640 | |
| 97.14 | 0.3580 | 0.6610 | |
| 104.00 | 0.3970 | 0.6460 | |
| 111.00 | 0.4510 | 0.6220 | |
| 112.93 | 0.4770 | 0.5970 | |
| 114.20 | 0.5400 | 0.5400 | CRIT |

Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to 12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

**T / K = 448.81**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 20.18 | 0.0090 | 0.0760 | |
| 25.47 | 0.0280 | 0.2220 | |
| 29.79 | 0.0450 | 0.3050 | |
| 36.38 | 0.0710 | 0.3910 | |
| 43.52 | 0.0990 | 0.4550 | |
| 51.01 | 0.1300 | 0.5020 | |
| 58.42 | 0.1590 | 0.5320 | |
| 65.56 | 0.1900 | 0.5550 | |
| 72.56 | 0.2210 | 0.5700 | |
| 80.04 | 0.2550 | 0.5790 | |
| 87.32 | 0.2920 | 0.5810 | |
| 95.01 | 0.3330 | 0.5750 | |
| 102.35 | 0.3840 | 0.5490 | |
| 105.10 | 0.4190 | 0.5140 | |
| 105.80 | 0.4680 | 0.4680 | CRIT |

Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to 12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

**T / K = 463.23**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 26.84 | 0.0150 | 0.1050 | |
| 32.06 | 0.0350 | 0.2030 | |
| 38.58 | 0.0600 | 0.2940 | |
| 45.59 | 0.0900 | 0.3610 | |
| 53.48 | 0.1210 | 0.4100 | |
| 61.44 | 0.1540 | 0.4450 | |
| 68.99 | 0.1860 | 0.4670 | |
| 76.47 | 0.2220 | 0.4790 | |
| 83.82 | 0.2600 | 0.4810 | |
| 90.82 | 0.3050 | 0.4670 | |
| 93.98 | 0.3330 | 0.4460 | |
| 95.20 | 0.3920 | 0.3920 | CRIT |

Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to 12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

**T / K = 478.17**

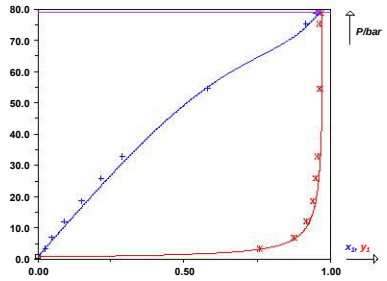
| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 31.03 | 0.0100 | 0.0540 |
| 36.11 | 0.0290 | 0.1370 |
| 43.18 | 0.0570 | 0.2200 |

| | | | |
|---|---|---|---|
| 50.46 | 0.0880 | 0.2790 | |
| 58.01 | 0.1200 | 0.3220 | |
| 64.53 | 0.1500 | 0.3460 | |
| 71.19 | 0.1840 | 0.3600 | |
| 77.57 | 0.2210 | 0.3570 | |
| 81.21 | 0.2540 | 0.3330 | |
| 81.90 | 0.2950 | 0.2950 | CRIT |

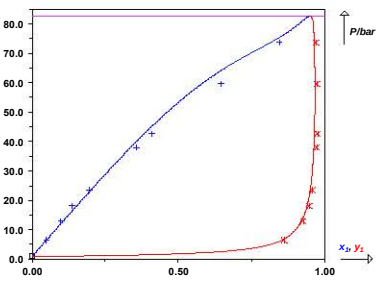
Shah, Nilesh N. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide + cyclopentane from 275 to 493 K at pressures to 12.2 MPa, Journal of Chemical & Engineering Data 2 (1991) 188-192. doi:10.1021/je00002a014

| **T / K =** | **493.11** | | |
|---|---|---|---|
| P / bar | $x_1$ | $y_1$ | |
| 38.79 | 0.0140 | 0.0490 | |
| 43.93 | 0.0350 | 0.1070 | |
| 56.98 | 0.0960 | 0.2110 | |
| 63.36 | 0.1300 | 0.2420 | |
| 66.40 | 0.2020 | 0.2020 | CRIT |

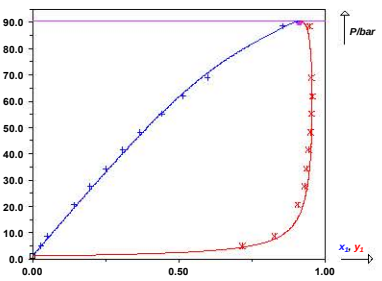
T/K = 313.08



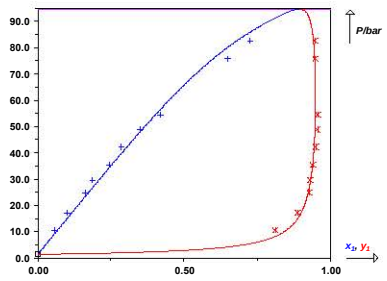

T/K = 318.15



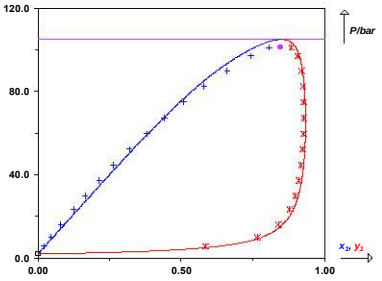

T/K = 328.23



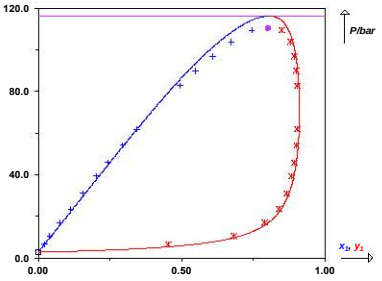

T/K = 333.15



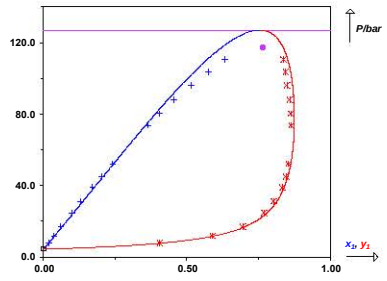

T/K = 344.70



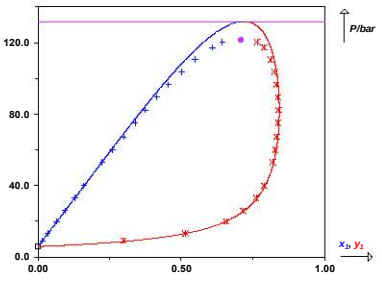

T/K = 358.06



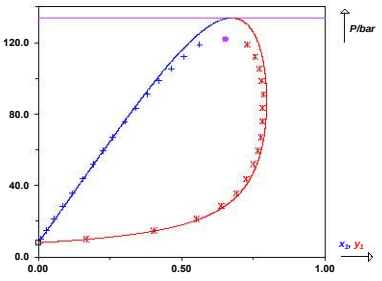

T/K = 375.15



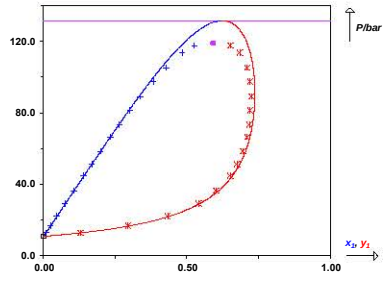

T/K = 388.11



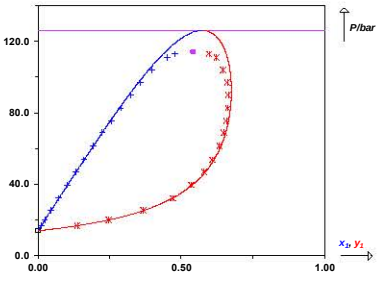

T/K = 403.07



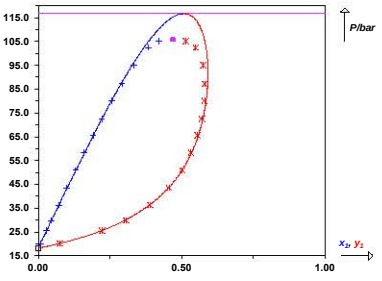

T/K = 419.15



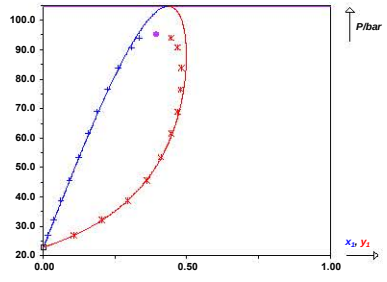

T/K = 433.21



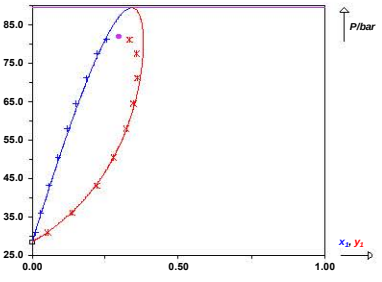

T/K = 448.81



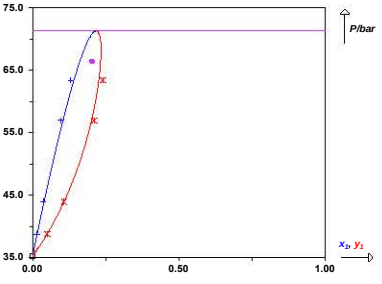

T/K = 463.23




T/K = 478.17




T/K = 493.11



## NITROGEN (1) + CARBON DIOXIDE (2)

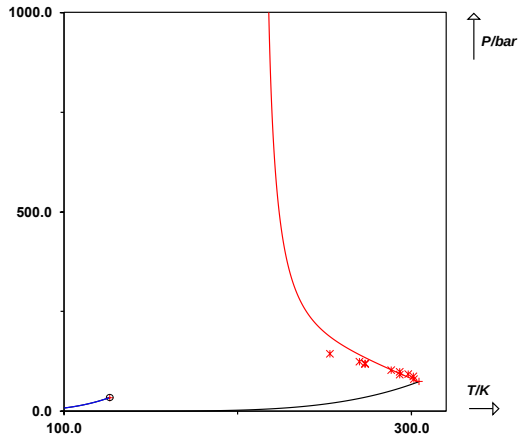
| | | |
|---|---|---|
| **CAS** | 7727-37-9 | 124-38-9 |
| **InChiKey** | MDFFNEOEWAXZRQ-UHFFFAOYSA-N | CURLTUGMZLYLDI-UHFFFAOYSA-N |
| **$T_c$ / K** | 126.20 | 304.21 |
| **$P_c$ / bar** | 34.00 | 73.83 |
| **ω** | 0.0380 | 0.2240 |

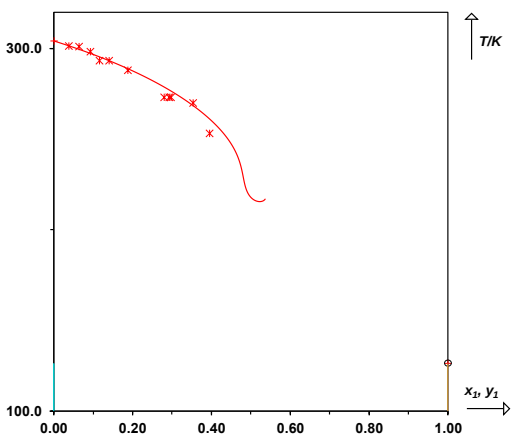
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 324
B/MPa = 1080

*Deviations*
MAPE on x = 12 %
MAPE on y = 4.3 %
MAPE on $x_c$ = 7 %
MAPE on $P_c$ = 10 %
MAPE on $h^M$ = 4.6 %



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**Isothermal phase equilibrium data**

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Fele, Ljudmila - Grilc, Viktor, Separation of Furfural from Ternary Mixtures, Journal of Chemical & Engineering Data 3 (2003) 564-570. doi:10.1021/je020117y

**T / K = 220.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.58 | 0.0067 | 0.4040 |
| 14.22 | 0.0121 | 0.5369 |
| 22.46 | 0.0243 | 0.6724 |
| 29.94 | 0.0358 | 0.7395 |
| 39.66 | 0.0510 | 0.7802 |
| 51.32 | 0.0689 | 0.8103 |
| 60.93 | 0.0848 | 0.8148 |
| 70.30 | 0.1034 | 0.8131 |
| 72.27 | 0.1133 | 0.8223 |
| 74.95 | 0.1124 | 0.8308 |
| 88.63 | 0.1290 | 0.8208 |
| 94.71 | 0.1426 | 0.8305 |
| 105.44 | 0.1634 | 0.8233 |
| 113.56 | 0.1782 | 0.8192 |
| 122.41 | 0.1983 | 0.8107 |
| 129.68 | 0.2127 | 0.8154 |
| 132.88 | 0.2204 | 0.7944 |
| 142.44 | 0.2438 | 0.7958 |

Brown, T.S. - Sloan, E.D. - Kidnay, A.J., Vapor-liquid equilibria in the nitrogen + carbon dioxide + ethane system, Fluid Phase Equilibria (1989) 299-313. doi:10.1016/0378-3812(89)80372-3

**T / K = 220.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.73 | 0.0108 | 0.5174 |
| 24.57 | 0.0269 | 0.6971 |
| 59.93 | 0.0830 | 0.8150 |
| 74.85 | 0.1092 | 0.8262 |
| 90.98 | 0.1338 | 0.8264 |
| 119.95 | 0.1903 | 0.8080 |

Al-Sahhaf, Taher A. - Kidnay, Arthur J. - Sloan, E. Dendy, Liquid + vapor equilibriums in the nitrogen + carbon dioxide + methane system, Industrial & Engineering Chemistry Fundamentals 4 (1983) 372-380. doi:10.1021/i100012a004

**T / K = 220.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.09 | 0.0132 | 0.5518 |
| 30.75 | 0.0362 | 0.7423 |
| 45.95 | 0.0601 | 0.7974 |
| 63.13 | 0.0883 | 0.8214 |
| 82.58 | 0.1209 | 0.8281 |
| 111.14 | 0.1742 | 0.8165 |
| 124.32 | 0.2016 | 0.8028 |
| 137.96 | 0.2324 | 0.7869 |
| 155.06 | 0.2771 | 0.7516 |
| 167.06 | 0.3155 | 0.7215 |

Zhang Zhanzhu - Guo Liping - Yang Xiadong - Knapp, H., Vapor And Liquid Equilibrium For Nitrogen - Ethane - Carbon Dioxide Ternary System, Huagong Xuebao 3 (1999) 392-398.

**T / K = 220.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.00 | 0.0209 | 0.6487 |
| 30.00 | 0.0363 | 0.7404 |
| 40.00 | 0.0515 | 0.7824 |
| 50.00 | 0.0731 | 0.8061 |

Yucelen, Belgin - Kidnay, Arthur J., Vapor−Liquid Equilibria in the Nitrogen + Carbon Dioxide + Propane System from 240 to 330 K at Pressures to 15 MPa, Journal of Chemical & Engineering Data 5 (1999) 926-931. doi:10.1021/je980321e

**T / K = 240.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.00 | 0.0130 | 0.3186 |
| 109.30 | 0.1830 | 0.6977 |
| 130.00 | 0.2467 | 0.6692 |

Al-Sahhaf, Taher A. - Kidnay, Arthur J. - Sloan, E. Dendy, Liquid + vapor equilibriums in the nitrogen + carbon dioxide + methane system, Industrial & Engineering Chemistry Fundamentals 4 (1983) 372-380. doi:10.1021/i100012a004

**T / K = 240.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 21.00 | 0.0129 | 0.3312 |
| 32.08 | 0.0307 | 0.5151 |
| 40.89 | 0.0454 | 0.5890 |
| 56.74 | 0.0734 | 0.6572 |
| 62.62 | 0.0838 | 0.6710 |
| 72.35 | 0.1022 | 0.6873 |
| 85.90 | 0.1297 | 0.6981 |
| 99.45 | 0.1592 | 0.6992 |
| 107.28 | 0.1775 | 0.6960 |
| 114.66 | 0.1958 | 0.6897 |
| 122.25 | 0.2165 | 0.6806 |
| 126.59 | 0.2296 | 0.6745 |
| 138.65 | 0.2696 | 0.6517 |
| 144.72 | 0.2944 | 0.6288 |

| | | |
|---|---|---|
| 154.24 | 0.3491 | 0.5929 |
| 157.68 | 0.3816 | 0.5633 |
| 161.47 | 0.4777 | 0.5202 |

Brown, T. S. - Sloan, E. D. - Kidnay, A. J., Vapor-liquid equilibria for the ternary system N2 + CO2 +n-C4H10 at 250 and 270 K1, International Journal of Thermophysics 6 (1994) 1211-1219. doi:10.1007/BF01458829

**T / K = 250.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 60.03 | 0.0755 | 0.5652 |
| 119.97 | 0.2192 | 0.6050 |
| 139.93 | 0.2980 | 0.5470 |

Brown, T.S. - Niesen, V.G. - Sloan, E.D. - Kidnay, A.J., Vapor-liquid equilibria for the binary systems of nitrogen, carbon dioxide, and n-butane at temperatures from 220 to 344 K., Fluid Phase Equilibria (1989) 7-14. doi:10.1016/0378-3812(89)80067-6

**T / K = 250.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 25.99 | 0.0136 | 0.2561 |
| 36.88 | 0.0331 | 0.4239 |
| 44.89 | 0.0488 | 0.5001 |
| 55.41 | 0.0664 | 0.5494 |
| 65.97 | 0.0870 | 0.5849 |
| 75.32 | 0.1069 | 0.6049 |
| 96.32 | 0.1532 | 0.6223 |
| 111.51 | 0.1931 | 0.6163 |
| 119.36 | 0.2173 | 0.6063 |
| 134.16 | 0.2708 | 0.5727 |
| 140.66 | 0.3008 | 0.5437 |

Al-Sahhaf, Taher A., Vapor—liquid equilibria for the ternary system N2 + CO2 + CH4 at 230 and 250 K, Fluid Phase Equilibria 1-2 (1990) 159-172. doi:10.1016/0378-3812(90)85010-8

**T / K = 250.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 89.63 | 0.1394 | 0.6142 |
| 103.42 | 0.1767 | 0.6162 |

Brown, T.S. - Niesen, V.G. - Sloan, E.D. - Kidnay, A.J., Vapor-liquid equilibria for the binary systems of nitrogen, carbon dioxide, and n-butane at temperatures from 220 to 344 K., Fluid Phase Equilibria (1989) 7-14. doi:10.1016/0378-3812(89)80067-6

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 48.57 | 0.0316 | 0.2423 |
| 60.84 | 0.0561 | 0.3309 |
| 76.50 | 0.0901 | 0.3942 |
| 91.02 | 0.1279 | 0.4205 |

Brown, T.S. - Sloan, E.D. - Kidnay, A.J., Vapor-liquid equilibria in the nitrogen + carbon dioxide + ethane system, Fluid Phase Equilibria (1989) 299-313. doi:10.1016/0378-3812(89)80372-3

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 57.79 | 0.0498 | 0.3087 |
| 61.82 | 0.0566 | 0.3322 |
| 71.65 | 0.0770 | 0.3747 |
| 75.46 | 0.0861 | 0.3879 |
| 82.89 | 0.1055 | 0.4049 |
| 84.76 | 0.1090 | 0.4095 |
| 90.01 | 0.1230 | 0.4148 |
| 95.86 | 0.1338 | 0.4186 |
| 101.93 | 0.1572 | 0.4192 |

Yucelen, Belgin - Kidnay, Arthur J., Vapor−Liquid Equilibria in the Nitrogen + Carbon Dioxide + Propane System from 240 to 330 K at Pressures to 15 MPa, Journal of Chemical & Engineering Data 5 (1999) 926-931. doi:10.1021/je980321e

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 35.67 | 0.0064 | 0.0759 |
| 37.19 | 0.0088 | 0.1036 |
| 50.76 | 0.0358 | 0.2629 |
| 60.00 | 0.0530 | 0.3250 |
| 119.70 | 0.2456 | 0.3822 |

Somait, Fahad A. - Kidnay, Arthur J., Liquid-vapor equilibriums at 270.00 K for systems containing nitrogen, methane, and carbon dioxide, Journal of Chemical & Engineering Data 4 (1978) 301-305. doi:10.1021/je60079a019

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 45.60 | 0.0250 | 0.2115 |
| 60.80 | 0.0560 | 0.3290 |
| 86.13 | 0.1142 | 0.4139 |
| 96.26 | 0.1430 | 0.4210 |
| 111.46 | 0.1950 | 0.4080 |
| 34.25 | 0.0040 | 0.0472 |
| 36.27 | 0.0078 | 0.0851 |
| 38.00 | 0.0108 | 0.1140 |
| 39.52 | 0.0135 | 0.1331 |
| 41.22 | 0.0168 | 0.1598 |
| 42.05 | 0.0182 | 0.1683 |
| 42.81 | 0.0197 | 0.1783 |

| | | | |
|---|---|---|---|
| 45.90 | 0.0263 | 0.2156 | |
| 47.60 | 0.0289 | 0.2323 | |
| 47.74 | 0.0292 | 0.2325 | |
| 51.52 | 0.0368 | 0.2674 | |
| 56.99 | 0.0476 | 0.3069 | |
| 60.49 | 0.0545 | 0.3280 | |
| 64.44 | 0.0630 | 0.3473 | |
| 70.93 | 0.0778 | 0.3770 | |
| 77.21 | 0.0921 | 0.3961 | |
| 83.80 | 0.1080 | 0.4126 | |
| 86.13 | 0.1142 | 0.4139 | |
| 89.83 | 0.1231 | 0.4190 | |
| 92.92 | 0.1319 | 0.4173 | |
| 96.26 | 0.1430 | 0.4210 | |
| 102.04 | 0.1585 | 0.4188 | |
| 107.14 | 0.1769 | 0.4134 | |
| 110.53 | 0.1904 | 0.4094 | |
| 112.52 | 0.1986 | 0.4061 | |
| 115.49 | 0.2142 | 0.3986 | |
| 119.48 | 0.2486 | 0.3762 | |
| 120.24 | 0.2454 | 0.3720 | |
| 120.73 | 0.2505 | 0.3664 | |
| 121.35 | 0.2556 | 0.3640 | |
| 123.41 | 0.3530 | 0.3530 | CRIT |

Yorizane, M. - Yoshimura, S. - Masuoka, H., Vapor liquid equilibrium at high pressures. N2-CO2, H2-CO2 systems, Kagaku Kogaku 9 (1970) 953-957. doi:10.1252/kakoronbunshu1953.34.953

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 40.53 | 0.0110 | 0.0910 | |
| 50.66 | 0.0310 | 0.2150 | |
| 60.80 | 0.0510 | 0.3000 | |
| 70.93 | 0.0710 | 0.3470 | |
| 91.19 | 0.1260 | 0.3920 | |
| 101.33 | 0.1580 | 0.3970 | |
| 111.46 | 0.2000 | 0.3900 | |
| 116.52 | 0.2510 | 0.3560 | |
| 117.54 | 0.2720 | 0.3380 | |
| 118.25 | 0.2970 | 0.2970 | CRIT |

Zenner, G.H. - Dana, L.I., Liquid-vapor equilibrium compositions of carbon dioxideoxygen-nitrogen mixtures, Chem. Eng. Progr. Symp. Ser. 44 (1963) 36-41.

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 48.33 | 0.0265 | 0.1980 |
| 60.29 | 0.0512 | 0.2920 |
| 60.39 | 0.0521 | 0.2885 |
| 63.13 | 0.0580 | 0.3100 |
| 79.95 | 0.0952 | 0.3730 |
| 95.85 | 0.1408 | 0.3960 |
| 109.73 | 0.1923 | 0.3845 |
| 116.62 | 0.2280 | 0.3540 |
| 118.55 | 0.2975 | 0.3045 |

Kaminishi, G.I. - Toriumi, T., Gas-liquid equilibrium under high pressures. VI. Vapor-liquid phase equilibrium in the CO2-H2, CO2-N2, and CO2-O2 systems, Kogyo Kagaku Zasshi (1966) 175-178.

**T / K = 288.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 74.17 | 0.0510 | 0.1750 |
| 84.40 | 0.0830 | 0.2020 |

Krichevskii, I.R. - Khazanova, N.E. - Lesnevskaya, L.S. - Sandalova, L.Yu., Liquid-gas equilibrium in the nitrogen-carbon dioxide system under elevated pressures, Khim. Promst. Moscow 3 (1962) 169-171.

**T / K = 288.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 60.80 | 0.0250 | 0.0900 | |
| 70.93 | 0.0500 | 0.1580 | |
| 81.06 | 0.0740 | 0.1950 | |
| 91.19 | 0.1020 | 0.2100 | |
| 101.33 | 0.1610 | 0.2050 | |
| 103.35 | 0.1870 | 0.1870 | CRIT |

Xu, Nanping - Dong, Junhang - Wang, Yanru - Shi, Jun, High pressure vapor liquid equilibria at 293 K for systems containing nitrogen, methane and carbon dioxide, Fluid Phase Equilibria (1992) 175-186. doi:10.1016/0378-3812(92)85150-7

**T / K = 293.30**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 60.00 | 0.0050 | 0.0230 | |
| 69.80 | 0.0290 | 0.0880 | |
| 74.20 | 0.0410 | 0.1110 | |
| 81.00 | 0.0610 | 0.1360 | |
| 87.00 | 0.0760 | 0.1370 | |
| 89.00 | 0.0860 | 0.1330 | |
| 90.30 | 0.0960 | 0.1290 | |
| 91.10 | 0.1160 | 0.1160 | CRIT |

Bian, Baigui - Wang, Yanru - Shi, Jun - Zhao, Ensheng - Lu, Benjamin C.-Y., Simultaneous determination of vapor-liquid equilibrium and molar volumes for coexisting phases up to the critical temperature with a static method, Fluid Phase Equilibria 1 (1993) 177-187. doi:10.1016/0378-3812(93)85012-B

| **T / K =** | **301.30** | | |
|---|---|---|---|
| P / bar | $x_1$ | $y_1$ | |
| 72.20 | 0.0069 | 0.0152 | |
| 73.30 | 0.0101 | 0.0206 | |
| 76.10 | 0.0182 | 0.0326 | |
| 79.00 | 0.0258 | 0.0390 | |
| 80.10 | 0.0348 | 0.0389 | |
| 80.50 | 0.0379 | 0.0379 | CRIT |

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**Enthalpy of mixing**

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Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

| **T / K =** | **283.15** |
|---|---|
| **P / bar =** | **10.13** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 21.00 | 0.1000 |
| 37.00 | 0.2000 |
| 47.00 | 0.3000 |
| 54.00 | 0.4000 |
| 59.00 | 0.5000 |
| 53.00 | 0.6000 |
| 44.00 | 0.7000 |
| 34.00 | 0.8000 |
| 18.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

| **T / K =** | **283.15** |
|---|---|
| **P / bar =** | **43.57** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 400.00 | 0.1000 |
| 530.00 | 0.2000 |
| 602.00 | 0.3000 |
| 620.00 | 0.4000 |
| 594.00 | 0.5000 |
| 543.00 | 0.6000 |
| 450.00 | 0.7000 |
| 335.00 | 0.8000 |
| 190.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

| **T / K =** | **293.15** |
|---|---|
| **P / bar =** | **40.53** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 185.00 | 0.1000 |
| 286.00 | 0.2000 |
| 346.00 | 0.3000 |
| 371.00 | 0.4000 |
| 363.00 | 0.5000 |
| 328.00 | 0.6000 |
| 270.00 | 0.7000 |
| 205.00 | 0.8000 |
| 112.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

| **T / K =** | **305.15** |
|---|---|
| **P / bar =** | **10.13** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 16.00 | 0.1000 |
| 30.00 | 0.2000 |
| 39.00 | 0.3000 |
| 44.00 | 0.4000 |
| 47.00 | 0.5000 |
| 43.00 | 0.6000 |
| 35.00 | 0.7000 |
| 26.00 | 0.8000 |
| 16.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

| **T / K =** | **305.15** |
|---|---|
| **P / bar =** | **50.66** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 234.00 | 0.1000 |
| 389.00 | 0.2000 |
| 452.00 | 0.3000 |
| 460.00 | 0.4000 |
| 439.00 | 0.5000 |
| 396.00 | 0.6000 |
| 329.00 | 0.7000 |
| 240.00 | 0.8000 |
| 133.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide,

Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 305.15**

**P / bar = 86.13**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 3980.0 | 0.1000 |
| 4340.0 | 0.2000 |
| 4170.0 | 0.3000 |
| 3740.0 | 0.4000 |
| 3240.0 | 0.5000 |
| 2705.0 | 0.6000 |
| 2085.0 | 0.7000 |
| 1405.0 | 0.8000 |
| 725.00 | 0.9000 |

Hejmadi, Arun V. - Katz, Donald L. - Powers, John E., Experimental determination of the enthalpy of mixing of N + CO2 under pressure, The Journal of Chemical Thermodynamics 4 (1971) 483-496. doi:10.1016/S0021-9614(71)80030-7

**T / K = 313.15**

**P / bar = 65.49**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 627.20 | 0.2200 |
| 705.50 | 0.3580 |
| 662.70 | 0.5160 |
| 444.00 | 0.7320 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 313.15**

**P / bar = 40.53**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 111.00 | 0.1000 |
| 187.00 | 0.2000 |
| 235.00 | 0.3000 |
| 256.00 | 0.4000 |
| 255.00 | 0.5000 |
| 230.00 | 0.6000 |
| 189.00 | 0.7000 |
| 130.00 | 0.8000 |
| 69.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 313.15**

**P / bar = 81.06**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 1021.0 | 0.1000 |
| 1292.0 | 0.2000 |
| 1416.0 | 0.3000 |
| 1370.0 | 0.4000 |
| 1243.0 | 0.5000 |
| 1097.0 | 0.6000 |
| 904.00 | 0.7000 |
| 668.00 | 0.8000 |
| 364.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 313.15**

**P / bar = 121.59**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 1883.0 | 0.1000 |
| 2940.0 | 0.2000 |
| 3291.0 | 0.3000 |
| 3244.0 | 0.4000 |
| 2879.0 | 0.5000 |
| 2391.0 | 0.6000 |
| 1787.0 | 0.7000 |
| 1138.0 | 0.8000 |
| 541.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 323.15**

**P / bar = 40.53**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 93.00 | 0.1000 |
| 156.00 | 0.2000 |
| 200.00 | 0.3000 |
| 225.00 | 0.4000 |
| 220.00 | 0.5000 |
| 195.00 | 0.6000 |
| 160.00 | 0.7000 |
| 115.00 | 0.8000 |
| 60.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 323.15**

**P / bar = 81.06**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 490.00 | 0.1000 |
| 720.00 | 0.2000 |
| 870.00 | 0.3000 |
| 890.00 | 0.4000 |
| 845.00 | 0.5000 |
| 760.00 | 0.6000 |
| 620.00 | 0.7000 |
| 465.00 | 0.8000 |
| 257.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 333.15**

**P / bar = 20.26**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 29.00 | 0.1000 |
| 48.00 | 0.2000 |
| 66.00 | 0.3000 |
| 76.00 | 0.4000 |
| 79.00 | 0.5000 |
| 76.00 | 0.6000 |
| 62.00 | 0.7000 |
| 45.00 | 0.8000 |
| 23.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 333.15**

**P / bar = 60.79**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 171.00 | 0.1000 |
| 272.00 | 0.2000 |
| 340.00 | 0.3000 |
| 370.00 | 0.4000 |
| 360.00 | 0.5000 |
| 325.00 | 0.6000 |
| 275.00 | 0.7000 |
| 200.00 | 0.8000 |
| 115.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 333.15**

**P / bar = 101.32**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 712.00 | 0.1000 |
| 1042.0 | 0.2000 |
| 1190.0 | 0.3000 |
| 1210.0 | 0.4000 |
| 1100.0 | 0.5000 |
| 955.00 | 0.6000 |
| 780.00 | 0.7000 |
| 556.00 | 0.8000 |
| 295.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 343.15**

**P / bar = 30.40**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 44.00 | 0.1000 |
| 76.00 | 0.2000 |
| 100.00 | 0.3000 |
| 113.00 | 0.4000 |
| 115.00 | 0.5000 |
| 110.00 | 0.6000 |
| 92.00 | 0.7000 |
| 68.00 | 0.8000 |
| 37.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 343.15**

**P / bar = 70.93**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 187.00 | 0.1000 |
| 310.00 | 0.2000 |
| 380.00 | 0.3000 |
| 415.00 | 0.4000 |
| 400.00 | 0.5000 |
| 350.00 | 0.6000 |
| 290.00 | 0.7000 |
| 215.00 | 0.8000 |
| 115.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide,

Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 353.15**

**P / bar = 10.13**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 9.000 | 0.1000 |
| 18.00 | 0.2000 |
| 24.00 | 0.3000 |
| 30.00 | 0.4000 |
| 32.00 | 0.5000 |
| 30.00 | 0.6000 |
| 24.00 | 0.7000 |
| 18.00 | 0.8000 |
| 9.000 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 353.15**

**P / bar = 50.66**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 82.00 | 0.1000 |
| 135.00 | 0.2000 |
| 176.00 | 0.3000 |
| 198.00 | 0.4000 |
| 203.00 | 0.5000 |
| 190.00 | 0.6000 |
| 164.00 | 0.7000 |
| 125.00 | 0.8000 |
| 67.00 | 0.9000 |

Lee, Jong Il - Mather, Alan E., Excess enthalpy of gaseous mixtures of nitrogen and carbon dioxide, Journal of Chemical & Engineering Data 2 (1972) 189-192. doi:10.1021/je60053a042

**T / K = 353.15**

**P / bar = 91.19**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 262.00 | 0.1000 |
| 412.00 | 0.2000 |
| 500.00 | 0.3000 |
| 540.00 | 0.4000 |
| 530.00 | 0.5000 |
| 470.00 | 0.6000 |
| 390.00 | 0.7000 |
| 285.00 | 0.8000 |
| 156.00 | 0.9000 |

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**Critical point**

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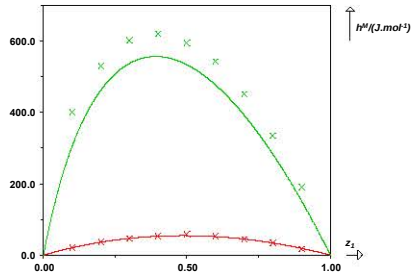
Krichevskii, I.R. - Khazanova, N.E. - Lesnevskaya, L.S. - Sandalova, L.Yu., Liquid-gas equilibrium in the nitrogen-carbon dioxide system under elevated pressures, Khim. Promst. Moscow 3 (1962) 169-171.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 293.15 | 98.79 | 0.1400 |
| 298.15 | 92.21 | 0.0930 |
| 301.15 | 87.14 | 0.0640 |

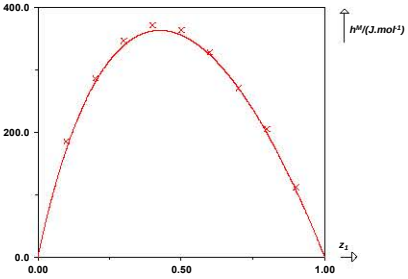
Arai, Yasuhiko - Kaminishi, Gen-Ichi - Saito, Shozaburo, The Experimental Determination Of The P-V-T-X Relations For The Carbon Dioxide-Nitrogen And The Carbon Dioxide-Methane Systems, Journal of Chemical Engineering of Japan 2 (1971) 113-122. doi:10.1252/jcej.4.113

| T / K | P / bar | $x_1$ |
|---|---|---|
| 253.15 | 144.39 | 0.3950 |

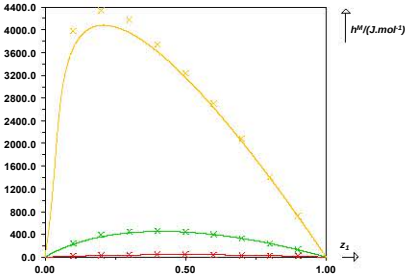
T/K = 283.15 - P/bar = 10.1300 43.5700



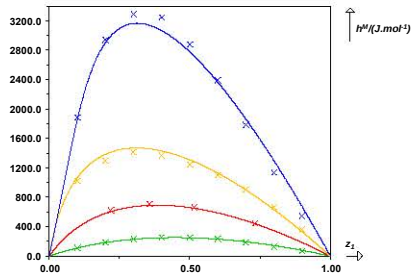

T/K = 293.15 - P/bar = 40.5300



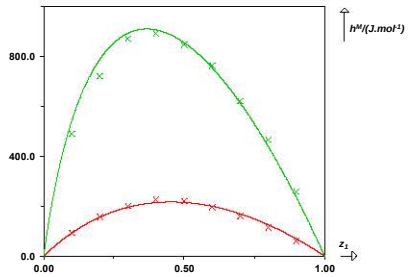

T/K = 305.15 - P/bar = 10.1300 50.6600 86.1300



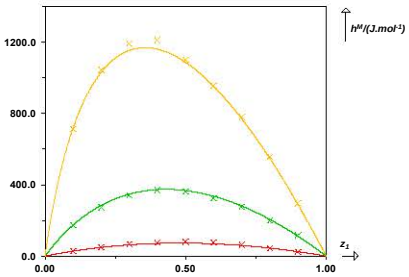

T/K = 313.15 - P/bar = 65.4900 40.5300 81.0600 121.5900



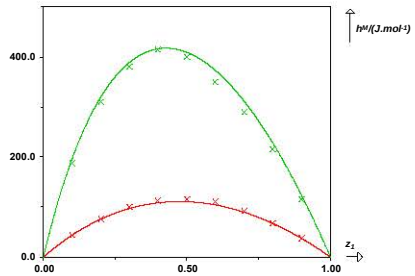

T/K = 323.15 - P/bar = 40.5300 81.0600



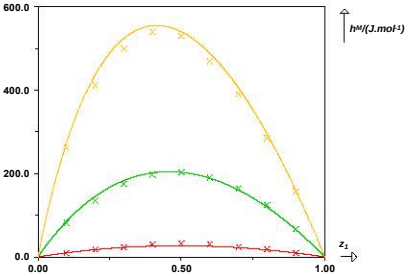

T/K = 333.15 - P/bar = 20.2600 60.7900 101.3200



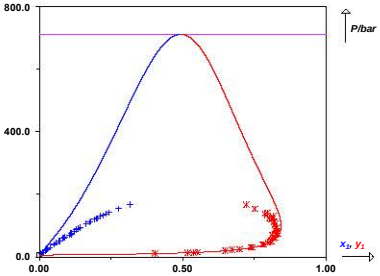

T/K = 343.15 - P/bar = 30.400 70.9300



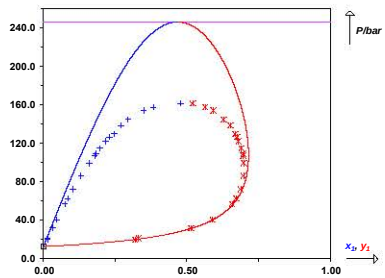

T/K = 353.15 - P/bar = 10.1300 50.6600 91.1900



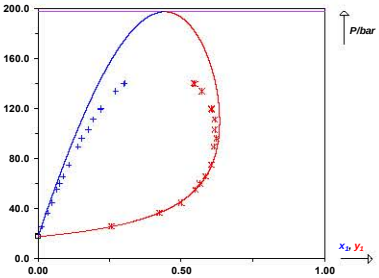

T/K = 220.00



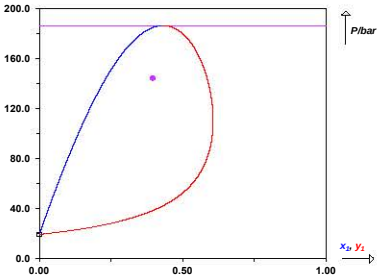

T/K = 240.00



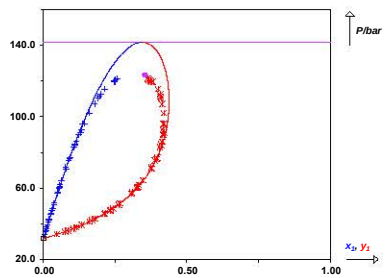

T/K = 250.00



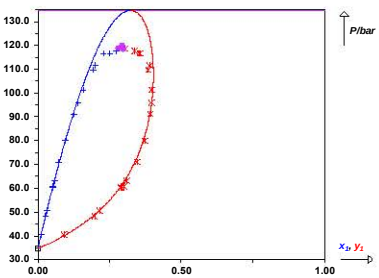

T/K = 253.15



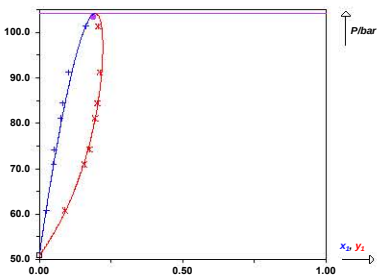

T/K = 270.00

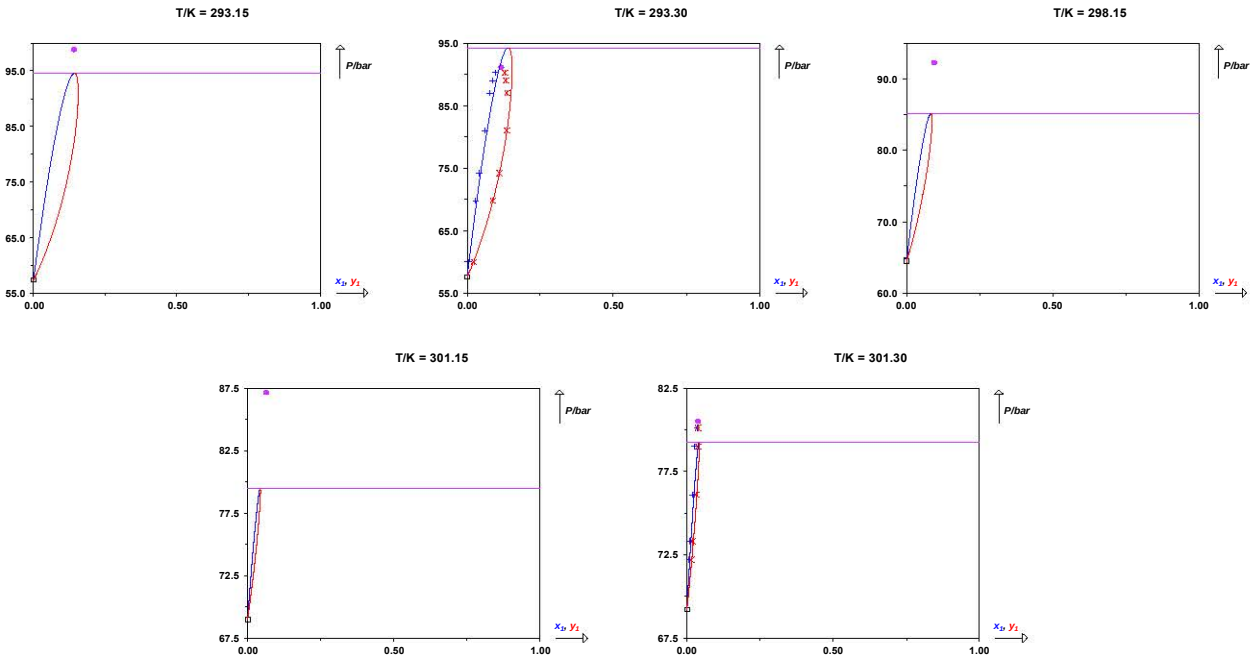



T/K = 273.15




T/K = 288.15




T/K = 293.15
P/bar
95.0
85.0
75.0
65.0
55.0
0.00
0.50
1.00
x1, y1
T/K = 293.30
P/bar
95.0
85.0
75.0
65.0
55.0
0.00
0.50
1.00
x1, y1
T/K = 298.15
P/bar
90.0
80.0
70.0
60.0
0.00
0.50
1.00
x1, y1
T/K = 301.15
P/bar
87.5
82.5
77.5
72.5
67.5
0.00
0.50
1.00
x1, y1
T/K = 301.30
P/bar
82.5
77.5
72.5
67.5
0.00
0.50
1.00
x1, y1

## METHANE (1) + HYDROGEN SULFIDE (2)

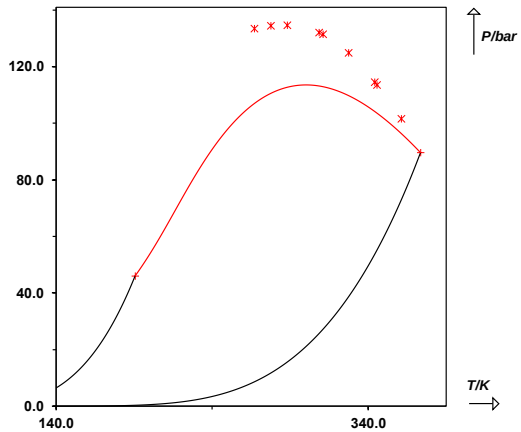
| | | |
|---|---|---|
| **CAS** | 74-82-8 | 7783-06-4 |
| **InChiKey** | VNWKTOKETHGBQD-UHFFFAOYSA-N | RWSOTUBLDIXVET-UHFFFAOYSA-N |
| **$T_c$ / K** | 190.56 | 373.53 |
| **$P_c$ / bar** | 45.99 | 89.63 |
| **ω** | 0.0120 | 0.0940 |

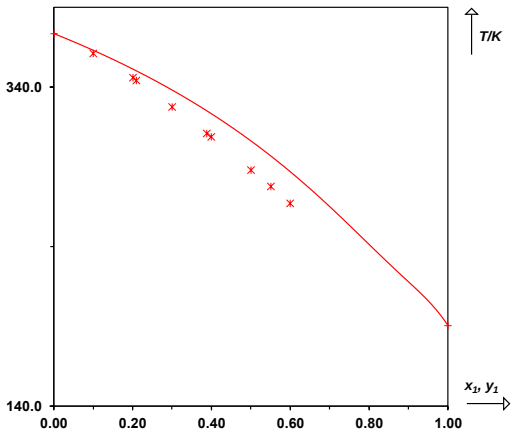
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 78
B/MPa = 134

*Deviations*
MAPE on x = 85 %
MAPE on y = 4.1 %
MAPE on $x_c$ = 16 %
MAPE on $P_c$ = 13 %
MAPE on $h^M$ = 88 %



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**Isothermal phase equilibrium data**

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Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems - Volumetric and Phase Behavior of the Methane-Hydrogen Sulfide System, Industrial & Engineering Chemistry 4 (1951) 976-981. doi:10.1021/ie50496a052

**T / K = 277.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 13.79 | 0.0057 | 0.1371 | |
| 17.24 | 0.0132 | 0.2783 | |
| 20.68 | 0.0212 | 0.3896 | |
| 24.13 | 0.0284 | 0.4604 | |
| 27.58 | 0.0354 | 0.5126 | |
| 31.03 | 0.0424 | 0.5551 | |
| 34.47 | 0.0493 | 0.5879 | |
| 41.37 | 0.0636 | 0.6394 | |
| 48.26 | 0.0783 | 0.6755 | |
| 55.16 | 0.0930 | 0.6989 | |
| 62.05 | 0.1083 | 0.7141 | |
| 68.95 | 0.1250 | 0.7242 | |
| 75.84 | 0.1433 | 0.7299 | |
| 82.74 | 0.1635 | 0.7321 | |
| 86.18 | 0.1750 | 0.7319 | |
| 89.63 | 0.1868 | 0.7306 | |
| 96.53 | 0.2137 | 0.7262 | |
| 103.42 | 0.2450 | 0.7185 | |
| 110.32 | 0.2798 | 0.7075 | |
| 117.21 | 0.3240 | 0.6931 | |
| 120.66 | 0.3492 | 0.6828 | |
| 124.11 | 0.3758 | 0.6686 | |
| 131.00 | 0.4401 | 0.6130 | |
| 134.38 | 0.5500 | 0.5500 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems - Volumetric and Phase Behavior of the Methane-Hydrogen Sulfide System, Industrial & Engineering Chemistry 4 (1951) 976-981. doi:10.1021/ie50496a052

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 27.58 | 0.0007 | 0.0117 | |
| 31.03 | 0.0067 | 0.0963 | |
| 34.47 | 0.0128 | 0.1642 | |
| 37.92 | 0.0190 | 0.2203 | |
| 41.37 | 0.0255 | 0.2688 | |
| 48.26 | 0.0385 | 0.3416 | |
| 55.16 | 0.0523 | 0.3976 | |
| 62.05 | 0.0670 | 0.4396 | |
| 68.95 | 0.0828 | 0.4707 | |
| 75.84 | 0.0996 | 0.4923 | |
| 82.74 | 0.1182 | 0.5079 | |
| 86.18 | 0.1282 | 0.5130 | |
| 89.63 | 0.1390 | 0.5182 | |
| 96.53 | 0.1620 | 0.5240 | |
| 103.42 | 0.1885 | 0.5255 | |
| 110.32 | 0.2192 | 0.5195 | |
| 117.21 | 0.2532 | 0.5058 | |
| 120.66 | 0.2725 | 0.4947 | |
| 124.11 | 0.2940 | 0.4797 | |
| 127.55 | 0.3185 | 0.4580 | |
| 131.00 | 0.3578 | 0.4190 | |
| 131.48 | 0.3880 | 0.3880 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems - Volumetric and Phase Behavior of the Methane-Hydrogen Sulfide System, Industrial & Engineering Chemistry 4 (1951) 976-981. doi:10.1021/ie50496a052

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 55.16 | 0.0031 | 0.0196 | |
| 58.61 | 0.0098 | 0.0592 | |
| 62.05 | 0.0167 | 0.0946 | |
| 68.95 | 0.0309 | 0.1553 | |
| 75.84 | 0.0459 | 0.2021 | |
| 82.74 | 0.0622 | 0.2367 | |
| 86.18 | 0.0720 | 0.2534 | |
| 89.63 | 0.0814 | 0.2646 | |
| 96.53 | 0.1021 | 0.2811 | |
| 103.42 | 0.1245 | 0.2775 | |
| 110.32 | 0.1547 | 0.2580 | |
| 113.76 | 0.1830 | 0.2295 | |
| 114.45 | 0.2090 | 0.2090 | CRIT |

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**Isobaric phase equilibrium data**

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Kohn, James P. - Kurata, Fred, Heterogeneous phase equilibria of the methane—hydrogen sulfide system, AIChE Journal 2 (1958) 211-217. doi:10.1002/aic.690040217

**P / bar = 13.79**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 277.59 | 0.0050 | 0.1400 |
| 255.38 | 0.0090 | 0.5220 |
| 233.15 | 0.0125 | 0.7540 |
| 210.93 | 0.0180 | 0.9060 |

Kohn, James P. - Kurata, Fred, Heterogeneous phase equilibria of the methane—hydrogen sulfide system, AIChE Journal 2 (1958) 211-217. doi:10.1002/aic.690040217

**P / bar = 27.58**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 299.81 | 0.0160 | 0.2510 |
| 277.59 | 0.0350 | 0.5130 |
| 255.38 | 0.0450 | 0.7200 |
| 233.15 | 0.0540 | 0.8620 |
| 210.93 | 0.0620 | 0.9350 |

Kohn, James P. - Kurata, Fred, Heterogeneous phase equilibria of the methane—hydrogen sulfide system, AIChE Journal 2 (1958) 211-217. doi:10.1002/aic.690040217

**P / bar = 41.37**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 322.03 | 0.0150 | 0.1430 |
| 299.81 | 0.0380 | 0.4060 |
| 277.59 | 0.0580 | 0.6280 |
| 255.38 | 0.0720 | 0.7920 |
| 233.15 | 0.0830 | 0.9000 |
| 210.93 | 0.0930 | 0.9470 |
| 199.82 | 0.1010 | 0.9550 |

Kohn, James P. - Kurata, Fred, Heterogeneous phase equilibria of the methane—hydrogen sulfide system, AIChE Journal 2 (1958) 211-217. doi:10.1002/aic.690040217

**P / bar = 55.15**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 338.70 | 0.0100 | 0.1040 |
| 322.03 | 0.0350 | 0.2900 |
| 310.92 | 0.0510 | 0.4050 |
| 299.81 | 0.0680 | 0.5010 |
| 288.70 | 0.0860 | 0.5960 |
| 277.59 | 0.0900 | 0.6900 |

Kohn, James P. - Kurata, Fred, Heterogeneous phase equilibria of the methane—hydrogen sulfide system, AIChE Journal 2 (1958) 211-217. doi:10.1002/aic.690040217

**P / bar = 82.73**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 366.48 | 0.0060 | 0.0250 |
| 344.26 | 0.0520 | 0.2380 |
| 322.03 | 0.0950 | 0.4320 |
| 299.81 | 0.1350 | 0.5820 |
| 277.59 | 0.1620 | 0.7270 |

Kohn, James P. - Kurata, Fred, Heterogeneous phase equilibria of the methane—hydrogen sulfide system, AIChE Journal 2 (1958) 211-217. doi:10.1002/aic.690040217

**P / bar = 110.31**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 344.26 | 0.1550 | 0.2500 |
| 322.03 | 0.1840 | 0.4410 |
| 310.92 | 0.2000 | 0.5200 |
| 299.81 | 0.2130 | 0.5860 |
| 277.59 | 0.2380 | 0.7050 |

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**Enthalpy of mixing**

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Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Excess enthalpies of the binary system methane-hydrogen sulfide by flow calorimetry, Journal of Chemical & Engineering Data 4 (1982) 436-439. doi:10.1021/je00030a020

**T / K = 293.15**

**P / bar = 5.070**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 28.30 | 0.2030 |
| 43.60 | 0.3990 |
| 44.80 | 0.5600 |
| 41.20 | 0.6720 |
| 40.50 | 0.7100 |
| 38.80 | 0.7770 |

Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Excess enthalpies of the binary system methane-hydrogen sulfide by flow calorimetry, Journal of Chemical & Engineering Data 4 (1982) 436-439. doi:10.1021/je00030a020

**T / K = 293.15**

**P / bar = 10.13**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 79.80 | 0.2650 |
| 101.10 | 0.4310 |
| 97.10 | 0.6590 |

Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Excess enthalpies of the binary system methane-hydrogen sulfide by flow calorimetry, Journal of Chemical & Engineering Data 4 (1982) 436-439. doi:10.1021/je00030a020

**T / K = 293.15**

**P / bar = 15.20**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 123.60 | 0.1840 |
| 149.50 | 0.2450 |

| | |
|---|---|
| 190.80 | 0.4830 |
| 184.60 | 0.5940 |
| 138.80 | 0.7930 |

Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Excess enthalpies of the binary system methane-hydrogen sulfide by flow calorimetry, Journal of Chemical & Engineering Data 4 (1982) 436-439. doi:10.1021/je00030a020

**T / K = 305.15**

**P / bar = 5.070**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 23.80 | 0.2060 |
| 39.70 | 0.4560 |
| 40.70 | 0.6210 |
| 37.00 | 0.7380 |

Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Excess enthalpies of the binary system methane-hydrogen sulfide by flow calorimetry, Journal of Chemical & Engineering Data 4 (1982) 436-439. doi:10.1021/je00030a020

**T / K = 305.15**

**P / bar = 10.13**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 60.40 | 0.1840 |
| 90.80 | 0.3920 |
| 95.00 | 0.4490 |
| 69.80 | 0.7820 |

Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Excess enthalpies of the binary system methane-hydrogen sulfide by flow calorimetry, Journal of Chemical & Engineering Data 4 (1982) 436-439. doi:10.1021/je00030a020

**T / K = 305.15**

**P / bar = 15.20**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 148.80 | 0.2740 |
| 163.80 | 0.4430 |
| 167.50 | 0.5680 |
| 83.30 | 0.8470 |

Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Excess enthalpies of the binary system methane-hydrogen sulfide by flow calorimetry, Journal of Chemical & Engineering Data 4 (1982) 436-439. doi:10.1021/je00030a020

**T / K = 313.15**

**P / bar = 5.070**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 34.60 | 0.3240 |
| 42.50 | 0.3860 |
| 43.90 | 0.4460 |
| 33.20 | 0.6930 |

Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Excess enthalpies of the binary system methane-hydrogen sulfide by flow calorimetry, Journal of Chemical & Engineering Data 4 (1982) 436-439. doi:10.1021/je00030a020

**T / K = 313.15**

**P / bar = 10.13**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 68.00 | 0.2370 |
| 78.80 | 0.3510 |
| 90.40 | 0.4830 |
| 83.60 | 0.6920 |
| 64.70 | 0.7800 |

Barry, Alpha O. - Kaliaguine, Serge C. - Ramalho, Rubens S., Excess enthalpies of the binary system methane-hydrogen sulfide by flow calorimetry, Journal of Chemical & Engineering Data 4 (1982) 436-439. doi:10.1021/je00030a020

**T / K = 313.15**

**P / bar = 15.20**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 119.20 | 0.2720 |
| 139.00 | 0.3240 |
| 135.50 | 0.6020 |
| 97.30 | 0.7780 |

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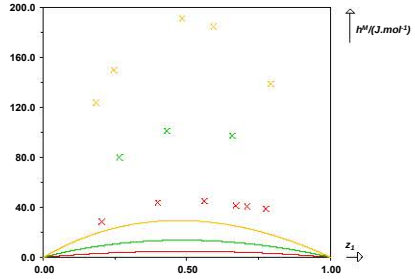
**Critical point**

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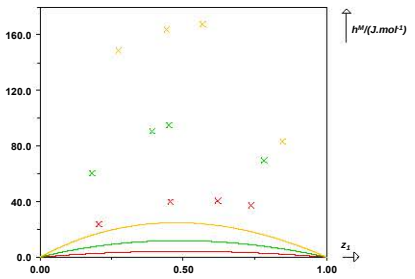
Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems - Volumetric and Phase Behavior of the Methane-Hydrogen Sulfide System, Industrial & Engineering Chemistry 4 (1951) 976-981. doi:10.1021/ie50496a052

| T / K | P / bar | $x_1$ |
|---|---|---|
| 361.09 | 101.56 | 0.1000 |
| 345.71 | 113.56 | 0.2000 |
| 327.59 | 124.93 | 0.3000 |
| 308.59 | 132.03 | 0.4000 |
| 288.09 | 134.72 | 0.5000 |
| 267.15 | 133.48 | 0.6000 |

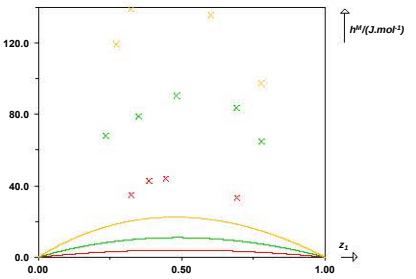
T/K = 293.15 - P/bar = 5.0700 10.1300 15.200



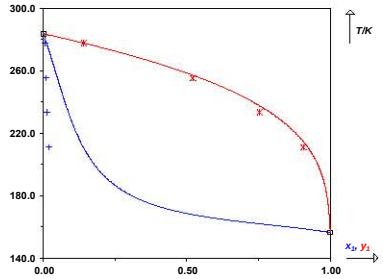

T/K = 305.15 - P/bar = 5.0700 10.1300 15.200



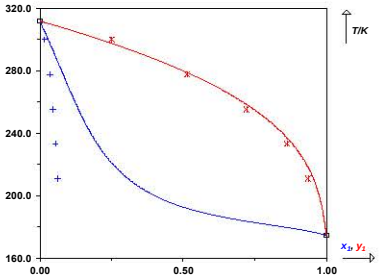

T/K = 313.15 - P/bar = 5.0700 10.1300 15.200



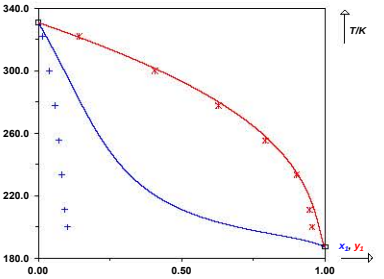

P/bar = 13.78800



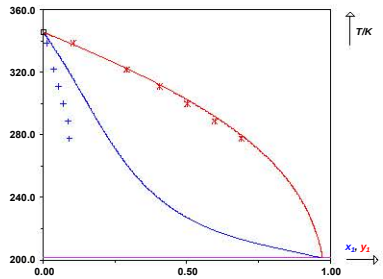

P/bar = 27.57600



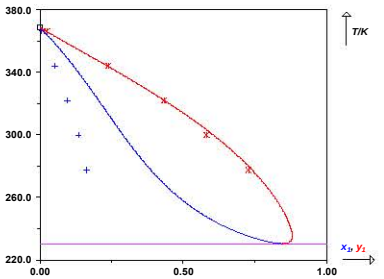

P/bar = 41.36500



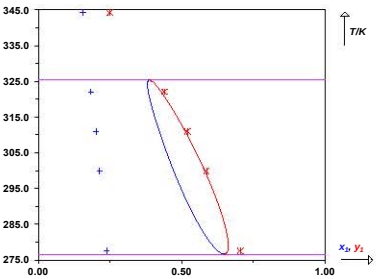

P/bar = 55.15300



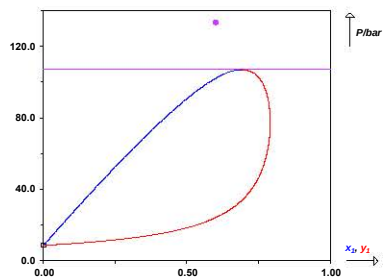

P/bar = 82.72900



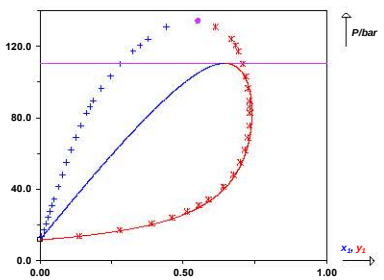

P/bar = 110.31000



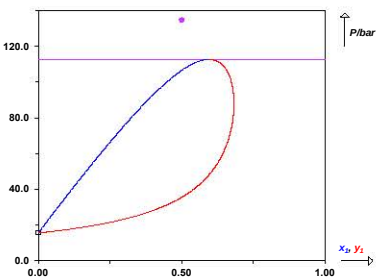

T/K = 267.15

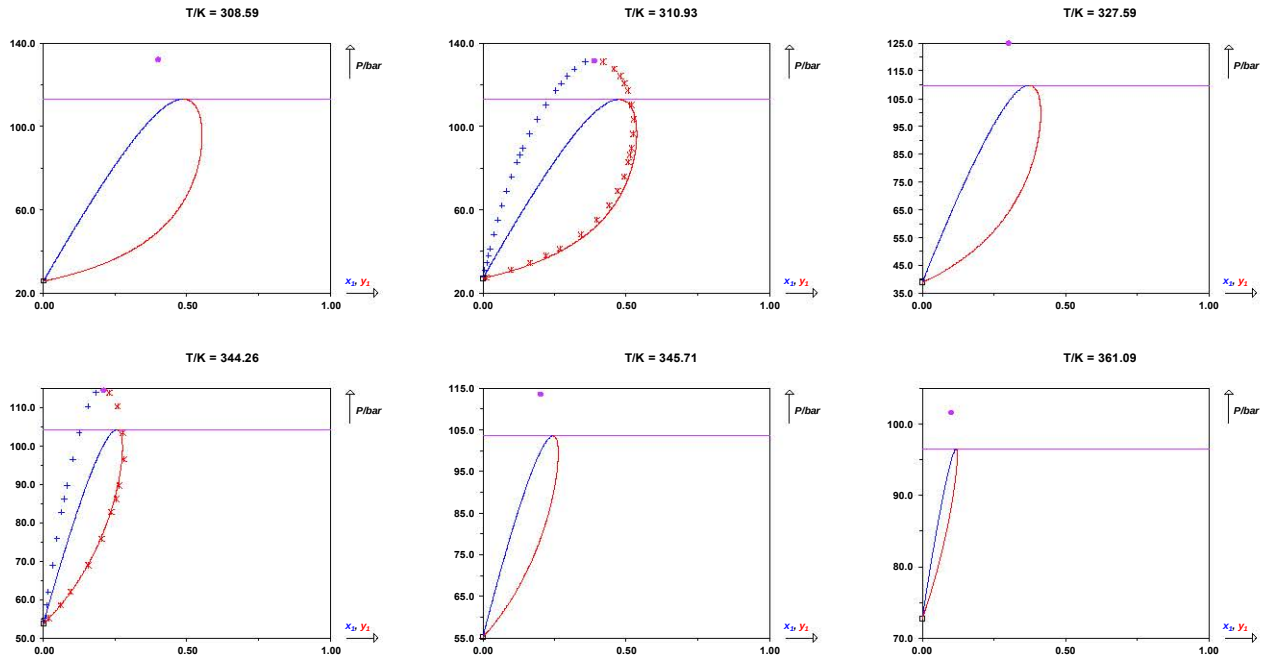



T/K = 277.59




T/K = 288.09




T/K = 308.59
T/K = 310.93
T/K = 327.59
T/K = 344.26
T/K = 345.71
T/K = 361.09
P/bar
x1, y1

## OXYGEN (1) + CARBON DIOXIDE (2)

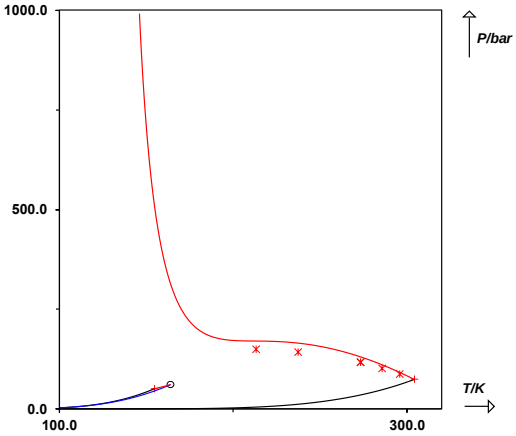
| | | |
|---|---|---|
| **CAS** | 7782-44-7 | 124-38-9 |
| **InChiKey** | XLYOFNOQVPJJNP-UHFFFAOYSA-N | CURLTUGMZLYLDI-UHFFFAOYSA-N |
| **$T_c$ / K** | 154.58 | 304.21 |
| **$P_c$ / bar** | 50.43 | 73.83 |
| **ω** | 0.0220 | 0.2240 |

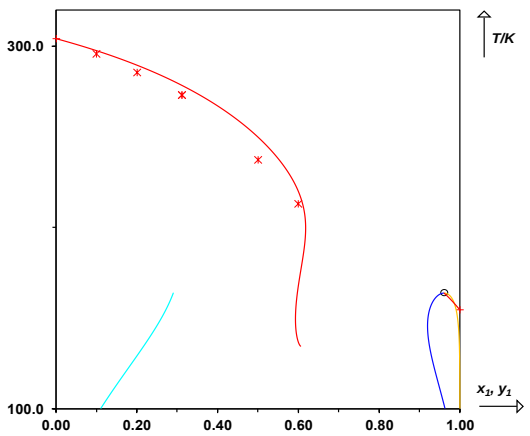
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 472
B/MPa = 441

*Deviations*
MAPE on x = 5.4 %
MAPE on y = 4 %
MAPE on $x_c$ = 10 %
MAPE on $P_c$ = 11 %



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**Isothermal phase equilibrium data**

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Zenner, G.H. - Dana, L.I., Liquid-vapor equilibrium compositions of carbon dioxideoxygen-nitrogen mixtures, Chem. Eng. Progr. Symp. Ser. 44 (1963) 36-41.

**T / K = 218.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 21.89 | 0.0330 | 0.7040 |
| 39.42 | 0.0720 | 0.8120 |
| 59.07 | 0.1190 | 0.8470 |
| 78.83 | 0.1740 | 0.8530 |
| 97.17 | 0.2340 | 0.8510 |
| 118.25 | 0.3120 | 0.8220 |
| 130.10 | 0.3820 | 0.7890 |
| 140.23 | 0.4680 | 0.7360 |

Fredenslund, Aage - Sather, G. A., Gas-liquid equilibrium of the oxygen-carbon dioxide system, Journal of Chemical & Engineering Data 1 (1970) 17-22. doi:10.1021/je60044a024

**T / K = 223.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.13 | 0.0080 | 0.3120 |
| 20.27 | 0.0250 | 0.6170 |
| 30.40 | 0.0490 | 0.7120 |
| 40.53 | 0.0710 | 0.7610 |
| 50.66 | 0.0960 | 0.7890 |
| 60.80 | 0.1170 | 0.8090 |
| 70.93 | 0.1500 | 0.8140 |
| 81.06 | 0.1890 | 0.8180 |
| 91.19 | 0.2200 | 0.8200 |
| 101.33 | 0.2670 | 0.8190 |
| 111.46 | 0.2930 | 0.7970 |
| 121.59 | 0.3340 | 0.7800 |
| 131.72 | 0.3930 | 0.7620 |

Zenner, G.H. - Dana, L.I., Liquid-vapor equilibrium compositions of carbon dioxideoxygen-nitrogen mixtures, Chem. Eng. Progr. Symp. Ser. 44 (1963) 36-41.

**T / K = 232.85**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 142.97 | 0.4970 | 0.6170 |
| 134.86 | 0.4030 | 0.7070 |
| 125.34 | 0.3400 | 0.7200 |
| 111.46 | 0.2760 | 0.7530 |
| 94.64 | 0.2170 | 0.7680 |
| 77.72 | 0.1645 | 0.7700 |
| 59.17 | 0.1130 | 0.7740 |

Fredenslund, Aage - Sather, G. A., Gas-liquid equilibrium of the oxygen-carbon dioxide system, Journal of Chemical & Engineering Data 1 (1970) 17-22. doi:10.1021/je60044a024

**T / K = 233.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.27 | 0.0210 | 0.4190 |
| 30.40 | 0.0410 | 0.5890 |
| 40.53 | 0.0640 | 0.6510 |
| 50.66 | 0.0870 | 0.6950 |
| 60.80 | 0.1200 | 0.7230 |
| 70.93 | 0.1410 | 0.7410 |
| 81.06 | 0.1670 | 0.7570 |
| 91.19 | 0.2050 | 0.7660 |
| 101.33 | 0.2480 | 0.7670 |
| 111.46 | 0.2740 | 0.7600 |
| 121.59 | 0.3280 | 0.7300 |
| 131.72 | 0.3800 | 0.7020 |

Fredenslund, Aage - Sather, G. A., Gas-liquid equilibrium of the oxygen-carbon dioxide system, Journal of Chemical & Engineering Data 1 (1970) 17-22. doi:10.1021/je60044a024

**T / K = 243.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.27 | 0.0100 | 0.2750 |
| 30.40 | 0.0310 | 0.4630 |
| 40.53 | 0.0520 | 0.5510 |
| 50.66 | 0.0800 | 0.6090 |
| 60.80 | 0.1040 | 0.6440 |
| 70.93 | 0.1400 | 0.6710 |
| 81.06 | 0.1620 | 0.6930 |
| 91.19 | 0.1910 | 0.6890 |
| 101.33 | 0.2360 | 0.6940 |
| 111.46 | 0.2660 | 0.6820 |
| 121.59 | 0.3060 | 0.6710 |

Kaminishi, G.I. - Toriumi, T., Gas-liquid equilibrium under high pressures. VI. Vapor-liquid phase equilibrium in the CO2-H2, CO2-N2, and CO2-O2 systems, Kogyo Kagaku Zasshi (1966) 175-178.

**T / K = 253.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 36.98 | 0.0360 | 0.3830 |
| 52.69 | 0.0720 | 0.5160 |
| 101.83 | 0.2180 | 0.6120 |
| 127.37 | 0.3710 | 0.5640 |

Fredenslund, Aage - Sather, G. A., Gas-liquid equilibrium of the oxygen-carbon dioxide system, Journal of Chemical & Engineering Data 1 (1970) 17-22. doi:10.1021/je60044a024

**T / K = 253.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.27 | 0.0060 | 0.0610 |
| 30.40 | 0.0300 | 0.3020 |
| 40.53 | 0.0420 | 0.4000 |
| 50.66 | 0.0620 | 0.5000 |
| 60.80 | 0.0920 | 0.5400 |
| 70.93 | 0.1250 | 0.5600 |
| 81.06 | 0.1410 | 0.5740 |
| 91.19 | 0.1700 | 0.6010 |
| 101.33 | 0.2200 | 0.5990 |
| 111.46 | 0.2550 | 0.6010 |
| 121.59 | 0.3000 | 0.5700 |

Fredenslund, Aage - Sather, G. A., Gas-liquid equilibrium of the oxygen-carbon dioxide system, Journal of Chemical & Engineering Data 1 (1970) 17-22. doi:10.1021/je60044a024

**T / K = 263.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 30.40 | 0.0090 | 0.0960 |
| 40.53 | 0.0350 | 0.2630 |
| 50.66 | 0.0560 | 0.3460 |
| 60.80 | 0.0790 | 0.4170 |
| 70.93 | 0.1100 | 0.4630 |
| 81.06 | 0.1340 | 0.4930 |
| 91.19 | 0.1620 | 0.4950 |
| 101.33 | 0.1950 | 0.5000 |
| 111.46 | 0.2430 | 0.4980 |
| 121.59 | 0.2990 | 0.4460 |

Kaminishi, G.I. - Toriumi, T., Gas-liquid equilibrium under high pressures. VI. Vapor-liquid phase equilibrium in the CO2-H2, CO2-N2, and CO2-O2 systems, Kogyo Kagaku Zasshi (1966) 175-178.

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 50.66 | 0.0360 | 0.2200 |
| 74.17 | 0.0960 | 0.3710 |
| 96.26 | 0.1660 | 0.4110 |
| 105.68 | 0.2060 | 0.4080 |

Chueh, P. L. - Muirbrook, N. K. - Prausnitz, J. M., Multicomponent vapor-liquid equilibria at high pressures: Part II. Thermodynamic analysis, AIChE Journal 6 (1965) 1097-1102. doi:10.1002/aic.690110625

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 55.16 | 0.0455 | 0.2520 | |
| 82.74 | 0.1205 | 0.3838 | |
| 103.42 | 0.1980 | 0.4065 | |
| 117.42 | 0.3120 | 0.3120 | CRIT |

Zenner, G.H. - Dana, L.I., Liquid-vapor equilibrium compositions of carbon dioxideoxygen-nitrogen mixtures, Chem. Eng. Progr. Symp. Ser. 44 (1963) 36-41.

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 60.19 | 0.0603 | 0.2980 |
| 53.20 | 0.0432 | 0.2540 |
| 69.71 | 0.0843 | 0.3530 |
| 84.91 | 0.1293 | 0.4070 |
| 94.23 | 0.1600 | 0.4205 |
| 104.06 | 0.1985 | 0.4220 |
| 111.05 | 0.2370 | 0.3990 |

Fredenslund, Aage - Sather, G. A., Gas-liquid equilibrium of the oxygen-carbon dioxide system, Journal of Chemical & Engineering Data 1 (1970) 17-22. doi:10.1021/je60044a024

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 40.53 | 0.0100 | 0.0990 |
| 50.66 | 0.0420 | 0.2140 |
| 60.80 | 0.0620 | 0.2980 |
| 70.93 | 0.0900 | 0.3360 |
| 81.06 | 0.1260 | 0.3720 |
| 91.19 | 0.1470 | 0.3980 |
| 101.33 | 0.1850 | 0.4010 |
| 111.46 | 0.2470 | 0.3620 |

Fredenslund, Aage - Sather, G. A., Gas-liquid equilibrium of the oxygen-carbon dioxide system, Journal of Chemical & Engineering Data 1 (1970) 17-22. doi:10.1021/je60044a024

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 50.66 | 0.0280 | 0.1150 |
| 60.80 | 0.0400 | 0.1610 |
| 70.93 | 0.0710 | 0.2180 |
| 81.06 | 0.0870 | 0.2630 |
| 91.19 | 0.1150 | 0.2940 |
| 101.33 | 0.1870 | 0.2630 |

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**Critical point**

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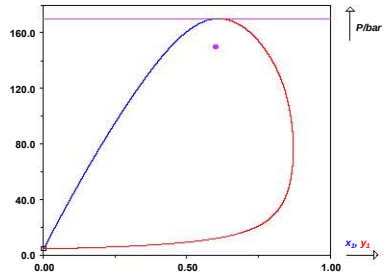
Muirbrook, N. K. - Prausnitz, J. M., Multicomponent vapor-liquid equilibria at high pressures: Part I. Experimental study of the nitrogen—oxygen—carbon dioxide system at 0°C, AIChE Journal 6 (1965) 1092-1096. doi:10.1002/aic.690110624

| T / K | P / bar | $x_1$ |
|---|---|---|
| 273.15 | 117.42 | 0.3120 |

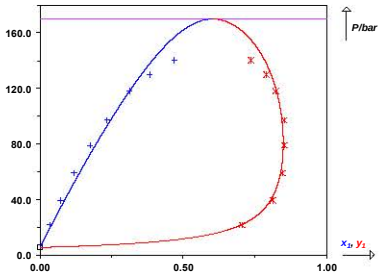
Leopold, G. H., Das Dreiphasengleichgewicht mit einem Druckminimum einer dissociabeln Verbindung zweier Komponenten. Dritte Mitteilung, Zeitschrift für Physikalische Chemie 1 (1910) doi:10.1515/zpch-1910-7106

| T / K | P / bar | $x_1$ |
|---|---|---|
| 295.66 | 87.14 | 0.1000 |
| 285.65 | 100.92 | 0.2000 |
| 237.45 | 142.56 | 0.5000 |
| 213.10 | 149.96 | 0.6000 |

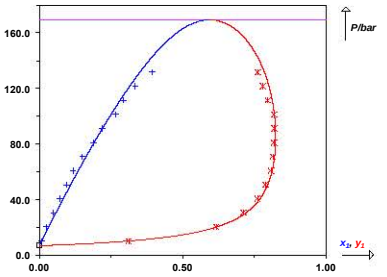
T/K = 213.10



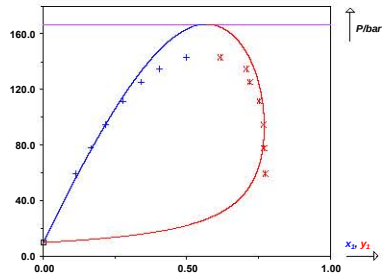

T/K = 218.15



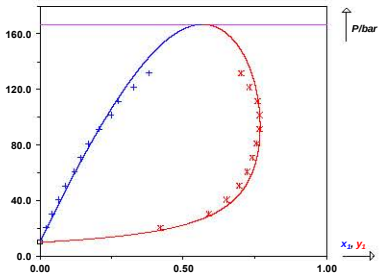

T/K = 223.15



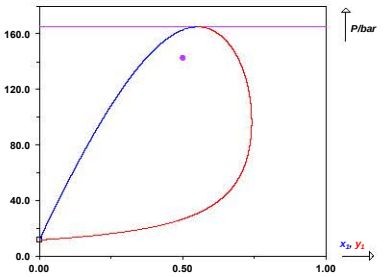

T/K = 232.85



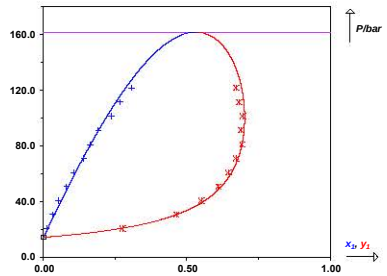

T/K = 233.15



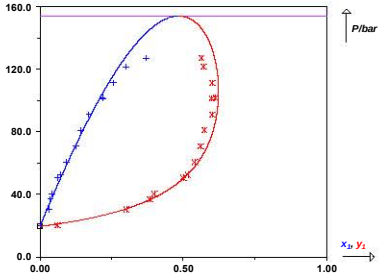

T/K = 237.45



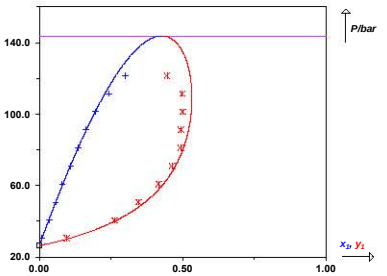

T/K = 243.15



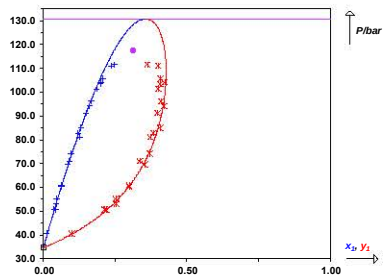

T/K = 253.15



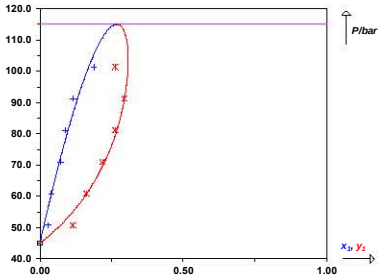

T/K = 263.15



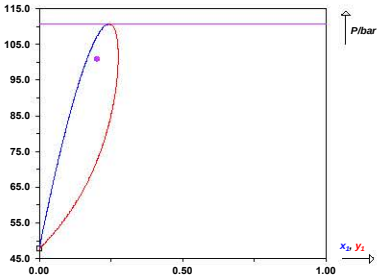

T/K = 273.15



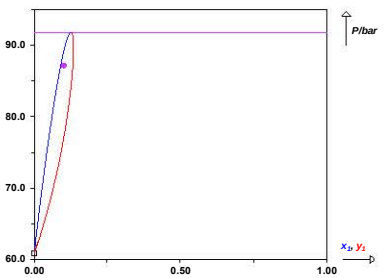

T/K = 283.15




T/K = 285.65




T/K = 295.66



## METHYL tert-BUTYL ETHER (1) + n-HEPTANE (2)

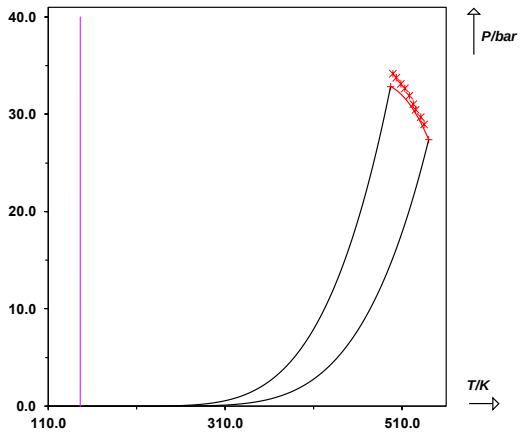
| | | |
|---|---|---|
| **CAS** | 1634-04-4 | 142-82-5 |
| **InChiKey** | BZLVMXJERCGZMT-UHFFFAOYSA-N | IMNFDUFMRHMDMM-UHFFFAOYSA-N |
| **$T_c$ / K** | 497.10 | 540.20 |
| **$P_c$ / bar** | 32.86 | 27.40 |
| **ω** | 0.2470 | 0.3490 |

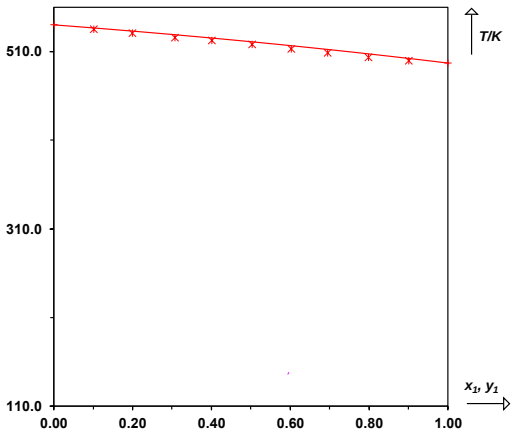
Ideal

**PPR78 results**

*Parameters*
A/MPa = 22.4
B/MPa = 71.2

*Deviations*
MAPE on x = 6.4 %
MAPE on y = 3.7 %
MAPE on $x_c$ = 21 %
MAPE on $P_c$ = 2.5 %
MAPE on $h^M$ = 3.1 %



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**Isothermal phase equilibrium data**

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Krevor, David H. - Prausnitz, John M., Vapor-liquid equilibria for model mixtures of coal-derived liquids. 1. Binary systems with 2-methylfuran, Journal of Chemical & Engineering Data 3 (1986) 349-353. doi:10.1021/je00045a027

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1550 | 0.0521 | 0.2426 |
| 0.1826 | 0.0996 | 0.3863 |
| 0.2107 | 0.1512 | 0.4970 |
| 0.2365 | 0.1990 | 0.5738 |
| 0.2658 | 0.2554 | 0.6440 |
| 0.2872 | 0.2988 | 0.6876 |
| 0.3116 | 0.3490 | 0.7301 |
| 0.3346 | 0.3976 | 0.7650 |
| 0.3354 | 0.3997 | 0.7665 |
| 0.3581 | 0.4483 | 0.7966 |
| 0.3584 | 0.4499 | 0.7975 |
| 0.3808 | 0.4982 | 0.8237 |
| 0.3809 | 0.4989 | 0.8241 |
| 0.4034 | 0.5487 | 0.8482 |
| 0.4037 | 0.5494 | 0.8485 |
| 0.4470 | 0.6490 | 0.8900 |
| 0.4687 | 0.6984 | 0.9081 |
| 0.4905 | 0.7501 | 0.9258 |
| 0.5120 | 0.8009 | 0.9421 |
| 0.5333 | 0.8490 | 0.9568 |
| 0.5544 | 0.8978 | 0.9711 |
| 0.5770 | 0.9514 | 0.9864 |

Lee, J.D. - Lee, T.J. - Park, S.J., Infinite dilution activity coefficients and vapor-liquid equilibria for the binary systems containing MTBE, Hwahak Konghak 5 (1995) 527-534.

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1551 | 0.0007 | 0.0052 |
| 0.1559 | 0.0019 | 0.0106 |
| 0.1598 | 0.0070 | 0.0405 |
| 0.1859 | 0.0416 | 0.1899 |
| 0.2124 | 0.0868 | 0.3280 |
| 0.2698 | 0.1768 | 0.5161 |
| 0.3135 | 0.2527 | 0.6206 |
| 0.3590 | 0.3316 | 0.7020 |
| 0.3949 | 0.3954 | 0.7536 |
| 0.4390 | 0.4768 | 0.8063 |
| 0.4901 | 0.5700 | 0.8559 |
| 0.5290 | 0.6567 | 0.8888 |
| 0.5661 | 0.7176 | 0.9165 |
| 0.6057 | 0.7895 | 0.9417 |
| 0.6422 | 0.8592 | 0.9625 |
| 0.6766 | 0.9252 | 0.9807 |
| 0.6982 | 0.9643 | 0.9912 |
| 0.7122 | 0.9906 | 0.9977 |
| 0.7158 | 0.9972 | 0.9993 |

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**Isobaric phase equilibrium data**

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Wisniak, Jaime - Magen, Erez - Shachar, Michal - Zeroni, Ilan - Reich, Ricardo - Segura, Hugo, Isobaric Vapor−Liquid Equilibria in the Systems Methyl 1,1-Dimethylethyl Ether + Hexane and + Heptane, Journal of Chemical & Engineering Data 2 (1997) 243-247. doi:10.1021/je960301h

**P / bar = 0.9400**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 366.45 | 0.0210 | 0.0780 |
| 365.35 | 0.0380 | 0.1340 |
| 364.25 | 0.0480 | 0.1670 |
| 363.65 | 0.0600 | 0.2020 |
| 360.55 | 0.1000 | 0.3140 |
| 359.95 | 0.1050 | 0.3230 |
| 356.25 | 0.1570 | 0.4290 |
| 350.55 | 0.2390 | 0.5510 |
| 349.25 | 0.2720 | 0.6000 |
| 348.55 | 0.2920 | 0.6180 |
| 346.25 | 0.3370 | 0.6770 |
| 342.85 | 0.4150 | 0.7430 |
| 340.75 | 0.4650 | 0.7820 |
| 340.65 | 0.4700 | 0.7860 |
| 336.55 | 0.5970 | 0.8530 |
| 334.85 | 0.6380 | 0.8760 |
| 333.75 | 0.6740 | 0.8920 |
| 332.15 | 0.7300 | 0.9150 |
| 331.15 | 0.7710 | 0.9290 |
| 330.45 | 0.8030 | 0.9410 |
| 329.15 | 0.8530 | 0.9570 |
| 328.15 | 0.8860 | 0.9670 |
| 327.85 | 0.8990 | 0.9710 |
| 326.85 | 0.9440 | 0.9840 |
| 326.45 | 0.9580 | 0.9880 |

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**Enthalpy of mixing**

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Tusel-Langer, E. - Garcia Alonso, J. M. - Villamañan Olfos, M. A. - Lichtenthaler, R. N., Excess enthalpies of mixtures containing n-heptane, methanol and methyl tert-butyl ether (MTBE), Journal of Solution Chemistry 1 (1991) 153-163. doi:10.1007/BF00651647

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 34.20 | 0.0245 |
| 82.30 | 0.0609 |
| 111.90 | 0.0809 |
| 155.30 | 0.1204 |
| 218.60 | 0.1785 |
| 270.10 | 0.2354 |
| 305.30 | 0.2911 |
| 327.10 | 0.3184 |
| 350.20 | 0.3723 |
| 368.80 | 0.3988 |
| 376.10 | 0.4509 |
| 383.20 | 0.5019 |
| 381.60 | 0.5519 |
| 373.10 | 0.6009 |
| 359.50 | 0.6488 |
| 334.60 | 0.6958 |
| 271.50 | 0.7870 |
| 194.90 | 0.8603 |
| 180.20 | 0.8747 |
| 65.20 | 0.9590 |

Tusel-Langer, E. - Garcia Alonso, J. M. - Villamañan Olfos, M. A. - Lichtenthaler, R. N., Excess enthalpies of mixtures containing n-heptane, methanol and methyl tert-butyl ether (MTBE), Journal of Solution Chemistry 1 (1991) 153-163. doi:10.1007/BF00651647

**T / K = 313.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 71.80 | 0.0609 |
| 147.20 | 0.1204 |
| 201.30 | 0.1785 |
| 292.40 | 0.2911 |
| 318.40 | 0.3455 |
| 346.50 | 0.3988 |
| 355.90 | 0.4509 |
| 363.80 | 0.5019 |
| 361.00 | 0.5519 |
| 354.00 | 0.6009 |
| 337.60 | 0.6488 |
| 317.80 | 0.6958 |
| 254.00 | 0.7870 |
| 186.90 | 0.8603 |
| 169.00 | 0.8747 |
| 61.30 | 0.9590 |

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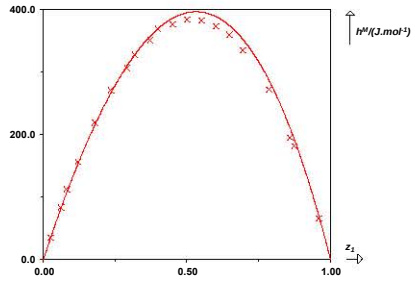
**Critical point**

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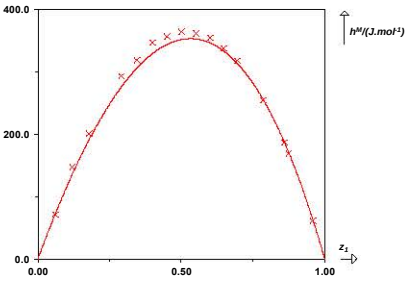
Han, Kewei - Xia, Shuqian - Ma, Peisheng - Yan, Fangyou - Liu, Tao, Measurement of critical temperatures and critical pressures for binary mixtures of methyl tert-butyl ether (MTBE)+alcohol and MTBE+alkane, The Journal of Chemical Thermodynamics (2013) 111-117. doi:10.1016/j.jct.2013.03.002

| T / K | P / bar | $x_1$ |
|---|---|---|
| 499.40 | 34.17 | 0.9000 |
| 503.70 | 33.75 | 0.7989 |
| 508.30 | 33.10 | 0.6944 |
| 513.10 | 32.67 | 0.6022 |
| 518.00 | 31.88 | 0.5030 |
| 522.60 | 31.05 | 0.4004 |
| 525.60 | 30.43 | 0.3067 |
| 530.90 | 29.69 | 0.1999 |
| 535.00 | 28.94 | 0.1016 |

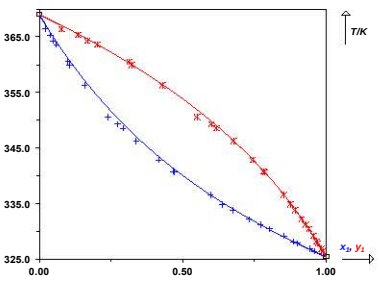
T/K = 298.15 - P/bar = 1.0100



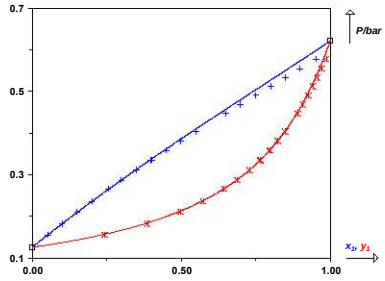

T/K = 313.15 - P/bar = 1.0100



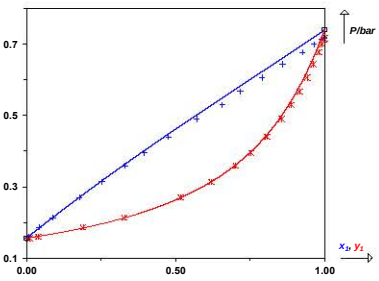

P/bar = 0.94000



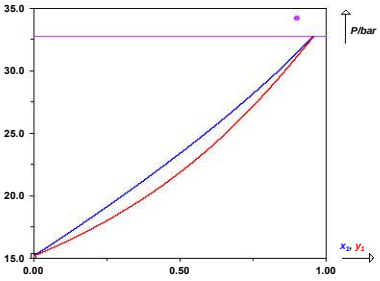

T/K = 313.15



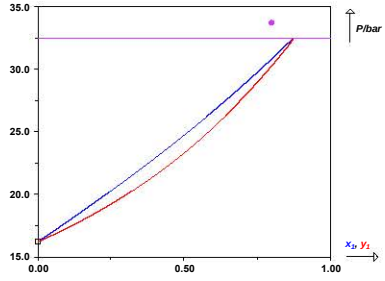

T/K = 318.15



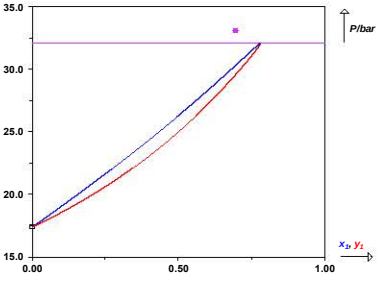

T/K = 499.40



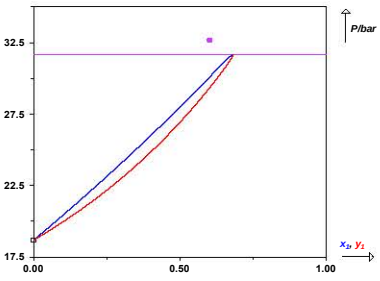

T/K = 503.70



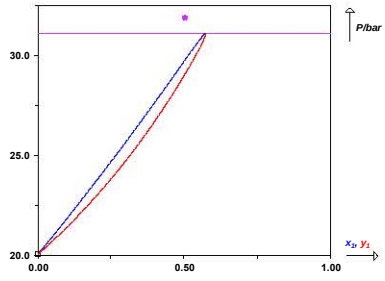

T/K = 508.30



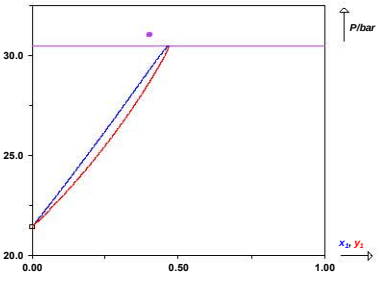

T/K = 513.10



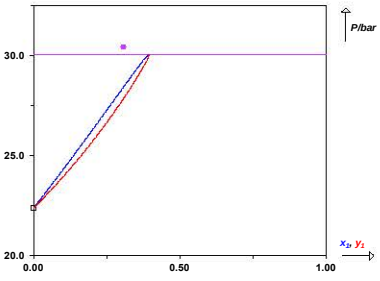

T/K = 518.00



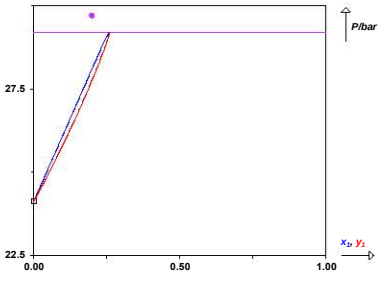

T/K = 522.60



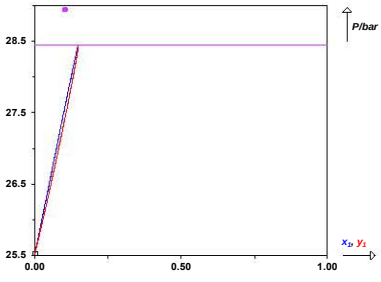

T/K = 525.60




T/K = 530.90




T/K = 535.00



## ETHYL ACETATE (1) + TOLUENE (2)

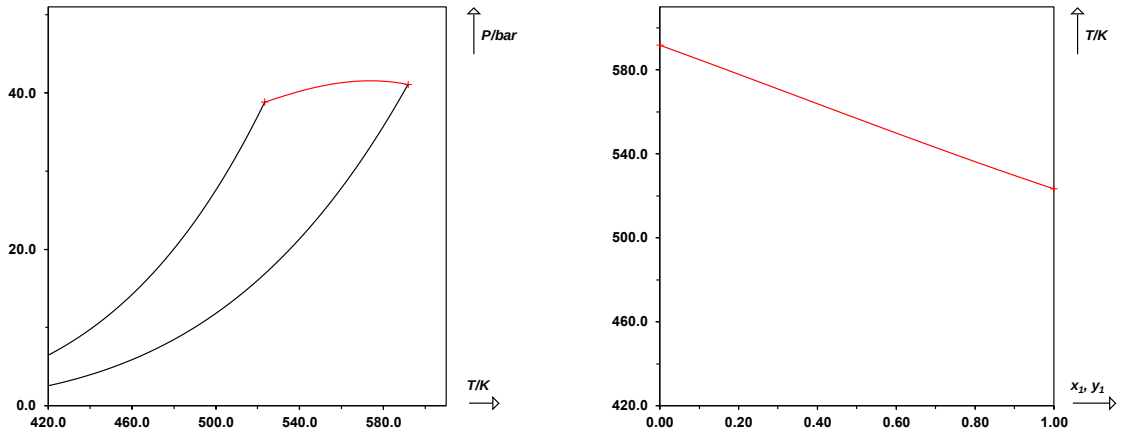
| | | |
|---|---|---|
| **CAS** | 141-78-6 | 108-88-3 |
| **InChiKey** | XEKOWRVHYACXOJ-UHFFFAOYSA-N | YXFVVABEGXRONW-UHFFFAOYSA-N |
| **$T_c$ / K** | 523.3 | 591.75 |
| **$P_c$ / bar** | 38.8 | 41.08 |
| **ω** | 0.3660 | 0.2640 |

Ideal

**PPR78 results**

*Parameters*
A/MPa = 26.2
B/MPa = 20.9

*Deviations*
MAPE on x = 6.1 %
MAPE on y = 3.9 %
MAPE on $h^M$ = 15 %
MAPE on $c_P^M$ = 100 %



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**Isobaric phase equilibrium data**

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Carr, A. D. - Kropholler, H. W., Vapor Liquid Equilibria at Atmospheric Pressure.Binary Systems of Ethyl Acetate-Benzene, Ethyl Acetate-Toluene, and Ethyl Acetate-p-Xylene, Journal of Chemical & Engineering Data 1 (1962) 26-28. doi:10.1021/je60012a007

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 381.97 | 0.0210 | 0.0640 |
| 381.02 | 0.0320 | 0.0970 |
| 380.09 | 0.0480 | 0.1370 |
| 376.61 | 0.1070 | 0.2650 |
| 372.95 | 0.1750 | 0.3910 |
| 368.66 | 0.2700 | 0.5280 |
| 368.17 | 0.2830 | 0.5450 |
| 365.24 | 0.3650 | 0.6290 |
| 362.37 | 0.4520 | 0.7030 |
| 358.31 | 0.5980 | 0.8000 |
| 356.70 | 0.6560 | 0.8370 |
| 355.40 | 0.7150 | 0.8670 |
| 354.29 | 0.7730 | 0.8990 |
| 353.06 | 0.8350 | 0.9280 |
| 351.95 | 0.8910 | 0.9530 |
| 351.54 | 0.9220 | 0.9670 |
| 350.96 | 0.9540 | 0.9800 |
| 350.75 | 0.9700 | 0.9870 |

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**Enthalpy of mixing**

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Delcros, S. - Jiménez, E. - Romaní, L. - Roux, A.H. - Grolier, J.-P.E. - Kehiaian, H.V., Linear alkanoates + aromatic hydrocarbon binary mixtures: new excess enthalpy measurements and DISQUAC analysis of thermodynamic properties, Fluid Phase Equilibria 1 (1995) 71-88. doi:10.1016/0378-3812(95)02838-6

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 4.200 | 0.0162 |
| 9.900 | 0.0388 |
| 23.90 | 0.0940 |
| 36.10 | 0.1446 |
| 47.90 | 0.1966 |
| 67.60 | 0.2969 |
| 81.90 | 0.3957 |
| 89.90 | 0.4900 |
| 90.00 | 0.4919 |
| 89.60 | 0.4919 |
| 91.50 | 0.5852 |
| 85.70 | 0.6798 |
| 72.30 | 0.7723 |
| 50.30 | 0.8641 |
| 36.10 | 0.9093 |
| 19.20 | 0.9550 |
| 11.50 | 0.9737 |
| 4.100 | 0.9911 |

Gmehling, J. - Meents, B., Excess enthalpy. Ethyl ethanoate-toluene system, Int. Data Ser. Sel. Data Mixtures Ser. A 3 (1992)

**T / K = 343.15**

**P / bar = 6.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 17.79 | 0.0543 |
| 33.97 | 0.1082 |
| 34.41 | 0.1082 |
| 48.48 | 0.1615 |
| 61.90 | 0.2144 |
| 72.81 | 0.2668 |
| 82.37 | 0.3187 |
| 95.46 | 0.4212 |
| 100.80 | 0.5218 |
| 99.21 | 0.5715 |
| 97.24 | 0.6208 |
| 85.45 | 0.7180 |
| 76.65 | 0.7660 |
| 65.89 | 0.8136 |
| 52.40 | 0.8608 |
| 37.74 | 0.9076 |
| 19.51 | 0.9540 |

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**Heat capacity of mixing**

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Jiménez, E, Excess heat capacities and excess volumes of (an n-alkylalkanoate + heptane or decane or toluene), The Journal of Chemical Thermodynamics 8 (1994) 817-827. doi:10.1006/jcht.1994.1098

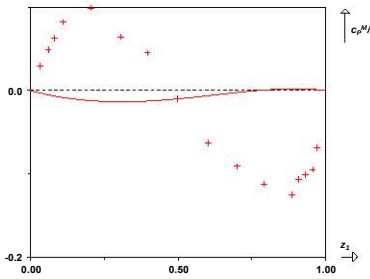
**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

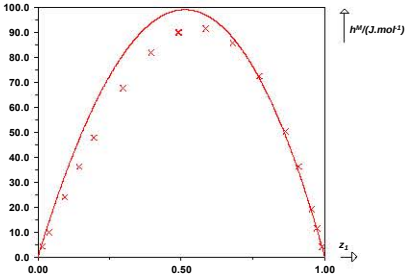
| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.0290 | 0.0313 |
| 0.0490 | 0.0593 |
| 0.0630 | 0.0804 |
| 0.0820 | 0.1109 |
| 0.0990 | 0.2056 |

| | |
|---|---|
| 0.0640 | 0.3049 |
| 0.0450 | 0.3964 |
| -0.0100 | 0.4975 |
| -0.0630 | 0.6037 |
| -0.0910 | 0.7006 |
| -0.1120 | 0.7913 |
| -0.1250 | 0.8860 |
| -0.1070 | 0.9092 |
| -0.1010 | 0.9310 |
| -0.0950 | 0.9570 |
| -0.0690 | 0.9717 |

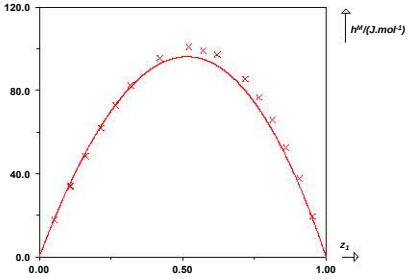
T/K = 298.15 - P/bar = 1.0132



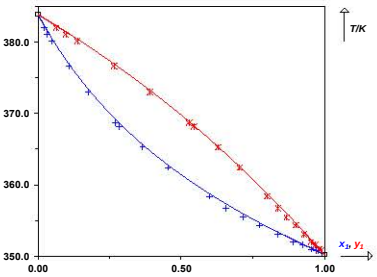

T/K = 298.15 - P/bar = 1.0100




T/K = 343.15 - P/bar = 6.00




P/bar = 1.01330



## CARBON TETRACHLORIDE (1) + 1,4-DIOXANE (2)

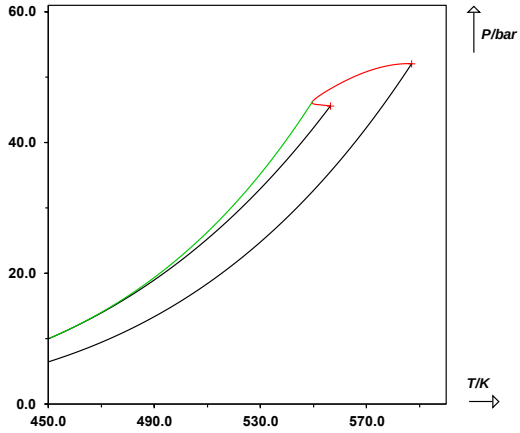
| | | |
|---|---|---|
| **CAS** | 56-23-5 | 123-91-1 |
| **InChiKey** | VZGDMQKNWNREIO-UHFFFAOYSA-N | RYHBNJHYFVUHQT-UHFFFAOYSA-N |
| **$T_c$ / K** | 556.35 | 587.00 |
| **$P_c$ / bar** | 45.60 | 52.08 |
| **ω** | 0.1930 | 0.2790 |

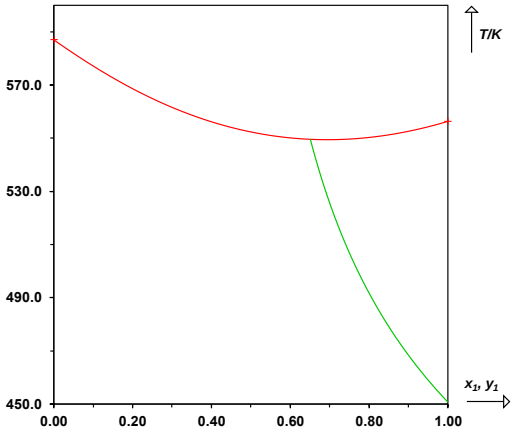
Ideal

**PPR78 results**

*Parameters*
A/MPa = 26.2
B/MPa = -71.9

*Deviations*
MAPE on x = 5.3 %
MAPE on y = 5.2 %
MAPE on $h^M$ = 12 %



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**Isothermal phase equilibrium data**

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Steinbrecher, M. - Bittrich, H.-J., Das isotherme Flüssigkeits-Dampf-Gleichgewicht der binären Systeme zwischen den Komponenten Tetrachlormethan, Äthylacetat und Dioxan, Zeitschrift für Physikalische Chemie 1 (1966) doi:10.1515/zpch-1966-23228

**T / K = 293.15**

| P / bar | $x_1$ |
|---|---|
| 0.0483 | 0.0930 |
| 0.0543 | 0.1550 |
| 0.0665 | 0.2620 |
| 0.0764 | 0.3690 |
| 0.0847 | 0.4690 |
| 0.0880 | 0.5030 |
| 0.0944 | 0.5820 |
| 0.1021 | 0.6780 |
| 0.1091 | 0.7820 |
| 0.1157 | 0.8840 |
| 0.1168 | 0.9030 |
| 0.1187 | 0.9430 |

Steinbrecher, M. - Bittrich, H.-J., Das isotherme Flüssigkeits-Dampf-Gleichgewicht der binären Systeme zwischen den Komponenten Tetrachlormethan, Äthylacetat und Dioxan, Zeitschrift für Physikalische Chemie 1 (1966) doi:10.1515/zpch-1966-23228

**T / K = 293.15**

| P / bar | $y_1$ |
|---|---|
| 0.1139 | 0.9430 |
| 0.1068 | 0.9030 |
| 0.1049 | 0.8840 |
| 0.0899 | 0.7820 |
| 0.0765 | 0.6780 |
| 0.0675 | 0.5820 |
| 0.0612 | 0.5030 |
| 0.0579 | 0.4690 |
| 0.0517 | 0.3690 |
| 0.0475 | 0.2620 |
| 0.0421 | 0.1550 |
| 0.0399 | 0.0930 |

Drobig, J. - Lindenau, E., A new apparatus to determine the isothermal liquid-vapor equilibrium, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 144-147.

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0697 | 0.0500 | 0.1550 |
| 0.0777 | 0.1000 | 0.2820 |
| 0.0857 | 0.1500 | 0.3860 |
| 0.0939 | 0.2000 | 0.4720 |
| 0.1017 | 0.2500 | 0.5440 |
| 0.1096 | 0.3000 | 0.6040 |
| 0.1171 | 0.3500 | 0.6540 |
| 0.1243 | 0.4000 | 0.6980 |
| 0.1311 | 0.4500 | 0.7350 |
| 0.1375 | 0.5000 | 0.7670 |
| 0.1436 | 0.5500 | 0.7960 |
| 0.1493 | 0.6000 | 0.8220 |
| 0.1547 | 0.6500 | 0.8450 |
| 0.1597 | 0.7000 | 0.8670 |
| 0.1645 | 0.7500 | 0.8880 |
| 0.1692 | 0.8000 | 0.9090 |
| 0.1740 | 0.8500 | 0.9300 |
| 0.1788 | 0.9000 | 0.9530 |

Drobig, J. - Lindenau, E., A new apparatus to determine the isothermal liquid-vapor equilibrium, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 144-147.

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1132 | 0.0500 | 0.1540 |
| 0.1255 | 0.1000 | 0.2760 |
| 0.1373 | 0.1500 | 0.3750 |
| 0.1491 | 0.2000 | 0.4570 |
| 0.1603 | 0.2500 | 0.5250 |
| 0.1712 | 0.3000 | 0.5830 |
| 0.1816 | 0.3500 | 0.6330 |
| 0.1916 | 0.4000 | 0.6760 |
| 0.2012 | 0.4500 | 0.7140 |
| 0.2103 | 0.5000 | 0.7480 |
| 0.2188 | 0.5500 | 0.7780 |
| 0.2271 | 0.6000 | 0.8060 |
| 0.2349 | 0.6500 | 0.8320 |
| 0.2424 | 0.7000 | 0.8560 |
| 0.2496 | 0.7500 | 0.8800 |
| 0.2567 | 0.8000 | 0.9030 |
| 0.2636 | 0.8500 | 0.9260 |
| 0.2705 | 0.9000 | 0.9500 |
| 0.2776 | 0.9500 | 0.9750 |

Drobig, J. - Lindenau, E., A new apparatus to determine the isothermal liquid-vapor equilibrium, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 144-147.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1764 | 0.0500 | 0.1480 |

| | | |
|---|---|---|
| 0.1940 | 0.1000 | 0.2660 |
| 0.2111 | 0.1500 | 0.3610 |
| 0.2273 | 0.2000 | 0.4400 |
| 0.2431 | 0.2500 | 0.5070 |
| 0.2581 | 0.3000 | 0.5640 |
| 0.2725 | 0.3500 | 0.6140 |
| 0.2862 | 0.4000 | 0.6570 |
| 0.2993 | 0.4500 | 0.6960 |
| 0.3120 | 0.5000 | 0.7310 |
| 0.3240 | 0.5500 | 0.7630 |
| 0.3354 | 0.6000 | 0.7930 |
| 0.3465 | 0.6500 | 0.8210 |
| 0.3572 | 0.7000 | 0.8470 |
| 0.3676 | 0.7500 | 0.8730 |
| 0.3776 | 0.8000 | 0.8980 |
| 0.3874 | 0.8500 | 0.9220 |
| 0.3972 | 0.9000 | 0.9480 |
| 0.4068 | 0.9500 | 0.9740 |

Drobig, J. - Lindenau, E., A new apparatus to determine the isothermal liquid-vapor equilibrium, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 144-147.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2657 | 0.0500 | 0.1410 |
| 0.2902 | 0.1000 | 0.2540 |
| 0.3136 | 0.1500 | 0.3460 |
| 0.3358 | 0.2000 | 0.4240 |
| 0.3572 | 0.2500 | 0.4890 |
| 0.3776 | 0.3000 | 0.5460 |
| 0.3970 | 0.3500 | 0.5960 |
| 0.4157 | 0.4000 | 0.6400 |
| 0.4334 | 0.4500 | 0.6800 |
| 0.4506 | 0.5000 | 0.7170 |
| 0.4669 | 0.5500 | 0.7500 |
| 0.4828 | 0.6000 | 0.7810 |
| 0.4978 | 0.6500 | 0.8110 |
| 0.5125 | 0.7000 | 0.8390 |
| 0.5268 | 0.7500 | 0.8660 |
| 0.5405 | 0.8000 | 0.8920 |
| 0.5538 | 0.8500 | 0.9180 |
| 0.5669 | 0.9000 | 0.9450 |
| 0.5798 | 0.9500 | 0.9720 |

Drobig, J. - Lindenau, E., A new apparatus to determine the isothermal liquid-vapor equilibrium, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 144-147.

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3889 | 0.0500 | 0.1340 |
| 0.4217 | 0.1000 | 0.2420 |
| 0.4530 | 0.1500 | 0.3320 |
| 0.4828 | 0.2000 | 0.4080 |
| 0.5112 | 0.2500 | 0.4730 |
| 0.5382 | 0.3000 | 0.5300 |
| 0.5640 | 0.3500 | 0.5800 |
| 0.5888 | 0.4000 | 0.6250 |
| 0.6124 | 0.4500 | 0.6660 |
| 0.6350 | 0.5000 | 0.7030 |
| 0.6569 | 0.5500 | 0.7380 |
| 0.6778 | 0.6000 | 0.7700 |
| 0.6981 | 0.6500 | 0.8010 |
| 0.7175 | 0.7000 | 0.8310 |
| 0.7363 | 0.7500 | 0.8590 |
| 0.7546 | 0.8000 | 0.8870 |
| 0.7722 | 0.8500 | 0.9140 |
| 0.7893 | 0.9000 | 0.9420 |
| 0.8058 | 0.9500 | 0.9700 |

Drobig, J. - Lindenau, E., A new apparatus to determine the isothermal liquid-vapor equilibrium, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 144-147.

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5546 | 0.0500 | 0.1270 |
| 0.5977 | 0.1000 | 0.2320 |
| 0.6385 | 0.1500 | 0.3190 |
| 0.6773 | 0.2000 | 0.3930 |
| 0.7142 | 0.2500 | 0.4580 |
| 0.7493 | 0.3000 | 0.5140 |
| 0.7829 | 0.3500 | 0.5650 |
| 0.8150 | 0.4000 | 0.6110 |
| 0.8457 | 0.4500 | 0.6520 |
| 0.8751 | 0.5000 | 0.6910 |
| 0.9035 | 0.5500 | 0.7260 |
| 0.9307 | 0.6000 | 0.7600 |
| 0.9569 | 0.6500 | 0.7920 |
| 0.9822 | 0.7000 | 0.8230 |
| 1.007 | 0.7500 | 0.8520 |
| 1.030 | 0.8000 | 0.8810 |
| 1.052 | 0.8500 | 0.9100 |
| 1.074 | 0.9000 | 0.9390 |
| 1.095 | 0.9500 | 0.9690 |

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**Enthalpy of mixing**

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Guillen, M.D. - Gutierrez Losa, C., Excess enthalpies and excess volumes of n-hexane + and of tetrachloromethane + furan, + 1,4-dioxane, + tetrahydrofuran, and + tetrahydropyran, The Journal of Chemical Thermodynamics 6 (1978) 567-576. doi:10.1016/0021-9614(78)90045-9

**T / K =** **283.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -133.00 | 0.1094 |
| -240.00 | 0.2252 |
| -354.00 | 0.3656 |
| -387.00 | 0.4585 |
| -389.00 | 0.5441 |
| -364.00 | 0.5903 |
| -323.00 | 0.6642 |
| -303.00 | 0.6910 |
| -192.00 | 0.8263 |
| -160.00 | 0.8579 |

Murakami, S. - Benson, G.C., An isothermal dilution calorimeter for measuring enthalpies of mixing, The Journal of Chemical Thermodynamics 6 (1969) 559-572. doi:10.1016/0021-9614(69)90016-0

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -25.37 | 0.0279 |
| -57.40 | 0.0641 |
| -92.53 | 0.1058 |
| -123.95 | 0.1480 |
| -158.76 | 0.2001 |
| -189.81 | 0.2552 |
| -214.16 | 0.3088 |
| -230.24 | 0.3536 |
| -230.02 | 0.3540 |
| -235.26 | 0.3702 |
| -236.97 | 0.3773 |
| -242.56 | 0.4027 |
| -243.63 | 0.4072 |
| -243.58 | 0.4098 |
| -247.85 | 0.4385 |
| -248.71 | 0.4428 |
| -250.86 | 0.4774 |
| -250.81 | 0.4869 |
| -250.26 | 0.4902 |
| -249.58 | 0.5190 |
| -248.07 | 0.5314 |
| -243.57 | 0.5654 |
| -241.64 | 0.5739 |
| -231.74 | 0.6159 |
| -229.10 | 0.6227 |
| -213.26 | 0.6691 |
| -205.46 | 0.6853 |
| -188.11 | 0.7238 |
| -182.17 | 0.7331 |
| -155.94 | 0.7810 |
| -152.71 | 0.7867 |
| -121.02 | 0.8349 |
| -120.78 | 0.8360 |
| -88.43 | 0.8814 |
| -85.89 | 0.8848 |
| -55.18 | 0.9261 |
| -51.11 | 0.9315 |
| -25.33 | 0.9659 |
| -21.48 | 0.9708 |

Becker, F. - Kiefer, M. - Koukol, H., Kontinuierliche Bestimmung von Mischungswärmen durch quasi-isotherme Wärmeflußkalorimetrie, Z. Phys. Chem. NF (1972) 29-43.

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

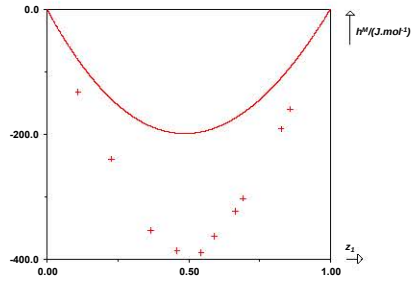
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -21.81 | 0.0250 |
| -43.59 | 0.0500 |
| -65.02 | 0.0750 |
| -85.75 | 0.1000 |
| -105.55 | 0.1250 |
| -124.26 | 0.1500 |
| -141.93 | 0.1750 |
| -158.39 | 0.2000 |
| -173.71 | 0.2250 |
| -187.86 | 0.2500 |
| -200.84 | 0.2750 |
| -212.69 | 0.3000 |
| -223.24 | 0.3250 |
| -232.45 | 0.3500 |
| -240.07 | 0.3750 |
| -246.02 | 0.4000 |
| -250.08 | 0.4250 |
| -252.42 | 0.4500 |
| -253.51 | 0.4750 |
| -252.67 | 0.5000 |
| -251.17 | 0.5250 |
| -248.24 | 0.5500 |
| -243.84 | 0.5750 |
| -238.02 | 0.6000 |
| -230.73 | 0.6250 |

| | |
|---|---|
| -222.07 | 0.6500 |
| -212.15 | 0.6750 |
| -200.88 | 0.7000 |
| -188.53 | 0.7250 |
| -175.13 | 0.7500 |
| -160.69 | 0.7750 |
| -145.32 | 0.8000 |
| -129.08 | 0.8250 |
| -112.08 | 0.8500 |
| -94.37 | 0.8750 |
| -76.03 | 0.9000 |
| -57.23 | 0.9250 |
| -38.18 | 0.9500 |
| -19.01 | 0.9750 |

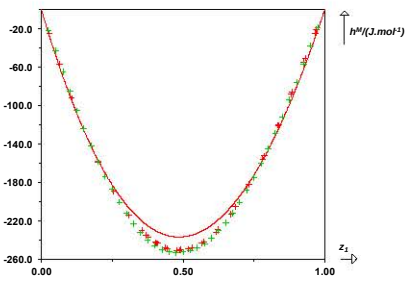
McKinnon, Ir - Williamson, Ag, Heats of mixing of CCl4 with dioxane, Australian Journal of Chemistry 12 (1964) doi:10.1071/CH9641374

| **T / K =** | **318.15** |
|---|---|
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| -96.00 | 0.2180 |
| -132.00 | 0.3140 |
| -150.00 | 0.4270 |
| -147.00 | 0.5070 |
| -131.00 | 0.6560 |
| -71.00 | 0.8120 |

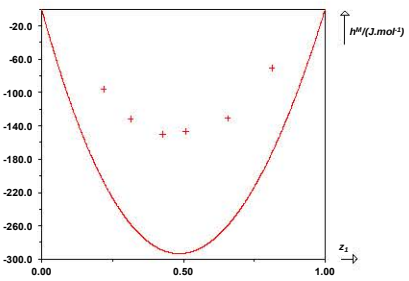
T/K = 283.15 - P/bar = 1.0132



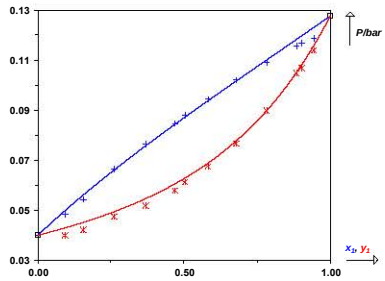

T/K = 298.15 - P/bar = 1.0132 1.0132



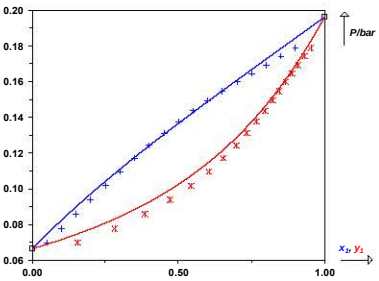

T/K = 318.15 - P/bar = 1.0132



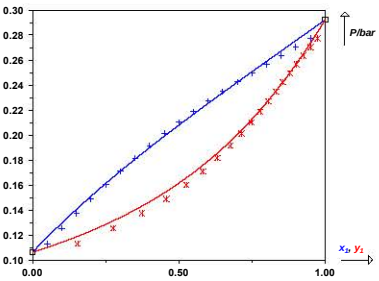

T/K = 293.15



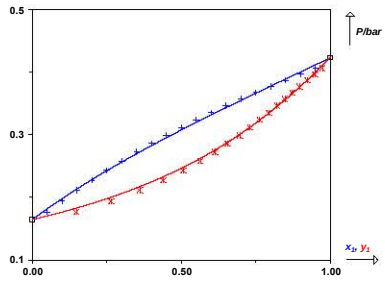

T/K = 303.15



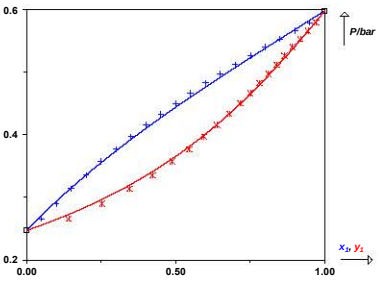

T/K = 313.15



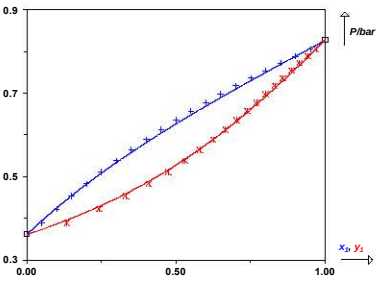

T/K = 323.15



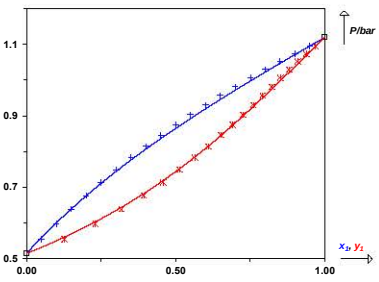

T/K = 333.15




T/K = 343.15




T/K = 353.15



## METHYL ETHYL KETONE (1) + BENZENE (2)

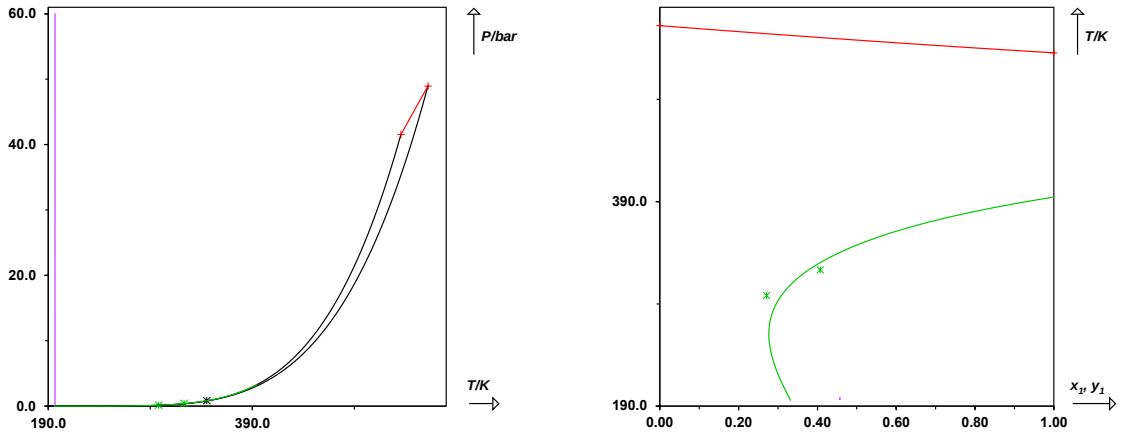
| | | |
|---|---|---|
| **CAS** | 78-93-3 | 71-43-2 |
| **InChiKey** | ZWEHNKRNPOVVGH-UHFFFAOYSA-N | UHOVQNZJYSORNB-UHFFFAOYSA-N |
| **$T_c$ / K** | 535.50 | 562.05 |
| **$P_c$ / bar** | 41.50 | 48.95 |
| **ω** | 0.3230 | 0.210 |

Ideal

**PPR78 results**

*Parameters*
A/MPa = 46.7
B/MPa = 214

*Deviations*
MAPE on x = 28 %
MAPE on y = 28 %
MAPE on $x_{az}$ = 23 %
MAPE on $P_{az}$ = 0.32 %
MAPE on $h^M$ = 3100 %



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**Isothermal phase equilibrium data**

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Ohta, Tatsuhiko - Koyabu, Jitsuo - Nagata, Isamu, Vapor—liquid equilibria for the ternary Ethanol—2-butanone—benzene system at 298.15 K, Fluid Phase Equilibria 1 (1981) 65-73. doi:10.1016/0378-3812(81)87006-9

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1321 | 0.0830 | 0.0940 | |
| 0.1328 | 0.1100 | 0.1220 | |
| 0.1339 | 0.2710 | 0.2710 | AZEO |
| 0.1333 | 0.4000 | 0.3870 | |
| 0.1315 | 0.5180 | 0.4980 | |
| 0.1289 | 0.6790 | 0.6520 | |
| 0.1269 | 0.7620 | 0.7360 | |
| 0.1245 | 0.8540 | 0.8350 | |
| 0.1219 | 0.9640 | 0.9580 | |

Diaz Peña, M - Crespo Colin, A - Compostizo, A, Isothermal liquid-vapour equilibria 2. The binary systems formed by benzene + acetone, + methyl ethyl ketone, + methyl propyl ketone, and + methyl isobutyl ketone, The Journal of Chemical Thermodynamics 11 (1978) 1101-1106. doi:10.1016/0021-9614(78)90084-8

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.3685 | 0.0774 | 0.0920 | |
| 0.3694 | 0.0903 | 0.1061 | |
| 0.3709 | 0.1135 | 0.1306 | |
| 0.3722 | 0.1328 | 0.1502 | |
| 0.3734 | 0.1554 | 0.1733 | |
| 0.3743 | 0.1769 | 0.1945 | |
| 0.3753 | 0.2117 | 0.2275 | |
| 0.3761 | 0.2458 | 0.2599 | |
| 0.3768 | 0.2737 | 0.2847 | |
| 0.3773 | 0.3056 | 0.3141 | |
| 0.3777 | 0.3357 | 0.3410 | |
| 0.3779 | 0.3539 | 0.3571 | |
| 0.3780 | 0.3737 | 0.3753 | |
| 0.3782 | 0.3928 | 0.3925 | |
| 0.3784 | 0.4072 | 0.4072 | AZEO |
| 0.3784 | 0.4109 | 0.4084 | |
| 0.3782 | 0.4767 | 0.4691 | |
| 0.3782 | 0.5001 | 0.4909 | |
| 0.3780 | 0.5271 | 0.5157 | |
| 0.3776 | 0.5514 | 0.5388 | |
| 0.3772 | 0.5737 | 0.5599 | |
| 0.3770 | 0.5892 | 0.5743 | |
| 0.3767 | 0.6068 | 0.5915 | |
| 0.3764 | 0.6255 | 0.6092 | |
| 0.3733 | 0.7247 | 0.7063 | |
| 0.3720 | 0.7572 | 0.7398 | |
| 0.3713 | 0.7749 | 0.7575 | |
| 0.3695 | 0.8191 | 0.8034 | |
| 0.3674 | 0.8676 | 0.8548 | |
| 0.3663 | 0.8887 | 0.8775 | |
| 0.3644 | 0.9262 | 0.9181 | |
| 0.3623 | 0.9652 | 0.9609 | |

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**Isobaric phase equilibrium data**

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Kumarkrishna Rao, V.N. - Swami, D.R. - Narasinga Rao, M., High-pressure vapor-liquid equilibriums of nonideal solutions. II. Benzene-methyl ethyl ketone system, J. Sci. Ind. Res. Sect. B (1957) 195-201.

**P / bar = 5.649**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 421.95 | 0.1000 | 0.1140 |
| 420.65 | 0.2000 | 0.2220 |
| 419.95 | 0.3000 | 0.3240 |
| 419.45 | 0.4000 | 0.4220 |
| 418.95 | 0.5000 | 0.5150 |
| 418.65 | 0.6000 | 0.6100 |
| 418.35 | 0.7000 | 0.7040 |

Kumarkrishna Rao, V.N. - Swami, D.R. - Narasinga Rao, M., High-pressure vapor-liquid equilibriums of nonideal solutions. II. Benzene-methyl ethyl ketone system, J. Sci. Ind. Res. Sect. B (1957) 195-201.

**P / bar = 7.516**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 435.95 | 0.1000 | 0.1180 |
| 434.75 | 0.2000 | 0.2230 |
| 434.05 | 0.3000 | 0.3230 |
| 433.55 | 0.4000 | 0.4210 |
| 433.15 | 0.5000 | 0.5160 |
| 432.85 | 0.6000 | 0.6120 |
| 432.55 | 0.7000 | 0.7100 |
| 432.35 | 0.8000 | 0.8060 |

Kumarkrishna Rao, V.N. - Swami, D.R. - Narasinga Rao, M., High-pressure vapor-liquid equilibriums of nonideal solutions. II. Benzene-methyl ethyl ketone system, J. Sci. Ind. Res. Sect. B (1957) 195-201.

**P / bar = 10.65**

| T / K | $x_1$ | $y_1$ |
|---|---|---|

| | | |
|---|---|---|
| 455.95 | 0.1000 | 0.1160 |
| 454.15 | 0.2000 | 0.2180 |
| 452.95 | 0.3000 | 0.3180 |
| 452.35 | 0.4000 | 0.4180 |
| 451.95 | 0.5000 | 0.5170 |
| 451.55 | 0.6000 | 0.6150 |
| 451.15 | 0.7000 | 0.7120 |
| 450.85 | 0.8000 | 0.8100 |
| 450.65 | 0.9000 | 0.9060 |

Kumarkrishna Rao, V.N. - Swami, D.R. - Narasinga Rao, M., High-pressure vapor-liquid equilibriums of nonideal solutions. II. Benzene-methyl ethyl ketone system, J. Sci. Ind. Res. Sect. B (1957) 195-201.

**P / bar = 13.98**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 471.75 | 0.1000 | 0.1170 |
| 470.15 | 0.2000 | 0.2220 |
| 469.25 | 0.3000 | 0.3230 |
| 468.65 | 0.4000 | 0.4220 |
| 468.05 | 0.5000 | 0.5190 |
| 467.55 | 0.6000 | 0.6160 |
| 467.05 | 0.7000 | 0.7110 |
| 466.65 | 0.8000 | 0.8070 |
| 466.35 | 0.9000 | 0.9050 |

Kumarkrishna Rao, V.N. - Swami, D.R. - Narasinga Rao, M., High-pressure vapor-liquid equilibriums of nonideal solutions. II. Benzene-methyl ethyl ketone system, J. Sci. Ind. Res. Sect. B (1957) 195-201.

**P / bar = 17.32**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 485.85 | 0.1000 | 0.1120 |
| 484.15 | 0.2000 | 0.2200 |
| 482.85 | 0.3000 | 0.3240 |
| 482.05 | 0.4000 | 0.4200 |
| 481.45 | 0.5000 | 0.5240 |
| 480.95 | 0.6000 | 0.6230 |
| 480.45 | 0.7000 | 0.7180 |
| 479.95 | 0.8000 | 0.8130 |
| 479.65 | 0.9000 | 0.9070 |

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**Enthalpy of mixing**

---

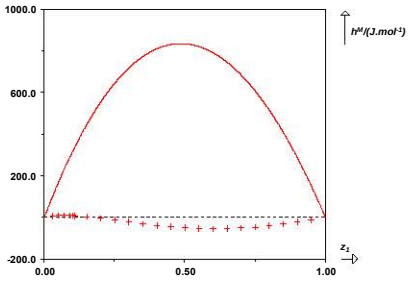
Grauer, F. - Kertes, A. S., Heats of mixing of tri-n-dodecylamine with n-octane, benzene, or chlorobenzene, Journal of Chemical & Engineering Data 4 (1973) 405-407. doi:10.1021/je60059a032

**T / K = 298.15**

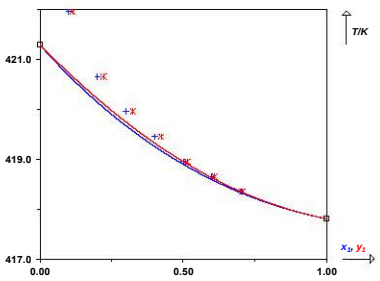
**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 6.260 | 0.0300 |
| 8.280 | 0.0500 |
| 9.050 | 0.0700 |
| 8.650 | 0.0900 |
| 8.270 | 0.1000 |
| 7.570 | 0.1100 |
| 3.520 | 0.1500 |
| -4.060 | 0.2000 |
| -12.83 | 0.2500 |
| -22.03 | 0.3000 |
| -30.66 | 0.3500 |
| -38.37 | 0.4000 |
| -44.71 | 0.4500 |
| -49.53 | 0.5000 |
| -52.70 | 0.5500 |
| -53.98 | 0.6000 |
| -53.29 | 0.6500 |
| -50.70 | 0.7000 |
| -50.65 | 0.7000 |
| -46.16 | 0.7500 |
| -39.91 | 0.8000 |
| -32.12 | 0.8500 |
| -22.75 | 0.9000 |
| -12.01 | 0.9500 |

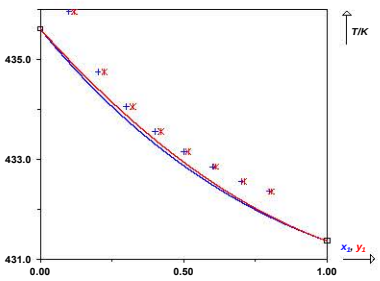
T/K = 298.15 - P/bar = 1.0132



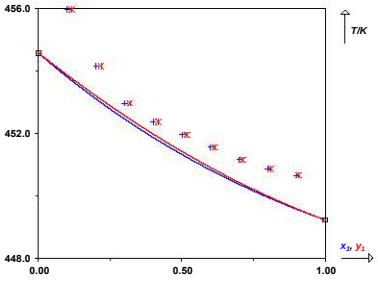

P/bar = 5.64860



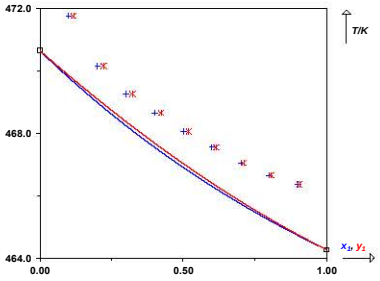

P/bar = 7.51580



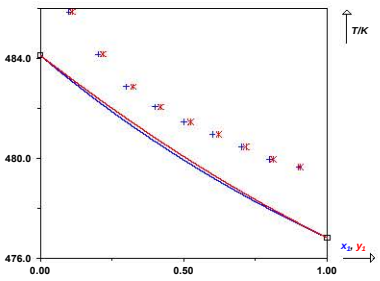

P/bar = 10.65000



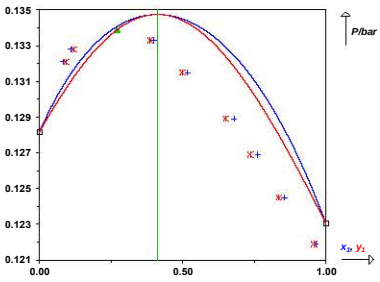

P/bar = 13.98400



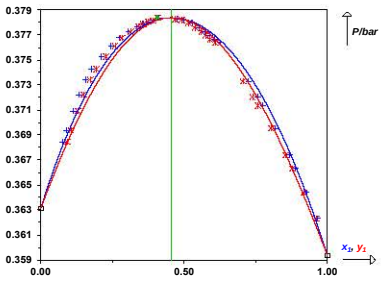

P/bar = 17.31900




T/K = 298.15




T/K = 323.15



## METHYL tert-PENTYL ETHER (1) + n-HEPTANE (2)

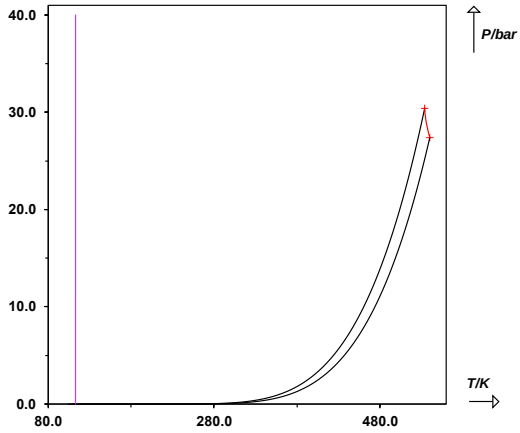
| | | |
|---|---|---|
| **CAS** | 994-05-8 | 142-82-5 |
| **InChiKey** | HVZJRWJGKQPSFL-UHFFFAOYSA-N | IMNFDUFMRHMDMM-UHFFFAOYSA-N |
| **$T_c$ / K** | 534 | 540.2 |
| **$P_c$ / bar** | 30.4 | 27.4 |
| **ω** | 0.298 | 0.349 |

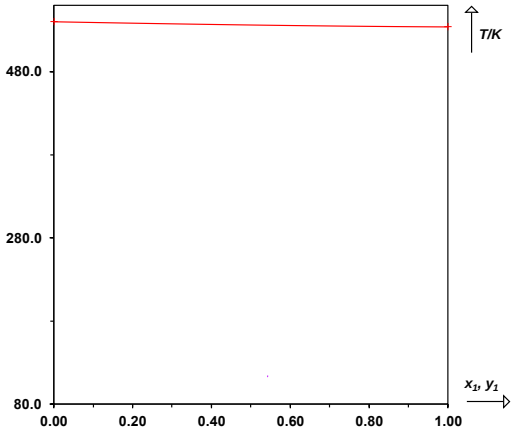
Ideal

**PPR78 results**

*Parameters*
A/MPa = 19.6
B/MPa = 46.7

*Deviations*
MAPE on x = 10 %
MAPE on y = 8.8 %
MAPE on $h^M$ = 2.6 %



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**Isothermal phase equilibrium data**

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Chamorro, César R - Segovia, José J - Martín, María C - Montero, Eduardo A - Villamañán, Miguel A, Phase equilibrium properties of binary and ternary systems containing tert-amylmethyl ether (TAME) as oxygenate additive and gasoline substitution hydrocarbons at 313.15 K, Fluid Phase Equilibria 1-2 (1999) 73-87. doi:10.1016/S0378-3812(99)00033-3

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1281 | 0.0440 | 0.0772 |
| 0.1335 | 0.0986 | 0.1637 |
| 0.1383 | 0.1499 | 0.2373 |
| 0.1428 | 0.1986 | 0.3013 |
| 0.1471 | 0.2484 | 0.3617 |
| 0.1513 | 0.2988 | 0.4182 |
| 0.1553 | 0.3491 | 0.4711 |
| 0.1628 | 0.4491 | 0.5670 |
| 0.1628 | 0.4493 | 0.5671 |
| 0.1698 | 0.5486 | 0.6536 |
| 0.1698 | 0.5495 | 0.6543 |
| 0.1731 | 0.5990 | 0.6951 |
| 0.1732 | 0.6009 | 0.6966 |
| 0.1763 | 0.6496 | 0.7354 |
| 0.1793 | 0.6988 | 0.7738 |
| 0.1821 | 0.7456 | 0.8096 |
| 0.1851 | 0.7986 | 0.8496 |
| 0.1878 | 0.8482 | 0.8867 |
| 0.1906 | 0.8999 | 0.9252 |
| 0.1927 | 0.9420 | 0.9566 |

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**Isobaric phase equilibrium data**

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Mejía, Andrés - Segura, Hugo - Cartes, Marcela, Vapor−Liquid Equilibrium in the Binary Systems 2-Butanol + tert-Amyl Methyl Ether, 2-Butanol + Heptane, and Heptane + tert-Amyl Methyl Ether, Journal of Chemical & Engineering Data 5 (2011) 2256-2265. doi:10.1021/je101250d

**P / bar = 0.5000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 347.05 | 0.1150 | 0.1770 |
| 346.23 | 0.1660 | 0.2450 |
| 345.44 | 0.2170 | 0.3090 |
| 344.74 | 0.2630 | 0.3620 |
| 344.01 | 0.3090 | 0.4140 |
| 343.45 | 0.3550 | 0.4630 |
| 342.88 | 0.4010 | 0.5090 |
| 342.28 | 0.4450 | 0.5560 |
| 341.85 | 0.4890 | 0.5920 |
| 341.31 | 0.5420 | 0.6390 |
| 340.79 | 0.5920 | 0.6820 |
| 340.25 | 0.6400 | 0.7230 |
| 339.81 | 0.6940 | 0.7660 |
| 339.44 | 0.7420 | 0.8040 |
| 339.06 | 0.7920 | 0.8410 |
| 338.73 | 0.8430 | 0.8800 |
| 338.35 | 0.8920 | 0.9170 |
| 338.02 | 0.9430 | 0.9560 |

Mejía, Andrés - Segura, Hugo - Cartes, Marcela, Vapor−Liquid Equilibrium in the Binary Systems 2-Butanol + tert-Amyl Methyl Ether, 2-Butanol + Heptane, and Heptane + tert-Amyl Methyl Ether, Journal of Chemical & Engineering Data 5 (2011) 2256-2265. doi:10.1021/je101250d

**P / bar = 0.7500**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 359.34 | 0.1150 | 0.1740 |
| 358.47 | 0.1660 | 0.2400 |
| 357.71 | 0.2170 | 0.3030 |
| 357.01 | 0.2620 | 0.3560 |
| 356.20 | 0.3090 | 0.4080 |
| 355.73 | 0.3550 | 0.4580 |
| 355.02 | 0.4000 | 0.5030 |
| 354.57 | 0.4440 | 0.5470 |
| 353.98 | 0.4890 | 0.5880 |
| 353.48 | 0.5410 | 0.6340 |
| 352.97 | 0.5920 | 0.6770 |
| 352.50 | 0.6400 | 0.7180 |
| 352.01 | 0.6930 | 0.7620 |
| 351.62 | 0.7420 | 0.8000 |
| 351.23 | 0.7920 | 0.8390 |
| 350.87 | 0.8420 | 0.8780 |
| 350.49 | 0.8910 | 0.9160 |
| 350.18 | 0.9410 | 0.9540 |

Mejía, Andrés - Segura, Hugo - Cartes, Marcela, Vapor−Liquid Equilibrium in the Binary Systems 2-Butanol + tert-Amyl Methyl Ether, 2-Butanol + Heptane, and Heptane + tert-Amyl Methyl Ether, Journal of Chemical & Engineering Data 5 (2011) 2256-2265. doi:10.1021/je101250d

**P / bar = 0.9400**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 366.70 | 0.1150 | 0.1700 |
| 365.80 | 0.1650 | 0.2370 |
| 364.88 | 0.2170 | 0.3000 |

| | | |
|---|---|---|
| 364.31 | 0.2620 | 0.3530 |
| 363.50 | 0.3090 | 0.4040 |
| 363.01 | 0.3540 | 0.4560 |
| 362.30 | 0.4000 | 0.4990 |
| 361.78 | 0.4430 | 0.5420 |
| 361.25 | 0.4890 | 0.5840 |
| 360.78 | 0.5410 | 0.6300 |
| 360.27 | 0.5910 | 0.6730 |
| 359.80 | 0.6390 | 0.7140 |
| 359.29 | 0.6930 | 0.7590 |
| 358.86 | 0.7410 | 0.7970 |
| 358.46 | 0.7910 | 0.8380 |
| 358.11 | 0.8420 | 0.8770 |
| 357.73 | 0.8900 | 0.9150 |
| 357.39 | 0.9410 | 0.9540 |

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**Enthalpy of mixing**

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Kammerer, K. - Lichtenthaler, R.N., Excess enthalpy HE of binary mixtures containing alkanes, methanol and tert-amyl-methyl ether (TAME), Thermochimica Acta (1996) 49-58. doi:10.1016/0040-6031(95)02588-X

**T / K =** **298.15**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 97.30 | 0.0930 |
| 183.40 | 0.1960 |
| 236.10 | 0.2840 |
| 275.40 | 0.3870 |
| 294.80 | 0.5150 |
| 283.10 | 0.5940 |
| 250.50 | 0.7060 |
| 200.20 | 0.7960 |
| 112.70 | 0.8970 |

Tsimering, L. - Kertes, A.S., Excess enthalpies of tri-n-butylphosphate + hydrocarbons, The Journal of Chemical Thermodynamics 5 (1974) 411-415. doi:10.1016/0021-9614(74)90001-9

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 56.70 | 0.0501 |
| 107.40 | 0.1001 |
| 152.20 | 0.1501 |
| 190.80 | 0.2001 |
| 222.00 | 0.2501 |
| 247.40 | 0.3001 |
| 267.80 | 0.3501 |
| 282.40 | 0.4002 |
| 290.70 | 0.4502 |
| 293.60 | 0.5003 |
| 293.80 | 0.5004 |
| 291.20 | 0.5500 |
| 282.70 | 0.6000 |
| 267.80 | 0.6503 |
| 247.20 | 0.7002 |
| 220.80 | 0.7500 |
| 187.70 | 0.8002 |
| 149.30 | 0.8502 |
| 104.90 | 0.9000 |
| 53.80 | 0.9500 |

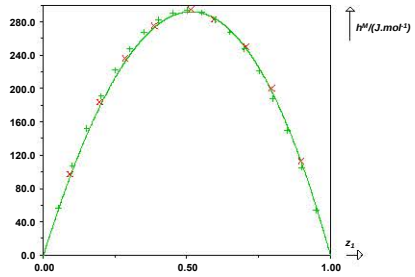
Kammerer, K. - Lichtenthaler, R.N., Excess enthalpy HE of binary mixtures containing alkanes, methanol and tert-amyl-methyl ether (TAME), Thermochimica Acta (1996) 49-58. doi:10.1016/0040-6031(95)02588-X

**T / K =** **313.15**

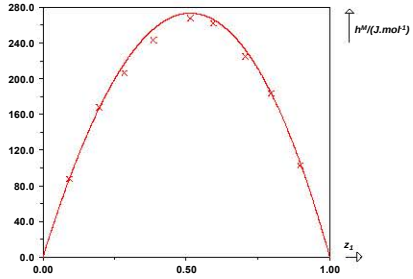
**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 87.70 | 0.0930 |
| 167.50 | 0.1960 |
| 206.00 | 0.2840 |
| 243.00 | 0.3870 |
| 267.80 | 0.5150 |
| 261.80 | 0.5940 |
| 224.60 | 0.7060 |
| 183.40 | 0.7960 |
| 102.70 | 0.8970 |

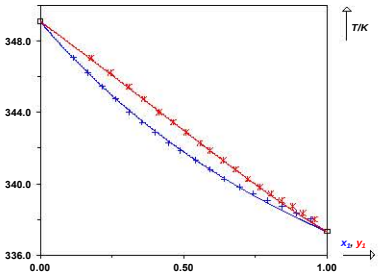
T/K = 298.15 - P/bar = 1.0130 1.0132



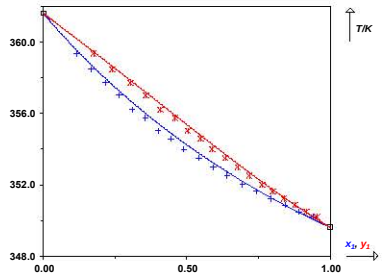

T/K = 313.15 - P/bar = 1.0130



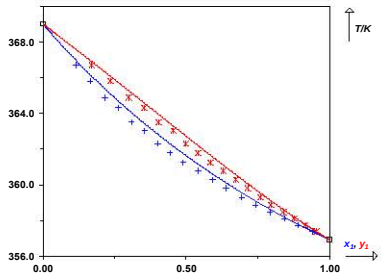

P/bar = 0.50000



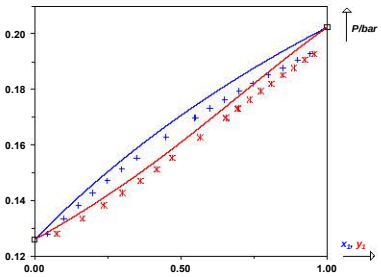

P/bar = 0.75001




P/bar = 0.94000




T/K = 313.15



## METHYL tert-BUTYL ETHER (1) + TOLUENE (2)

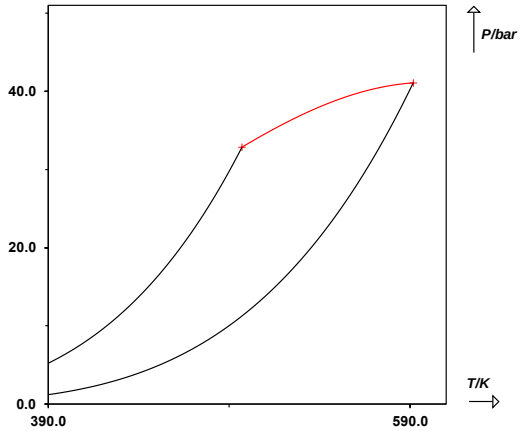
| | | |
|---|---|---|
| **CAS** | 1634-04-4 | 108-88-3 |
| **InChiKey** | BZLVMXJERCGZMT-UHFFFAOYSA-N | YXFVVABEGXRONW-UHFFFAOYSA-N |
| **$T_c$ / K** | 497.10 | 591.75 |
| **$P_c$ / bar** | 32.86 | 41.08 |
| **ω** | 0.2470 | 0.2640 |

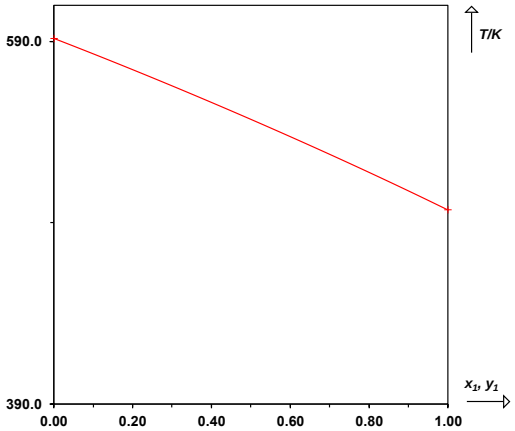
Ideal

**PPR78 results**

*Parameters*
A/MPa = 15.1
B/MPa = 4.17

*Deviations*
MAPE on x = 16 %
MAPE on y = 5.8 %
MAPE on $h^M$ = 76 %



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**Isothermal phase equilibrium data**

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Vorenberg, Daniel G. - Raal, J. David - Ramjugernath, Deresh, Vapor–Liquid Equilibrium Measurements of MTBE and TAME with Toluene, Journal of Chemical & Engineering Data 1 (2005) 56-59. doi:10.1021/je049867t

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0712 | 0.0180 | 0.1470 |
| 0.0744 | 0.0240 | 0.1850 |
| 0.0804 | 0.0370 | 0.2510 |
| 0.1032 | 0.0820 | 0.4340 |
| 0.1650 | 0.2120 | 0.6980 |
| 0.2628 | 0.4330 | 0.8600 |
| 0.3606 | 0.6710 | 0.9360 |
| 0.4360 | 0.8590 | 0.9770 |
| 0.4614 | 0.9210 | 0.9880 |
| 0.4805 | 0.9660 | 0.9950 |
| 0.4883 | 0.9840 | 0.9970 |

Vorenberg, Daniel G. - Raal, J. David - Ramjugernath, Deresh, Vapor–Liquid Equilibrium Measurements of MTBE and TAME with Toluene, Journal of Chemical & Engineering Data 1 (2005) 56-59. doi:10.1021/je049867t

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1099 | 0.0150 | 0.1140 |
| 0.1157 | 0.0230 | 0.1650 |
| 0.1246 | 0.0360 | 0.2340 |
| 0.1605 | 0.0880 | 0.4350 |
| 0.2527 | 0.2240 | 0.6930 |
| 0.3736 | 0.4170 | 0.8410 |
| 0.5124 | 0.6560 | 0.9290 |
| 0.6173 | 0.8390 | 0.9700 |
| 0.6687 | 0.9260 | 0.9870 |
| 0.6961 | 0.9710 | 0.9950 |
| 0.7074 | 0.9890 | 0.9980 |

Vorenberg, Daniel G. - Raal, J. David - Ramjugernath, Deresh, Vapor–Liquid Equilibrium Measurements of MTBE and TAME with Toluene, Journal of Chemical & Engineering Data 1 (2005) 56-59. doi:10.1021/je049867t

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1320 | 0.0110 | 0.0800 |
| 0.1465 | 0.0280 | 0.1810 |
| 0.1589 | 0.0430 | 0.2540 |
| 0.1818 | 0.0710 | 0.3660 |
| 0.2519 | 0.1580 | 0.5840 |
| 0.4278 | 0.3930 | 0.8200 |
| 0.5676 | 0.5940 | 0.9010 |
| 0.7255 | 0.8260 | 0.9660 |
| 0.7992 | 0.9310 | 0.9870 |
| 0.8321 | 0.9770 | 0.9960 |
| 0.8380 | 0.9850 | 0.9970 |

Hsieh, Cheng-Ting - Lee, Ming-Jer - Lin, Ho-mu - Cheng, Ju-Chun - Ji, Wan-Yun, Multiphase equilibria for mixtures containing water, isopropanol, propionic acid, and isopropyl propionate, Fluid Phase Equilibria 1 (2011) 53-61. doi:10.1016/j.fluid.2011.03.003

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2952 | 0.0970 | 0.4300 |
| 0.3812 | 0.1770 | 0.5910 |
| 0.4513 | 0.2430 | 0.6820 |
| 0.5247 | 0.3170 | 0.7530 |
| 0.6895 | 0.4890 | 0.8540 |
| 0.7775 | 0.5790 | 0.8960 |
| 0.8545 | 0.6560 | 0.9100 |
| 0.8910 | 0.6950 | 0.9350 |
| 0.9628 | 0.7730 | 0.9540 |
| 1.010 | 0.8180 | 0.9620 |

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**Isobaric phase equilibrium data**

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Reich, Ricardo - Cartes, Marcela - Wisniak, Jaime - Segura, Hugo, Phase Equilibria in the Systems Methyl 1,1-Dimethylethyl Ether + Benzene and + Toluene, Journal of Chemical & Engineering Data 3 (1998) 299-303. doi:10.1021/je970248c

**P / bar = 0.9400**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 380.47 | 0.0040 | 0.0210 |
| 378.74 | 0.0170 | 0.0830 |
| 377.24 | 0.0290 | 0.1320 |
| 375.24 | 0.0460 | 0.1930 |
| 373.00 | 0.0640 | 0.2600 |
| 370.62 | 0.0850 | 0.3280 |
| 369.13 | 0.0980 | 0.3660 |
| 367.07 | 0.1180 | 0.4200 |
| 364.86 | 0.1410 | 0.4740 |
| 362.89 | 0.1630 | 0.5160 |
| 360.71 | 0.1870 | 0.5570 |
| 358.93 | 0.2090 | 0.5950 |
| 357.55 | 0.2250 | 0.6210 |

| | | |
|---|---|---|
| 355.77 | 0.2520 | 0.6530 |
| 353.12 | 0.2910 | 0.6960 |
| 350.83 | 0.3260 | 0.7310 |
| 348.83 | 0.3630 | 0.7670 |
| 345.66 | 0.4280 | 0.8090 |
| 342.41 | 0.4890 | 0.8490 |
| 340.53 | 0.5300 | 0.8730 |
| 337.28 | 0.6110 | 0.9060 |
| 335.18 | 0.6700 | 0.9280 |
| 332.81 | 0.7490 | 0.9490 |
| 330.53 | 0.8110 | 0.9670 |
| 329.21 | 0.8660 | 0.9760 |
| 327.79 | 0.9190 | 0.9850 |
| 327.06 | 0.9540 | 0.9900 |
| 326.37 | 0.9790 | 0.9930 |
| 326.05 | 0.9900 | 0.9950 |

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**Enthalpy of mixing**

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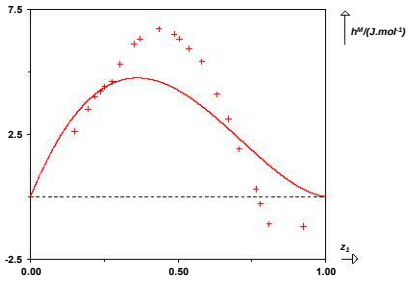
Letcher, Trevor M - Domańska, Urszula, Excess molar enthalpies of (2,2,4-trimethylpentane, or 1-heptene, or 1-hexene, or toluene+methyl 1,1-dimethylethyl ether) and of (1-heptene, or 1-hexene, or toluene+1,1-dimethylpropyl ether) at the temperatures 298.15 K and 308.15 K, The Journal of Chemical Thermodynamics 7 (1997) 721-730. doi:10.1006/jcht.1997.0198

| | |
|---|---|
| **T / K =** | **298.15** |
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| 2.600 | 0.1493 |
| 3.500 | 0.1950 |
| 4.000 | 0.2188 |
| 4.200 | 0.2372 |
| 4.400 | 0.2523 |
| 4.600 | 0.2758 |
| 5.300 | 0.3030 |
| 6.100 | 0.3510 |
| 6.300 | 0.3704 |
| 6.700 | 0.4360 |
| 6.500 | 0.4865 |
| 6.300 | 0.5036 |
| 5.900 | 0.5379 |
| 5.400 | 0.5808 |
| 4.100 | 0.6325 |
| 3.100 | 0.6712 |
| 1.900 | 0.7079 |
| 0.3000 | 0.7643 |
| -0.3000 | 0.7798 |
| -1.100 | 0.8088 |
| -1.200 | 0.9250 |

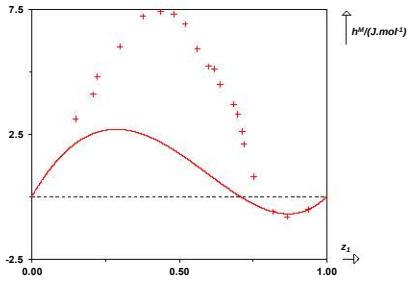
Letcher, Trevor M - Domańska, Urszula, Excess molar enthalpies of (2,2,4-trimethylpentane, or 1-heptene, or 1-hexene, or toluene+methyl 1,1-dimethylethyl ether) and of (1-heptene, or 1-hexene, or toluene+1,1-dimethylpropyl ether) at the temperatures 298.15 K and 308.15 K, The Journal of Chemical Thermodynamics 7 (1997) 721-730. doi:10.1006/jcht.1997.0198

| | |
|---|---|
| **T / K =** | **308.15** |
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| 3.100 | 0.1480 |
| 4.100 | 0.2084 |
| 4.800 | 0.2230 |
| 6.000 | 0.2981 |
| 7.200 | 0.3764 |
| 7.400 | 0.4362 |
| 7.300 | 0.4814 |
| 6.900 | 0.5187 |
| 5.900 | 0.5620 |
| 5.200 | 0.5998 |
| 5.100 | 0.6187 |
| 4.500 | 0.6380 |
| 3.700 | 0.6835 |
| 3.300 | 0.6986 |
| 2.600 | 0.7120 |
| 2.100 | 0.7187 |
| 0.8000 | 0.7537 |
| -0.6000 | 0.8168 |
| -0.8000 | 0.8649 |
| -0.5000 | 0.9375 |

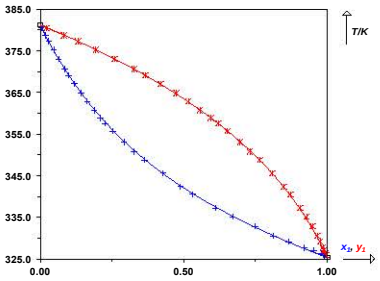
T/K = 298.15 - P/bar = 1.0132



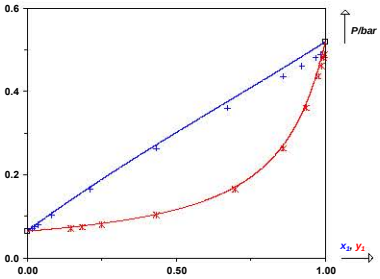

T/K = 308.15 - P/bar = 1.0132



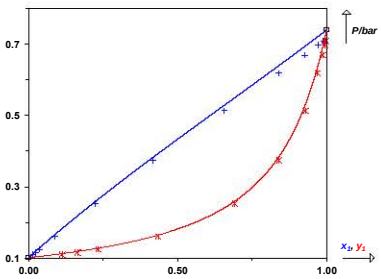

P/bar = 0.94000



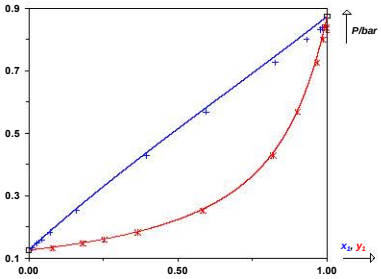

T/K = 308.15



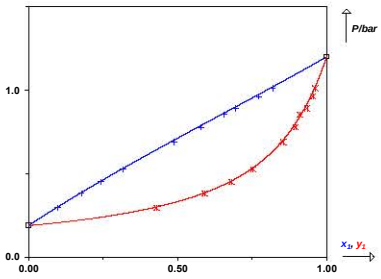

T/K = 318.15




T/K = 323.15




T/K = 333.15



## ETHYLENE (1) + CARBON DIOXIDE (2)

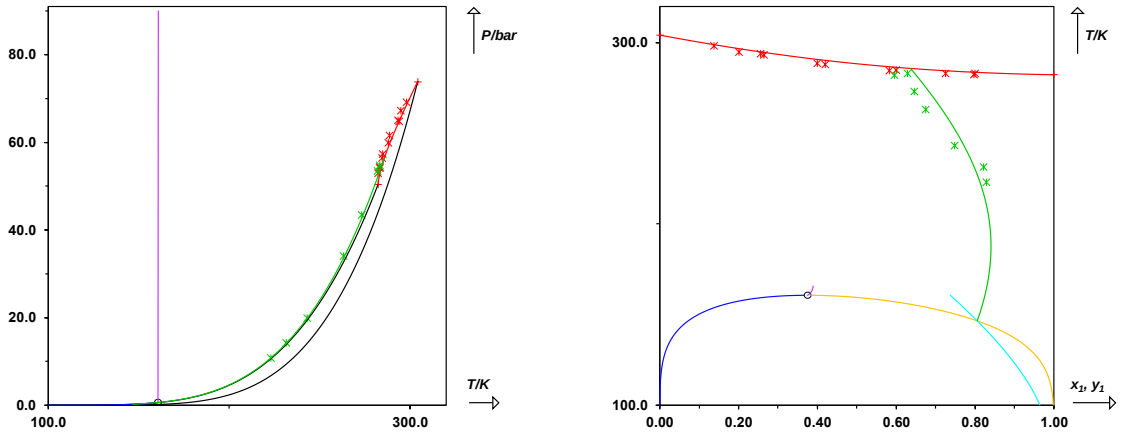
| | | |
|---|---|---|
| **CAS** | 74-85-1 | 124-38-9 |
| **InChiKey** | VGGSQFUCUMXWEO-UHFFFAOYSA-N | CURLTUGMZLYLDI-UHFFFAOYSA-N |
| **$T_c$ / K** | 282.34 | 304.21 |
| **$P_c$ / bar** | 50.41 | 73.83 |
| **ω** | 0.0860 | 0.2240 |

Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 159
B/MPa = 432

*Deviations*
MAPE on x = 17 %
MAPE on y = 20 %
MAPE on $x_c$ = 22 %
MAPE on $P_c$ = 2.4 %
MAPE on $x^{az}$ = 7.6 %
MAPE on $P^{az}$ = 1.5 %
MAPE on $h^M$ = 17 %



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**Isothermal phase equilibrium data**

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Mollerup, Jørgen, Vapour/liquid equilibrium in ethylene + carbon dioxide and ethane + carbon dioxide, Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases 0 (1975) doi:10.1039/f19757102351

**T / K = 223.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 7.321 | 0.0365 | 0.0946 | |
| 8.028 | 0.0985 | 0.2088 | |
| 8.828 | 0.1941 | 0.3354 | |
| 9.494 | 0.3018 | 0.4360 | |
| 9.936 | 0.4029 | 0.5120 | |
| 10.35 | 0.5305 | 0.6035 | |
| 10.54 | 0.6093 | 0.6573 | |
| 10.69 | 0.7149 | 0.7363 | |
| 10.74 | 0.8280 | 0.8280 | AZEO |
| 10.73 | 0.8641 | 0.8619 | |
| 10.65 | 0.9633 | 0.9604 | |

Nagahama, Kunio - Konishi, Hitoshi - Hoshino, Daisuke - Hirata, Mitsuho, Binary Vapor-Liquid Equilibria Of Carbon Dioxide-Light Hydrocarbons At Low Temperature, Journal of Chemical Engineering of Japan 5 (1974) 323-328. doi:10.1252/jcej.7.323

**T / K = 231.55**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 10.44 | 0.0520 | 0.1150 | |
| 10.94 | 0.0860 | 0.1810 | |
| 11.86 | 0.1670 | 0.2800 | |
| 12.62 | 0.2650 | 0.3850 | |
| 13.32 | 0.4280 | 0.4980 | |
| 13.68 | 0.4900 | 0.5620 | |
| 13.98 | 0.5870 | 0.6350 | |
| 14.14 | 0.7250 | 0.7350 | |
| 14.19 | 0.8210 | 0.8210 | AZEO |
| 14.19 | 0.8240 | 0.8220 | |
| 14.03 | 0.9210 | 0.9160 | |

Mollerup, Jørgen, Vapour/liquid equilibrium in ethylene + carbon dioxide and ethane + carbon dioxide, Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases 0 (1975) doi:10.1039/f19757102351

**T / K = 243.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 15.88 | 0.0872 | 0.1563 | |
| 17.17 | 0.1807 | 0.2775 | |
| 17.95 | 0.2596 | 0.3528 | |
| 18.73 | 0.3650 | 0.4391 | |
| 19.26 | 0.4593 | 0.5152 | |
| 19.94 | 0.7432 | 0.7382 | |
| 19.94 | 0.7480 | 0.7480 | AZEO |
| 19.59 | 0.9254 | 0.9156 | |

Nagahama, Kunio - Konishi, Hitoshi - Hoshino, Daisuke - Hirata, Mitsuho, Binary Vapor-Liquid Equilibria Of Carbon Dioxide-Light Hydrocarbons At Low Temperature, Journal of Chemical Engineering of Japan 5 (1974) 323-328. doi:10.1252/jcej.7.323

**T / K = 252.95**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.92 | 0.0600 | 0.1050 |
| 22.04 | 0.1130 | 0.1800 |
| 23.71 | 0.2330 | 0.3150 |
| 24.62 | 0.3240 | 0.3960 |
| 25.59 | 0.4530 | 0.5010 |
| 25.69 | 0.4940 | 0.5390 |
| 25.94 | 0.5340 | 0.5670 |
| 26.14 | 0.6380 | 0.6530 |
| 25.99 | 0.8250 | 0.8170 |
| 25.84 | 0.8730 | 0.8640 |
| 25.48 | 0.9290 | 0.9280 |

Bae, Hyo Kwang - Nagahama, Kunio - Hirata, Mitsuho, Isothermal vapor-liquid equilibriums for the ethylene-carbon dioxide system at high pressure, Journal of Chemical & Engineering Data 1 (1982) 25-27. doi:10.1021/je00027a007

**T / K = 263.14**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 27.82 | 0.0490 | 0.0840 | |
| 29.21 | 0.1060 | 0.1660 | |
| 30.79 | 0.2040 | 0.2680 | |
| 32.23 | 0.3100 | 0.3650 | |
| 33.02 | 0.4050 | 0.4440 | |
| 33.53 | 0.4850 | 0.5240 | |
| 33.96 | 0.6000 | 0.6130 | |
| 33.98 | 0.6690 | 0.6700 | |
| 34.00 | 0.6750 | 0.6750 | AZEO |
| 33.89 | 0.7640 | 0.7500 | |
| 33.54 | 0.8370 | 0.8250 | |

Bae, Hyo Kwang - Nagahama, Kunio - Hirata, Mitsuho, Isothermal vapor-liquid equilibriums for the ethylene-carbon dioxide system at high pressure, Journal of Chemical & Engineering Data 1 (1982) 25-27. doi:10.1021/je00027a007

**T / K = 273.16**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|

| | | | |
|---|---|---|---|
| 36.00 | 0.0390 | 0.0560 | |
| 37.36 | 0.0890 | 0.1250 | |
| 38.86 | 0.1550 | 0.2020 | |
| 40.21 | 0.2260 | 0.2730 | |
| 41.46 | 0.3160 | 0.3550 | |
| 42.63 | 0.4330 | 0.4580 | |
| 43.19 | 0.5260 | 0.5390 | |
| 43.38 | 0.5940 | 0.5980 | |
| 43.40 | 0.6460 | 0.6460 | AZEO |
| 43.42 | 0.6670 | 0.6660 | |
| 43.40 | 0.6840 | 0.6810 | |
| 43.15 | 0.7540 | 0.7510 | |
| 42.75 | 0.8170 | 0.8090 | |
| 42.21 | 0.8840 | 0.8780 | |
| 41.42 | 0.9520 | 0.9500 | |

Bae, Hyo Kwang - Nagahama, Kunio - Hirata, Mitsuho, Isothermal vapor-liquid equilibriums for the ethylene-carbon dioxide system at high pressure, Journal of Chemical & Engineering Data 1 (1982) 25-27. doi:10.1021/je00027a007

**T / K = 283.16**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 46.98 | 0.0600 | 0.0810 | |
| 48.27 | 0.1050 | 0.1390 | |
| 49.86 | 0.1590 | 0.2060 | |
| 51.86 | 0.2610 | 0.2970 | |
| 52.99 | 0.3380 | 0.3670 | |
| 54.10 | 0.4530 | 0.4660 | |
| 54.51 | 0.5350 | 0.5390 | |
| 54.79 | 0.6170 | 0.6180 | |
| 54.49 | 0.7070 | 0.7050 | |
| 54.41 | 0.7200 | 0.7190 | |
| 54.38 | 0.7250 | 0.7250 | CRIT |

Bae, Hyo Kwang - Nagahama, Kunio - Hirata, Mitsuho, Isothermal vapor-liquid equilibriums for the ethylene-carbon dioxide system at high pressure, Journal of Chemical & Engineering Data 1 (1982) 25-27. doi:10.1021/je00027a007

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 65.47 | 0.0330 | 0.0400 | |
| 66.98 | 0.0710 | 0.0810 | |
| 68.56 | 0.1130 | 0.1230 | |
| 69.01 | 0.1300 | 0.1350 | |
| 69.18 | 0.1370 | 0.1370 | CRIT |

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**Isobaric phase equilibrium data**

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Haselden, G. G. - Newitt, D. M. - Shah, S. M., Two-Phase Equilibrium in Binary and Ternary Systems. V. Carbon Dioxide-Ethylene. VI. Carbon Dioxide-Propylene, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 1096 (1951) 1-14. doi:10.1098/rspa.1951.0183

**P / bar = 30.40**

| T / K | $x_1$ |
|---|---|
| 264.97 | 0.0940 |
| 262.47 | 0.2113 |
| 260.86 | 0.3004 |
| 259.78 | 0.4025 |
| 259.12 | 0.5015 |
| 258.73 | 0.6327 |
| 258.57 | 0.7059 |
| 258.83 | 0.7904 |
| 258.98 | 0.8470 |
| 259.20 | 0.8933 |

Haselden, G. G. - Newitt, D. M. - Shah, S. M., Two-Phase Equilibrium in Binary and Ternary Systems. V. Carbon Dioxide-Ethylene. VI. Carbon Dioxide-Propylene, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 1096 (1951) 1-14. doi:10.1098/rspa.1951.0183

**P / bar = 30.40**

| T / K | $y_1$ |
|---|---|
| 266.30 | 0.0940 |
| 264.37 | 0.2113 |
| 262.62 | 0.3004 |
| 261.01 | 0.4025 |
| 259.81 | 0.5015 |
| 258.95 | 0.6327 |
| 258.66 | 0.7059 |
| 259.08 | 0.7904 |
| 259.38 | 0.8470 |
| 259.75 | 0.8933 |

Haselden, G. G. - Newitt, D. M. - Shah, S. M., Two-Phase Equilibrium in Binary and Ternary Systems. V. Carbon Dioxide-Ethylene. VI. Carbon Dioxide-Propylene, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 1096 (1951) 1-14. doi:10.1098/rspa.1951.0183

**P / bar = 40.53**

| T / K | $x_1$ |
|---|---|
| 275.96 | 0.0940 |
| 273.63 | 0.2113 |
| 272.05 | 0.3004 |
| 271.15 | 0.4025 |
| 270.40 | 0.5015 |

| | |
|---|---|
| 270.11 | 0.6327 |
| 270.03 | 0.7059 |
| 270.35 | 0.7904 |
| 270.67 | 0.8470 |
| 270.92 | 0.8933 |

Haselden, G. G. - Newitt, D. M. - Shah, S. M., Two-Phase Equilibrium in Binary and Ternary Systems. V. Carbon Dioxide-Ethylene. VI. Carbon Dioxide-Propylene, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 1096 (1951) 1-14. doi:10.1098/rspa.1951.0183

**P / bar = 40.53**

| T / K | $y_1$ |
|---|---|
| 276.78 | 0.0940 |
| 274.84 | 0.2113 |
| 272.98 | 0.3004 |
| 271.78 | 0.4025 |
| 270.78 | 0.5015 |
| 270.19 | 0.6327 |
| 270.13 | 0.7059 |
| 270.51 | 0.7904 |
| 270.95 | 0.8470 |
| 271.35 | 0.8933 |

Haselden, G. G. - Newitt, D. M. - Shah, S. M., Two-Phase Equilibrium in Binary and Ternary Systems. V. Carbon Dioxide-Ethylene. VI. Carbon Dioxide-Propylene, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 1096 (1951) 1-14. doi:10.1098/rspa.1951.0183

**P / bar = 45.60**

| T / K | $x_1$ |
|---|---|
| 280.67 | 0.0940 |
| 278.37 | 0.2113 |
| 276.83 | 0.3004 |
| 275.75 | 0.4025 |
| 275.23 | 0.5015 |
| 274.93 | 0.6327 |
| 274.97 | 0.7059 |
| 275.40 | 0.7904 |
| 275.77 | 0.8470 |
| 276.12 | 0.8933 |

Haselden, G. G. - Newitt, D. M. - Shah, S. M., Two-Phase Equilibrium in Binary and Ternary Systems. V. Carbon Dioxide-Ethylene. VI. Carbon Dioxide-Propylene, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 1096 (1951) 1-14. doi:10.1098/rspa.1951.0183

**P / bar = 45.60**

| T / K | $y_1$ |
|---|---|
| 281.70 | 0.0940 |
| 279.36 | 0.2113 |
| 277.65 | 0.3004 |
| 276.43 | 0.4025 |
| 275.53 | 0.5015 |
| 274.95 | 0.6327 |
| 275.05 | 0.7059 |
| 275.53 | 0.7904 |
| 276.00 | 0.8470 |
| 276.38 | 0.8933 |

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**Enthalpy of mixing**

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Wormald, C.J. - Eyears, J.M., Excess molar enthalpies of (carbon dioxide + ethene) in the liquid and near-critical regions, The Journal of Chemical Thermodynamics 7 (2001) 775-786. doi:10.1006/jcht.2000.0778

**T / K = 260.95**

**P / bar = 35.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 562.00 | 0.2370 |
| 685.00 | 0.3160 |
| 779.00 | 0.3960 |
| 793.00 | 0.4750 |
| 805.00 | 0.5170 |
| 800.00 | 0.5570 |
| 783.00 | 0.5950 |
| 716.00 | 0.6380 |
| 643.00 | 0.6780 |

Wormald, C.J. - Eyears, J.M., Excess molar enthalpies of (carbon dioxide + ethene) in the liquid and near-critical regions, The Journal of Chemical Thermodynamics 7 (2001) 775-786. doi:10.1006/jcht.2000.0778

**T / K = 276.65**

**P / bar = 110.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 126.00 | 0.0520 |
| 246.00 | 0.1010 |
| 377.00 | 0.1510 |
| 499.00 | 0.2010 |
| 584.00 | 0.2500 |
| 631.00 | 0.3010 |
| 688.00 | 0.3520 |
| 722.00 | 0.4020 |
| 734.00 | 0.4520 |
| 734.00 | 0.5030 |

| | |
|---|---|
| 720.00 | 0.5530 |
| 700.00 | 0.6610 |
| 645.00 | 0.6510 |
| 602.00 | 0.7030 |
| 338.00 | 0.8510 |

Wormald, C.J. - Eyears, J.M., Excess molar enthalpies of (carbon dioxide + ethene) in the liquid and near-critical regions, The Journal of Chemical Thermodynamics 7 (2001) 775-786. doi:10.1006/jcht.2000.0778

**T / K = 276.65**

**P / bar = 47.50**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 102.00 | 0.0410 |
| 217.00 | 0.0800 |
| 332.00 | 0.1200 |
| 429.00 | 0.1590 |
| 500.00 | 0.1980 |
| 590.00 | 0.2380 |
| 646.00 | 0.2770 |
| 720.00 | 0.3180 |
| 780.00 | 0.3570 |
| 811.00 | 0.3980 |
| 855.00 | 0.4370 |
| 858.00 | 0.4770 |
| 886.00 | 0.5160 |
| 885.00 | 0.5530 |
| 853.00 | 0.5970 |
| 851.00 | 0.6400 |
| 822.00 | 0.6800 |
| 691.00 | 0.7610 |
| 604.00 | 0.8010 |
| 507.00 | 0.8420 |

Wormald, C.J. - Eyears, J.M., Excess molar enthalpies of (carbon dioxide + ethene) in the liquid and near-critical regions, The Journal of Chemical Thermodynamics 7 (2001) 775-786. doi:10.1006/jcht.2000.0778

**T / K = 285.85**

**P / bar = 110.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 98.00 | 0.0490 |
| 295.00 | 0.1000 |
| 399.00 | 0.1530 |
| 503.00 | 0.2010 |
| 600.00 | 0.2510 |
| 682.00 | 0.3030 |
| 750.00 | 0.4020 |
| 741.00 | 0.5010 |
| 730.00 | 0.5510 |
| 703.00 | 0.5950 |
| 660.00 | 0.6380 |
| 620.00 | 0.6900 |
| 555.00 | 0.7400 |
| 448.00 | 0.8020 |
| 361.00 | 0.8520 |

Wormald, C.J. - Eyears, J.M., Excess molar enthalpies of (carbon dioxide + ethene) in the liquid and near-critical regions, The Journal of Chemical Thermodynamics 7 (2001) 775-786. doi:10.1006/jcht.2000.0778

**T / K = 285.85**

**P / bar = 62.50**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 410.00 | 0.1610 |
| 547.00 | 0.1990 |
| 648.00 | 0.2400 |
| 737.00 | 0.2790 |
| 829.00 | 0.3200 |
| 892.00 | 0.3590 |
| 957.00 | 0.4000 |
| 1007.0 | 0.4390 |
| 1053.0 | 0.4790 |
| 1059.0 | 0.5220 |
| 1074.0 | 0.5610 |
| 1055.0 | 0.5990 |
| 1024.0 | 0.6420 |
| 936.00 | 0.6820 |
| 820.00 | 0.7190 |
| 703.00 | 0.7620 |
| 595.00 | 0.8020 |
| 490.00 | 0.8430 |

Wormald, C.J. - Eyears, J.M., Excess molar enthalpies of (carbon dioxide + ethene) in the liquid and near-critical regions, The Journal of Chemical Thermodynamics 7 (2001) 775-786. doi:10.1006/jcht.2000.0778

**T / K = 300.45**

**P / bar = 110.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 139.00 | 0.0520 |
| 300.00 | 0.1010 |
| 452.00 | 0.1510 |
| 561.00 | 0.2010 |
| 659.00 | 0.2500 |
| 726.00 | 0.3010 |

| | |
|---|---|
| 812.00 | 0.3520 |
| 847.00 | 0.4020 |
| 830.00 | 0.4510 |
| 831.00 | 0.5030 |
| 830.00 | 0.5530 |
| 792.00 | 0.6010 |
| 730.00 | 0.6510 |
| 665.00 | 0.7030 |
| 592.00 | 0.7530 |
| 473.00 | 0.8010 |
| 373.00 | 0.8510 |
| 229.00 | 0.9020 |
| 103.00 | 0.9510 |

Wormald, C.J. - Eyears, J.M., Excess molar enthalpies of (carbon dioxide + ethene) in the liquid and near-critical regions, The Journal of Chemical Thermodynamics 7 (2001) 775-786. doi:10.1006/jcht.2000.0778

**T / K = 300.45**

**P / bar = 75.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 210.00 | 0.0420 |
| 415.00 | 0.0810 |
| 675.00 | 0.1220 |
| 954.00 | 0.1610 |
| 1295.0 | 0.2010 |
| 1639.0 | 0.2410 |
| 1925.0 | 0.2810 |
| 2148.0 | 0.3210 |
| 2249.0 | 0.3610 |
| 2309.0 | 0.4020 |
| 2286.0 | 0.4410 |
| 2200.0 | 0.4810 |
| 2131.0 | 0.5230 |
| 2043.0 | 0.5630 |
| 1895.0 | 0.6010 |
| 1762.0 | 0.6430 |
| 1586.0 | 0.6830 |
| 1422.0 | 0.7210 |
| 1242.0 | 0.7630 |
| 1021.0 | 0.8030 |
| 768.00 | 0.8440 |
| 600.00 | 0.8810 |
| 328.00 | 0.9250 |
| 131.00 | 0.9640 |

Wormald, C.J. - Eyears, J.M., Excess molar enthalpies of (carbon dioxide + ethene) in the liquid and near-critical regions, The Journal of Chemical Thermodynamics 7 (2001) 775-786. doi:10.1006/jcht.2000.0778

**T / K = 300.45**

**P / bar = 65.70**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 247.00 | 0.1010 |
| 340.00 | 0.1500 |
| 418.00 | 0.2010 |
| 471.00 | 0.2500 |
| 539.00 | 0.3310 |
| 582.00 | 0.3480 |
| 610.00 | 0.3980 |
| 630.00 | 0.4990 |
| 631.00 | 0.5490 |
| 585.00 | 0.6520 |

Wormald, C.J. - Eyears, J.M., Excess molar enthalpies of (carbon dioxide + ethene) in the liquid and near-critical regions, The Journal of Chemical Thermodynamics 7 (2001) 775-786. doi:10.1006/jcht.2000.0778

**T / K = 305.75**

**P / bar = 80.50**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 887.00 | 0.0720 |
| 1254.0 | 0.0840 |
| 1764.0 | 0.1250 |
| 2028.0 | 0.1670 |
| 2176.0 | 0.2090 |
| 2223.0 | 0.2500 |
| 2340.0 | 0.2930 |
| 2204.0 | 0.3340 |
| 2194.0 | 0.3740 |
| 2157.0 | 0.4150 |
| 2076.0 | 0.4580 |
| 1943.0 | 0.5000 |
| 1833.0 | 0.5420 |
| 1681.0 | 0.5830 |
| 1580.0 | 0.6250 |
| 1360.0 | 0.6680 |
| 1304.0 | 0.7090 |
| 991.00 | 0.7510 |
| 904.00 | 0.7950 |
| 613.00 | 0.8350 |

Wormald, C.J. - Eyears, J.M., Excess molar enthalpies of (carbon dioxide + ethene) in the liquid and near-critical regions, The Journal of Chemical Thermodynamics 7 (2001) 775-786. doi:10.1006/jcht.2000.0778

**T / K =** **306.62**
**P / bar =** **110.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 155.00 | 0.0500 |
| 337.00 | 0.1010 |
| 599.00 | 0.1530 |
| 701.00 | 0.2010 |
| 799.00 | 0.2510 |
| 898.00 | 0.3010 |
| 968.00 | 0.3500 |
| 989.00 | 0.4010 |
| 981.00 | 0.5010 |
| 940.00 | 0.5530 |
| 880.00 | 0.6010 |
| 824.00 | 0.6520 |
| 739.00 | 0.7020 |
| 641.00 | 0.7510 |
| 544.00 | 0.8010 |
| 442.00 | 0.8520 |
| 305.00 | 0.9010 |

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**Critical point**

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Rowlinson, J.S. - Sutton, J.R. - Weston, J.F., Liquid-vapor equilibrium in the ternary system carbon dioxide-nitrous oxide-ethylene, Proceedings (1958) 10-14.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 294.95 | 67.28 | 0.2000 |
| 288.55 | 61.50 | 0.4000 |
| 284.75 | 57.35 | 0.6000 |
| 283.15 | 54.11 | 0.8000 |

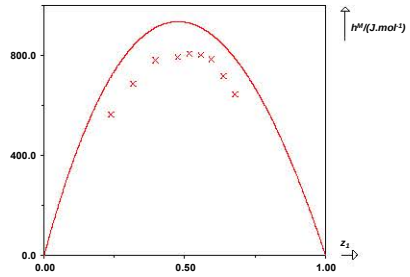
Bae, Hyo Kwang - Nagahama, Kunio - Hirata, Mitsuho, Isothermal vapor-liquid equilibriums for the ethylene-carbon dioxide system at high pressure, Journal of Chemical & Engineering Data 1 (1982) 25-27. doi:10.1021/je00027a007

| T / K | P / bar | $x_1$ |
|---|---|---|
| 293.18 | 65.05 | 0.2640 |

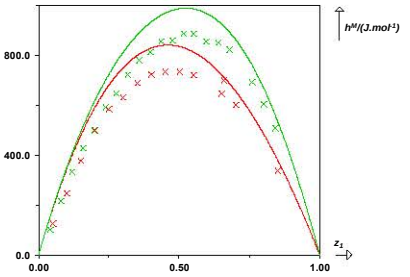
Khazanova, N.E. - Sominskaya, E.E. - Zakharova, A.V. - Rozovskii, M.B. - Nechimailo, N.L., Systems with azeotropism at high pressures. X. Phase and volume relations in the ethylene-carbon dioxide system, Zh. Fiz. Khim. 6 (1979) 1594-1597.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 282.39 | 52.89 | 0.7970 |
| 284.65 | 56.39 | 0.5820 |
| 288.09 | 59.83 | 0.4190 |
| 293.95 | 64.75 | 0.2560 |

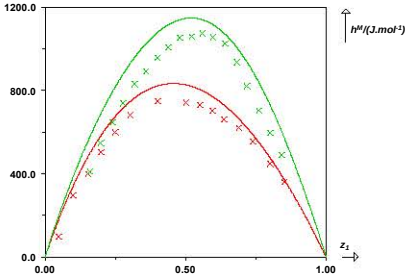
T/K = 260.95 - P/bar = 35.00



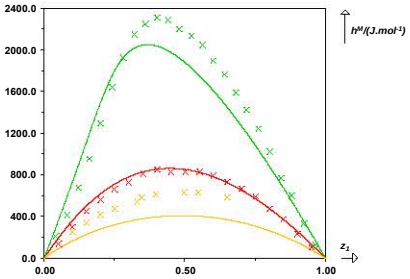

T/K = 276.65 - P/bar = 110.00 47.500



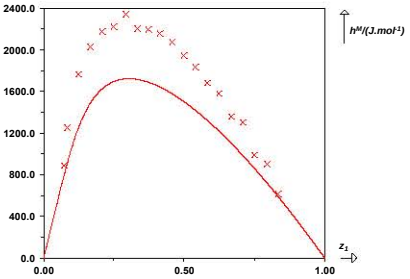

T/K = 285.85 - P/bar = 110.00 62.500



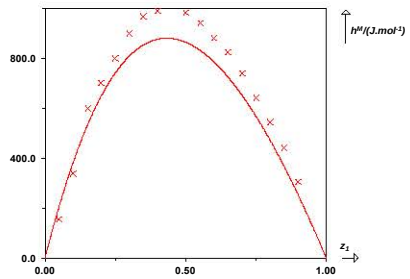

T/K = 300.45 - P/bar = 110.00 75.00 65.700



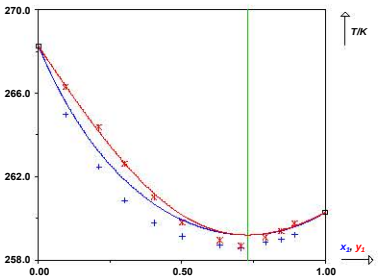

T/K = 305.75 - P/bar = 80.500



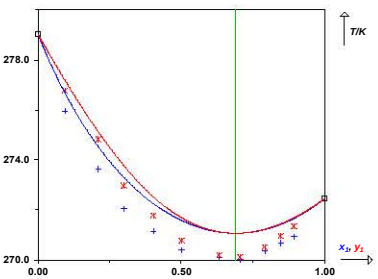

T/K = 306.62 - P/bar = 110.00



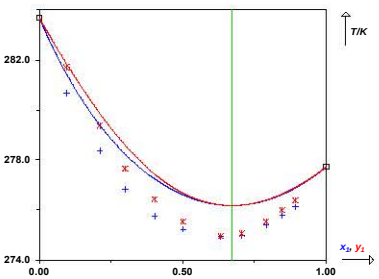

P/bar = 30.39800



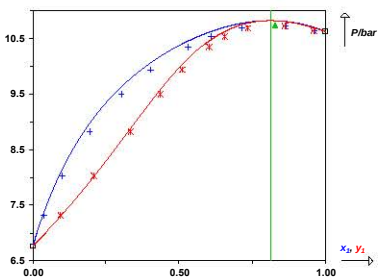

P/bar = 40.53000



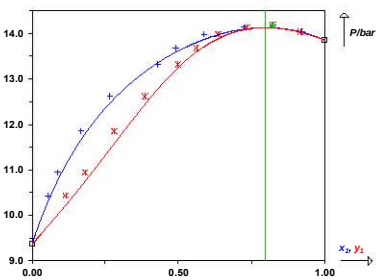

P/bar = 45.59600



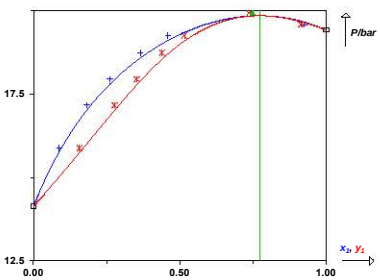

T/K = 223.15



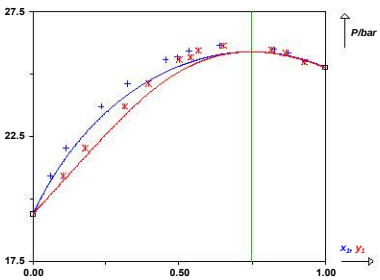

T/K = 231.55



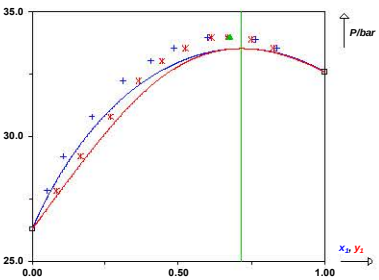

T/K = 243.15



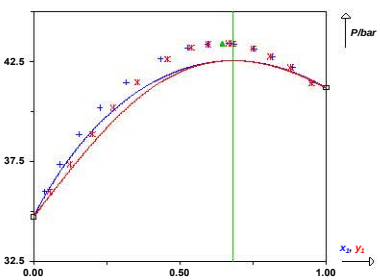

T/K = 252.95



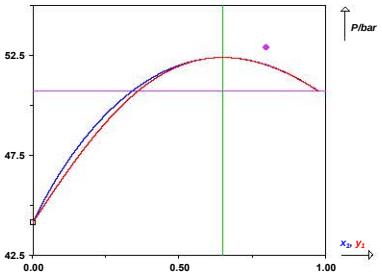

T/K = 263.14



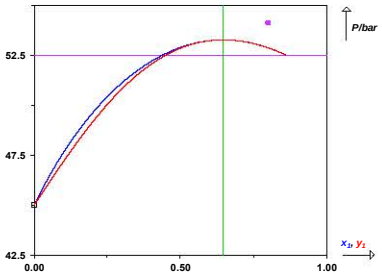

T/K = 273.16



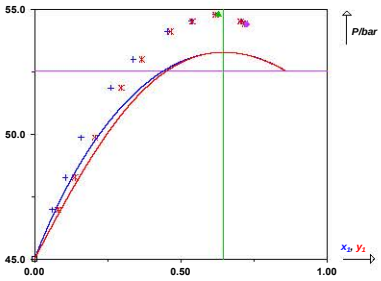
T/K = 282.39



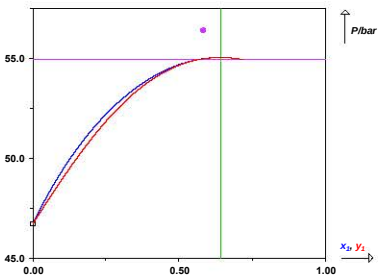

T/K = 283.15



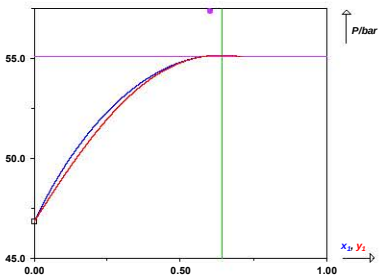

T/K = 283.16



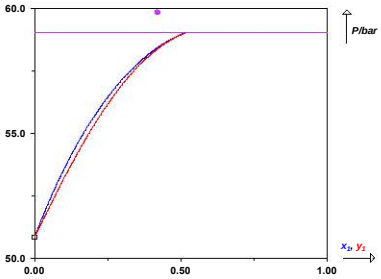

T/K = 284.65



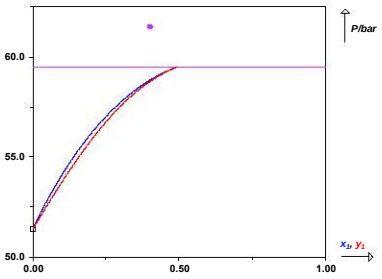

T/K = 284.75



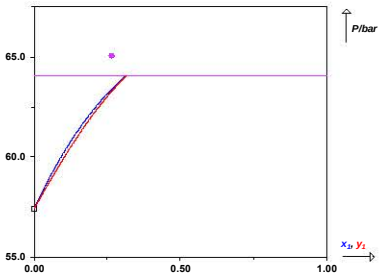

T/K = 288.09



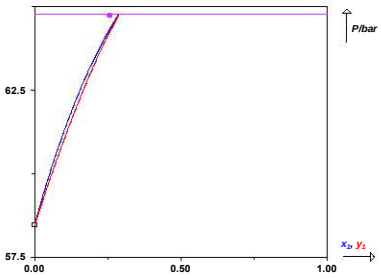

T/K = 288.55



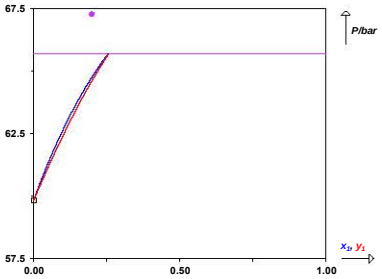

T/K = 293.18



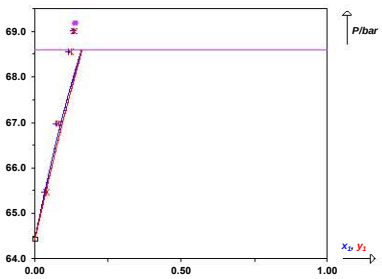

T/K = 293.95




T/K = 294.95




T/K = 298.15



## CARBON DIOXIDE (1) + PROPANE (2)

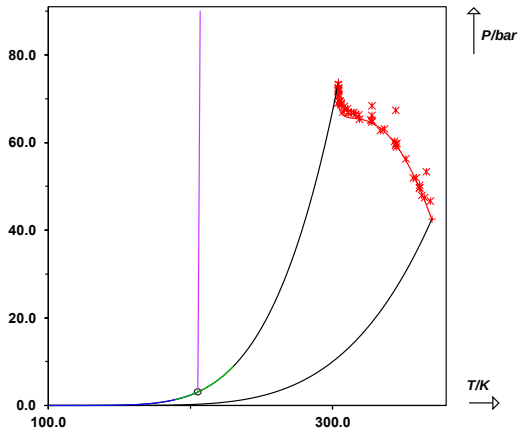
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 74-98-6 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | ATUOYWHBWRKTHZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 369.83 |
| **$P_c$ / bar** | 73.83 | 42.48 |
| **ω** | 0.2240 | 0.1520 |

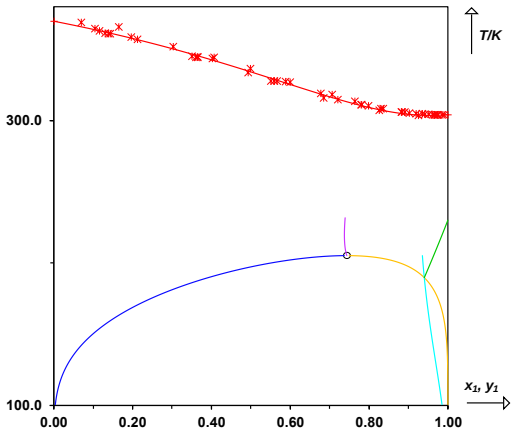
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 394
B/MPa = 690

*Deviations*
MAPE on x = 3.8 %
MAPE on y = 3.1 %
MAPE on $x_c$ = 87 %
MAPE on $P_c$ = 24 %



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**Isothermal phase equilibrium data**

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Yucelen, Belgin - Kidnay, Arthur J., Vapor–Liquid Equilibria in the Nitrogen + Carbon Dioxide + Propane System from 240 to 330 K at Pressures to 15 MPa, Journal of Chemical & Engineering Data 5 (1999) 926-931. doi:10.1021/je980321e

**T / K = 240.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.160 | 0.0604 | 0.5424 |
| 4.480 | 0.1203 | 0.6787 |
| 4.640 | 0.1282 | 0.6935 |
| 7.440 | 0.2727 | 0.8184 |
| 8.370 | 0.3354 | 0.8488 |
| 8.811 | 0.3736 | 0.8583 |
| 10.17 | 0.5165 | 0.8902 |
| 10.57 | 0.5700 | 0.8933 |
| 12.00 | 0.8206 | 0.9302 |

Kim, Ju Hyok - Kim, Min Soo, Vapor–liquid equilibria for the carbon dioxide+propane system over a temperature range from 253.15 to 323.15K, Fluid Phase Equilibria 1 (2005) 13-19. doi:10.1016/j.fluid.2005.09.006

**T / K = 253.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.092 | 0.0160 | 0.1910 |
| 4.075 | 0.0420 | 0.3880 |
| 5.560 | 0.0840 | 0.5440 |
| 8.199 | 0.1700 | 0.6930 |
| 11.01 | 0.2790 | 0.7830 |
| 11.62 | 0.3050 | 0.7980 |
| 12.82 | 0.3850 | 0.8340 |
| 14.03 | 0.4550 | 0.8550 |
| 14.73 | 0.5000 | 0.8660 |
| 15.19 | 0.5360 | 0.8750 |
| 15.75 | 0.5820 | 0.8820 |
| 16.57 | 0.6570 | 0.8950 |
| 18.04 | 0.8150 | 0.9240 |
| 18.48 | 0.8700 | 0.9350 |

Webster, Leigh A. - Kidnay, Arthur J., Vapor–Liquid Equilibria for the Methane–Propane–Carbon Dioxide Systems at 230 K and 270 K, Journal of Chemical & Engineering Data 3 (2001) 759-764. doi:10.1021/je000307d

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.040 | 0.0337 | 0.2915 |
| 6.410 | 0.0409 | 0.3347 |
| 6.790 | 0.0490 | 0.3735 |
| 7.180 | 0.0569 | 0.4061 |
| 7.500 | 0.0630 | 0.4380 |
| 8.180 | 0.0757 | 0.4786 |
| 9.770 | 0.1139 | 0.5638 |
| 10.96 | 0.1407 | 0.6142 |
| 12.51 | 0.1722 | 0.6651 |
| 13.87 | 0.2169 | 0.7001 |
| 15.98 | 0.2820 | 0.7444 |
| 17.58 | 0.3231 | 0.7721 |
| 19.18 | 0.3742 | 0.7953 |
| 20.79 | 0.4443 | 0.8214 |
| 22.30 | 0.5051 | 0.8373 |
| 23.17 | 0.5408 | 0.8489 |
| 24.06 | 0.5820 | 0.8585 |
| 24.70 | 0.6110 | 0.8645 |
| 26.01 | 0.6730 | 0.8804 |
| 26.76 | 0.7089 | 0.8900 |
| 27.99 | 0.7716 | 0.9066 |
| 27.83 | 0.7730 | 0.9054 |
| 28.79 | 0.8174 | 0.9196 |
| 29.60 | 0.8620 | 0.9339 |
| 30.35 | 0.9003 | 0.9493 |
| 31.03 | 0.9403 | 0.9656 |
| 31.34 | 0.9565 | 0.9745 |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Propane-Carbon Dioxide System, Industrial & Engineering Chemistry 11 (1951) 2515-2520. doi:10.1021/ie50503a035

**T / K = 277.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0247 | 0.2056 |
| 10.34 | 0.0884 | 0.4676 |
| 13.79 | 0.1602 | 0.6036 |
| 17.24 | 0.2402 | 0.6864 |
| 20.69 | 0.3316 | 0.7431 |
| 24.13 | 0.4361 | 0.7876 |
| 27.58 | 0.5532 | 0.8309 |
| 31.03 | 0.6714 | 0.8688 |
| 34.48 | 0.7956 | 0.9102 |
| 37.92 | 0.9401 | 0.9702 |

Tanaka, Katsuyuki - Higashi, Yukihiro - Akasaka, Ryo - Kayukawa, Yohei - Fujii, Kenich, Measurements of the Vapor–Liquid Equilibrium for the CO2 + R290 Mixture, Journal of Chemical & Engineering Data 3 (2009) 1029-1033. doi:10.1021/je800938s

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.610 | 0.0610 | 0.3250 |
| 17.57 | 0.2060 | 0.6300 |
| 23.98 | 0.3520 | 0.7280 |
| 27.94 | 0.4490 | 0.7730 |
| 39.21 | 0.7810 | 0.8910 |

Kim, Ju Hyok - Kim, Min Soo, Vapor–liquid equilibria for the carbon dioxide+propane system over a temperature range from 253.15 to 323.15K, Fluid Phase Equilibria 1 (2005) 13-19. doi:10.1016/j.fluid.2005.09.006

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.718 | 0.0210 | 0.1580 |
| 8.950 | 0.0410 | 0.2650 |
| 11.29 | 0.0810 | 0.4130 |
| 15.86 | 0.1620 | 0.5770 |
| 17.97 | 0.2080 | 0.6300 |
| 21.28 | 0.2730 | 0.6870 |
| 22.23 | 0.2950 | 0.7010 |
| 24.90 | 0.3680 | 0.7460 |
| 28.29 | 0.4530 | 0.7750 |
| 29.42 | 0.4830 | 0.7930 |
| 30.69 | 0.5210 | 0.8090 |
| 32.86 | 0.5900 | 0.8290 |
| 35.69 | 0.6750 | 0.8520 |
| 39.65 | 0.8080 | 0.8970 |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Propane-Carbon Dioxide System, Industrial & Engineering Chemistry 11 (1951) 2515-2520. doi:10.1021/ie50503a035

**T / K = 294.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.34 | 0.0245 | 0.1618 |
| 13.79 | 0.0742 | 0.3589 |
| 17.24 | 0.1274 | 0.4812 |
| 20.69 | 0.1834 | 0.5634 |
| 24.13 | 0.2423 | 0.6235 |
| 27.58 | 0.3048 | 0.6718 |
| 31.03 | 0.3727 | 0.7148 |
| 34.48 | 0.4443 | 0.7518 |
| 37.92 | 0.5178 | 0.7814 |
| 41.37 | 0.5937 | 0.8092 |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Propane-Carbon Dioxide System, Industrial & Engineering Chemistry 11 (1951) 2515-2520. doi:10.1021/ie50503a035

**T / K = 294.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 44.82 | 0.6722 | 0.8368 |
| 48.26 | 0.7516 | 0.8673 |
| 51.71 | 0.8275 | 0.9011 |
| 55.16 | 0.9046 | 0.9417 |
| 58.61 | 0.9805 | 0.9874 |

Niesen, Vicki G - Rainwater, James C, Critical locus, (vapor + liquid) equilibria, and coexisting densities of (carbon dioxide + propane) at temperatures from 311 K to 361 K, The Journal of Chemical Thermodynamics 8 (1990) 777-795. doi:10.1016/0021-9614(90)90070-7

**T / K = 311.05**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 14.89 | 0.0199 | 0.1100 |
| 16.07 | 0.0343 | 0.1673 |
| 17.49 | 0.0505 | 0.2280 |
| 18.96 | 0.0692 | 0.2817 |
| 20.30 | 0.0858 | 0.3243 |
| 21.62 | 0.1014 | 0.3636 |
| 22.80 | 0.1166 | 0.3921 |
| 24.25 | 0.1347 | 0.4243 |
| 25.92 | 0.1573 | 0.4589 |
| 27.60 | 0.1774 | 0.4888 |
| 29.55 | 0.2048 | 0.5198 |
| 31.41 | 0.2285 | 0.5454 |
| 33.29 | 0.2542 | 0.5699 |
| 35.37 | 0.2831 | 0.5920 |
| 37.01 | 0.3076 | 0.6088 |
| 39.62 | 0.3458 | 0.6383 |
| 41.51 | 0.3729 | 0.6529 |
| 43.22 | 0.3988 | 0.6680 |
| 45.12 | 0.4262 | 0.6800 |
| 47.04 | 0.4564 | 0.6933 |
| 48.97 | 0.4853 | 0.7055 |
| 50.97 | 0.5187 | 0.7162 |
| 52.68 | 0.5435 | 0.7265 |
| 53.18 | 0.5520 | 0.7290 |
| 54.84 | 0.5780 | 0.7386 |
| 54.86 | 0.5794 | 0.7384 |
| 57.04 | 0.6117 | 0.7488 |
| 57.20 | 0.6143 | 0.7507 |
| 58.87 | 0.6403 | 0.7602 |
| 59.02 | 0.6412 | 0.7606 |
| 60.91 | 0.6703 | 0.7705 |
| 62.97 | 0.7049 | 0.7811 |

| | | | |
|---|---|---|---|
| 64.12 | 0.7205 | 0.7820 | |
| 65.29 | 0.7405 | 0.7894 | |
| 66.40 | 0.7600 | 0.7910 | |
| 66.78 | 0.7695 | 0.7867 | |
| 67.02 | 0.7800 | 0.7800 | CRIT |

Kim, Ju Hyok - Kim, Min Soo, Vapor–liquid equilibria for the carbon dioxide+propane system over a temperature range from 253.15 to 323.15K, Fluid Phase Equilibria 1 (2005) 13-19. doi:10.1016/j.fluid.2005.09.006

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 19.11 | 0.0210 | 0.0880 |
| 21.24 | 0.0440 | 0.1640 |
| 24.58 | 0.0790 | 0.2570 |
| 32.30 | 0.1650 | 0.4070 |
| 35.63 | 0.2040 | 0.4550 |
| 41.27 | 0.2690 | 0.5130 |
| 48.42 | 0.3570 | 0.5750 |
| 52.91 | 0.4160 | 0.6020 |
| 57.38 | 0.4780 | 0.6210 |
| 60.75 | 0.5250 | 0.6320 |
| 62.81 | 0.5590 | 0.6360 |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Propane-Carbon Dioxide System, Industrial & Engineering Chemistry 11 (1951) 2515-2520. doi:10.1021/ie50503a035

**T / K = 327.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 20.69 | 0.0176 | 0.0734 | |
| 24.13 | 0.0526 | 0.1873 | |
| 27.58 | 0.0882 | 0.2739 | |
| 31.03 | 0.1246 | 0.3425 | |
| 34.48 | 0.1618 | 0.3980 | |
| 37.92 | 0.1992 | 0.4426 | |
| 41.37 | 0.2376 | 0.4804 | |
| 44.82 | 0.2770 | 0.5124 | |
| 48.26 | 0.3171 | 0.5394 | |
| 51.71 | 0.3577 | 0.5619 | |
| 55.16 | 0.3996 | 0.5806 | |
| 58.61 | 0.4403 | 0.5896 | |
| 62.05 | 0.4840 | 0.5968 | |
| 65.50 | 0.5306 | 0.5980 | |
| 68.40 | 0.5880 | 0.5880 | CRIT |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Propane-Carbon Dioxide System, Industrial & Engineering Chemistry 11 (1951) 2515-2520. doi:10.1021/ie50503a035

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 27.58 | 0.0099 | 0.0315 | |
| 31.03 | 0.0409 | 0.1153 | |
| 34.48 | 0.0726 | 0.1832 | |
| 37.92 | 0.1043 | 0.2377 | |
| 41.37 | 0.1370 | 0.2840 | |
| 44.82 | 0.1698 | 0.3218 | |
| 48.26 | 0.2019 | 0.3513 | |
| 51.71 | 0.2338 | 0.3743 | |
| 55.16 | 0.2666 | 0.3930 | |
| 58.61 | 0.2998 | 0.4068 | |
| 62.05 | 0.3348 | 0.4162 | |
| 65.50 | 0.3735 | 0.4202 | |
| 67.29 | 0.4070 | 0.4070 | CRIT |

Niesen, Vicki G - Rainwater, James C, Critical locus, (vapor + liquid) equilibria, and coexisting densities of (carbon dioxide + propane) at temperatures from 311 K to 361 K, The Journal of Chemical Thermodynamics 8 (1990) 777-795. doi:10.1016/0021-9614(90)90070-7

**T / K = 344.43**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 28.91 | 0.0214 | 0.0650 | |
| 29.85 | 0.0293 | 0.0860 | |
| 31.38 | 0.0430 | 0.1200 | |
| 32.89 | 0.0566 | 0.1478 | |
| 35.30 | 0.0800 | 0.1934 | |
| 35.75 | 0.0833 | 0.2031 | |
| 38.13 | 0.1065 | 0.2365 | |
| 40.22 | 0.1265 | 0.2655 | |
| 42.37 | 0.1451 | 0.2902 | |
| 43.43 | 0.1562 | 0.3025 | |
| 44.89 | 0.1703 | 0.3168 | |
| 47.61 | 0.1981 | 0.3417 | |
| 49.59 | 0.2190 | 0.3598 | |
| 50.54 | 0.2274 | 0.3640 | |
| 51.79 | 0.2420 | 0.3740 | |
| 53.90 | 0.2653 | 0.3820 | |
| 55.89 | 0.2862 | 0.3885 | |
| 57.14 | 0.3038 | 0.3910 | |
| 58.29 | 0.3237 | 0.3854 | |
| 58.94 | 0.3341 | 0.3839 | |
| 59.19 | 0.3410 | 0.3755 | |
| 59.80 | 0.3643 | 0.3643 | CRIT |
| 59.32 | 0.3711 | 0.3740 | |

Niesen, Vicki G - Rainwater, James C, Critical locus, (vapor + liquid) equilibria, and coexisting densities of (carbon dioxide + propane) at temperatures from 311 K to 361 K, The Journal of Chemical Thermodynamics 8 (1990) 777-795. doi:10.1016/0021-9614(90)90070-7

**T / K = 361.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 38.00 | 0.0125 | 0.0306 | |
| 40.62 | 0.0354 | 0.0701 | |
| 43.10 | 0.0584 | 0.1004 | |
| 44.54 | 0.0720 | 0.1176 | |
| 47.33 | 0.1000 | 0.1423 | |
| 48.60 | 0.1149 | 0.1505 | |
| 49.26 | 0.1255 | 0.1535 | |
| 49.60 | 0.1394 | 0.1394 | CRIT |
| 49.75 | 0.1444 | 0.1448 | |

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**Isobaric phase equilibrium data**

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Poettmann, Fred H. - Katz, D. L., Phase Behavior of Binary Carbon Dioxide-Paraffin Systems, Industrial & Engineering Chemistry 9 (1945) 847-853. doi:10.1021/ie50429a017

**P / bar = 46.68**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 288.15 | 0.9000 | 0.9480 |
| 292.55 | 0.8000 | 0.9030 |
| 298.15 | 0.7000 | 0.8510 |
| 304.85 | 0.6000 | 0.7940 |
| 312.05 | 0.5000 | 0.7320 |
| 319.25 | 0.4000 | 0.6580 |
| 331.45 | 0.3000 | 0.5400 |
| 346.45 | 0.2000 | 0.3720 |
| 363.15 | 0.1000 | 0.1780 |

Poettmann, Fred H. - Katz, D. L., Phase Behavior of Binary Carbon Dioxide-Paraffin Systems, Industrial & Engineering Chemistry 9 (1945) 847-853. doi:10.1021/ie50429a017

**P / bar = 53.35**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 295.35 | 0.9000 | 0.9380 |
| 299.25 | 0.8000 | 0.8840 |
| 305.95 | 0.7000 | 0.8200 |
| 313.15 | 0.6000 | 0.7520 |
| 320.95 | 0.5000 | 0.6780 |
| 328.75 | 0.4000 | 0.6030 |
| 340.35 | 0.3000 | 0.4870 |
| 358.15 | 0.2000 | 0.2730 |

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**Critical point**

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Roof, J. G. - Baron, J. D., Critical loci of binary mixtures of propane with methane, carbon dioxide, and nitrogen, Journal of Chemical & Engineering Data 3 (1967) 292-293. doi:10.1021/je60034a003

| T / K | P / bar | $x_1$ |
|---|---|---|
| 361.26 | 50.19 | 0.1300 |
| 345.15 | 59.78 | 0.3500 |
| 327.76 | 66.19 | 0.5500 |
| 308.21 | 68.19 | 0.8300 |
| 305.87 | 68.95 | 0.8900 |
| 304.98 | 69.29 | 0.9200 |

Morrison, G. - Kincaid, J. M., Critical point measurements on nearly polydisperse fluids, AIChE Journal 2 (1984) 257-262. doi:10.1002/aic.690300213

| T / K | P / bar | $x_1$ |
|---|---|---|
| 304.17 | 73.24 | 0.9895 |
| 304.15 | 72.43 | 0.9857 |
| 304.13 | 72.29 | 0.9739 |
| 304.13 | 72.30 | 0.9734 |
| 304.14 | 72.00 | 0.9718 |
| 304.14 | 71.83 | 0.9667 |
| 304.15 | 71.78 | 0.9659 |
| 304.17 | 71.58 | 0.9609 |
| 304.28 | 71.08 | 0.9504 |
| 305.35 | 69.50 | 0.9015 |

Van Poolen, Lambert J. - Holcomb, Cynthia D., Critical temperatures, pressures, and densities for the mixtures CO2–C3H8, CO2–nC4H10, C2H6–C3H8, and C3H8–nC4H10, Fluid Phase Equilibria 2 (1999) 157-168. doi:10.1016/S0378-3812(99)00275-7

| T / K | P / bar | $x_1$ |
|---|---|---|
| 311.04 | 66.86 | 0.7805 |
| 327.74 | 64.97 | 0.5659 |
| 344.41 | 59.41 | 0.3612 |
| 361.13 | 49.68 | 0.1428 |

Juntarachat, Niramol - Bello, Salma - Privat, Romain - Jaubert, Jean-Noël, Validation of a New Apparatus Using the Dynamic Method for Determining the Critical Properties of Binary Gas/Gas Mixtures, Journal of Chemical & Engineering Data 3 (2013) 671-676. doi:10.1021/je301209u

| T / K | P / bar | $x_1$ |
|---|---|---|
| 362.84 | 47.91 | 0.1157 |
| 356.93 | 51.93 | 0.2129 |

| | | |
|---|---|---|
| 344.98 | 58.99 | 0.3654 |
| 333.78 | 62.76 | 0.4928 |
| 319.00 | 65.29 | 0.6773 |
| 307.12 | 66.90 | 0.8254 |
| 303.46 | 68.94 | 0.9252 |

Horstmann, S. - Fischer, K. - Gmehling, J., Experimental Determination of Critical Points of Pure Components and Binary Mixtures Using a Flow Apparatus, Chemical Engineering & Technology 10 (1999) 839-842. doi:10.1002/(SICI)1521-4125(199910)22:10<839::AID-CEAT839>3.0.CO;2-L

| T / K | P / bar | $x_1$ |
|---|---|---|
| 364.76 | 47.44 | 0.1041 |
| 358.67 | 51.87 | 0.1965 |
| 351.77 | 56.26 | 0.3029 |
| 343.59 | 60.29 | 0.4017 |
| 336.37 | 63.08 | 0.4986 |
| 326.98 | 65.20 | 0.5999 |
| 318.40 | 66.37 | 0.7060 |
| 313.45 | 66.81 | 0.7640 |
| 308.47 | 67.65 | 0.8353 |
| 306.10 | 68.59 | 0.8814 |
| 304.34 | 70.73 | 0.9410 |

Niesen, Vicki G - Rainwater, James C, Critical locus, (vapor + liquid) equilibria, and coexisting densities of (carbon dioxide + propane) at temperatures from 311 K to 361 K, The Journal of Chemical Thermodynamics 8 (1990) 777-795. doi:10.1016/0021-9614(90)90070-7

| T / K | P / bar | $x_1$ |
|---|---|---|
| 327.75 | 64.60 | 0.5594 |

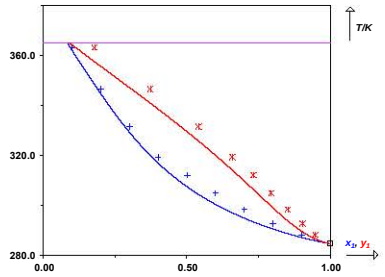
Ke, Jie - George, Michael W. - Poliakoff, Martyn - Han, Buxing - Yan, Haike, How Does the Critical Point Change during the Hydrogenation of Propene in Supercritical Carbon Dioxide?, The Journal of Physical Chemistry B 17 (2002) 4496-4502. doi:10.1021/jp0129333

| T / K | P / bar | $x_1$ |
|---|---|---|
| 304.70 | 70.70 | 0.9356 |
| 306.10 | 69.00 | 0.8833 |
| 310.30 | 67.70 | 0.7988 |
| 314.70 | 66.80 | 0.7204 |
| 316.10 | 66.50 | 0.6851 |

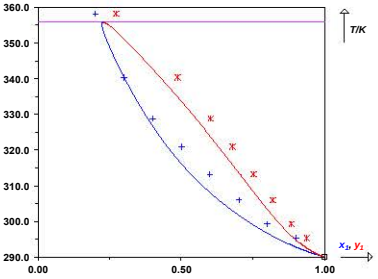
Poettmann, Fred H. - Katz, D. L., Phase Behavior of Binary Carbon Dioxide-Paraffin Systems, Industrial & Engineering Chemistry 9 (1945) 847-853. doi:10.1021/ie50429a017

| T / K | P / bar | $x_1$ |
|---|---|---|
| 368.95 | 46.68 | 0.0700 |
| 365.95 | 53.35 | 0.1650 |

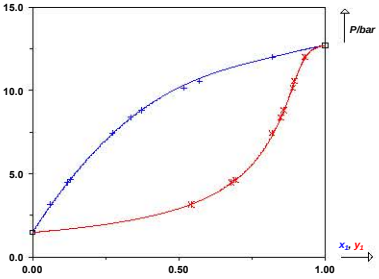
P/bar = 46.68000



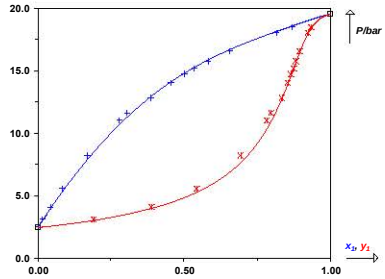

P/bar = 53.34800



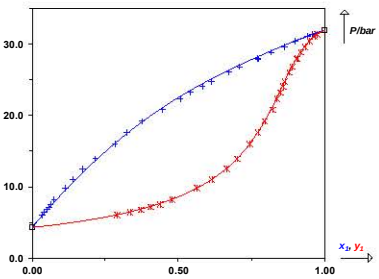

T/K = 240.00



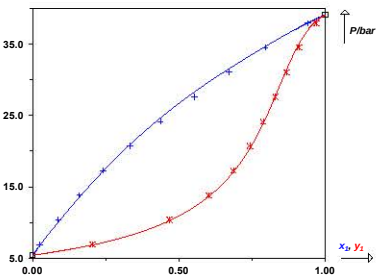

T/K = 253.15



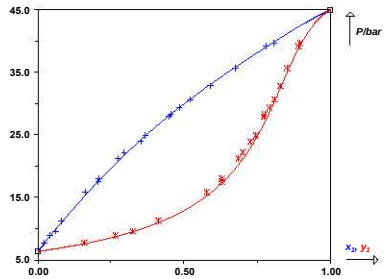

T/K = 270.00



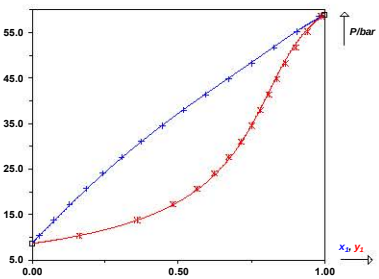

T/K = 277.59



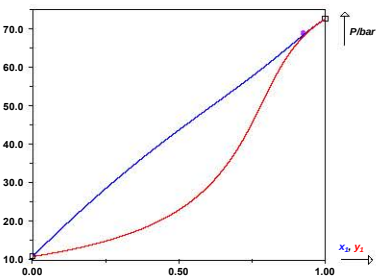

T/K = 283.15



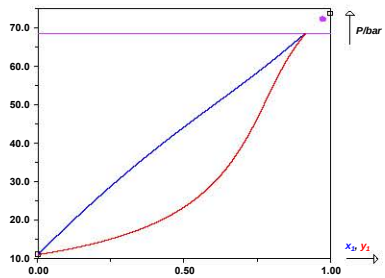

T/K = 294.26



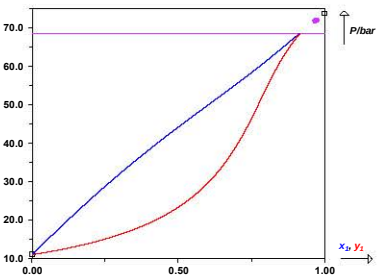

T/K = 303.46



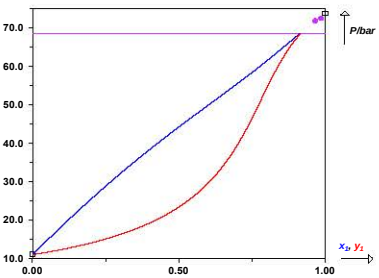

T/K = 304.13



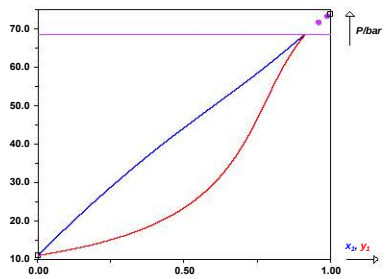

T/K = 304.14



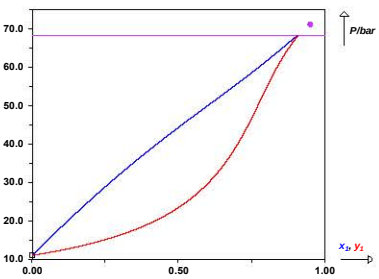

T/K = 304.15



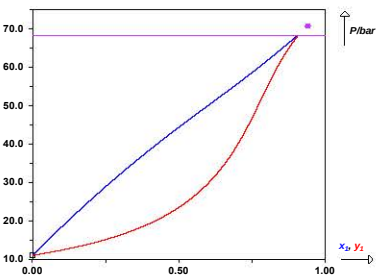

T/K = 304.17



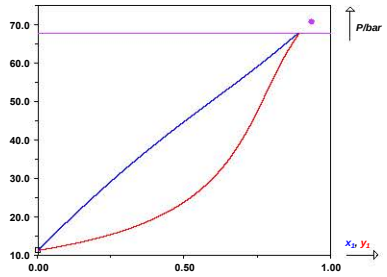

T/K = 304.28



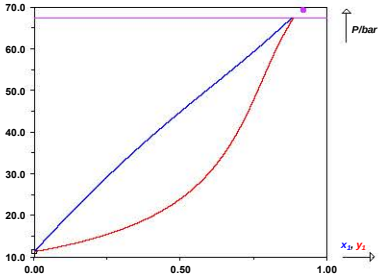

T/K = 304.34



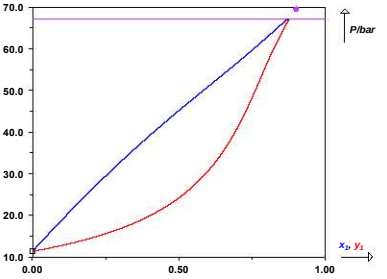
T/K = 304.70



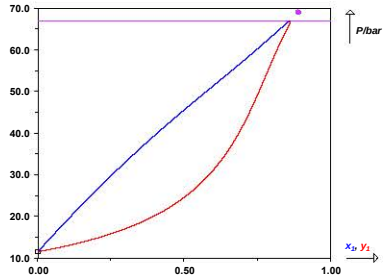

T/K = 304.98



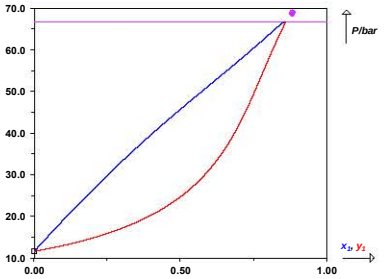

T/K = 305.35



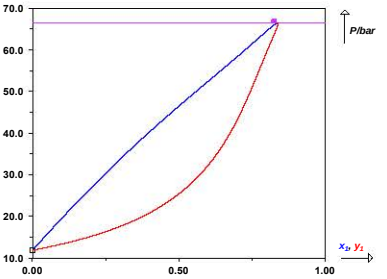

T/K = 305.87



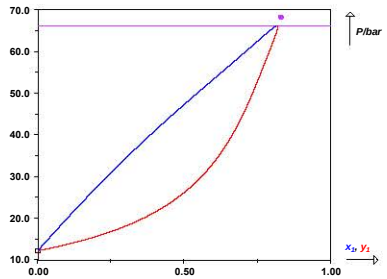

T/K = 306.10



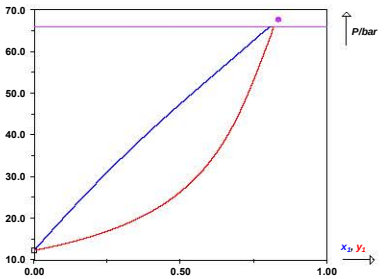

T/K = 307.12



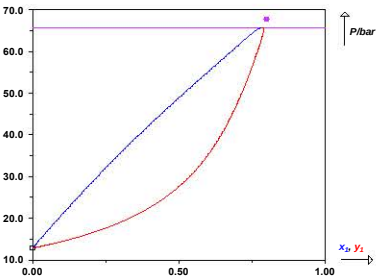

T/K = 308.21



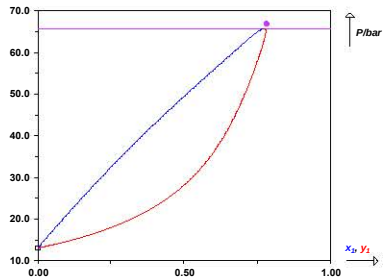

T/K = 308.47



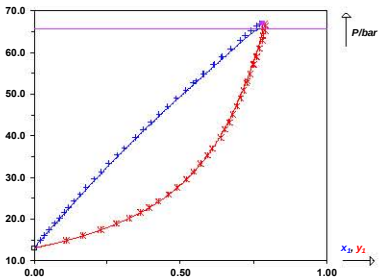

T/K = 310.30



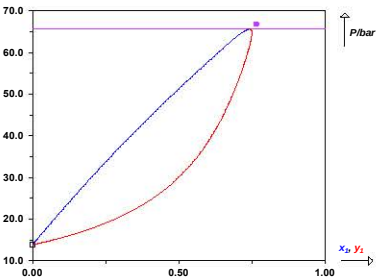

T/K = 311.04



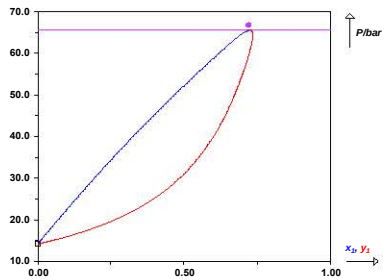

T/K = 311.05



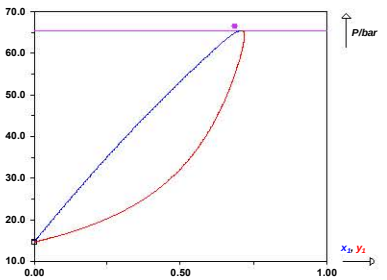

T/K = 313.45



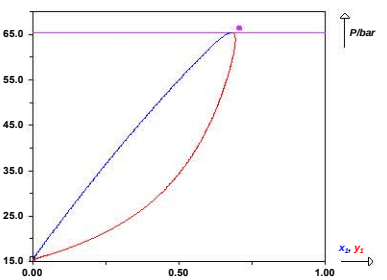

T/K = 314.70



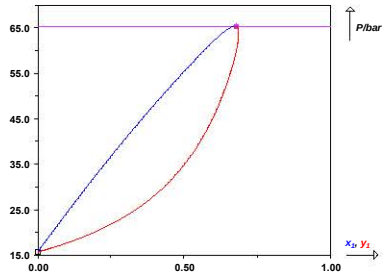

T/K = 316.10



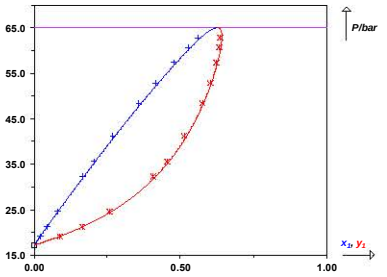

T/K = 318.40



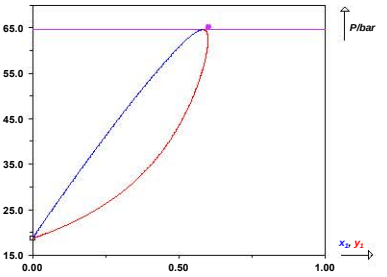
T/K = 319.00



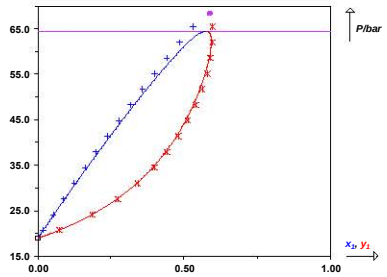

T/K = 323.15



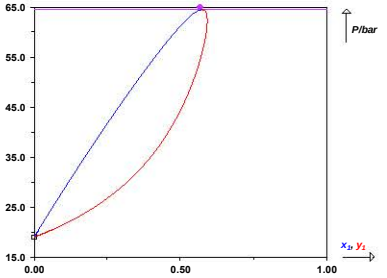

T/K = 326.98



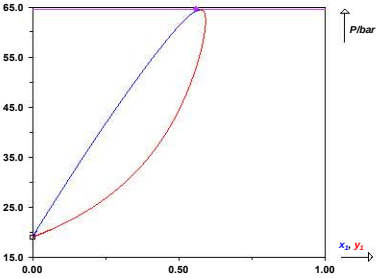

T/K = 327.59



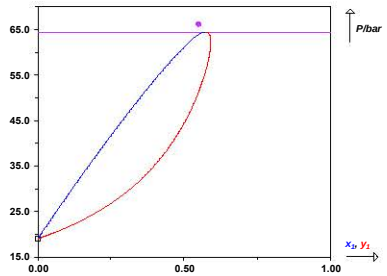

T/K = 327.74



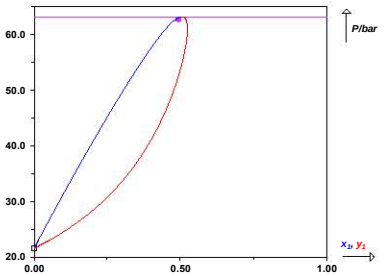

T/K = 327.75



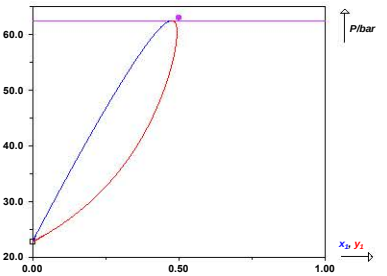

T/K = 327.76



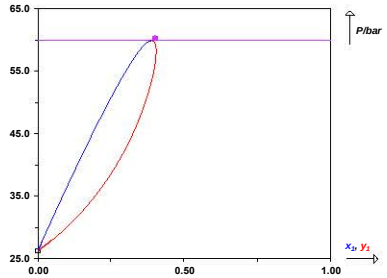

T/K = 333.78



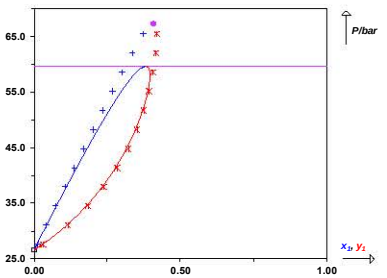

T/K = 336.37



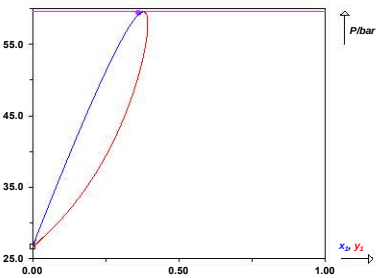

T/K = 343.59



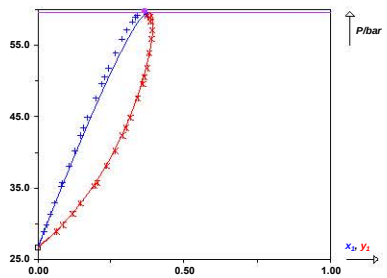

T/K = 344.26



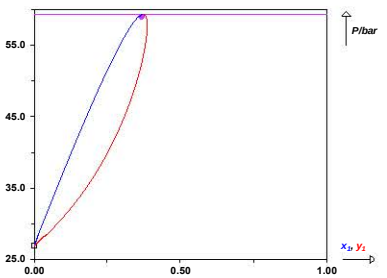

T/K = 344.41



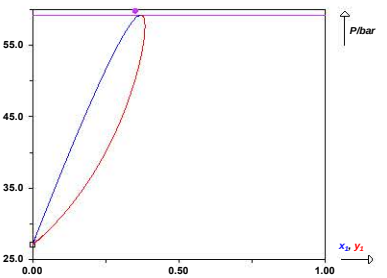

T/K = 344.43



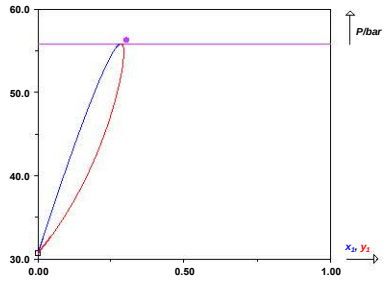

T/K = 344.98



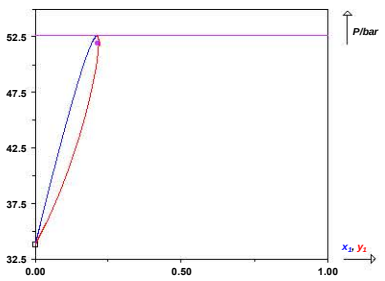

T/K = 345.15



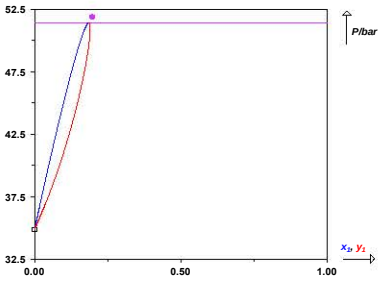
T/K = 351.77



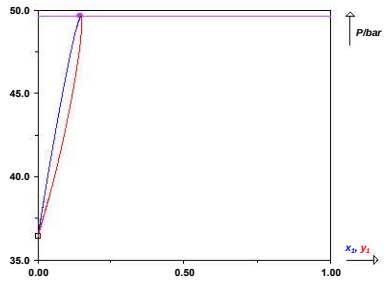

T/K = 356.93



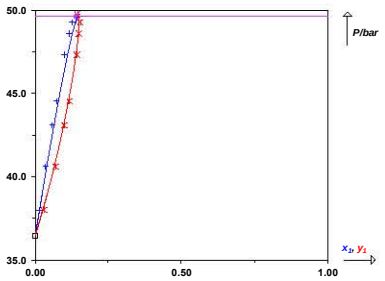

T/K = 358.67



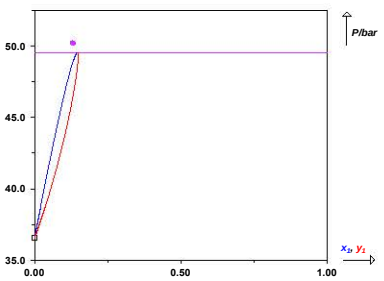

T/K = 361.13



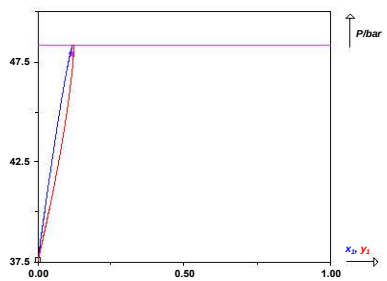

T/K = 361.15



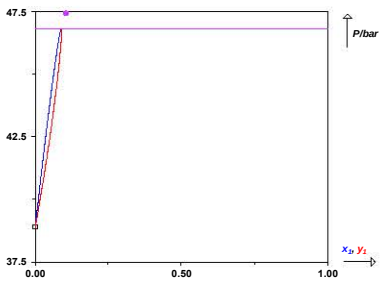

T/K = 361.26



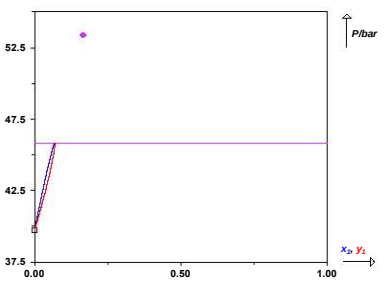

T/K = 362.84




T/K = 364.76




T/K = 365.95



## ACETONE (1) + n-HEXANE (2)

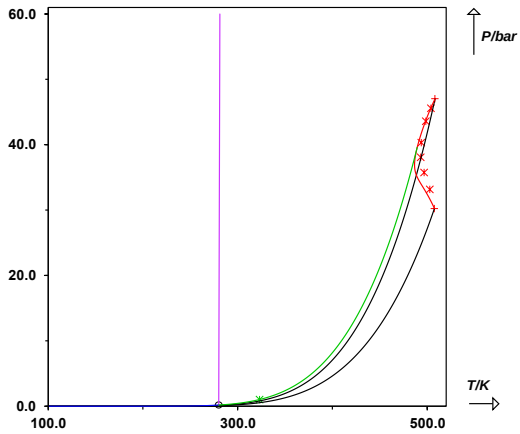
| | | |
|---|---|---|
| **CAS** | 67-64-1 | 110-54-3 |
| **InChiKey** | CSCPPACGZOOCGX-UHFFFAOYSA-N | VLKZOEOYAKHREP-UHFFFAOYSA-N |
| **$T_c$ / K** | 508.20 | 507.60 |
| **$P_c$ / bar** | 47.01 | 30.25 |
| **ω** | 0.3070 | 0.3010 |

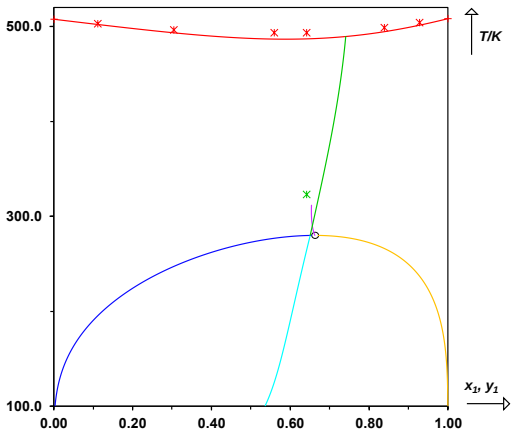
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 287
B/MPa = 329

*Deviations*
MAPE on x = 17 %
MAPE on y = 6.5 %
MAPE on $x_{az}$ = 6.8 %
MAPE on $P_{az}$ = 0.052 %
MAPE on $h^M$ = 16 %



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**Isothermal phase equilibrium data**

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Rall, W. - Schäfer, K., Thermodynamische Untersuchungen an flüssigen Mischsystemen von Aceton und n-Pentan sowie von Aceton und n-Hexan, Z. Elektrochem. 9-10 (1959) 1019-1024.

**T / K = 268.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0777 | 0.0839 | 0.4372 |
| 0.0937 | 0.2618 | 0.5688 |
| 0.0955 | 0.3402 | 0.5827 |
| 0.0966 | 0.4172 | 0.5935 |
| 0.0971 | 0.4569 | 0.5988 |
| 0.0980 | 0.5230 | 0.6057 |
| 0.0977 | 0.6039 | 0.6161 |
| 0.0973 | 0.7250 | 0.6389 |
| 0.0945 | 0.8535 | 0.6851 |
| 0.0865 | 0.9337 | 0.7738 |
| 0.0779 | 0.9768 | 0.8900 |

Kato, Ryo - Gmehling, Jürgen, Systems with ionic liquids: Measurement of VLE and γ∞ data and prediction of their thermodynamic behavior using original UNIFAC, mod. UNIFAC(Do) and COSMO-RS(Ol), The Journal of Chemical Thermodynamics 6 (2005) 603-619. doi:10.1016/j.jct.2005.04.010

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4421 | 0.0862 | 0.3240 |
| 0.5309 | 0.1902 | 0.4760 |
| 0.5672 | 0.2945 | 0.5400 |
| 0.5834 | 0.3917 | 0.5780 |
| 0.5945 | 0.4945 | 0.6000 |
| 0.5953 | 0.5996 | 0.6280 |
| 0.5956 | 0.6995 | 0.6480 |
| 0.5853 | 0.8049 | 0.7000 |
| 0.5540 | 0.9060 | 0.7800 |

Kolasińska, G. - Góral, M. - Giza, J., Vapour-Liquid Equilibria and Excess Gibbs Free Energy in Binary Systems of Acetone with Aliphatic and Aromatic Hydrocarbons at 313 15 K, Zeitschrift für Physikalische Chemie 1 (1982) doi:10.1515/zpch-1982-26317

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4719 | 0.0385 | 0.2328 |
| 0.5017 | 0.0540 | 0.2869 |
| 0.5391 | 0.0782 | 0.3490 |
| 0.5891 | 0.1224 | 0.4222 |
| 0.6079 | 0.1417 | 0.4446 |
| 0.6397 | 0.1916 | 0.4874 |
| 0.6415 | 0.1950 | 0.4898 |
| 0.6615 | 0.2369 | 0.5149 |
| 0.6654 | 0.2469 | 0.5200 |
| 0.6674 | 0.2534 | 0.5231 |
| 0.6810 | 0.2964 | 0.5418 |
| 0.6838 | 0.3140 | 0.5485 |
| 0.6931 | 0.3497 | 0.5609 |
| 0.7057 | 0.4366 | 0.5864 |
| 0.7122 | 0.4948 | 0.6013 |
| 0.7153 | 0.5550 | 0.6160 |
| 0.7172 | 0.6145 | 0.6309 |
| 0.7172 | 0.6633 | 0.6441 |
| 0.7070 | 0.7897 | 0.6921 |
| 0.6809 | 0.8760 | 0.7543 |
| 0.6524 | 0.9262 | 0.8175 |
| 0.6395 | 0.9401 | 0.8412 |
| 0.6147 | 0.9645 | 0.8925 |

Kato, Ryo - Gmehling, Jürgen, Systems with ionic liquids: Measurement of VLE and γ∞ data and prediction of their thermodynamic behavior using original UNIFAC, mod. UNIFAC(Do) and COSMO-RS(Ol), The Journal of Chemical Thermodynamics 6 (2005) 603-619. doi:10.1016/j.jct.2005.04.010

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.6405 | 0.0894 | 0.3300 |
| 0.7649 | 0.1958 | 0.4890 |
| 0.8153 | 0.2967 | 0.5400 |
| 0.8413 | 0.3950 | 0.5840 |
| 0.8579 | 0.4955 | 0.6080 |
| 0.8617 | 0.5997 | 0.6220 |
| 0.8633 | 0.6997 | 0.6540 |
| 0.8482 | 0.8035 | 0.7000 |
| 0.8055 | 0.9045 | 0.7870 |

Kato, Ryo - Gmehling, Jürgen, Systems with ionic liquids: Measurement of VLE and γ∞ data and prediction of their thermodynamic behavior using original UNIFAC, mod. UNIFAC(Do) and COSMO-RS(Ol), The Journal of Chemical Thermodynamics 6 (2005) 603-619. doi:10.1016/j.jct.2005.04.010

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.8930 | 0.0926 | 0.3300 |
| 1.041 | 0.1846 | 0.4760 |
| 1.136 | 0.2989 | 0.5400 |
| 1.165 | 0.3933 | 0.5780 |
| 1.191 | 0.4975 | 0.6020 |

| | | |
|---|---|---|
| 1.207 | 0.5998 | 0.6280 |
| 1.200 | 0.6993 | 0.6610 |
| 1.178 | 0.8021 | 0.7000 |
| 1.122 | 0.9090 | 0.7950 |

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**Isobaric phase equilibrium data**

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Acosta, Jhoany - Arce, Alberto - Martínez-Ageitos, José - Rodil, Eva - Soto, Ana, Vapor−Liquid Equilibrium of the Ternary System Ethyl Acetate + Hexane + Acetone at 101.32 kPa, Journal of Chemical & Engineering Data 4 (2002) 849-854. doi:10.1021/je0102917

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 340.07 | 0.0106 | 0.0575 |
| 338.78 | 0.0132 | 0.0994 |
| 336.35 | 0.0295 | 0.1811 |
| 333.36 | 0.0631 | 0.2749 |
| 330.00 | 0.1032 | 0.3764 |
| 326.82 | 0.1796 | 0.4666 |
| 325.08 | 0.2451 | 0.5173 |
| 324.16 | 0.3050 | 0.5446 |
| 323.43 | 0.3746 | 0.5773 |
| 322.88 | 0.4834 | 0.6042 |
| 322.78 | 0.5131 | 0.6102 |
| 322.69 | 0.5450 | 0.6172 |
| 322.69 | 0.6931 | 0.6570 |
| 322.82 | 0.7315 | 0.6706 |
| 322.93 | 0.7592 | 0.6829 |
| 323.16 | 0.7953 | 0.7012 |
| 323.83 | 0.8580 | 0.7428 |
| 324.60 | 0.8999 | 0.7840 |
| 325.73 | 0.9378 | 0.8386 |
| 327.02 | 0.9681 | 0.8999 |
| 327.84 | 0.9826 | 0.9383 |
| 328.67 | 0.9950 | 0.9763 |

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**Enthalpy of mixing**

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Schaefer, K., Excess enthalpies of acetone + n-alkane (C3-C6) binary mixtures, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1978) 74-77.

**T / K = 243.20**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 334.00 | 0.0407 |
| 618.00 | 0.0932 |
| 806.00 | 0.1395 |
| 1048.0 | 0.2324 |
| 1179.0 | 0.3314 |
| 1232.0 | 0.3803 |
| 1252.0 | 0.4318 |
| 1267.0 | 0.5278 |
| 1236.0 | 0.6030 |
| 1112.0 | 0.7206 |
| 980.00 | 0.7872 |
| 955.00 | 0.7936 |
| 883.00 | 0.8182 |
| 718.00 | 0.8670 |
| 534.00 | 0.9087 |
| 216.00 | 0.9679 |

Schaefer, K., Excess enthalpies of acetone + n-alkane (C3-C6) binary mixtures, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1978) 74-77.

**T / K = 253.20**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 587.00 | 0.0850 |
| 934.00 | 0.1712 |
| 1148.0 | 0.2565 |
| 1301.0 | 0.3584 |
| 1331.0 | 0.4225 |
| 1357.0 | 0.4599 |
| 1379.0 | 0.4902 |
| 1326.0 | 0.5526 |
| 1328.0 | 0.5604 |
| 1316.0 | 0.5900 |
| 1274.0 | 0.6365 |
| 1261.0 | 0.6607 |
| 1100.0 | 0.7480 |
| 1093.0 | 0.7535 |
| 815.00 | 0.8450 |
| 623.00 | 0.8921 |
| 559.00 | 0.9062 |
| 223.00 | 0.9502 |

Schaefer, K., Excess enthalpies of acetone + n-alkane (C3-C6) binary mixtures, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1978) 74-77.

**T / K = 273.20**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 405.00 | 0.0509 |
| 428.00 | 0.0531 |
| 919.00 | 0.1517 |
| 1070.0 | 0.1979 |

| | |
|---|---|
| 1206.0 | 0.2540 |
| 1356.0 | 0.3181 |
| 1426.0 | 0.3819 |
| 1451.0 | 0.4466 |
| 1462.0 | 0.4587 |
| 1472.0 | 0.5243 |
| 1406.0 | 0.6057 |
| 1399.0 | 0.6121 |
| 1181.0 | 0.7341 |
| 1002.0 | 0.8079 |
| 802.00 | 0.8490 |
| 515.00 | 0.9163 |
| 213.00 | 0.9680 |

Schaefer, K., Excess enthalpies of acetone + n-alkane (C3-C6) binary mixtures, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1978) 74-77.

**T / K =** **293.20**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 460.00 | 0.0580 |
| 813.00 | 0.1188 |
| 1067.0 | 0.1821 |
| 1276.0 | 0.2487 |
| 1425.0 | 0.3183 |
| 1534.0 | 0.3864 |
| 1572.0 | 0.4772 |
| 1549.0 | 0.5152 |
| 1513.0 | 0.5741 |
| 1491.0 | 0.5868 |
| 1459.0 | 0.6185 |
| 1374.0 | 0.6719 |
| 1359.0 | 0.6918 |
| 1218.0 | 0.7489 |
| 887.00 | 0.8402 |
| 482.00 | 0.9260 |

Singh, Prem P. - Malik, Renu - Maken, S. - Acree, William E. - Tucker, Sheryl A., Thermochemical investigations of associated solutions. 10. Excess enthalpies and excess volumes of ternary acetone + bromoform + n-hexane mixtures, Thermochimica Acta 2 (1990) 291-309. doi:10.1016/0040-6031(90)80350-8

**T / K =** **308.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 590.00 | 0.9042 |
| 603.00 | 0.9005 |
| 1060.0 | 0.8069 |
| 1171.0 | 0.7809 |
| 1185.0 | 0.7771 |
| 1622.0 | 0.6349 |
| 1629.0 | 0.6345 |
| 1659.0 | 0.6169 |
| 1668.0 | 0.6120 |
| 1825.0 | 0.4449 |
| 1824.0 | 0.4349 |
| 1780.0 | 0.3781 |
| 1430.0 | 0.2323 |
| 1423.0 | 0.2287 |
| 943.00 | 0.1286 |

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**Critical point**

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Kay, Webster B., P-T-x Diagrams in the Critical Region. Acetone-n-Alkane Systems, The Journal of Physical Chemistry 4 (1964) 827-831. doi:10.1021/j100786a021

| T / K | P / bar | $x_1$ |
|---|---|---|
| 503.75 | 45.60 | 0.9280 |
| 498.65 | 43.57 | 0.8390 |
| 493.55 | 40.33 | 0.6410 |
| 493.05 | 38.10 | 0.5590 |
| 496.35 | 35.77 | 0.3040 |
| 502.55 | 33.13 | 0.1110 |

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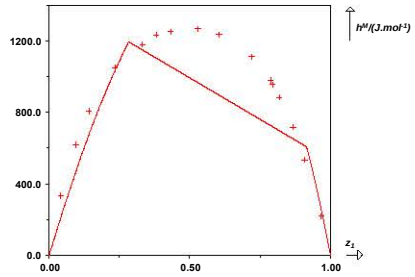
**Azeotropic point**

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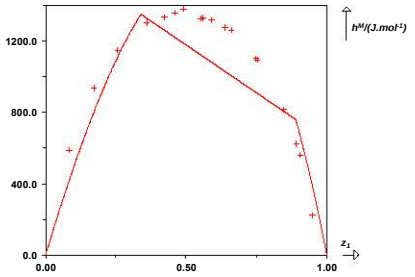
Acosta, Jhoany - Arce, Alberto - Martínez-Ageitos, José - Rodil, Eva - Soto, Ana, Vapor−Liquid Equilibrium of the Ternary System Ethyl Acetate + Hexane + Acetone at 101.32 kPa, Journal of Chemical & Engineering Data 4 (2002) 849-854. doi:10.1021/je0102917

| T / K | P / bar | $x_1$ |
|---|---|---|
| 322.70 | 1.013 | 0.6420 |

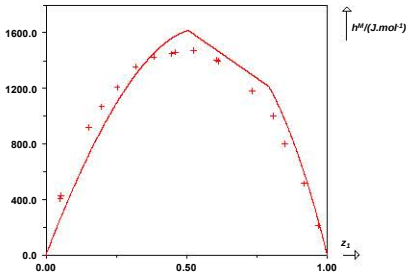
T/K = 243.20 - P/bar = 1.0132



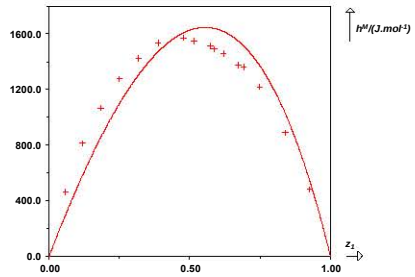

T/K = 253.20 - P/bar = 1.0132



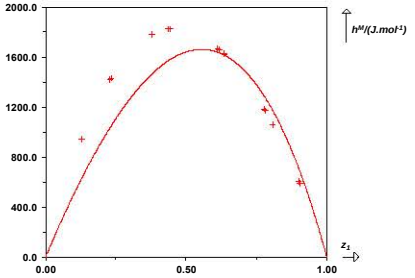

T/K = 273.20 - P/bar = 1.0132



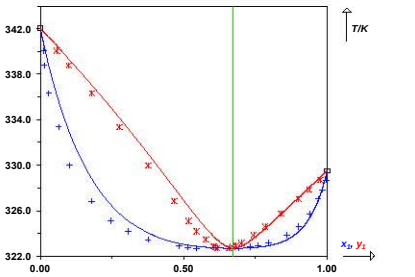

T/K = 293.20 - P/bar = 1.0132



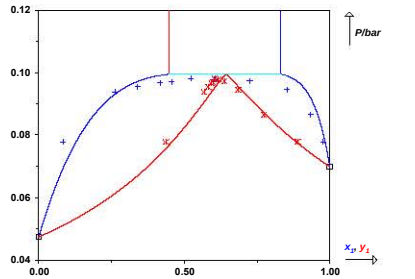

T/K = 308.15 - P/bar = 1.0132



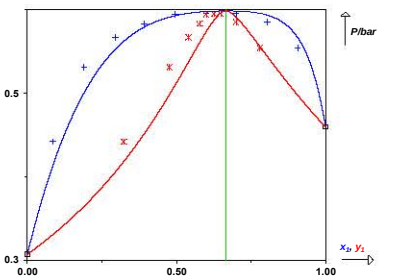

P/bar = 1.01320



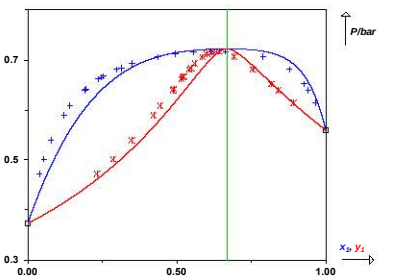

T/K = 268.15



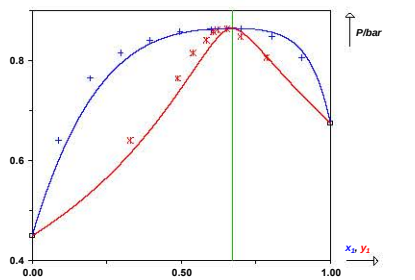

T/K = 308.15



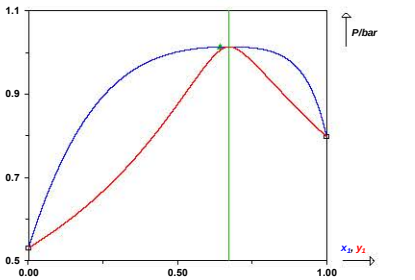

T/K = 313.15



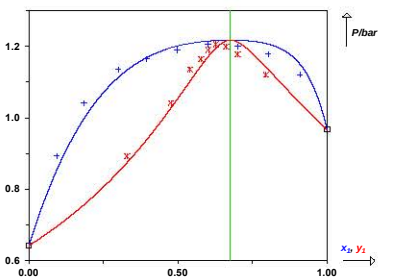

T/K = 318.15

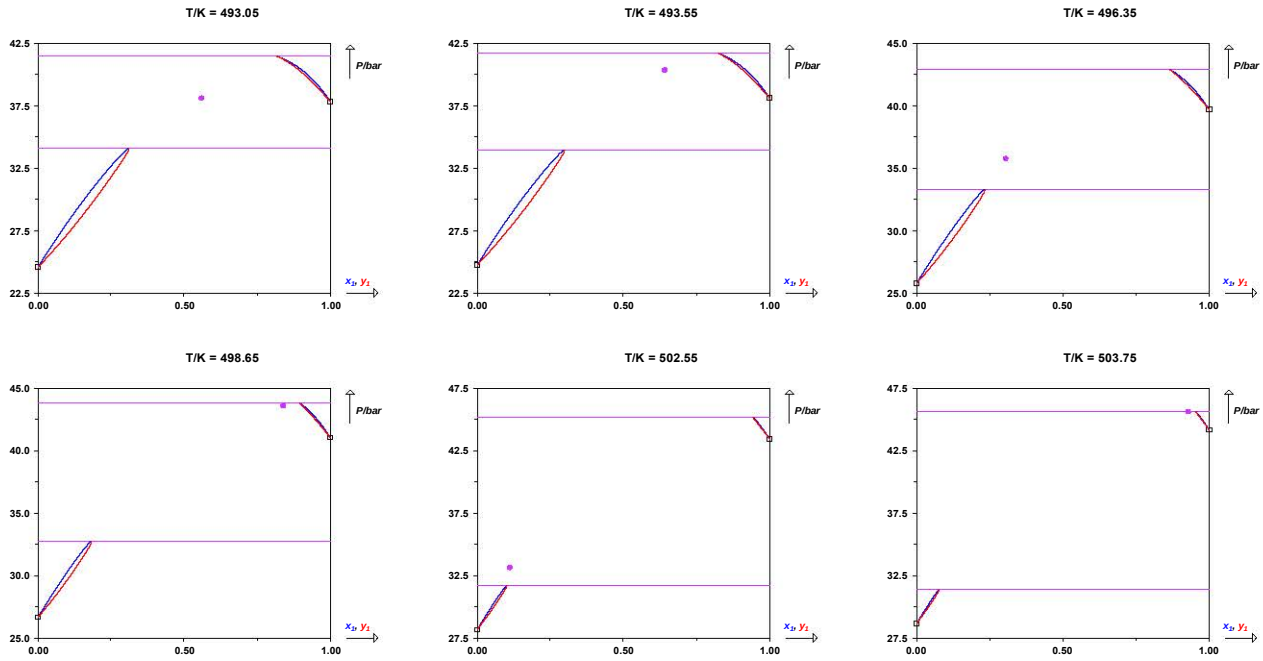



T/K = 322.70




T/K = 328.15




T/K = 493.05
T/K = 493.55
T/K = 496.35
T/K = 498.65
T/K = 502.55
T/K = 503.75
P/bar
x1, y1

## n-PENTANE (1) + ACETONE (2)

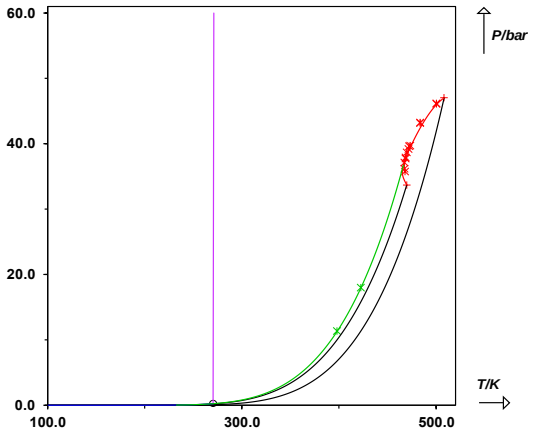
| | | |
|---|---|---|
| **CAS** | 109-66-0 | 67-64-1 |
| **InChiKey** | OFBQJSOFQDEBGM-UHFFFAOYSA-N | CSCPPACGZOOCGX-UHFFFAOYSA-N |
| **$T_c$ / K** | 469.70 | 508.20 |
| **$P_c$ / bar** | 33.70 | 47.01 |
| **ω** | 0.2520 | 0.3070 |

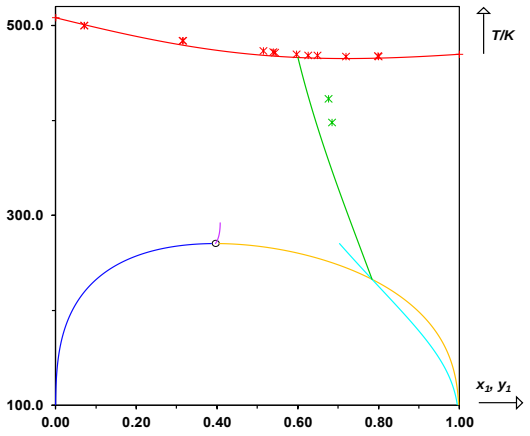
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 295
B/MPa = 359

*Deviations*
MAPE on x = 20 %
MAPE on y = 9.9 %
MAPE on $x_c$ = 16 %
MAPE on $P_c$ = 1.2 %
MAPE on $x_{az}$ = 10 %
MAPE on $P_{az}$ = 0.61 %
MAPE on $h^M$ = 14 %



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**Isothermal phase equilibrium data**

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Rall, W. - Schäfer, K., Thermodynamische Untersuchungen an flüssigen Mischsystemen von Aceton und n-Pentan sowie von Aceton und n-Hexan, Z. Elektrochem. 9-10 (1959) 1019-1024.

**T / K = 258.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0779 | 0.0497 | 0.5079 |
| 0.1072 | 0.1269 | 0.6617 |
| 0.1171 | 0.1639 | 0.6890 |
| 0.1291 | 0.2851 | 0.7319 |
| 0.1332 | 0.3857 | 0.7442 |
| 0.1351 | 0.4730 | 0.7490 |
| 0.1353 | 0.5459 | 0.7550 |
| 0.1365 | 0.6580 | 0.7650 |
| 0.1371 | 0.7173 | 0.7689 |
| 0.1372 | 0.8325 | 0.7933 |
| 0.1329 | 0.9287 | 0.8490 |

Rall, W. - Schäfer, K., Thermodynamische Untersuchungen an flüssigen Mischsystemen von Aceton und n-Pentan sowie von Aceton und n-Hexan, Z. Elektrochem. 9-10 (1959) 1019-1024.

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3408 | 0.0094 | 0.1055 |
| 0.4581 | 0.0540 | 0.3633 |
| 0.5285 | 0.0887 | 0.4592 |
| 0.6245 | 0.1600 | 0.5648 |
| 0.7330 | 0.3741 | 0.6654 |
| 0.7305 | 0.3880 | 0.6658 |
| 0.7561 | 0.4721 | 0.6865 |
| 0.7666 | 0.5689 | 0.7074 |
| 0.7763 | 0.6548 | 0.7274 |
| 0.7767 | 0.7192 | 0.7442 |
| 0.7782 | 0.7787 | 0.7623 |
| 0.7529 | 0.9223 | 0.8486 |

Campbell, Scott W. - Wilsak, Richard A. - Thodos, George, Isothermal vapor-liquid equilibrium measurements for the n-pentane-acetone system at 372.7, 397.7, and 422.6 K, Journal of Chemical & Engineering Data 4 (1986) 424-430. doi:10.1021/je00046a016

**T / K = 372.70**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.781 | 0.0840 | 0.2650 |
| 5.516 | 0.1800 | 0.3740 |
| 6.133 | 0.3150 | 0.5100 |
| 6.422 | 0.4220 | 0.5460 |
| 6.609 | 0.5320 | 0.6160 |
| 6.722 | 0.6490 | 0.6710 |
| 6.681 | 0.7850 | 0.7530 |
| 6.378 | 0.9160 | 0.8690 |

Campbell, Scott W. - Wilsak, Richard A. - Thodos, George, Isothermal vapor-liquid equilibrium measurements for the n-pentane-acetone system at 372.7, 397.7, and 422.6 K, Journal of Chemical & Engineering Data 4 (1986) 424-430. doi:10.1021/je00046a016

**T / K = 397.70**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 7.601 | 0.0440 | 0.1350 | |
| 8.208 | 0.0870 | 0.2080 | |
| 8.863 | 0.1330 | 0.2940 | |
| 9.680 | 0.2100 | 0.3920 | |
| 10.47 | 0.3310 | 0.4780 | |
| 10.84 | 0.4120 | 0.5330 | |
| 11.10 | 0.4950 | 0.5690 | |
| 11.28 | 0.5760 | 0.6210 | |
| 11.36 | 0.6840 | 0.6840 | AZEO |
| 11.35 | 0.7020 | 0.7010 | |
| 11.15 | 0.8240 | 0.7900 | |
| 10.68 | 0.9190 | 0.8820 | |

Campbell, Scott W. - Wilsak, Richard A. - Thodos, George, Isothermal vapor-liquid equilibrium measurements for the n-pentane-acetone system at 372.7, 397.7, and 422.6 K, Journal of Chemical & Engineering Data 4 (1986) 424-430. doi:10.1021/je00046a016

**T / K = 422.60**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 13.62 | 0.1140 | 0.2080 | |
| 14.81 | 0.1800 | 0.2980 | |
| 15.87 | 0.2570 | 0.3810 | |
| 17.39 | 0.4450 | 0.5370 | |
| 17.99 | 0.6580 | 0.6630 | |
| 17.99 | 0.6760 | 0.6760 | AZEO |
| 17.82 | 0.7940 | 0.7700 | |
| 17.22 | 0.8790 | 0.8470 | |
| 16.36 | 0.9560 | 0.9310 | |

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**Enthalpy of mixing**

---

Schaefer, K., Excess enthalpies of acetone + n-alkane (C3-C6) binary mixtures, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1978) 74-77.

**T / K =** **243.20**
**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 284.00 | 0.0507 |
| 583.00 | 0.1153 |
| 814.00 | 0.1822 |
| 1030.0 | 0.2677 |
| 1148.0 | 0.3481 |
| 1207.0 | 0.4312 |
| 1223.0 | 0.4710 |
| 1229.0 | 0.4868 |
| 1236.0 | 0.5635 |
| 1174.0 | 0.6552 |
| 1120.0 | 0.7009 |
| 968.00 | 0.7892 |
| 789.00 | 0.8634 |
| 611.00 | 0.9047 |
| 396.00 | 0.9462 |

Schaefer, K., Excess enthalpies of acetone + n-alkane (C3-C6) binary mixtures, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1978) 74-77.

**T / K =** **253.20**
**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 463.00 | 0.0859 |
| 791.00 | 0.1716 |
| 1029.0 | 0.2544 |
| 1170.0 | 0.3324 |
| 1256.0 | 0.4298 |
| 1276.0 | 0.5061 |
| 1280.0 | 0.5727 |
| 1268.0 | 0.6168 |
| 1179.0 | 0.6868 |
| 1084.0 | 0.7513 |
| 946.00 | 0.8129 |
| 714.00 | 0.8854 |
| 402.00 | 0.9474 |

Schaefer, K., Excess enthalpies of acetone + n-alkane (C3-C6) binary mixtures, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1978) 74-77.

**T / K =** **273.20**
**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 335.00 | 0.0584 |
| 623.00 | 0.1181 |
| 922.00 | 0.2006 |
| 1096.0 | 0.2643 |
| 1251.0 | 0.3332 |
| 1327.0 | 0.4073 |
| 1367.0 | 0.4672 |
| 1374.0 | 0.5456 |
| 1345.0 | 0.6301 |
| 1239.0 | 0.7056 |
| 1068.0 | 0.7920 |
| 802.00 | 0.8743 |
| 519.00 | 0.9290 |
| 292.00 | 0.9664 |

Schaefer, K., Excess enthalpies of acetone + n-alkane (C3-C6) binary mixtures, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1978) 74-77.

**T / K =** **293.20**
**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 314.00 | 0.0534 |
| 745.00 | 0.1452 |
| 1037.0 | 0.2256 |
| 1254.0 | 0.3026 |
| 1387.0 | 0.3805 |
| 1426.0 | 0.4292 |
| 1440.0 | 0.4883 |
| 1450.0 | 0.5704 |
| 1386.0 | 0.6553 |
| 1282.0 | 0.7261 |
| 1133.0 | 0.7882 |
| 892.00 | 0.8567 |
| 540.00 | 0.9290 |

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**Critical point**

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Kay, Webster B., P-T-x Diagrams in the Critical Region. Acetone-n-Alkane Systems, The Journal of Physical Chemistry 4 (1964) 827-831. doi:10.1021/j100786a021

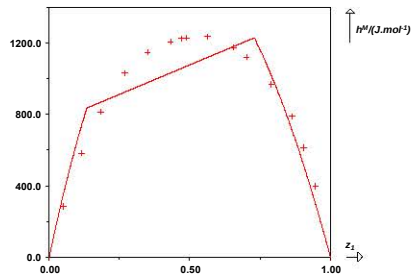
| T / K | P / bar | $x_1$ |
|---|---|---|
| 483.65 | 43.27 | 0.3150 |
| 472.25 | 39.62 | 0.5390 |
| 468.65 | 37.69 | 0.6260 |
| 467.65 | 35.77 | 0.7990 |

Hajjar, Raja F. - Cherry, R.H. - Kay, W.B., Critical properties of the vapor—liquid equilibria of the binary system acetone—n-pentane, Fluid Phase Equilibria 2 (1986) 137-146. doi:10.1016/0378-3812(86)80011-5

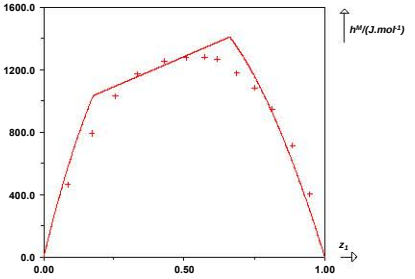
| T / K | P / bar | $x_1$ |
|---|---|---|
| 499.95 | 46.10 | 0.0708 |

| | | |
|---|---|---|
| 483.65 | 43.20 | 0.3154 |
| 472.99 | 39.73 | 0.5141 |
| 471.31 | 39.23 | 0.5430 |
| 469.81 | 38.64 | 0.5967 |
| 468.66 | 37.91 | 0.6490 |
| 467.42 | 37.13 | 0.7188 |
| 467.07 | 36.17 | 0.8003 |

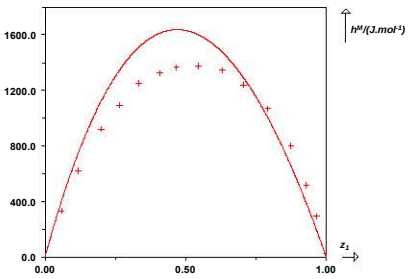
T/K = 243.20 - P/bar = 1.0132



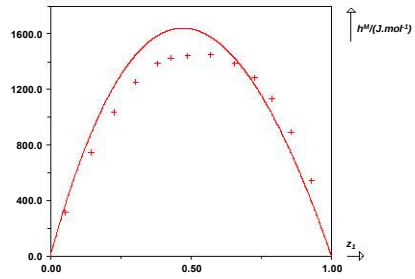

T/K = 253.20 - P/bar = 1.0132



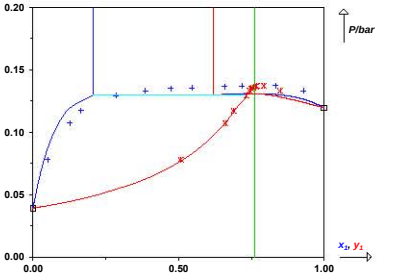

T/K = 273.20 - P/bar = 1.0132



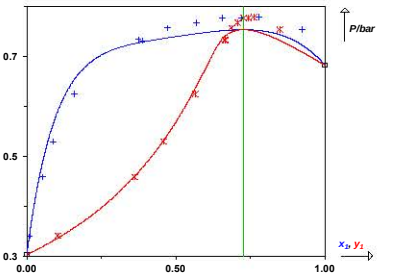

T/K = 293.20 - P/bar = 1.0132



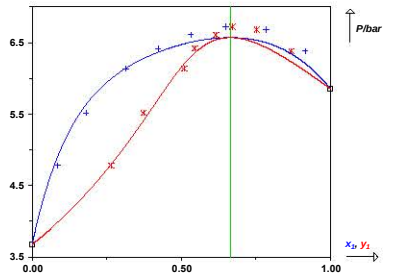

T/K = 258.15



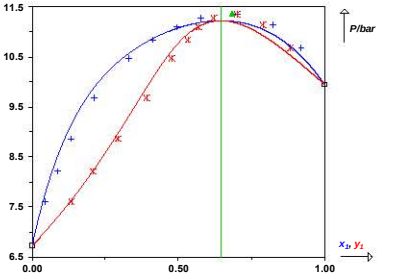

T/K = 298.15



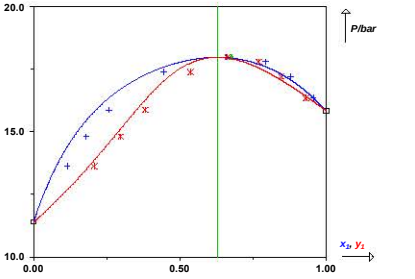

T/K = 372.70



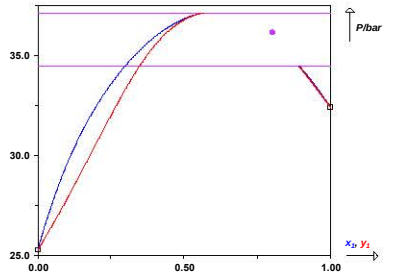

T/K = 397.70



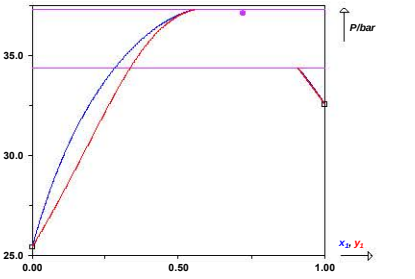

T/K = 422.60



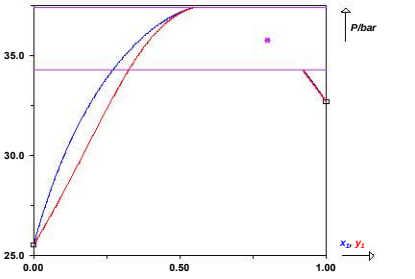

T/K = 467.07



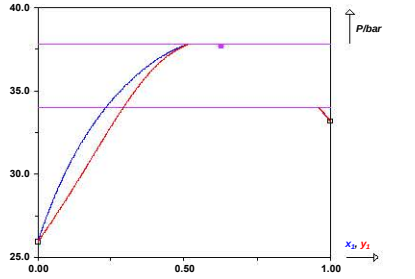

T/K = 467.42



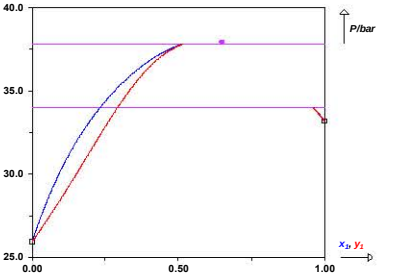

T/K = 467.65



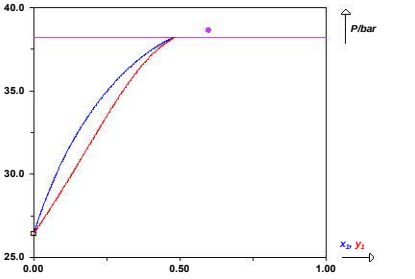

T/K = 468.65

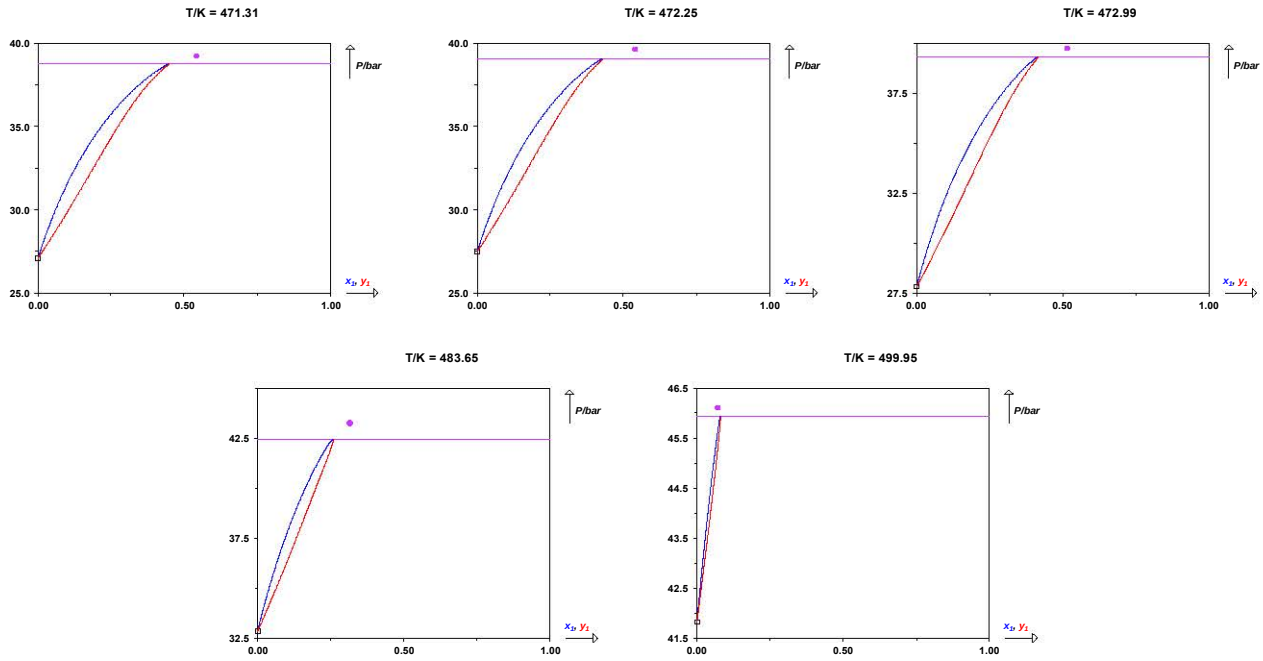



T/K = 468.66




T/K = 469.81




T/K = 471.31
T/K = 472.25
T/K = 472.99
T/K = 483.65
T/K = 499.95
P/bar
x₁, y₁

## ACETONE (1) + CYCLOHEXANE (2)

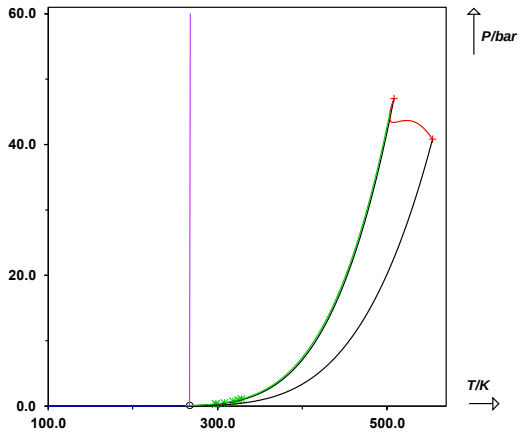
| | | |
|---|---|---|
| **CAS** | 67-64-1 | 110-82-7 |
| **InChiKey** | CSCPPACGZOOCGX-UHFFFAOYSA-N | XDTMQSROBMDMFD-UHFFFAOYSA-N |
| **$T_c$ / K** | 508.20 | 553.80 |
| **$P_c$ / bar** | 47.01 | 40.80 |
| **ω** | 0.3070 | 0.2080 |

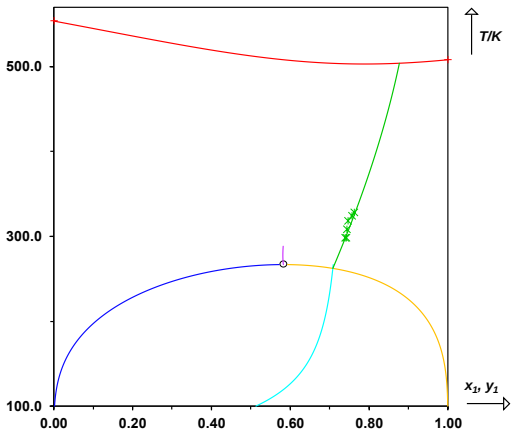
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 293
B/MPa = 351

*Deviations*
MAPE on x = 9.9 %
MAPE on y = 3.3 %
MAPE on $x_{az}$ = 1.1 %
MAPE on $P_{az}$ = 0.49 %
MAPE on $h^M$ = 14 %



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**Isothermal phase equilibrium data**

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Tasić, Aleksandar - Djordjević, Bojan - Grozdanić, Dušan - Afgan, Naim - Malić, Dragomir, Vapour—liquid equilibria of the systems acetone—benzene, benzene—cyclohexane and acetone—cyclohexane at 25°C, Chemical Engineering Science 2 (1978) 189-197. doi:10.1016/0009-2509(78)85053-2

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1574 | 0.0115 | 0.1810 | |
| 0.1666 | 0.0160 | 0.2250 | |
| 0.1839 | 0.0250 | 0.3040 | |
| 0.1933 | 0.0300 | 0.3450 | |
| 0.2137 | 0.0440 | 0.4100 | |
| 0.2305 | 0.0575 | 0.4580 | |
| 0.2609 | 0.0890 | 0.5330 | |
| 0.2769 | 0.1125 | 0.5670 | |
| 0.3036 | 0.1775 | 0.6110 | |
| 0.3171 | 0.2330 | 0.6325 | |
| 0.3284 | 0.3090 | 0.6550 | |
| 0.3385 | 0.4235 | 0.6800 | |
| 0.3432 | 0.5105 | 0.6940 | |
| 0.3458 | 0.5760 | 0.7050 | |
| 0.3473 | 0.6250 | 0.7095 | |
| 0.3481 | 0.6605 | 0.7170 | |
| 0.3486 | 0.6920 | 0.7250 | |
| 0.3493 | 0.7390 | 0.7390 | AZEO |
| 0.3492 | 0.7575 | 0.7460 | |
| 0.3449 | 0.8605 | 0.8030 | |
| 0.3409 | 0.8930 | 0.8280 | |
| 0.3360 | 0.9250 | 0.8580 | |
| 0.3250 | 0.9625 | 0.9160 | |

Puri, Pushpinder S. - Polak, Jiri - Ruether, John A., Vapor-liquid equilibriums of acetone-cyclohexane and acetone-isopropanol systems at 25°C, Journal of Chemical & Engineering Data 1 (1974) 87-89. doi:10.1021/je60060a007

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.3092 | 0.2077 | 0.6184 | |
| 0.3238 | 0.2868 | 0.6452 | |
| 0.3322 | 0.3520 | 0.6609 | |
| 0.3374 | 0.4158 | 0.6737 | |
| 0.3418 | 0.4847 | 0.6867 | |
| 0.3455 | 0.5654 | 0.7025 | |
| 0.3477 | 0.6311 | 0.7156 | |
| 0.3487 | 0.6809 | 0.7272 | |
| 0.3494 | 0.7316 | 0.7403 | |
| 0.3494 | 0.7420 | 0.7420 | AZEO |
| 0.3483 | 0.7990 | 0.7681 | |
| 0.3453 | 0.8610 | 0.7976 | |
| 0.3380 | 0.9209 | 0.8536 | |

Marinichev, A.N. - Susarev, M.P., Liquid-vapor equilibriums in the systems acetone-methanol and acetone-cyclohexane at 35, 45, and 55° and a pressure of 760 mm, J. Appl. Chem. USSR 2 (1965) 371-375.

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.4548 | 0.1980 | 0.6010 | |
| 0.4797 | 0.2830 | 0.6350 | |
| 0.4949 | 0.3870 | 0.6650 | |
| 0.5032 | 0.4890 | 0.6860 | |
| 0.5097 | 0.5980 | 0.7090 | |
| 0.5130 | 0.7000 | 0.7320 | |
| 0.5146 | 0.7430 | 0.7430 | AZEO |
| 0.5141 | 0.7710 | 0.7540 | |
| 0.5020 | 0.8950 | 0.8410 | |

Marinichev, A.N. - Susarev, M.P., Liquid-vapor equilibriums in the systems acetone-methanol and acetone-cyclohexane at 35, 45, and 55° and a pressure of 760 mm, J. Appl. Chem. USSR 2 (1965) 371-375.

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.6509 | 0.1970 | 0.5870 | |
| 0.6917 | 0.2810 | 0.6290 | |
| 0.7161 | 0.3840 | 0.6580 | |
| 0.7290 | 0.4910 | 0.6800 | |
| 0.7415 | 0.5980 | 0.7040 | |
| 0.7509 | 0.7000 | 0.7340 | |
| 0.7513 | 0.7470 | 0.7470 | AZEO |
| 0.7478 | 0.7710 | 0.7590 | |
| 0.7318 | 0.8950 | 0.8510 | |

Crespo Colin, A. - Compostizo, A. - Díaz Peña, M., Excess Gibbs energy and excess volume of (cyclohexane + 2-propanone) and of (cyclohexane+2-butanone), The Journal of Chemical Thermodynamics 5 (1984) 497-502. doi:10.1016/0021-9614(84)90208-8

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5275 | 0.0501 | 0.3381 |
| 0.7167 | 0.1546 | 0.5450 |
| 0.7681 | 0.2087 | 0.5869 |
| 0.7925 | 0.2434 | 0.6055 |
| 0.8067 | 0.2695 | 0.6166 |
| 0.8357 | 0.3350 | 0.6404 |

| | | |
|---|---|---|
| 0.8464 | 0.3666 | 0.6504 |
| 0.8678 | 0.4491 | 0.6711 |
| 0.8747 | 0.4812 | 0.6790 |
| 0.8800 | 0.5122 | 0.6854 |
| 0.8825 | 0.5226 | 0.6897 |
| 0.8856 | 0.5470 | 0.6952 |
| 0.8922 | 0.5922 | 0.7054 |
| 0.8957 | 0.6197 | 0.7111 |
| 0.8981 | 0.6418 | 0.7212 |
| 0.9007 | 0.6770 | 0.7276 |
| 0.9022 | 0.6916 | 0.7356 |
| 0.9041 | 0.7161 | 0.7435 |
| 0.9050 | 0.7463 | 0.7556 |
| 0.9045 | 0.7751 | 0.7675 |
| 0.9043 | 0.7931 | 0.7765 |
| 0.9011 | 0.8309 | 0.7981 |
| 0.8952 | 0.8677 | 0.8220 |
| 0.8863 | 0.8985 | 0.8496 |
| 0.8647 | 0.9495 | 0.9036 |

Marinichev, A.N. - Susarev, M.P., Liquid-vapor equilibriums in the systems acetone-methanol and acetone-cyclohexane at 35, 45, and 55° and a pressure of 760 mm, J. Appl. Chem. USSR 2 (1965) 371-375.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.7474 | 0.0900 | 0.4320 | |
| 0.9110 | 0.1950 | 0.5760 | |
| 0.9721 | 0.2780 | 0.6230 | |
| 1.004 | 0.3800 | 0.6500 | |
| 1.036 | 0.4930 | 0.6770 | |
| 1.052 | 0.5980 | 0.7030 | |
| 1.067 | 0.7000 | 0.7380 | |
| 1.070 | 0.7620 | 0.7620 | AZEO |
| 1.070 | 0.7700 | 0.7660 | |
| 1.046 | 0.8950 | 0.8650 | |

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**Isobaric phase equilibrium data**

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Mejía, Andrés - Segura, Hugo - Cartes, Marcela - Calvo, Catherine, Vapor–liquid equilibria and interfacial tensions for the ternary system acetone+2,2′-oxybis[propane]+cyclohexane and its constituent binary systems, Fluid Phase Equilibria 1-2 (2008) 75-86. doi:10.1016/j.fluid.2008.06.006

**P / bar = 0.9400**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 345.05 | 0.0240 | 0.1990 |
| 339.48 | 0.0530 | 0.3490 |
| 334.38 | 0.0990 | 0.4740 |
| 331.43 | 0.1440 | 0.5390 |
| 329.52 | 0.1910 | 0.5800 |
| 328.01 | 0.2460 | 0.6140 |
| 327.05 | 0.2960 | 0.6340 |
| 326.40 | 0.3450 | 0.6500 |
| 325.85 | 0.3990 | 0.6640 |
| 325.39 | 0.4530 | 0.6780 |
| 325.05 | 0.5010 | 0.6880 |
| 324.80 | 0.5520 | 0.6990 |
| 324.57 | 0.6090 | 0.7120 |
| 324.38 | 0.6590 | 0.7250 |
| 324.33 | 0.8230 | 0.7900 |
| 324.65 | 0.8790 | 0.8300 |
| 325.36 | 0.9350 | 0.8870 |
| 326.11 | 0.9690 | 0.9380 |

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**Enthalpy of mixing**

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Pfeffer, Thomas - Löwen, Burkhard - Schulz, Siegfried, Calorimetric measurement of the partial molar excess enthalpy at infinite dilution iE,∞ and its meaning for the calculation of the concentration and temperature dependence of the molar excess enthalpy hE, Fluid Phase Equilibria 1-2 (1995) 139-167. doi:10.1016/0378-3812(94)02630-J

**T / K = 283.15**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 6.730 | 0.0007 |
| 13.40 | 0.0015 |
| 19.88 | 0.0022 |
| 26.21 | 0.0029 |
| 32.67 | 0.0036 |
| 38.98 | 0.0042 |

Löwen, B. - Schulz, S., Excess molar enthalpies of acetone + water, cyclohexane, methanol, 1-propanol, 2-propanol, 1-butanol and 1-pentanol at 283.15, 298.15, 323.15, 343.15 and 363.15 K, Thermochimica Acta (1995) 69-82. doi:10.1016/0040-6031(95)02278-A

**T / K = 283.15**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 376.40 | 0.0480 |
| 728.00 | 0.1050 |
| 966.20 | 0.1530 |
| 1145.8 | 0.1990 |
| 1293.0 | 0.2490 |

| | |
|---|---|
| 1416.2 | 0.2970 |
| 1494.4 | 0.3450 |
| 1536.9 | 0.3950 |
| 1553.2 | 0.4460 |
| 1546.4 | 0.4910 |
| 1525.4 | 0.5440 |
| 1475.7 | 0.5920 |
| 1383.0 | 0.6550 |
| 1278.9 | 0.7030 |
| 1148.8 | 0.7530 |
| 995.10 | 0.7990 |
| 784.00 | 0.8530 |
| 566.70 | 0.9010 |
| 318.30 | 0.9480 |

Marongiu, B., Excess enthalpy. 2-Propanone-cyclohexane system, Int. DATA Ser., Sel. Data Mixtures, Ser. A 1 (1987) 1-6.

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 477.00 | 0.0639 |
| 781.00 | 0.1153 |
| 1100.0 | 0.1832 |
| 1405.0 | 0.2873 |
| 1538.0 | 0.3775 |
| 1567.0 | 0.5072 |
| 1466.0 | 0.5987 |
| 1275.0 | 0.6939 |
| 1147.0 | 0.7388 |
| 828.00 | 0.8341 |
| 524.00 | 0.9025 |

Löwen, B. - Schulz, S., Excess molar enthalpies of acetone + water, cyclohexane, methanol, 1-propanol, 2-propanol, 1-butanol and 1-pentanol at 283.15, 298.15, 323.15, 343.15 and 363.15 K, Thermochimica Acta (1995) 69-82. doi:10.1016/0040-6031(95)02278-A

**T / K = 298.15**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 417.80 | 0.0480 |
| 759.10 | 0.1050 |
| 973.70 | 0.1530 |
| 1138.6 | 0.1990 |
| 1289.2 | 0.2490 |
| 1378.4 | 0.2970 |
| 1448.0 | 0.3450 |
| 1502.0 | 0.3950 |
| 1532.3 | 0.4460 |
| 1531.2 | 0.4910 |
| 1509.9 | 0.5440 |
| 1462.6 | 0.5920 |
| 1364.6 | 0.6550 |
| 1259.6 | 0.7030 |
| 1125.6 | 0.7530 |
| 973.30 | 0.7990 |
| 766.80 | 0.8530 |
| 550.80 | 0.9010 |
| 307.10 | 0.9480 |

Singh, Prem P. - Malik, Renu - Maken, S. - Acree, William E. - Zvaigzni, Anita I., Thermochemical investigations of associated solutions, Thermochimica Acta 1 (1990) 113-127. doi:10.1016/0040-6031(90)80211-G

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 806.00 | 0.1086 |
| 1280.0 | 0.1965 |
| 1290.0 | 0.1997 |
| 1725.0 | 0.3339 |
| 1805.0 | 0.3882 |
| 1817.0 | 0.3979 |
| 1810.0 | 0.5654 |
| 1802.0 | 0.5704 |
| 1770.0 | 0.5887 |
| 1776.0 | 0.5891 |
| 1380.0 | 0.7419 |
| 1363.0 | 0.7461 |
| 1258.0 | 0.7751 |
| 755.00 | 0.8818 |
| 727.00 | 0.8862 |

Löwen, B. - Schulz, S., Excess molar enthalpies of acetone + water, cyclohexane, methanol, 1-propanol, 2-propanol, 1-butanol and 1-pentanol at 283.15, 298.15, 323.15, 343.15 and 363.15 K, Thermochimica Acta (1995) 69-82. doi:10.1016/0040-6031(95)02278-A

**T / K = 323.15**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 415.10 | 0.0480 |
| 782.10 | 0.1050 |
| 1022.8 | 0.1530 |
| 1201.3 | 0.1990 |
| 1345.7 | 0.2490 |

| | |
|---|---|
| 1460.6 | 0.2970 |
| 1550.4 | 0.3450 |
| 1603.9 | 0.3950 |
| 1627.5 | 0.4460 |
| 1633.9 | 0.4910 |
| 1597.9 | 0.5440 |
| 1538.8 | 0.5920 |
| 1422.8 | 0.6550 |
| 1306.1 | 0.7030 |
| 1157.8 | 0.7530 |
| 993.70 | 0.7990 |
| 775.90 | 0.8530 |
| 553.50 | 0.9010 |
| 305.90 | 0.9480 |

Löwen, B. - Schulz, S., Excess molar enthalpies of acetone + water, cyclohexane, methanol, 1-propanol, 2-propanol, 1-butanol and 1-pentanol at 283.15, 298.15, 323.15, 343.15 and 363.15 K, Thermochimica Acta (1995) 69-82. doi:10.1016/0040-6031(95)02278-A

| **T / K =** | **343.15** |
|---|---|
| **P / bar =** | **4.000** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 379.80 | 0.0480 |
| 740.80 | 0.1050 |
| 976.50 | 0.1530 |
| 1162.7 | 0.1990 |
| 1312.0 | 0.2490 |
| 1432.4 | 0.2970 |
| 1518.1 | 0.3450 |
| 1573.3 | 0.3950 |
| 1601.2 | 0.4460 |
| 1608.4 | 0.4910 |
| 1582.6 | 0.5440 |
| 1531.7 | 0.5920 |
| 1426.6 | 0.6550 |
| 1312.5 | 0.7030 |
| 1169.1 | 0.7530 |
| 1005.3 | 0.7990 |
| 785.80 | 0.8530 |
| 560.10 | 0.9010 |
| 310.00 | 0.9480 |

Löwen, B. - Schulz, S., Excess molar enthalpies of acetone + water, cyclohexane, methanol, 1-propanol, 2-propanol, 1-butanol and 1-pentanol at 283.15, 298.15, 323.15, 343.15 and 363.15 K, Thermochimica Acta (1995) 69-82. doi:10.1016/0040-6031(95)02278-A

| **T / K =** | **363.15** |
|---|---|
| **P / bar =** | **4.000** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 385.10 | 0.0480 |
| 743.50 | 0.1050 |
| 989.40 | 0.1530 |
| 1184.5 | 0.1990 |
| 1345.9 | 0.2490 |
| 1463.8 | 0.2970 |
| 1551.2 | 0.3450 |
| 1608.7 | 0.3950 |
| 1640.7 | 0.4460 |
| 1648.5 | 0.4910 |
| 1627.0 | 0.5440 |
| 1575.3 | 0.5920 |
| 1467.2 | 0.6550 |
| 1349.3 | 0.7030 |
| 1202.2 | 0.7530 |
| 1034.6 | 0.7990 |
| 808.80 | 0.8530 |
| 577.20 | 0.9010 |
| 319.20 | 0.9480 |

Gmehling, J. - Krentscher, B., Excess enthalpies of 12 binary liquid mixtures containing cyclohexane at elevated temperatures and pressures (up to 416 K and 1.9 MPa), ELDATA Int. Electron. J. Phys.-Chem. Data 3 (1995) 181-190.

| **T / K =** | **413.21** |
|---|---|
| **P / bar =** | **17.54** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 997.16 | 0.1410 |
| 1517.9 | 0.2698 |
| 1759.2 | 0.3878 |
| 1818.1 | 0.4963 |
| 1729.5 | 0.5964 |
| 1539.2 | 0.6891 |
| 1254.4 | 0.7752 |
| 909.06 | 0.8553 |
| 490.00 | 0.9301 |

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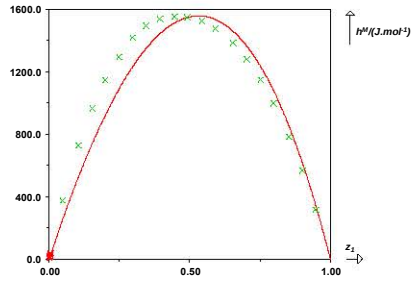
**Azeotropic point**

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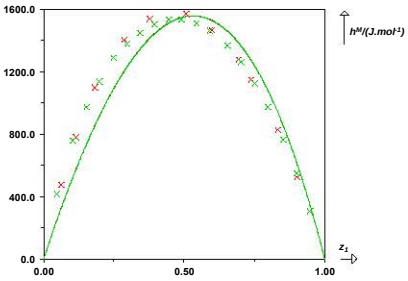
Mejía, Andrés - Segura, Hugo - Cartes, Marcela - Calvo, Catherine, Vapor–liquid equilibria and interfacial tensions for the ternary system acetone+2,2′-oxybis[propane]+cyclohexane and its constituent binary systems, Fluid Phase Equilibria 1-2 (2008) 75-86. doi:10.1016/j.fluid.2008.06.006

| T / K | P / bar | $x_1$ |
|---|---|---|
| 324.25 | 0.9400 | 0.7570 |

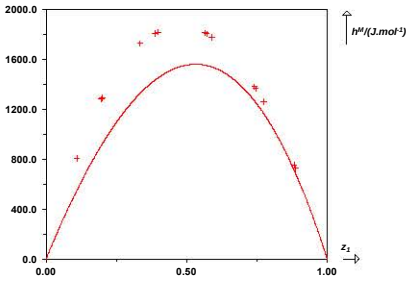
T/K = 283.15 - P/bar = 4.00 4.00



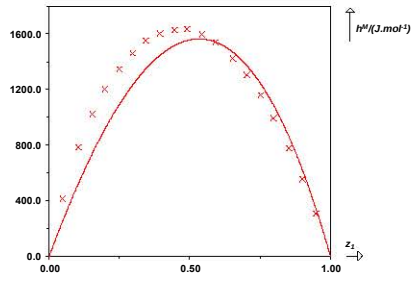

T/K = 298.15 - P/bar = 1.0100 4.00



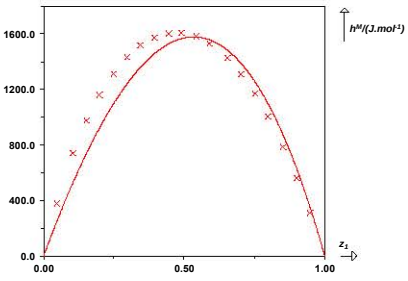

T/K = 308.15 - P/bar = 1.0132



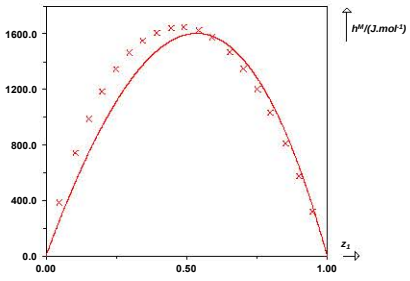

T/K = 323.15 - P/bar = 4.00



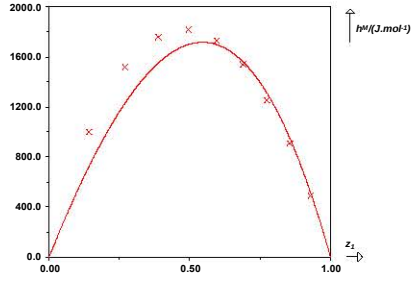

T/K = 343.15 - P/bar = 4.00



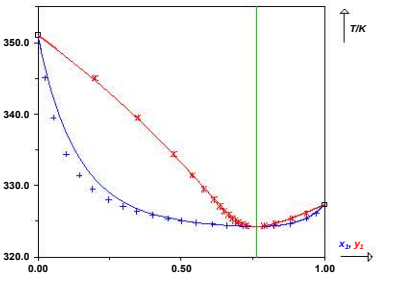

T/K = 363.15 - P/bar = 4.00



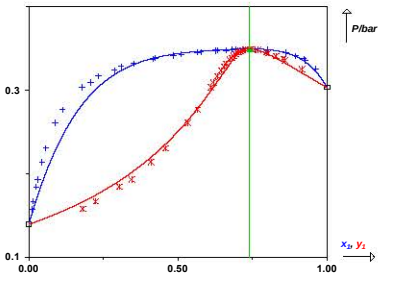

T/K = 413.21 - P/bar = 17.5400



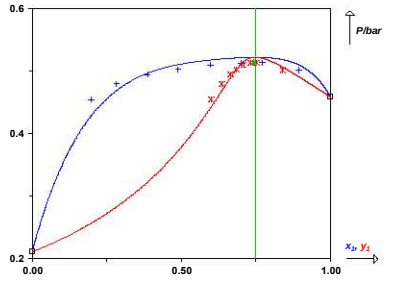

P/bar = 0.94000



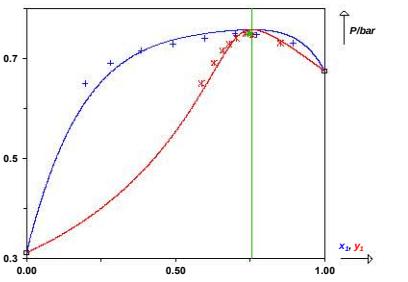

T/K = 298.15



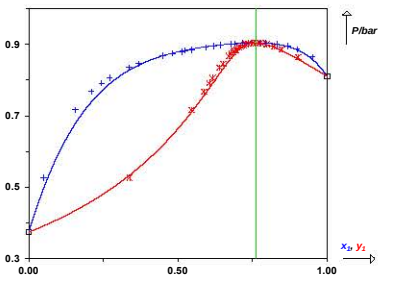

T/K = 308.15



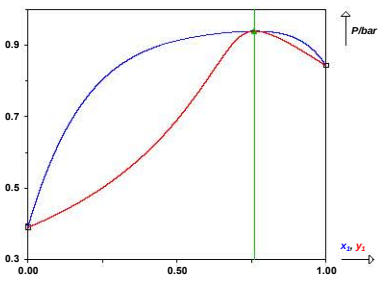

T/K = 318.15



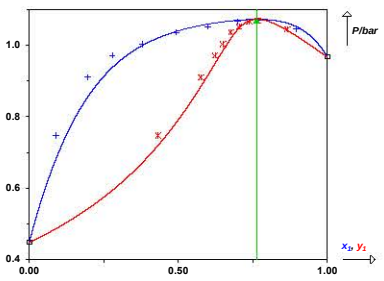

T/K = 323.15




T/K = 324.25




T/K = 328.15



## CARBON DIOXIDE (1) + ETHANE (2)

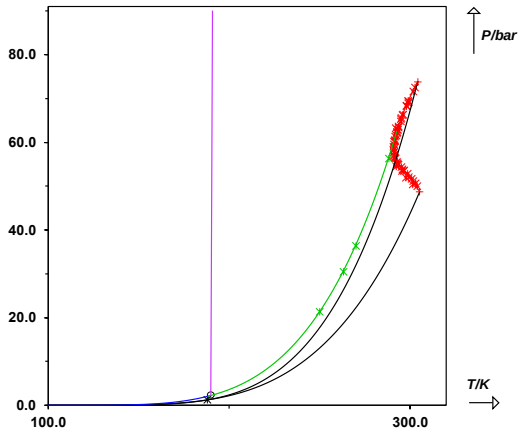
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 74-84-0 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | OTMSDBZUPAUEDD-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 305.32 |
| **$P_c$ / bar** | 73.83 | 48.72 |
| **ω** | 0.2240 | 0.0990 |

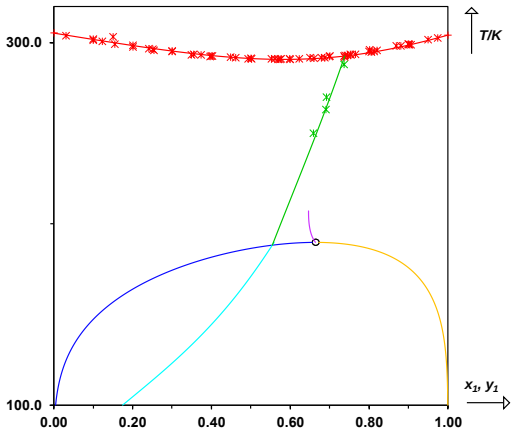
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 402
B/MPa = 681

*Deviations*
MAPE on x = 6.2 %
MAPE on y = 3.4 %
MAPE on $x_c$ = 6 %
MAPE on $P_c$ = 2.3 %
MAPE on $x_{az}$ = 1.4 %
MAPE on $P_{az}$ = 0.41 %
MAPE on $h^M$ = 27 %



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**Isothermal phase equilibrium data**

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Wei, Michael S.-W. - Brown, Trent S. - Kidnay, Arthur J. - Sloan, E. Dendy, Vapor + Liquid Equilibria for the Ternary System Methane + Ethane + Carbon Dioxide at 230 K and Its Constituent Binaries at Temperatures from 207 to 270 K, Journal of Chemical & Engineering Data 4 (1995) 726-731. doi:10.1021/je00020a002

**T / K = 207.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.710 | 0.3738 | 0.5104 |
| 4.650 | 0.3364 | 0.4937 |
| 4.620 | 0.3111 | 0.4786 |
| 4.610 | 0.3028 | 0.4759 |
| 4.590 | 0.2923 | 0.4699 |
| 4.560 | 0.2744 | 0.4592 |
| 4.440 | 0.2285 | 0.4292 |
| 4.190 | 0.1638 | 0.3714 |
| 3.720 | 0.0778 | 0.2624 |

Wei, Michael S.-W. - Brown, Trent S. - Kidnay, Arthur J. - Sloan, E. Dendy, Vapor + Liquid Equilibria for the Ternary System Methane + Ethane + Carbon Dioxide at 230 K and Its Constituent Binaries at Temperatures from 207 to 270 K, Journal of Chemical & Engineering Data 4 (1995) 726-731. doi:10.1021/je00020a002

**T / K = 210.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.380 | 0.7093 | 0.6213 |
| 5.400 | 0.6963 | 0.6172 |
| 5.410 | 0.6844 | 0.6149 |
| 5.430 | 0.6651 | 0.6097 |
| 5.450 | 0.6566 | 0.6053 |
| 5.460 | 0.6150 | 0.5924 |
| 5.470 | 0.5572 | 0.5698 |
| 5.450 | 0.4965 | 0.5506 |
| 5.410 | 0.4316 | 0.5288 |
| 5.390 | 0.4093 | 0.5203 |
| 5.370 | 0.3842 | 0.5129 |
| 5.220 | 0.2961 | 0.4737 |
| 4.980 | 0.2153 | 0.4185 |
| 4.540 | 0.1254 | 0.3194 |
| 4.260 | 0.0877 | 0.2571 |
| 3.800 | 0.0358 | 0.1322 |

Wei, Michael S.-W. - Brown, Trent S. - Kidnay, Arthur J. - Sloan, E. Dendy, Vapor + Liquid Equilibria for the Ternary System Methane + Ethane + Carbon Dioxide at 230 K and Its Constituent Binaries at Temperatures from 207 to 270 K, Journal of Chemical & Engineering Data 4 (1995) 726-731. doi:10.1021/je00020a002

**T / K = 213.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.640 | 0.8678 | 0.7327 |
| 5.760 | 0.8317 | 0.7055 |
| 5.940 | 0.7601 | 0.6588 |
| 6.040 | 0.6982 | 0.6319 |
| 6.100 | 0.6503 | 0.6022 |
| 6.130 | 0.6089 | 0.5911 |
| 6.160 | 0.5557 | 0.5800 |
| 6.130 | 0.4789 | 0.5531 |
| 6.070 | 0.4282 | 0.5302 |
| 5.830 | 0.3075 | 0.4770 |
| 5.320 | 0.1706 | 0.3725 |
| 5.080 | 0.1306 | 0.3185 |
| 4.710 | 0.0837 | 0.2401 |
| 4.320 | 0.0442 | 0.1458 |

Brown, T.S. - Kidnay, A.J. - Sloan, E.D., Vapor—liquid equilibria in the carbon dioxide-ethane system, Fluid Phase Equilibria 1-2 (1988) 169-184. doi:10.1016/0378-3812(88)80028-1

**T / K = 220.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.220 | 0.0150 | 0.0706 |
| 5.480 | 0.0317 | 0.1239 |
| 5.790 | 0.0532 | 0.1846 |
| 6.130 | 0.0812 | 0.2418 |
| 6.600 | 0.1332 | 0.3178 |
| 6.860 | 0.1608 | 0.3592 |
| 7.200 | 0.2186 | 0.4120 |
| 7.420 | 0.2564 | 0.4454 |
| 7.650 | 0.3190 | 0.4850 |
| 7.800 | 0.3693 | 0.5114 |
| 7.960 | 0.4631 | 0.5518 |
| 8.030 | 0.5641 | 0.5866 |
| 8.020 | 0.6552 | 0.6186 |
| 7.880 | 0.7782 | 0.6692 |
| 7.630 | 0.8572 | 0.7195 |
| 7.360 | 0.9035 | 0.7668 |
| 7.000 | 0.9428 | 0.8247 |
| 6.540 | 0.9772 | 0.9006 |

Brown, T.S. - Kidnay, A.J. - Sloan, E.D., Vapor—liquid equilibria in the carbon dioxide-ethane system, Fluid Phase Equilibria 1-2 (1988) 169-184. doi:10.1016/0378-3812(88)80028-1

**T / K = 230.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.990 | 0.0485 | 0.1513 |
| 8.330 | 0.0681 | 0.1910 |

| | | |
|---|---|---|
| 8.410 | 0.0745 | 0.1982 |
| 8.830 | 0.1035 | 0.2452 |
| 8.950 | 0.1106 | 0.2670 |
| 9.210 | 0.1280 | 0.2862 |
| 9.480 | 0.1548 | 0.3225 |
| 9.650 | 0.1712 | 0.3482 |
| 10.38 | 0.2538 | 0.4280 |
| 10.80 | 0.3300 | 0.4782 |
| 10.98 | 0.3605 | 0.5022 |
| 11.12 | 0.4092 | 0.5227 |
| 11.22 | 0.4422 | 0.5402 |
| 11.38 | 0.5195 | 0.5750 |
| 11.45 | 0.6844 | 0.6484 |
| 11.00 | 0.8438 | 0.7403 |
| 10.23 | 0.9326 | 0.8389 |
| 9.360 | 0.9828 | 0.9451 |

Wallis, Kevin P - Clancy, Paulette - Zollweg, John A - Streett, William B, Excess thermodynamic properties for {xCO2 + (1 − x)C2H6} (I): experiment and theory, The Journal of Chemical Thermodynamics 9 (1984) 811-823. doi:10.1016/0021-9614(84)90028-4

**T / K = 243.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.56 | 0.0330 | 0.0960 |
| 12.44 | 0.0710 | 0.1770 |
| 14.14 | 0.1660 | 0.3160 |
| 15.34 | 0.2530 | 0.4100 |
| 16.38 | 0.3760 | 0.5000 |
| 17.07 | 0.5040 | 0.5730 |
| 17.29 | 0.5760 | 0.6100 |
| 17.29 | 0.7230 | 0.6910 |
| 16.73 | 0.8440 | 0.7760 |
| 15.46 | 0.9480 | 0.8940 |

Brown, T.S. - Kidnay, A.J. - Sloan, E.D., Vapor—liquid equilibria in the carbon dioxide-ethane system, Fluid Phase Equilibria 1-2 (1988) 169-184. doi:10.1016/0378-3812(88)80028-1

**T / K = 250.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 14.35 | 0.0424 | 0.1092 |
| 14.82 | 0.0571 | 0.1442 |
| 15.50 | 0.0865 | 0.1944 |
| 15.76 | 0.0974 | 0.2109 |
| 16.49 | 0.1280 | 0.2576 |
| 16.92 | 0.1489 | 0.2885 |
| 17.50 | 0.1783 | 0.3216 |
| 18.67 | 0.2501 | 0.3988 |
| 19.73 | 0.3373 | 0.4688 |
| 20.22 | 0.3884 | 0.5023 |
| 20.24 | 0.3922 | 0.5038 |
| 20.81 | 0.4754 | 0.5561 |
| 21.00 | 0.5170 | 0.5807 |
| 21.10 | 0.5344 | 0.5930 |
| 21.16 | 0.5525 | 0.6001 |
| 21.20 | 0.5720 | 0.6107 |
| 21.28 | 0.6046 | 0.6287 |
| 21.34 | 0.6583 | 0.6583 AZEO |
| 21.34 | 0.6601 | 0.6589 |
| 20.82 | 0.8279 | 0.7685 |
| 19.91 | 0.9048 | 0.8497 |
| 19.05 | 0.9589 | 0.9170 |
| 18.21 | 0.9891 | 0.9790 |

Wallis, Kevin P - Clancy, Paulette - Zollweg, John A - Streett, William B, Excess thermodynamic properties for {xCO2 + (1 − x)C2H6} (I): experiment and theory, The Journal of Chemical Thermodynamics 9 (1984) 811-823. doi:10.1016/0021-9614(84)90028-4

**T / K = 263.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.18 | 0.0450 | 0.1040 |
| 24.11 | 0.1650 | 0.2860 |
| 26.60 | 0.2730 | 0.3970 |
| 27.80 | 0.3390 | 0.4530 |
| 28.95 | 0.4250 | 0.5140 |
| 30.08 | 0.5480 | 0.5960 |
| 30.50 | 0.6540 | 0.6660 |
| 30.46 | 0.6900 | 0.6900 AZEO |
| 30.28 | 0.7730 | 0.7450 |
| 29.60 | 0.8580 | 0.8160 |
| 28.23 | 0.9370 | 0.9000 |

Brown, T.S. - Kidnay, A.J. - Sloan, E.D., Vapor—liquid equilibria in the carbon dioxide-ethane system, Fluid Phase Equilibria 1-2 (1988) 169-184. doi:10.1016/0378-3812(88)80028-1

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 24.34 | 0.0517 | 0.1056 |
| 25.72 | 0.0858 | 0.1641 |
| 26.35 | 0.1036 | 0.1898 |
| 27.34 | 0.1332 | 0.2297 |
| 28.70 | 0.1751 | 0.2824 |
| 29.76 | 0.2116 | 0.3227 |
| 30.83 | 0.2527 | 0.3632 |
| 31.81 | 0.2931 | 0.4014 |
| 32.65 | 0.3328 | 0.4362 |
| 33.60 | 0.3819 | 0.4751 |

| | | | |
|---|---|---|---|
| 35.19 | 0.4967 | 0.5594 | |
| 35.81 | 0.5616 | 0.6036 | |
| 36.10 | 0.6076 | 0.6360 | |
| 36.36 | 0.6893 | 0.6914 | |
| 36.36 | 0.6925 | 0.6925 | AZEO |
| 36.27 | 0.7392 | 0.7261 | |
| 36.21 | 0.7690 | 0.7494 | |
| 36.13 | 0.7783 | 0.7550 | |
| 35.85 | 0.8182 | 0.7864 | |
| 34.86 | 0.8940 | 0.8608 | |
| 34.49 | 0.9142 | 0.8788 | |
| 34.16 | 0.9328 | 0.9002 | |
| 32.82 | 0.9797 | 0.9645 | |

Wei, Michael S.-W. - Brown, Trent S. - Kidnay, Arthur J. - Sloan, E. Dendy, Vapor + Liquid Equilibria for the Ternary System Methane + Ethane + Carbon Dioxide at 230 K and Its Constituent Binaries at Temperatures from 207 to 270 K, Journal of Chemical & Engineering Data 4 (1995) 726-731. doi:10.1021/je00020a002

**T / K = 270.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 33.44 | 0.9642 | 0.9337 |
| 35.67 | 0.8418 | 0.8095 |
| 31.51 | 0.2907 | 0.4116 |
| 27.97 | 0.1568 | 0.2689 |
| 25.43 | 0.0801 | 0.1633 |

Ohgaki, Kazunari - Katayama, Takashi, Isothermal vapor-liquid equilibrium data for the ethane—carbon dioxide system at high pressures, Fluid Phase Equilibria 1 (1977) 27-32. doi:10.1016/0378-3812(77)80023-X

**T / K = 288.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 38.59 | 0.0850 | 0.1379 | |
| 40.48 | 0.1202 | 0.1836 | |
| 41.70 | 0.1473 | 0.2153 | |
| 45.27 | 0.2227 | 0.2980 | |
| 46.67 | 0.2552 | 0.3317 | |
| 48.66 | 0.3201 | 0.3897 | |
| 54.87 | 0.5596 | 0.5858 | |
| 55.90 | 0.6172 | 0.6333 | |
| 56.36 | 0.6846 | 0.6888 | |
| 56.34 | 0.6977 | 0.6967 | |
| 56.32 | 0.7367 | 0.7367 | AZEO |
| 56.32 | 0.7403 | 0.7379 | |
| 56.31 | 0.7711 | 0.7508 | |
| 56.02 | 0.8351 | 0.8105 | |
| 54.87 | 0.8965 | 0.8708 | |
| 53.00 | 0.9591 | 0.9426 | |

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**Enthalpy of mixing**

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Wallis, Kevin P - Clancy, Paulette - Zollweg, John A - Streett, William B, Excess thermodynamic properties for {xCO2 + (1 − x)C2H6} (l): experiment and theory, The Journal of Chemical Thermodynamics 9 (1984) 811-823. doi:10.1016/0021-9614(84)90028-4

**T / K = 217.00**

**P / bar = UNKNOWN (10.5067)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 1019.6 | 0.8029 |
| 1345.7 | 0.6975 |
| 1422.6 | 0.6118 |
| 1464.4 | 0.5367 |
| 1363.0 | 0.4116 |
| 1322.1 | 0.3574 |
| 1164.5 | 0.2889 |

Wormald, C.J - Eyears, J.M, Excess molar enthalpies and excess molar volumes of {xCO2 + (1 − x)C2H6} up to 308.4 K and 11.0 MPa, The Journal of Chemical Thermodynamics 3 (1988) 323-331. doi:10.1016/0021-9614(88)90129-2

**T / K = 248.10**

**P / bar = 30.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 519.00 | 0.9040 |
| 1048.0 | 0.8070 |
| 1365.0 | 0.7090 |
| 1514.0 | 0.6090 |
| 1509.0 | 0.5090 |
| 1465.0 | 0.4590 |
| 1301.0 | 0.4100 |
| 671.00 | 0.1530 |

Wormald, C.J - Eyears, J.M, Excess molar enthalpies and excess molar volumes of {xCO2 + (1 − x)C2H6} up to 308.4 K and 11.0 MPa, The Journal of Chemical Thermodynamics 3 (1988) 323-331. doi:10.1016/0021-9614(88)90129-2

**T / K = 272.10**

**P / bar = 45.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 194.00 | 0.9590 |
| 432.00 | 0.9180 |
| 725.00 | 0.8700 |
| 906.00 | 0.8380 |
| 1075.0 | 0.7960 |
| 1416.0 | 0.7138 |

| | |
|---|---|
| 1475.0 | 0.6730 |
| 1595.0 | 0.6330 |
| 1626.0 | 0.5920 |
| 1702.0 | 0.5250 |
| 1670.0 | 0.5080 |
| 1655.0 | 0.4650 |
| 1641.0 | 0.4250 |
| 1519.0 | 0.3400 |
| 1328.0 | 0.2990 |
| 1264.0 | 0.2560 |
| 1055.0 | 0.2130 |
| 792.00 | 0.1720 |
| 429.00 | 0.1250 |
| 137.00 | 0.0410 |

Wormald, C.J. - Hodgetts, R.W., Excess enthalpies and volumes for (carbon dioxide + ethane) atT= 291.6 K, close to the minimum in the critical locus, The Journal of Chemical Thermodynamics 1 (1997) 75-85. doi:10.1006/jcht.1996.0141

| **T / K =** | **291.60** |
|---|---|
| **P / bar =** | **40.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 235.00 | 0.9780 |
| 462.00 | 0.9520 |
| 942.00 | 0.8930 |
| 1431.0 | 0.8340 |
| 1899.0 | 0.7750 |
| 2339.0 | 0.7160 |
| 2781.0 | 0.6560 |
| 3219.0 | 0.5970 |
| 3607.0 | 0.5370 |
| 4003.0 | 0.4760 |
| 4352.0 | 0.4170 |
| 4656.0 | 0.3580 |
| 4923.0 | 0.2960 |
| 5220.0 | 0.2370 |
| 5424.0 | 0.1780 |
| 5431.0 | 0.1190 |
| 27.00 | 0.0610 |

Wormald, C.J. - Hodgetts, R.W., Excess enthalpies and volumes for (carbon dioxide + ethane) atT= 291.6 K, close to the minimum in the critical locus, The Journal of Chemical Thermodynamics 1 (1997) 75-85. doi:10.1006/jcht.1996.0141

| **T / K =** | **291.60** |
|---|---|
| **P / bar =** | **54.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 207.00 | 0.9790 |
| 243.00 | 0.9780 |
| 242.00 | 0.9770 |
| 460.00 | 0.9420 |
| 877.00 | 0.8820 |
| 1277.0 | 0.8230 |
| 1624.0 | 0.7620 |
| 1931.0 | 0.7030 |
| 2179.0 | 0.6440 |
| 2379.0 | 0.5840 |
| 2473.0 | 0.5250 |
| 2414.0 | 0.4640 |
| -346.00 | 0.3820 |
| -366.00 | 0.3460 |
| -373.00 | 0.2870 |
| -274.00 | 0.2250 |
| -184.00 | 0.1660 |
| -138.00 | 0.1070 |

Wormald, C.J. - Hodgetts, R.W., Excess enthalpies and volumes for (carbon dioxide + ethane) atT= 291.6 K, close to the minimum in the critical locus, The Journal of Chemical Thermodynamics 1 (1997) 75-85. doi:10.1006/jcht.1996.0141

| **T / K =** | **291.60** |
|---|---|
| **P / bar =** | **58.50** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 509.00 | 0.9460 |
| 4872.0 | 0.8690 |
| 6123.0 | 0.8310 |
| 6055.0 | 0.7730 |
| 5904.0 | 0.7150 |
| 5530.0 | 0.6560 |
| 4867.0 | 0.5960 |
| 2473.0 | 0.5060 |
| 2264.0 | 0.4760 |
| 1957.0 | 0.4160 |
| 1699.0 | 0.3570 |
| 1431.0 | 0.2960 |
| 1151.0 | 0.2350 |
| 863.00 | 0.1730 |
| 538.00 | 0.1110 |

Wormald, C.J. - Hodgetts, R.W., Excess enthalpies and volumes for (carbon dioxide + ethane) atT= 291.6 K, close to the minimum in the critical locus, The Journal of Chemical Thermodynamics 1 (1997) 75-85. doi:10.1006/jcht.1996.0141

| **T / K =** | **291.60** |
|---|---|
| **P / bar =** | **31.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |

| | |
|---|---|
| 49.00 | 0.9780 |
| 200.00 | 0.8930 |
| 217.00 | 0.8340 |
| 256.00 | 0.7740 |
| 324.00 | 0.7140 |
| 377.00 | 0.6550 |
| 434.00 | 0.5350 |
| 437.00 | 0.4760 |
| 438.00 | 0.4140 |
| 434.00 | 0.3550 |
| 394.00 | 0.2970 |
| 354.00 | 0.2350 |
| 310.00 | 0.1760 |
| 233.00 | 0.1180 |
| 129.00 | 0.0560 |

Wormald, C.J - Eyears, J.M, Excess molar enthalpies and excess molar volumes of {xCO2 + (1 − x)C2H6} up to 308.4 K and 11.0 MPa, The Journal of Chemical Thermodynamics 3 (1988) 323-331. doi:10.1016/0021-9614(88)90129-2

| **T / K =** | **300.10** |
|---|---|
| **P / bar =** | **40.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 219.00 | 0.8500 |
| 343.00 | 0.7490 |
| 398.00 | 0.6980 |
| 435.00 | 0.6500 |
| 473.00 | 0.6000 |
| 510.00 | 0.5480 |
| 522.00 | 0.4990 |
| 545.00 | 0.4000 |
| 511.00 | 0.2980 |
| 474.00 | 0.2470 |
| 399.00 | 0.1970 |
| 218.00 | 0.0980 |

Wormald, C.J - Eyears, J.M, Excess molar enthalpies and excess molar volumes of {xCO2 + (1 − x)C2H6} up to 308.4 K and 11.0 MPa, The Journal of Chemical Thermodynamics 3 (1988) 323-331. doi:10.1016/0021-9614(88)90129-2

| **T / K =** | **308.40** |
|---|---|
| **P / bar =** | **40.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 133.00 | 0.9030 |
| 249.00 | 0.8090 |
| 340.00 | 0.7110 |
| 402.00 | 0.6160 |
| 433.00 | 0.5120 |
| 436.00 | 0.3130 |
| 356.00 | 0.2100 |
| 236.00 | 0.1060 |

Wormald, C.J - Eyears, J.M, Excess molar enthalpies and excess molar volumes of {xCO2 + (1 − x)C2H6} up to 308.4 K and 11.0 MPa, The Journal of Chemical Thermodynamics 3 (1988) 323-331. doi:10.1016/0021-9614(88)90129-2

| **T / K =** | **308.40** |
|---|---|
| **P / bar =** | **65.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 424.00 | 0.9170 |
| 685.00 | 0.8860 |
| 670.00 | 0.8680 |
| 1156.0 | 0.7720 |
| 1503.0 | 0.7220 |
| 1559.0 | 0.6730 |
| 1740.0 | 0.6220 |
| 1794.0 | 0.5720 |
| 2014.0 | 0.5680 |
| 2008.0 | 0.5190 |
| 2016.0 | 0.5190 |
| 2046.0 | 0.5190 |
| 2201.0 | 0.4730 |
| 2160.0 | 0.4240 |
| 2156.0 | 0.3740 |
| 1998.0 | 0.2940 |
| 1680.0 | 0.2430 |
| 659.00 | 0.1480 |
| 317.00 | 0.0980 |

Wormald, C.J - Eyears, J.M, Excess molar enthalpies and excess molar volumes of {xCO2 + (1 − x)C2H6} up to 308.4 K and 11.0 MPa, The Journal of Chemical Thermodynamics 3 (1988) 323-331. doi:10.1016/0021-9614(88)90129-2

| **T / K =** | **308.40** |
|---|---|
| **P / bar =** | **83.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 1684.0 | 0.8980 |
| 2039.0 | 0.8470 |
| 2354.0 | 0.7480 |
| 2418.0 | 0.6970 |
| 2365.0 | 0.6690 |
| 2280.0 | 0.5950 |
| 2159.0 | 0.5460 |
| 2010.0 | 0.4950 |
| 1861.0 | 0.4460 |
| 1401.0 | 0.3420 |

| | |
|---|---|
| 1266.0 | 0.2940 |
| 1053.0 | 0.2420 |
| 897.00 | 0.1960 |
| 685.00 | 0.1480 |
| 440.00 | 0.0980 |
| 204.00 | 0.0460 |

Wormald, C.J - Eyears, J.M, Excess molar enthalpies and excess molar volumes of {xCO2 + (1 − x)C2H6} up to 308.4 K and 11.0 MPa, The Journal of Chemical Thermodynamics 3 (1988) 323-331. doi:10.1016/0021-9614(88)90129-2

**T / K = 308.40**

**P / bar = 110.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 527.00 | 0.8980 |
| 1121.0 | 0.7950 |
| 1355.0 | 0.6940 |
| 1454.0 | 0.6430 |
| 1454.0 | 0.6180 |
| 1478.0 | 0.5930 |
| 1476.0 | 0.5700 |
| 1470.0 | 0.5430 |
| 1465.0 | 0.5200 |
| 1438.0 | 0.4950 |
| 1404.0 | 0.4860 |
| 1397.0 | 0.4450 |
| 1307.0 | 0.3920 |
| 1061.0 | 0.2920 |
| 759.00 | 0.1930 |
| 393.00 | 0.0950 |

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**Critical point**

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Khazanova, N.E. - Lesnevskaya, L.S. - Zakharova, A.V., Liquid-vapor equilibrium in the ethane-CO2 system, Khim. Promst. Moscow (1966) 364-365.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 299.05 | 69.41 | 0.9000 |
| 295.25 | 65.56 | 0.8000 |
| 292.55 | 62.01 | 0.7000 |
| 290.95 | 58.97 | 0.6000 |
| 290.75 | 58.26 | 0.5730 |
| 291.35 | 56.54 | 0.5000 |
| 292.75 | 55.02 | 0.4000 |
| 295.45 | 53.40 | 0.3000 |
| 297.75 | 51.88 | 0.2000 |
| 301.45 | 50.36 | 0.1000 |

Gil, Laura - Otín, Santos F. - Embid, Jose Muñoz - Gallardo, M. Asunción - Blanco, Sofía - Artal, Manuela - Velasco, Inmaculada, Experimental setup to measure critical properties of pure and binary mixtures and their densities at different pressures and temperatures, The Journal of Supercritical Fluids 2 (2008) 123-138. doi:10.1016/j.supflu.2007.11.003

| T / K | P / bar | $x_1$ |
|---|---|---|
| 304.01 | 50.01 | 0.0305 |
| 301.84 | 51.08 | 0.1005 |
| 299.12 | 52.06 | 0.1540 |
| 298.56 | 52.85 | 0.2008 |
| 295.83 | 53.83 | 0.2546 |
| 295.18 | 54.37 | 0.3006 |
| 293.25 | 54.95 | 0.3493 |
| 292.56 | 55.47 | 0.4024 |
| 291.90 | 56.34 | 0.4484 |
| 291.00 | 57.02 | 0.5016 |
| 291.08 | 57.76 | 0.5517 |
| 291.09 | 59.49 | 0.5988 |
| 291.63 | 60.22 | 0.6493 |
| 292.31 | 61.54 | 0.6991 |
| 293.65 | 63.35 | 0.7526 |
| 296.12 | 66.32 | 0.8019 |
| 298.15 | 68.19 | 0.8688 |
| 299.15 | 69.12 | 0.8988 |
| 301.80 | 71.62 | 0.9495 |

Morrison, G. - Kincaid, J. M., Critical point measurements on nearly polydisperse fluids, AIChE Journal 2 (1984) 257-262. doi:10.1002/aic.690300213

| T / K | P / bar | $x_1$ |
|---|---|---|
| 302.66 | 72.50 | 0.9739 |
| 298.92 | 69.35 | 0.9025 |

Khazanova, N.E. - Sominskaya, E.E. - Zakharova, A.V. - Rozovski, M.B., Thermodynamic properties of the ethane-carbon dioxide system and the pressure-volume-temperature-normality data, Teplofiz. Svoistva Veshchestv Mater. (1976) 213-219.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 299.00 | 68.90 | 0.9060 |
| 295.03 | 65.25 | 0.8130 |
| 294.77 | 64.75 | 0.8050 |
| 293.19 | 62.87 | 0.7540 |
| 292.95 | 62.39 | 0.7450 |
| 292.72 | 62.28 | 0.7360 |
| 291.59 | 60.59 | 0.6790 |
| 290.70 | 58.16 | 0.5690 |
| 292.45 | 54.51 | 0.3960 |

| | | |
|---|---|---|
| 303.19 | 50.66 | 0.1500 |

Goodwin, Anthony R.H. - Moldover, Michael R., Phase border and density determinations in the critical region of (carbon dioxide+ethane) determined from dielectric permittivity measurements, The Journal of Chemical Thermodynamics 12 (1997) 1481-1494. doi:10.1006/jcht.1997.0257

| T / K | P / bar | $x_1$ |
|---|---|---|
| 292.98 | 62.78 | 0.7398 |
| 291.13 | 56.84 | 0.4924 |
| 296.51 | 53.47 | 0.2517 |

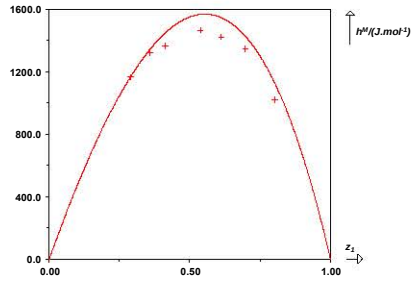
Horstmann, Sven - Fischer, Kai - Gmehling, Jürgen - Kolář, Petr, Experimental determination of the critical line for (carbon dioxide + ethane) and calculation of various thermodynamic properties for (carbon dioxide +n-alkane) using the PSRK model, The Journal of Chemical Thermodynamics 4 (2000) 451-464. doi:10.1006/jcht.2000.0611

| T / K | P / bar | $x_1$ |
|---|---|---|
| 300.70 | 51.62 | 0.1223 |
| 296.82 | 53.52 | 0.2403 |
| 293.66 | 54.85 | 0.3548 |
| 291.80 | 56.44 | 0.4607 |
| 291.04 | 57.87 | 0.5605 |
| 291.48 | 60.26 | 0.6601 |
| 293.71 | 63.58 | 0.7657 |
| 298.16 | 68.31 | 0.8805 |

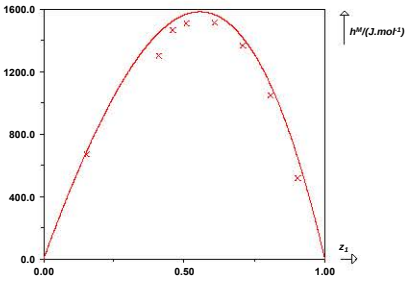
Ohgaki, Kazunari - Katayama, Takashi, Isothermal vapor-liquid equilibrium data for the ethane—carbon dioxide system at high pressures, Fluid Phase Equilibria 1 (1977) 27-32. doi:10.1016/0378-3812(77)80023-X

| T / K | P / bar | $x_1$ |
|---|---|---|
| 293.15 | 55.29 | 0.3735 |
| 290.96 | 58.60 | 0.5767 |
| 290.97 | 60.11 | 0.6222 |
| 291.60 | 61.28 | 0.6871 |
| 292.04 | 63.21 | 0.7372 |
| 295.90 | 66.17 | 0.8202 |

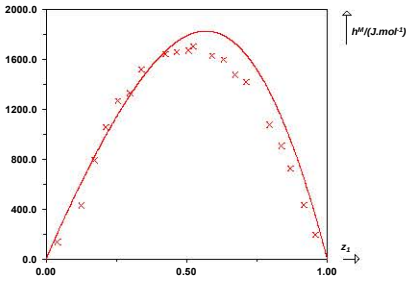
T/K = 217.00 - P/bar = 10.5067



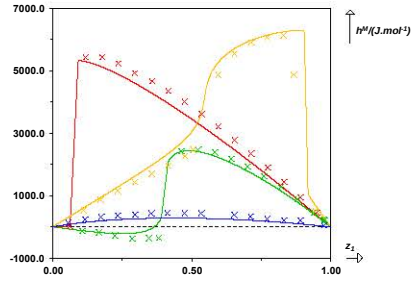

T/K = 248.10 - P/bar = 30.00



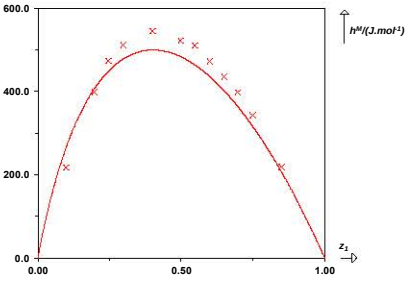

T/K = 272.10 - P/bar = 45.00



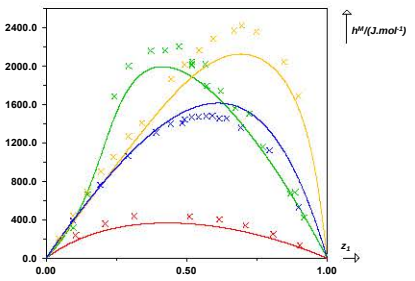

T/K = 291.60 - P/bar = 40.00 54.00 58.500 31.00



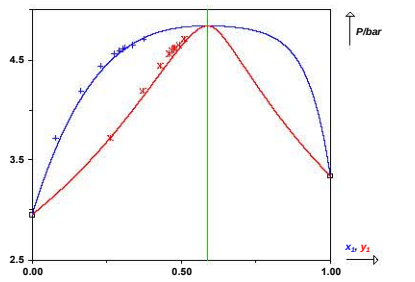

T/K = 300.10 - P/bar = 40.00



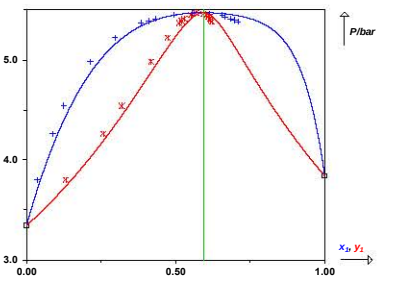

T/K = 308.40 - P/bar = 40.00 65.00 83.00 110.00



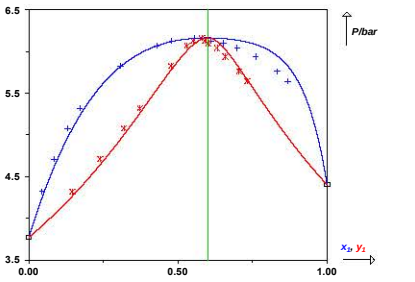

T/K = 207.00



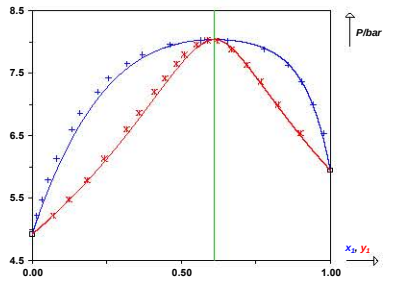

T/K = 210.00



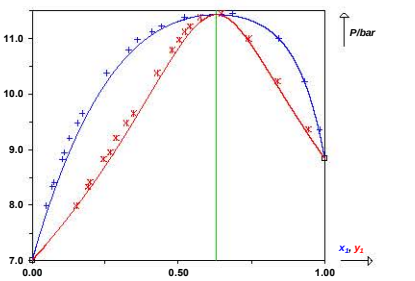

T/K = 213.00



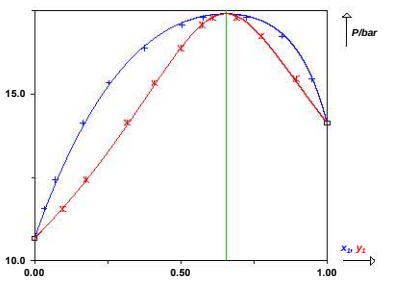

T/K = 220.00



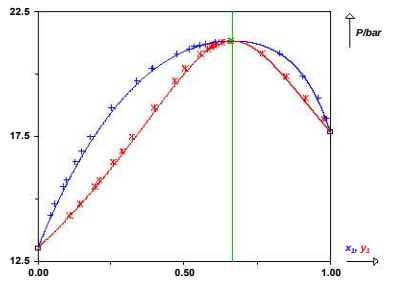

T/K = 230.00



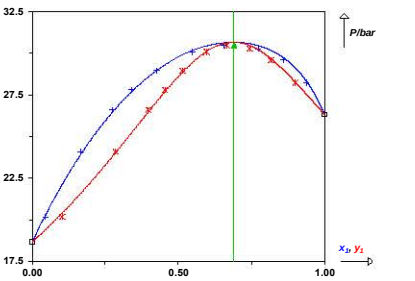

T/K = 243.15



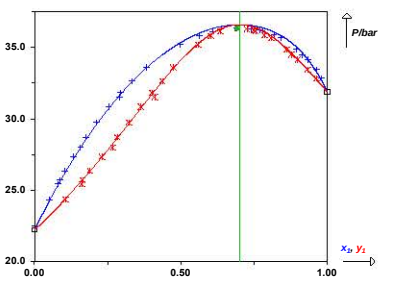

T/K = 250.00



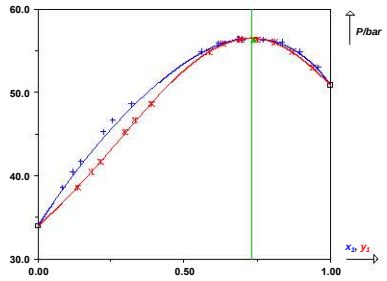

T/K = 263.15



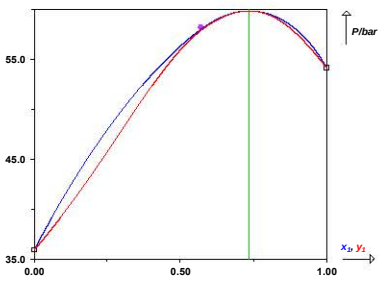

T/K = 270.00



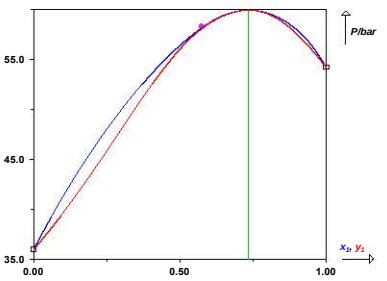
T/K = 288.15



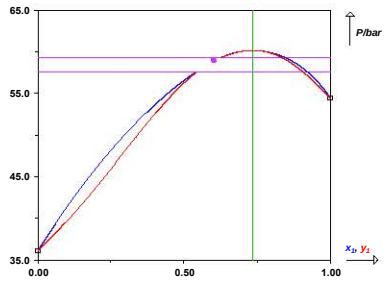

T/K = 290.70



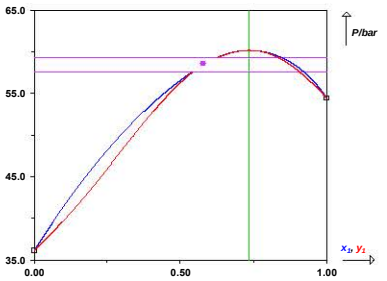

T/K = 290.75



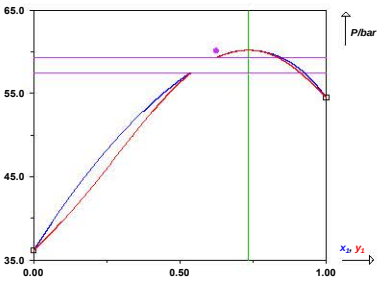

T/K = 290.95



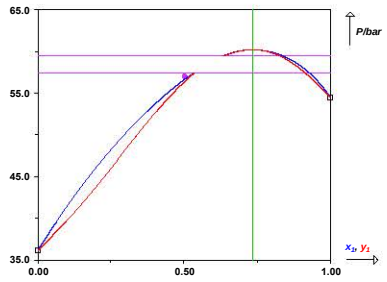

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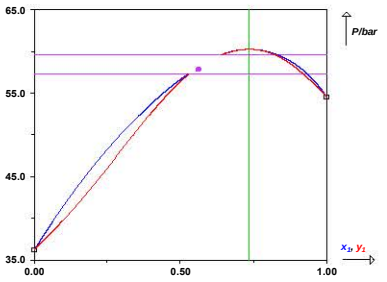

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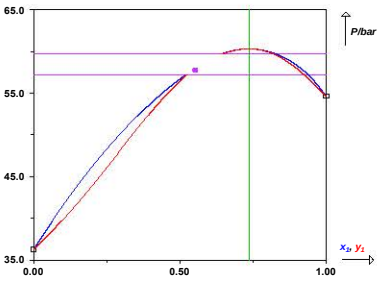

T/K = 291.00



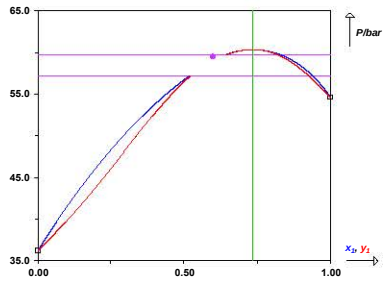

T/K = 291.04



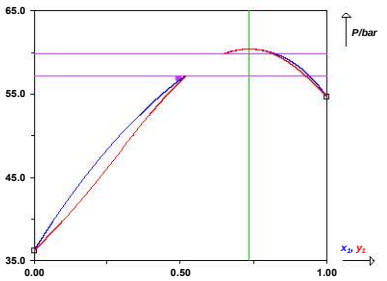

T/K = 291.08



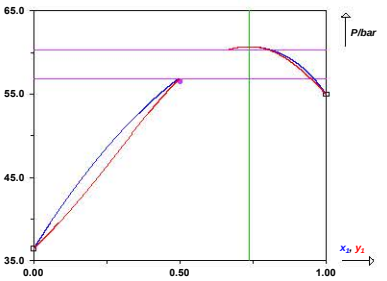

T/K = 291.09



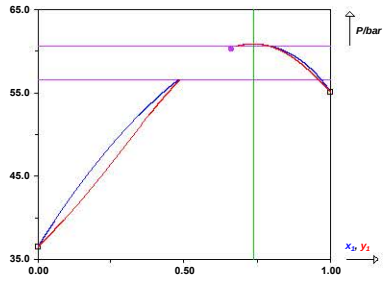

T/K = 291.13



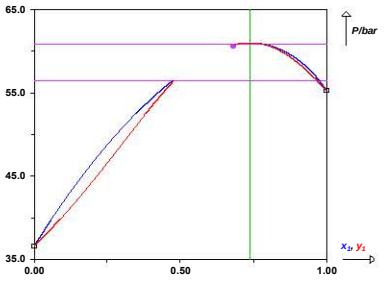

T/K = 291.35



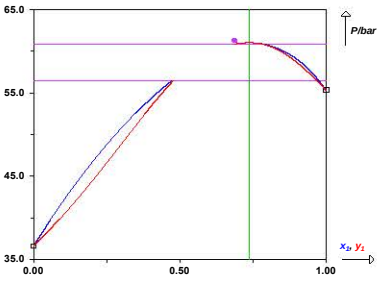

T/K = 291.48



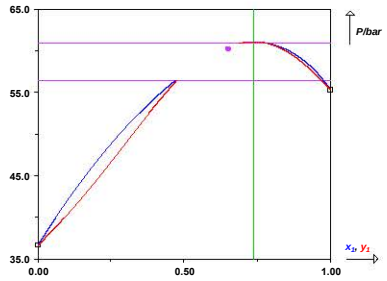

T/K = 291.59



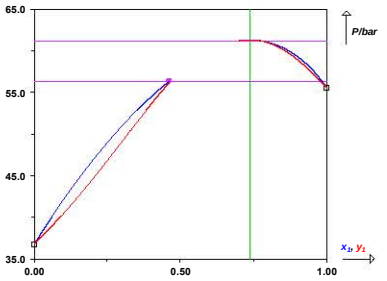

T/K = 291.60



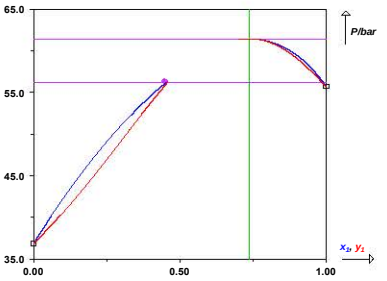
T/K = 291.63



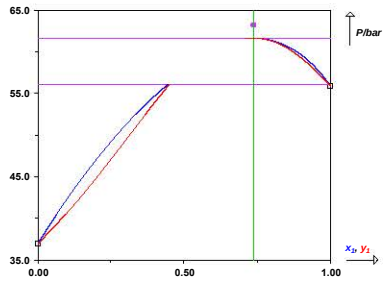

T/K = 291.80



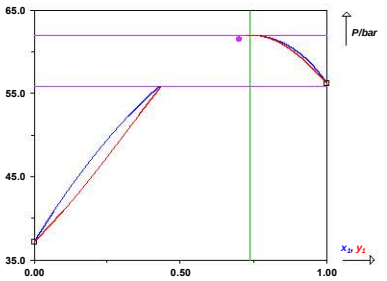

T/K = 291.90



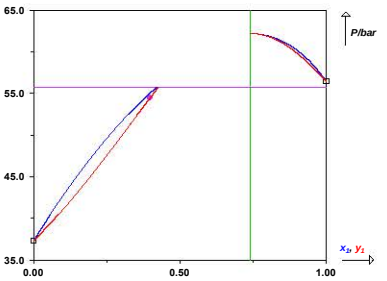

T/K = 292.04



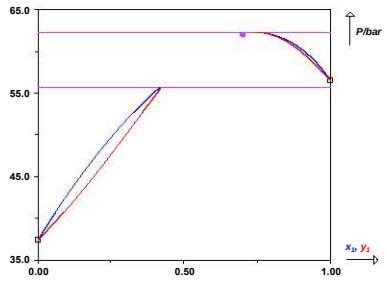

T/K = 292.31



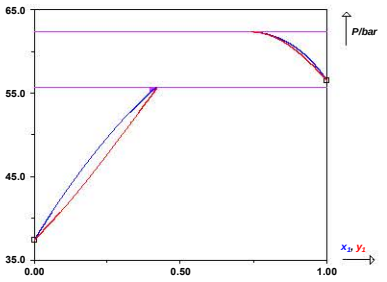

T/K = 292.45



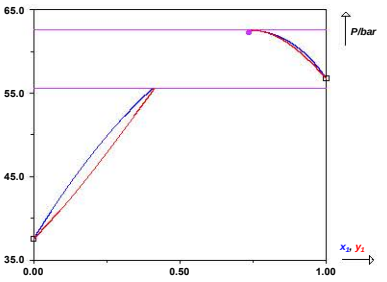

T/K = 292.55



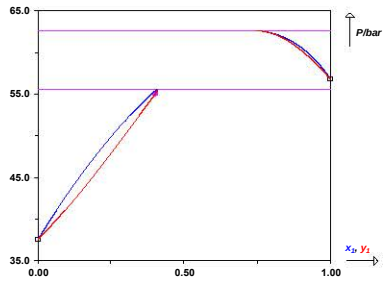

T/K = 292.56



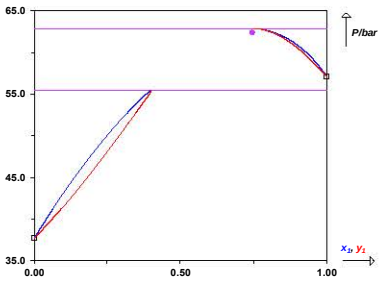

T/K = 292.72



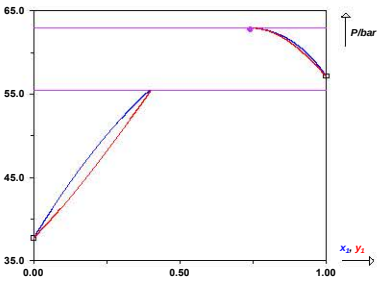

T/K = 292.75



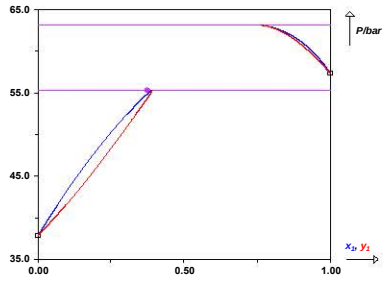

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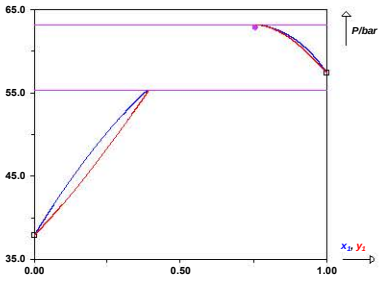

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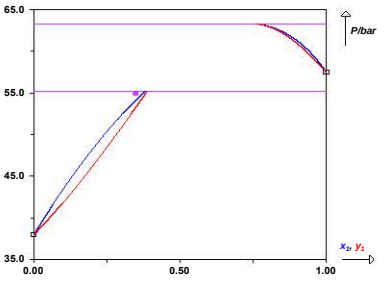

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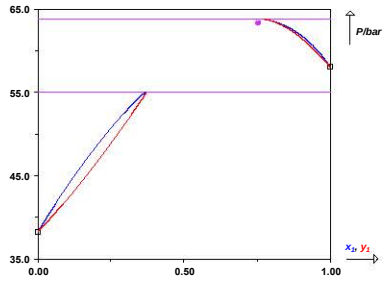

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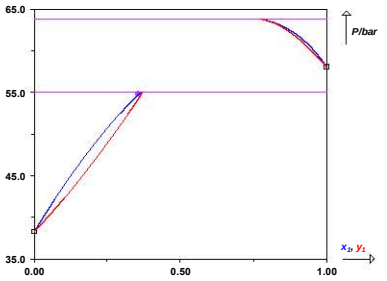

T/K = 293.25



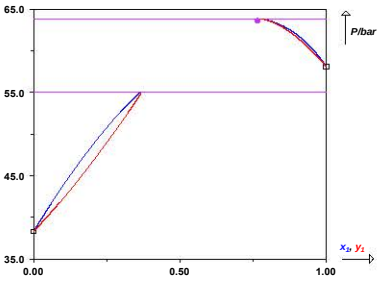
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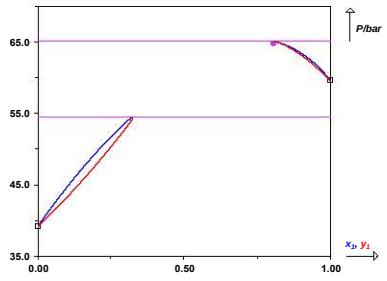

T/K = 293.66



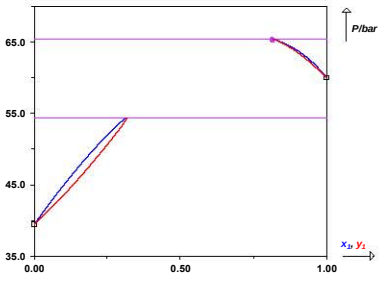

T/K = 293.71



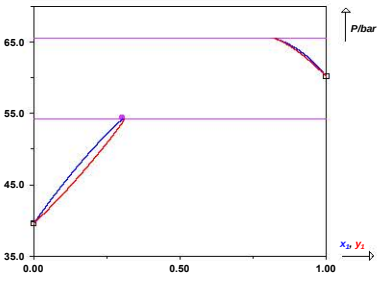

T/K = 294.77



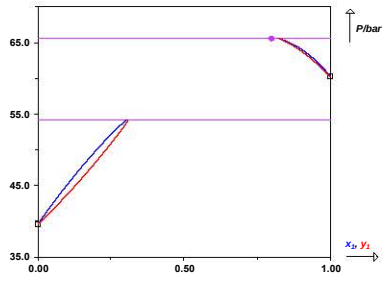

T/K = 295.03



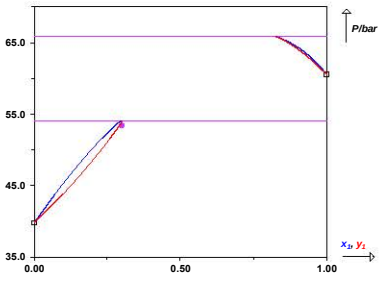

T/K = 295.18



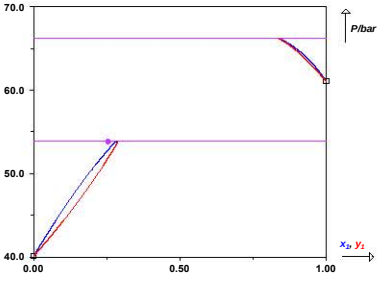

T/K = 295.25



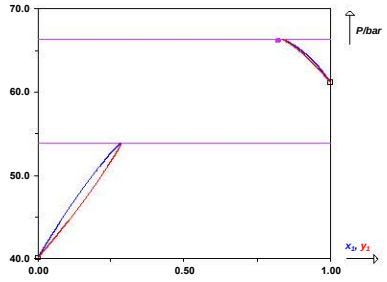

T/K = 295.45



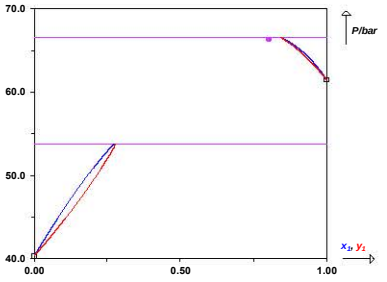

T/K = 295.83



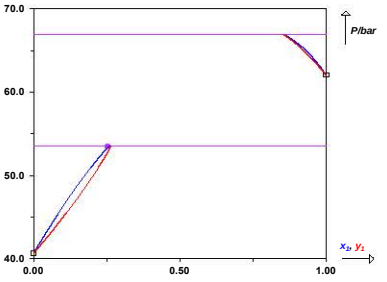

T/K = 295.90



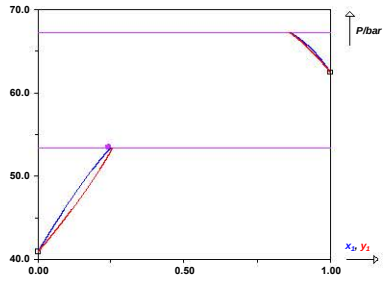

T/K = 296.12



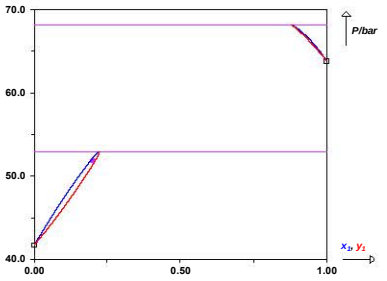

T/K = 296.51



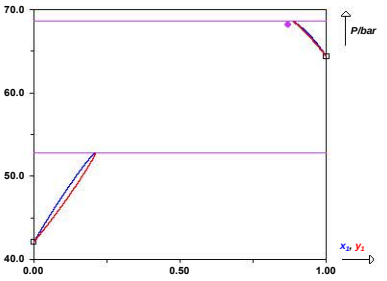

T/K = 296.82



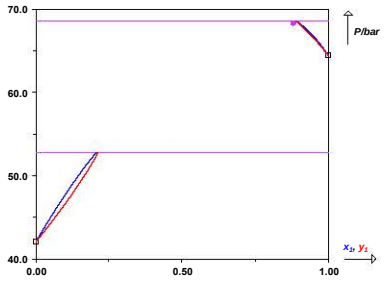

T/K = 297.75



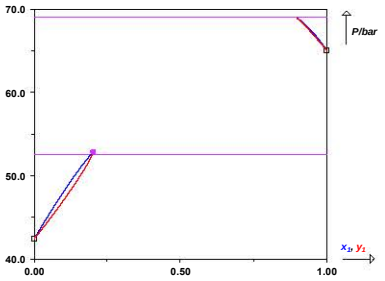

T/K = 298.15



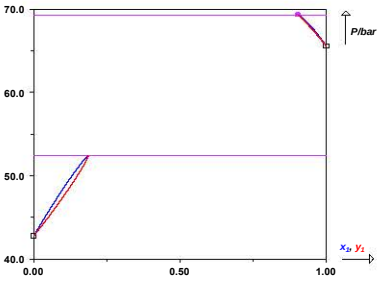
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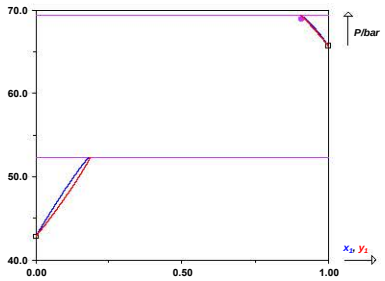

T/K = 298.56



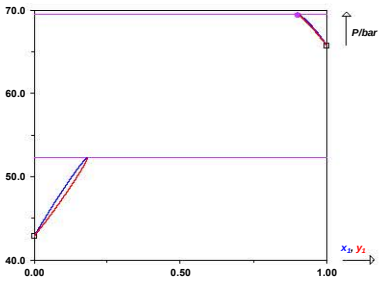

T/K = 298.92



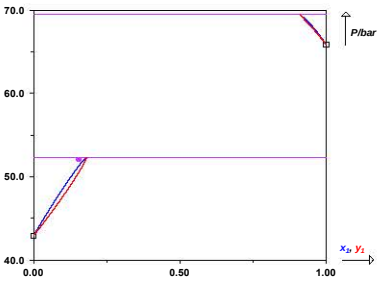

T/K = 299.00



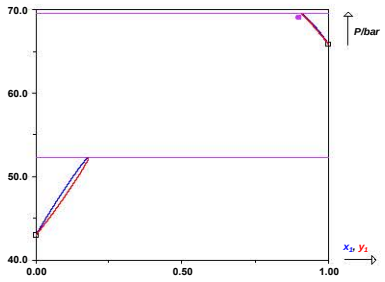

T/K = 299.05



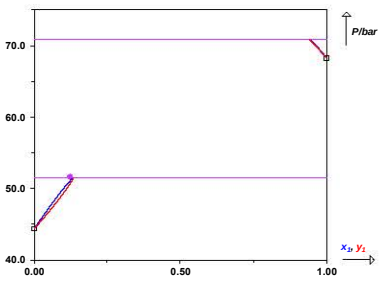

T/K = 299.12



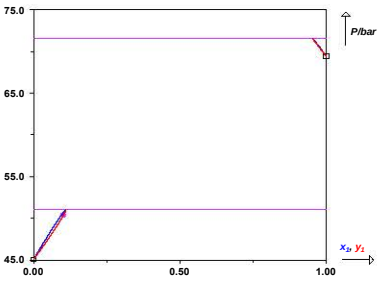

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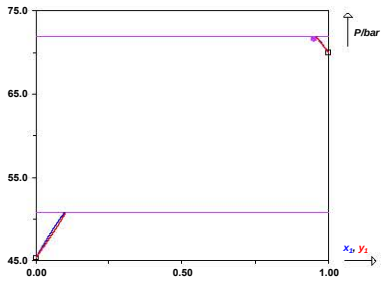

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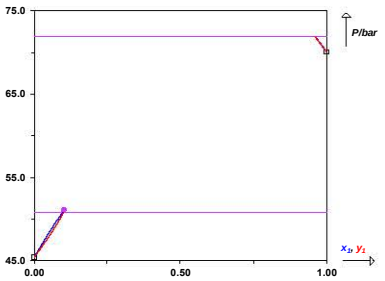

T/K = 301.45



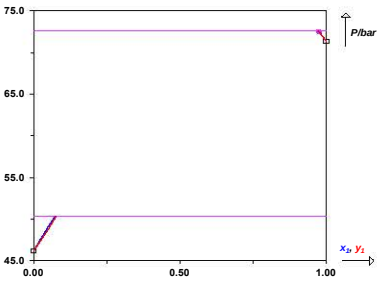

T/K = 301.80



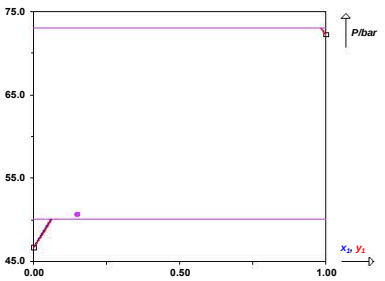

T/K = 301.84



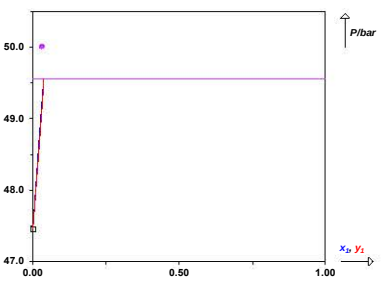

T/K = 302.66




T/K = 303.19




T/K = 304.01



## CARBON DIOXIDE (1) + n-BUTANE (2)

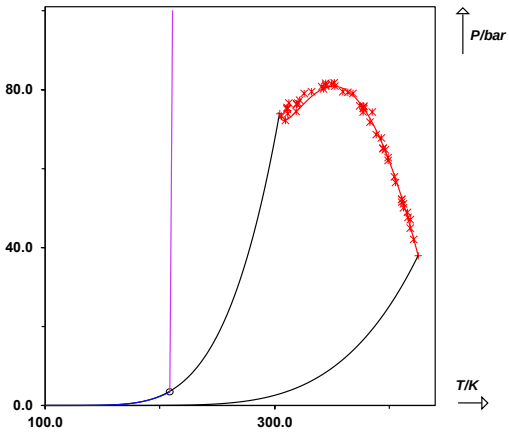
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 106-97-8 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | IJDNQMDRQITEOD-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 425.12 |
| **$P_c$ / bar** | 73.83 | 37.96 |
| **ω** | 0.2240 | 0.2000 |

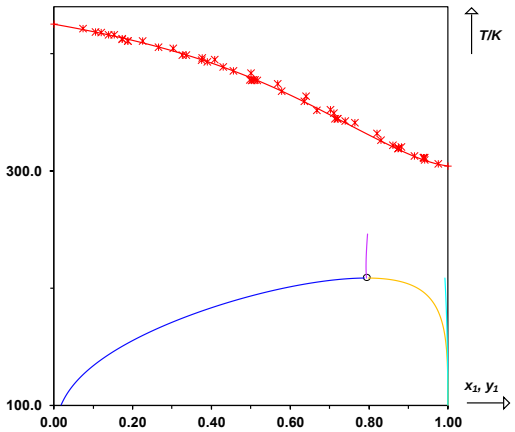
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 390
B/MPa = 578

*Deviations*
MAPE on x = 3.4 %
MAPE on y = 3.1 %
MAPE on $x_c$ = 4.1 %
MAPE on $P_c$ = 1.4 %



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**Isothermal phase equilibrium data**

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Brown, T.S. - Niesen, V.G. - Sloan, E.D. - Kidnay, A.J., Vapor-liquid equilibria for the binary systems of nitrogen, carbon dioxide, and n-butane at temperatures from 220 to 344 K., Fluid Phase Equilibria (1989) 7-14. doi:10.1016/0378-3812(89)80067-6

**T / K = 250.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.760 | 0.0603 | 0.8567 |
| 3.260 | 0.0743 | 0.8775 |
| 4.049 | 0.0972 | 0.9019 |
| 5.253 | 0.1330 | 0.9246 |
| 6.433 | 0.1728 | 0.9384 |
| 8.267 | 0.2407 | 0.9524 |
| 8.425 | 0.2459 | 0.9533 |
| 11.38 | 0.4097 | 0.9673 |
| 12.65 | 0.5063 | 0.9715 |
| 13.53 | 0.5780 | 0.9746 |
| 14.18 | 0.6356 | 0.9768 |
| 14.73 | 0.7003 | 0.9789 |
| 14.76 | 0.7171 | 0.9794 |
| 15.20 | 0.7639 | 0.9810 |
| 15.76 | 0.8229 | 0.9838 |
| 16.45 | 0.9024 | 0.9880 |
| 16.49 | 0.9001 | 0.9873 |

Kalra, Harish - Krishnana, Thamra R. - Robinson, Donald B., Equilibrium-phase properties of carbon dioxide-butane and nitrogen-hydrogen sulfide systems at subambient temperatures, Journal of Chemical & Engineering Data 2 (1976) 222-225. doi:10.1021/je60069a027

**T / K = 255.98**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.048 | 0.0109 | 0.5112 |
| 1.544 | 0.0223 | 0.6634 |
| 2.317 | 0.0387 | 0.7804 |
| 3.475 | 0.0686 | 0.8505 |
| 5.537 | 0.1233 | 0.9104 |
| 7.674 | 0.1888 | 0.9406 |
| 9.742 | 0.2634 | 0.9526 |
| 12.56 | 0.3831 | 0.9654 |
| 14.93 | 0.5225 | 0.9716 |
| 17.64 | 0.7387 | 0.9794 |
| 18.86 | 0.8150 | 0.9833 |

Weber, L.A., Vapour-liquid equilibria measurements for carbon dioxide with normal and isobutane from 250 to 280 K, Cryogenics 6 (1985) 338-342. doi:10.1016/0011-2275(85)90019-0

**T / K = 260.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.070 | 0.0530 | 0.7970 |
| 5.520 | 0.1110 | 0.8860 |
| 7.650 | 0.1670 | 0.9180 |
| 9.110 | 0.2110 | 0.9310 |
| 10.81 | 0.2560 | 0.9420 |
| 12.33 | 0.3230 | 0.9500 |
| 13.93 | 0.3850 | 0.9570 |
| 15.31 | 0.4590 | 0.9610 |
| 16.48 | 0.5200 | 0.9650 |
| 17.32 | 0.5650 | 0.9670 |
| 18.40 | 0.6460 | 0.9710 |
| 19.61 | 0.7340 | 0.9750 |
| 20.50 | 0.8020 | 0.9780 |
| 21.11 | 0.8410 | 0.9800 |
| 21.66 | 0.8740 | 0.9830 |
| 21.98 | 0.9050 | 0.9840 |

Nagahama, Kunio - Konishi, Hitoshi - Hoshino, Daisuke - Hirata, Mitsuho, Binary Vapor-Liquid Equilibria Of Carbon Dioxide-Light Hydrocarbons At Low Temperature, Journal of Chemical Engineering of Japan 5 (1974) 323-328. doi:10.1252/jcej.7.323

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.432 | 0.0300 | 0.5880 |
| 3.952 | 0.0570 | 0.7410 |
| 5.877 | 0.0940 | 0.8260 |
| 8.410 | 0.1440 | 0.8770 |
| 10.74 | 0.2000 | 0.9000 |
| 13.07 | 0.2750 | 0.9160 |
| 15.50 | 0.3340 | 0.9200 |
| 18.04 | 0.3980 | 0.9320 |
| 20.27 | 0.4690 | 0.9420 |
| 23.20 | 0.5680 | 0.9510 |
| 26.04 | 0.6810 | 0.9630 |
| 28.98 | 0.8040 | 0.9740 |
| 31.92 | 0.9110 | 0.9830 |

Weber, L.A., Vapour-liquid equilibria measurements for carbon dioxide with normal and isobutane from 250 to 280 K, Cryogenics 6 (1985) 338-342. doi:10.1016/0011-2275(85)90019-0

**T / K = 280.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.620 | 0.0300 | 0.6180 |
| 4.026 | 0.0420 | 0.6600 |

| | | |
|---|---|---|
| 5.940 | 0.0680 | 0.7640 |
| 5.980 | 0.0720 | 0.7690 |
| 6.240 | 0.0690 | 0.7810 |
| 7.450 | 0.0880 | 0.8130 |
| 12.02 | 0.1750 | 0.8810 |
| 14.30 | 0.2170 | 0.9010 |
| 17.13 | 0.2710 | 0.9170 |
| 23.18 | 0.4400 | 0.9370 |
| 27.05 | 0.5640 | 0.9400 |
| 30.16 | 0.6590 | 0.9470 |
| 32.25 | 0.7310 | 0.9500 |
| 34.18 | 0.8100 | 0.9550 |

Niesen, Vicki G., (Vapor + liquid) equilibria and coexisting densities of (carbon dioxide + n-butane) at 311 to 395 K, The Journal of Chemical Thermodynamics 9 (1989) 915-923. doi:10.1016/0021-9614(89)90150-X

**T / K = 311.09**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.900 | 0.0245 | 0.3711 |
| 7.590 | 0.0444 | 0.4936 |
| 9.880 | 0.0722 | 0.6062 |
| 12.07 | 0.0998 | 0.6768 |
| 14.22 | 0.1227 | 0.7226 |
| 15.28 | 0.1361 | 0.7390 |
| 16.82 | 0.1540 | 0.7623 |
| 17.98 | 0.1675 | 0.7734 |
| 18.51 | 0.1756 | 0.7804 |
| 18.97 | 0.1805 | 0.7862 |
| 20.44 | 0.1998 | 0.7995 |
| 21.97 | 0.2190 | 0.8115 |
| 22.63 | 0.2283 | 0.8157 |
| 23.22 | 0.2352 | 0.8195 |
| 24.69 | 0.2535 | 0.8282 |
| 26.79 | 0.2810 | 0.8394 |
| 27.80 | 0.2948 | 0.8467 |
| 29.99 | 0.3231 | 0.8544 |
| 30.89 | 0.3393 | 0.8568 |
| 32.09 | 0.3552 | 0.8611 |
| 33.39 | 0.3757 | 0.8664 |
| 35.24 | 0.4010 | 0.8725 |
| 37.09 | 0.4255 | 0.8781 |
| 38.35 | 0.4456 | 0.8813 |
| 40.24 | 0.4720 | 0.8865 |
| 41.49 | 0.4903 | 0.8896 |
| 43.15 | 0.5171 | 0.8937 |
| 45.59 | 0.5527 | 0.8994 |
| 47.91 | 0.5873 | 0.9050 |
| 50.25 | 0.6235 | 0.9078 |
| 51.99 | 0.6493 | 0.9099 |
| 53.99 | 0.6806 | 0.9120 |
| 55.81 | 0.7065 | 0.9142 |
| 57.59 | 0.7330 | 0.9165 |
| 60.49 | 0.7723 | 0.9206 |
| 63.03 | 0.8045 | 0.9243 |
| 64.47 | 0.8247 | 0.9265 |
| 66.82 | 0.8527 | 0.9303 |
| 68.19 | 0.8677 | 0.9335 |
| 69.02 | 0.8750 | 0.9354 |
| 69.99 | 0.8866 | 0.9362 |
| 71.16 | 0.8976 | 0.9398 |
| 72.07 | 0.9072 | 0.9415 |
| 73.79 | 0.9240 | 0.9424 |
| 74.55 | 0.9300 | 0.9405 |
| 75.23 | 0.9377 | 0.9377 CRIT |
| 75.23 | 0.9388 | 0.9410 |

Hsu, Jack J. C. - Nagarajan, N. - Robinson, R. L., Equilibrium phase compositions, phase densities, and interfacial tensions for carbon dioxide + hydrocarbon systems. 1. Carbon dioxide + n-butane, Journal of Chemical & Engineering Data 4 (1985) 485-491. doi:10.1021/je00042a036

**T / K = 319.30**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 21.80 | 0.1880 | 0.7450 |
| 25.85 | 0.2320 | 0.7780 |
| 34.25 | 0.3350 | 0.8260 |
| 35.45 | 0.3460 | 0.8300 |
| 42.05 | 0.4280 | 0.8560 |
| 48.95 | 0.5150 | 0.8730 |
| 54.75 | 0.5920 | 0.8850 |
| 66.05 | 0.7350 | 0.8960 |
| 71.55 | 0.8000 | 0.8990 |
| 72.60 | 0.8110 | 0.8980 |
| 73.55 | 0.8240 | 0.8970 |
| 74.35 | 0.8350 | 0.8960 |
| 75.85 | 0.8550 | 0.8880 |
| 76.20 | 0.8640 | 0.8820 |
| 76.40 | 0.8730 | 0.8760 |
| 76.25 | 0.8750 | 0.8750 CRIT |

Pozo de Fernandez, Maria E. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the binary system carbon dioxide + n-butane, Journal of Chemical & Engineering Data 3 (1989) 324-328. doi:10.1021/je00057a019

**T / K = 325.01**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.136 | 0.0288 | 0.2622 |
| 10.34 | 0.0506 | 0.3960 |
| 13.93 | 0.0863 | 0.5577 |
| 17.24 | 0.1204 | 0.6362 |
| 20.68 | 0.1553 | 0.6956 |
| 24.27 | 0.1918 | 0.7325 |
| 27.72 | 0.2273 | 0.7634 |
| 31.03 | 0.2665 | 0.7856 |
| 34.47 | 0.3022 | 0.8034 |
| 38.61 | 0.3497 | 0.8203 |
| 44.89 | 0.4179 | 0.8388 |
| 52.06 | 0.5017 | 0.8544 |
| 58.61 | 0.5789 | 0.8657 |
| 65.64 | 0.6620 | 0.8720 |
| 68.95 | 0.7053 | 0.8722 |
| 72.40 | 0.7433 | 0.8724 |
| 75.57 | 0.7817 | 0.8687 |
| 77.50 | 0.8063 | 0.8608 |

Weber, Lloyd A., Simple apparatus for vapor-liquid equilibrium measurements with data for the binary systems of carbon dioxide with n-butane and isobutane, Journal of Chemical & Engineering Data 2 (1989) 171-175. doi:10.1021/je00056a007

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.330 | 0.0091 | 0.0842 |
| 12.77 | 0.0391 | 0.2980 |
| 13.42 | 0.0446 | 0.3400 |
| 16.38 | 0.0699 | 0.4370 |
| 17.90 | 0.0822 | 0.4770 |
| 20.80 | 0.1083 | 0.5367 |
| 25.83 | 0.1520 | 0.6120 |
| 27.40 | 0.1660 | 0.6290 |
| 31.07 | 0.1980 | 0.6630 |
| 40.56 | 0.2820 | 0.7210 |
| 47.93 | 0.3510 | 0.7580 |
| 57.92 | 0.4430 | 0.7800 |
| 62.30 | 0.4830 | 0.7840 |
| 67.53 | 0.5350 | 0.7910 |
| 72.92 | 0.5900 | 0.7920 |
| 76.98 | 0.6320 | 0.7840 |
| 79.44 | 0.6640 | 0.7740 |
| 80.46 | 0.6810 | 0.7580 |
| 81.10 | 0.6940 | 0.7460 |

Olds, R. H. - Reamer, H. H. - Sage, B. H. - Lacey, W. N., The n-Butane–Carbon Dioxide System, Industrial & Engineering Chemistry 3 (1949) 475-482. doi:10.1021/ie50471a011

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 8.619 | 0.0020 | 0.0300 | |
| 10.34 | 0.0170 | 0.1730 | |
| 12.07 | 0.0310 | 0.2770 | |
| 13.79 | 0.0450 | 0.3550 | |
| 17.24 | 0.0740 | 0.4620 | |
| 20.68 | 0.1030 | 0.5360 | |
| 24.13 | 0.1320 | 0.5920 | |
| 27.58 | 0.1620 | 0.6350 | |
| 31.03 | 0.1920 | 0.6680 | |
| 34.47 | 0.2220 | 0.6940 | |
| 41.37 | 0.2830 | 0.7320 | |
| 48.26 | 0.3450 | 0.7540 | |
| 55.16 | 0.4090 | 0.7700 | |
| 62.05 | 0.4740 | 0.7800 | |
| 68.95 | 0.5430 | 0.7840 | |
| 75.84 | 0.6180 | 0.7780 | |
| 79.29 | 0.6610 | 0.7580 | |
| 81.63 | 0.7130 | 0.7130 | CRIT |

Olds, R. H. - Reamer, H. H. - Sage, B. H. - Lacey, W. N., The n-Butane–Carbon Dioxide System, Industrial & Engineering Chemistry 3 (1949) 475-482. doi:10.1021/ie50471a011

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 8.619 | 0.0020 | 0.0300 | |
| 10.34 | 0.0170 | 0.1730 | |
| 12.07 | 0.0310 | 0.2770 | |
| 13.79 | 0.0450 | 0.3550 | |
| 17.24 | 0.0740 | 0.4620 | |
| 20.69 | 0.1030 | 0.5360 | |
| 24.13 | 0.1320 | 0.5920 | |
| 27.58 | 0.1620 | 0.6350 | |
| 31.03 | 0.1920 | 0.6680 | |
| 34.48 | 0.2220 | 0.6940 | |
| 41.37 | 0.2830 | 0.7320 | |
| 48.26 | 0.3450 | 0.7540 | |
| 55.16 | 0.4090 | 0.7700 | |
| 62.05 | 0.4740 | 0.7800 | |
| 68.95 | 0.5430 | 0.7840 | |
| 75.84 | 0.6180 | 0.7780 | |
| 79.29 | 0.6610 | 0.7580 | |
| 81.63 | 0.7130 | 0.7130 | CRIT |

Pozo de Fernandez, Maria E. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the

binary system carbon dioxide + n-butane, Journal of Chemical & Engineering Data 3 (1989) 324-328. doi:10.1021/je00057a019

**T / K = 357.77**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 14.82 | 0.0297 | 0.2165 | |
| 19.03 | 0.0623 | 0.3622 | |
| 23.51 | 0.0959 | 0.4577 | |
| 27.44 | 0.1283 | 0.5182 | |
| 31.16 | 0.1567 | 0.5645 | |
| 36.40 | 0.1964 | 0.6028 | |
| 42.89 | 0.2503 | 0.6469 | |
| 49.57 | 0.3042 | 0.6785 | |
| 56.40 | 0.3590 | 0.6973 | |
| 63.57 | 0.4187 | 0.7107 | |
| 70.67 | 0.4926 | 0.7139 | |
| 75.43 | 0.5352 | 0.7116 | |
| 77.91 | 0.5647 | 0.6986 | |
| 79.29 | 0.5745 | 0.6893 | |

Leu, Ah Dong - Robinson, Donald B., Equilibrium phase properties of the n-butane-carbon dioxide and isobutane-carbon dioxide binary systems, Journal of Chemical & Engineering Data 4 (1987) 444-447. doi:10.1021/je00050a017

**T / K = 368.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 15.31 | 0.0099 | 0.0764 | |
| 17.37 | 0.0243 | 0.1683 | |
| 20.82 | 0.0478 | 0.2750 | |
| 26.41 | 0.0878 | 0.4026 | |
| 35.30 | 0.1568 | 0.5225 | |
| 50.06 | 0.2631 | 0.6286 | |
| 64.05 | 0.3782 | 0.6652 | |
| 71.02 | 0.4320 | 0.6643 | |
| 74.60 | 0.4811 | 0.6571 | |
| 77.98 | 0.5394 | 0.6206 | |
| 79.01 | 0.5783 | 0.5783 | CRIT |

Hsu, Jack J. C. - Nagarajan, N. - Robinson, R. L., Equilibrium phase compositions, phase densities, and interfacial tensions for carbon dioxide + hydrocarbon systems. 1. Carbon dioxide + n-butane, Journal of Chemical & Engineering Data 4 (1985) 485-491. doi:10.1021/je00042a036

**T / K = 377.60**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 28.80 | 0.0880 | 0.3400 | |
| 34.35 | 0.1290 | 0.4140 | |
| 41.65 | 0.1810 | 0.4810 | |
| 48.40 | 0.2300 | 0.5250 | |
| 55.45 | 0.2840 | 0.5560 | |
| 59.50 | 0.3150 | 0.5650 | |
| 62.65 | 0.3410 | 0.5710 | |
| 66.00 | 0.3680 | 0.5750 | |
| 69.15 | 0.3980 | 0.5730 | |
| 70.20 | 0.4060 | 0.5720 | |
| 71.75 | 0.4230 | 0.5690 | |
| 72.95 | 0.4340 | 0.5650 | |
| 74.25 | 0.4520 | 0.5540 | |
| 75.30 | 0.4730 | 0.5390 | |
| 75.65 | 0.4850 | 0.5270 | |
| 75.80 | 0.5100 | 0.5100 | CRIT |

Pozo de Fernandez, Maria E. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the binary system carbon dioxide + n-butane, Journal of Chemical & Engineering Data 3 (1989) 324-328. doi:10.1021/je00057a019

**T / K = 387.62**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 26.27 | 0.0424 | 0.1789 |
| 29.79 | 0.0673 | 0.2425 |
| 35.99 | 0.1072 | 0.3283 |
| 41.51 | 0.1503 | 0.3858 |
| 46.33 | 0.1823 | 0.4213 |
| 51.37 | 0.2175 | 0.4483 |
| 56.12 | 0.2544 | 0.4691 |
| 62.12 | 0.3059 | 0.4812 |
| 64.95 | 0.3280 | 0.4811 |
| 67.22 | 0.3528 | 0.4750 |
| 68.05 | 0.3590 | 0.4685 |

Leu, Ah Dong - Robinson, Donald B., Equilibrium phase properties of the n-butane-carbon dioxide and isobutane-carbon dioxide binary systems, Journal of Chemical & Engineering Data 4 (1987) 444-447. doi:10.1021/je00050a017

**T / K = 393.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 23.92 | 0.0109 | 0.0506 | |
| 25.92 | 0.0236 | 0.1016 | |
| 29.51 | 0.0496 | 0.1828 | |
| 34.82 | 0.0844 | 0.2661 | |
| 43.99 | 0.1480 | 0.3686 | |
| 59.36 | 0.2670 | 0.4495 | |
| 65.36 | 0.3293 | 0.4422 | |
| 65.84 | 0.3361 | 0.4304 | |
| 67.71 | 0.3895 | 0.3895 | CRIT |

Niesen, Vicki G., (Vapor + liquid) equilibria and coexisting densities of (carbon dioxide + n-butane) at 311 to 395 K, The Journal of Chemical Thermodynamics 9 (1989) 915-923. doi:10.1016/0021-9614(89)90150-X

**T / K = 394.60**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 24.79 | 0.0110 | 0.0678 |
| 25.28 | 0.0156 | 0.0779 |
| 27.81 | 0.0321 | 0.1440 |
| 29.37 | 0.0440 | 0.1736 |
| 31.18 | 0.0560 | 0.2051 |
| 33.11 | 0.0687 | 0.2344 |
| 34.25 | 0.0769 | 0.2511 |
| 38.48 | 0.1082 | 0.3025 |
| 40.41 | 0.1224 | 0.3165 |
| 42.82 | 0.1379 | 0.3421 |
| 44.62 | 0.1515 | 0.3542 |
| 46.84 | 0.1685 | 0.3694 |
| 48.66 | 0.1822 | 0.3808 |
| 51.24 | 0.2016 | 0.3940 |
| 53.12 | 0.2180 | 0.4014 |
| 54.47 | 0.2273 | 0.4070 |
| 56.68 | 0.2440 | 0.4121 |
| 58.28 | 0.2573 | 0.4144 |
| 59.78 | 0.2721 | 0.4170 |
| 61.29 | 0.2867 | 0.4142 |
| 63.18 | 0.3086 | 0.4084 |
| 64.14 | 0.3230 | 0.3971 |
| 64.71 | 0.3342 | 0.3918 |
| 65.09 | 0.3535 | 0.3879 |

Olds, R. H. - Reamer, H. H. - Sage, B. H. - Lacey, W. N., The n-Butane–Carbon Dioxide System, Industrial & Engineering Chemistry 3 (1949) 475-482. doi:10.1021/ie50471a011

**T / K = 410.93**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 31.03 | 0.0060 | 0.0190 | |
| 34.48 | 0.0270 | 0.0770 | |
| 37.92 | 0.0490 | 0.1240 | |
| 41.37 | 0.0730 | 0.1610 | |
| 44.82 | 0.1000 | 0.1910 | |
| 48.26 | 0.1310 | 0.2100 | |
| 51.71 | 0.1690 | 0.2050 | |
| 52.26 | 0.1880 | 0.1880 | CRIT |

Leu, Ah Dong - Robinson, Donald B., Equilibrium phase properties of the n-butane-carbon dioxide and isobutane-carbon dioxide binary systems, Journal of Chemical & Engineering Data 4 (1987) 444-447. doi:10.1021/je00050a017

**T / K = 418.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 34.82 | 0.0131 | 0.0320 | |
| 37.16 | 0.0282 | 0.0632 | |
| 40.20 | 0.0494 | 0.0959 | |
| 43.58 | 0.0756 | 0.1209 | |
| 44.95 | 0.0858 | 0.1277 | |
| 46.26 | 0.1030 | 0.1314 | |
| 47.02 | 0.1206 | 0.1206 | CRIT |

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**Isobaric phase equilibrium data**

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Pozo de Fernandez, Maria E. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the binary system carbon dioxide + n-butane, Journal of Chemical & Engineering Data 3 (1989) 324-328. doi:10.1021/je00057a019

**P / bar = 41.37**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 418.48 | 0.0500 | 0.0870 |
| 410.93 | 0.0720 | 0.1610 |
| 397.89 | 0.1180 | 0.2840 |
| 387.62 | 0.1480 | 0.3850 |
| 377.55 | 0.1750 | 0.4810 |
| 357.17 | 0.2380 | 0.6380 |
| 344.25 | 0.2820 | 0.7220 |
| 325.01 | 0.3850 | 0.8250 |
| 292.60 | 0.7230 | 0.9450 |

Pozo de Fernandez, Maria E. - Zollweg, John A. - Streett, William B., Vapor-liquid equilibrium in the binary system carbon dioxide + n-butane, Journal of Chemical & Engineering Data 3 (1989) 324-328. doi:10.1021/je00057a019

**P / bar = 62.05**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 397.89 | 0.2750 | 0.3690 |
| 387.62 | 0.3000 | 0.4800 |
| 377.55 | 0.3260 | 0.5690 |
| 357.17 | 0.4090 | 0.7060 |
| 344.25 | 0.4730 | 0.7700 |
| 325.01 | 0.6200 | 0.8690 |

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**Critical point**

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Poettmann, Fred H. - Katz, D. L., Phase Behavior of Binary Carbon Dioxide-Paraffin Systems, Industrial &

Engineering Chemistry 9 (1945) 847-853. doi:10.1021/ie50429a017

| T / K | P / bar | $x_1$ |
|---|---|---|
| 385.09 | 74.26 | 0.4551 |
| 349.26 | 81.43 | 0.7102 |
| 321.76 | 77.36 | 0.8609 |
| 396.48 | 64.81 | 0.3761 |
| 415.82 | 48.88 | 0.1393 |

Morrison, G. - Kincaid, J. M., Critical point measurements on nearly polydisperse fluids, AIChE Journal 2 (1984) 257-262. doi:10.1002/aic.690300213

| T / K | P / bar | $x_1$ |
|---|---|---|
| 306.15 | 73.36 | 0.9748 |
| 312.48 | 76.63 | 0.9144 |

Van Poolen, Lambert J. - Holcomb, Cynthia D., Critical temperatures, pressures, and densities for the mixtures CO2–C3H8, CO2–nC4H10, C2H6–C3H8, and C3H8–nC4H10, Fluid Phase Equilibria 2 (1999) 157-168. doi:10.1016/S0378-3812(99)00275-7

| T / K | P / bar | $x_1$ |
|---|---|---|
| 311.08 | 75.10 | 0.9403 |
| 319.29 | 76.27 | 0.8741 |
| 344.41 | 80.85 | 0.7190 |
| 377.57 | 75.77 | 0.5067 |
| 394.57 | 65.00 | 0.3746 |
| 410.90 | 51.49 | 0.1883 |

Juntarachat, Niramol - Bello, Salma - Privat, Romain - Jaubert, Jean-Noël, Validation of a New Apparatus Using the Dynamic Method for Determining the Critical Properties of Binary Gas/Gas Mixtures, Journal of Chemical & Engineering Data 3 (2013) 671-676. doi:10.1021/je301209u

| T / K | P / bar | $x_1$ |
|---|---|---|
| 418.38 | 44.94 | 0.1052 |
| 412.48 | 50.00 | 0.1736 |
| 405.58 | 56.42 | 0.2651 |
| 398.71 | 62.04 | 0.3365 |
| 388.66 | 68.68 | 0.4303 |
| 377.29 | 74.26 | 0.5160 |
| 359.42 | 79.44 | 0.6355 |
| 342.29 | 80.12 | 0.7394 |
| 318.81 | 74.49 | 0.8732 |
| 309.41 | 72.24 | 0.9403 |

Horstmann, S. - Fischer, K. - Gmehling, J., Experimental Determination of Critical Points of Pure Components and Binary Mixtures Using a Flow Apparatus, Chemical Engineering & Technology 10 (1999) 839-842. doi:10.1002/(SICI)1521-4125(199910)22:10<839::AID-CEAT839>3.0.CO;2-L

| T / K | P / bar | $x_1$ |
|---|---|---|
| 421.28 | 42.10 | 0.0743 |
| 416.09 | 47.65 | 0.1533 |
| 410.60 | 52.26 | 0.2248 |
| 404.39 | 57.95 | 0.3025 |
| 394.68 | 65.13 | 0.4076 |
| 383.17 | 71.79 | 0.5008 |
| 374.35 | 75.95 | 0.5676 |
| 363.71 | 79.32 | 0.6403 |
| 352.20 | 80.94 | 0.7021 |
| 341.13 | 80.75 | 0.7637 |
| 331.99 | 79.41 | 0.8195 |
| 320.20 | 76.60 | 0.8814 |
| 311.42 | 73.96 | 0.9386 |

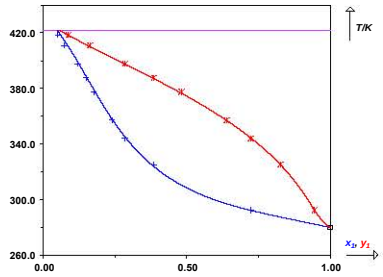
Olds, R. H. - Reamer, H. H. - Sage, B. H. - Lacey, W. N., The n-Butane–Carbon Dioxide System, Industrial & Engineering Chemistry 3 (1949) 475-482. doi:10.1021/ie50471a011

| T / K | P / bar | $x_1$ |
|---|---|---|
| 310.93 | 75.50 | 0.9400 |
| 377.59 | 75.15 | 0.4980 |
| 325.93 | 79.08 | 0.8306 |
| 351.71 | 81.70 | 0.6666 |
| 377.21 | 75.36 | 0.5016 |
| 398.76 | 62.81 | 0.3260 |
| 412.26 | 51.09 | 0.1727 |

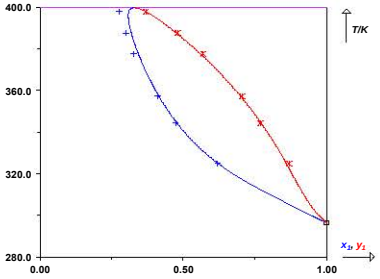
Hsu, Jack J. C. - Nagarajan, N. - Robinson, R. L., Equilibrium phase compositions, phase densities, and interfacial tensions for carbon dioxide + hydrocarbon systems. 1. Carbon dioxide + n-butane, Journal of Chemical & Engineering Data 4 (1985) 485-491. doi:10.1021/je00042a036

| T / K | P / bar | $x_1$ |
|---|---|---|
| 319.26 | 76.26 | 0.8750 |
| 344.26 | 81.22 | 0.7200 |

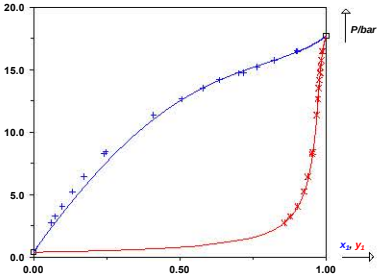
P/bar = 41.37000



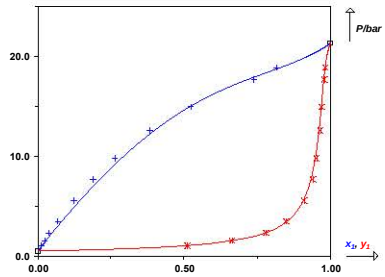

P/bar = 62.05000



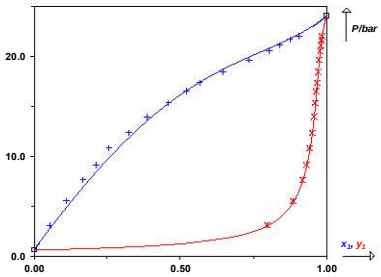

T/K = 250.00



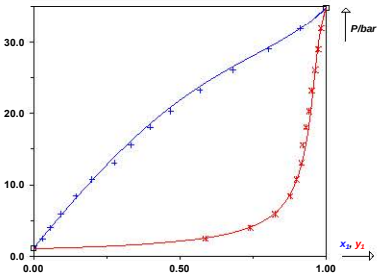

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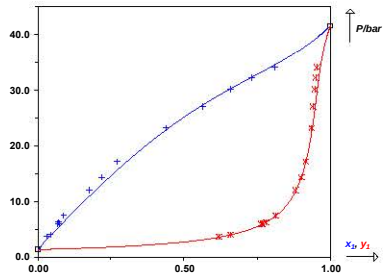

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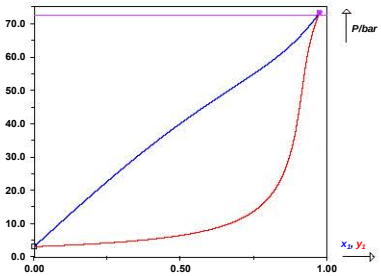

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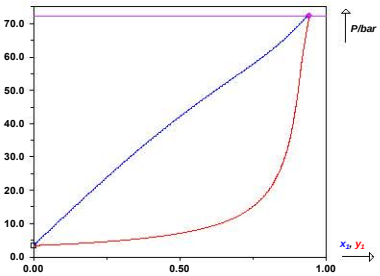

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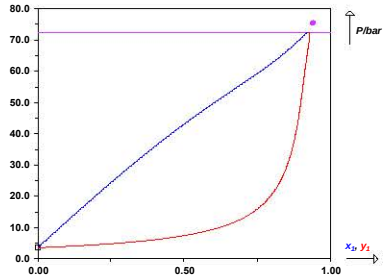

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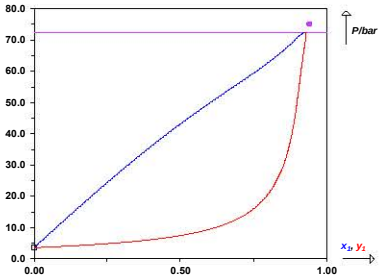

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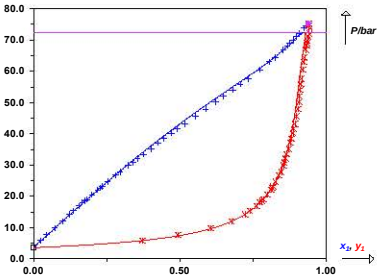

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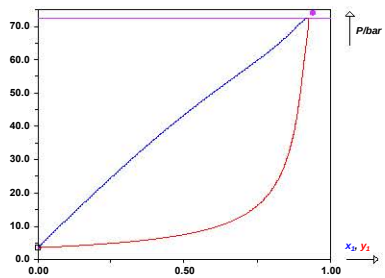

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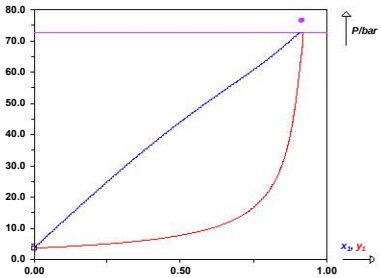

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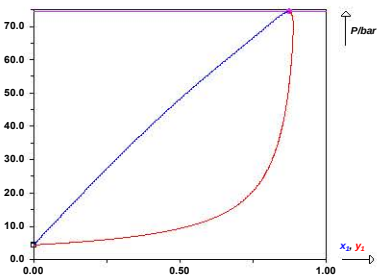

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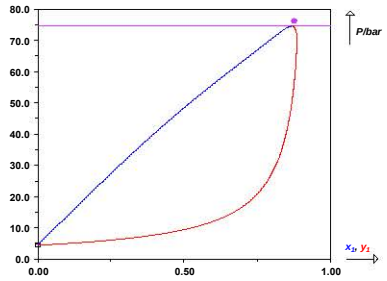

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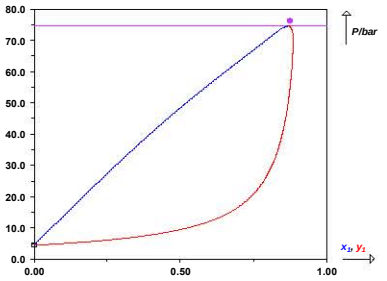

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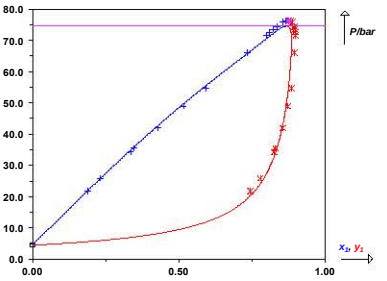
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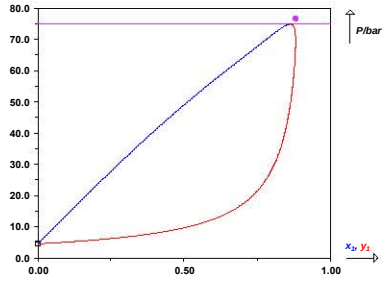

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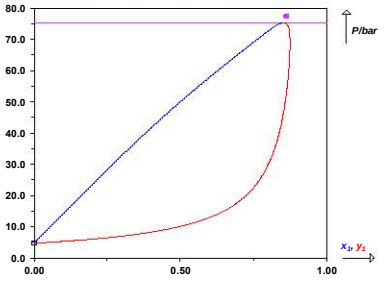

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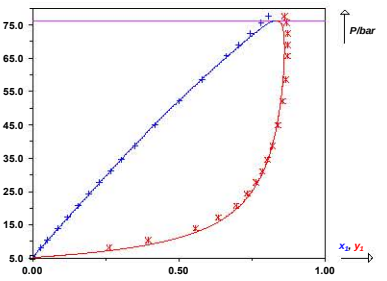

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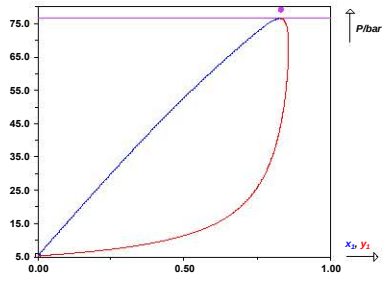

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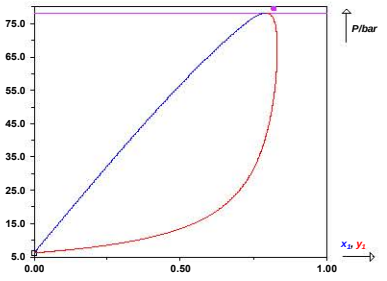

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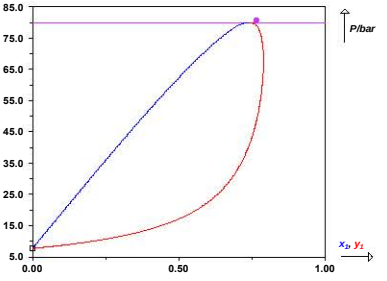

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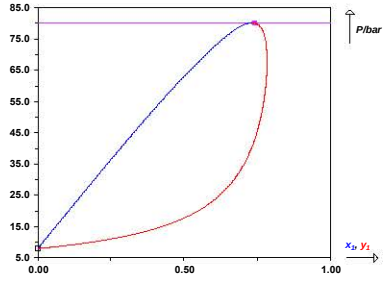

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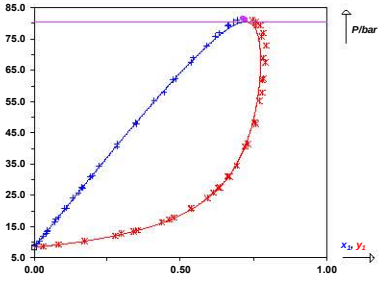

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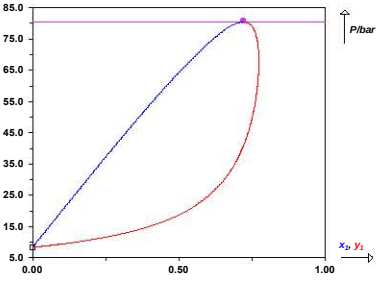

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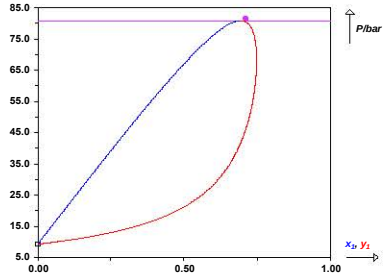

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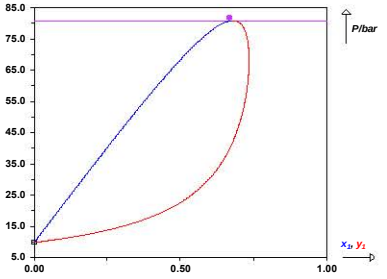

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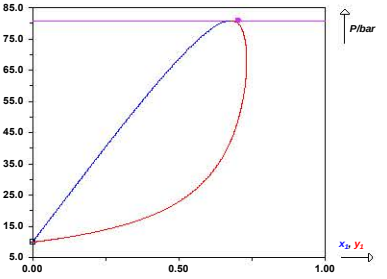

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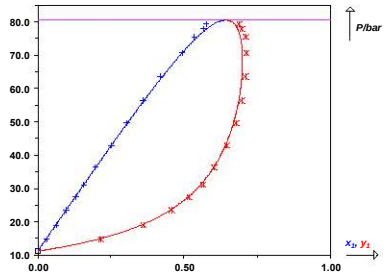

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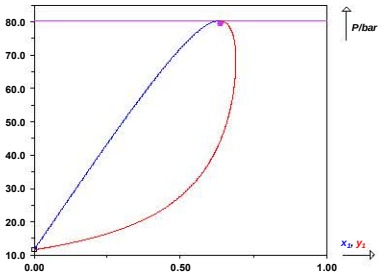

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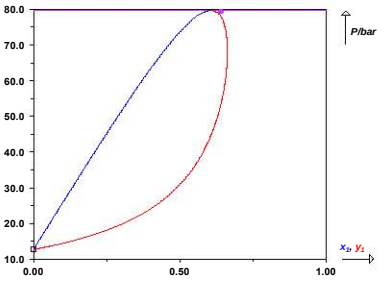
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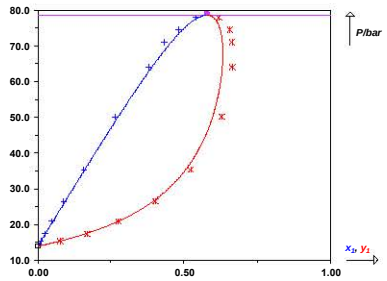

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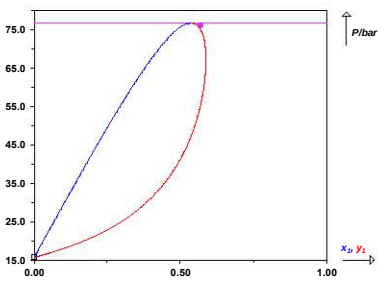

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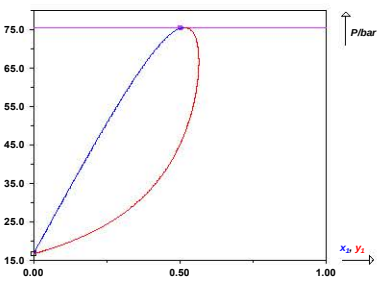

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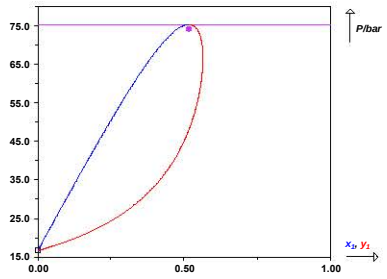

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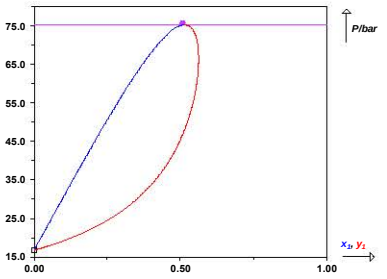

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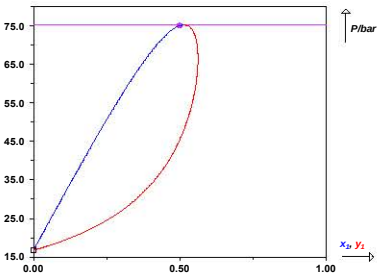

T/K = 377.29



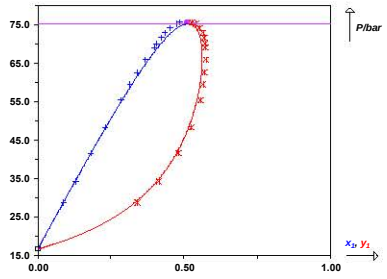

T/K = 377.57



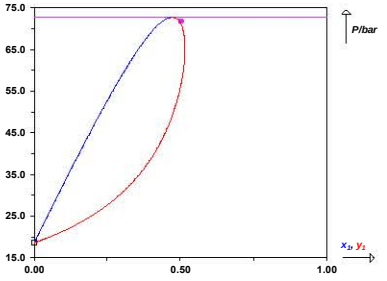

T/K = 377.59



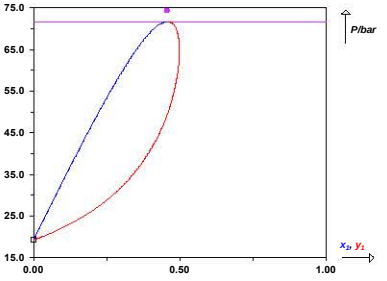

T/K = 377.60



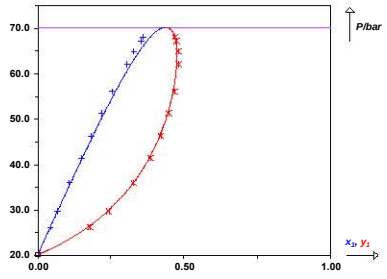

T/K = 383.17



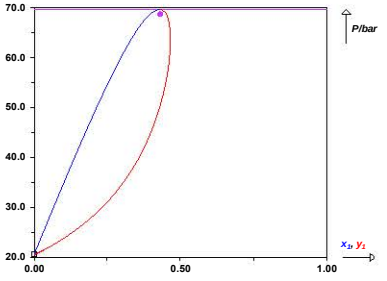

T/K = 385.09



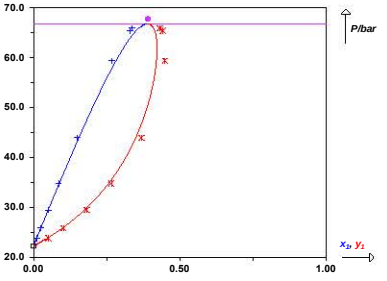

T/K = 387.62



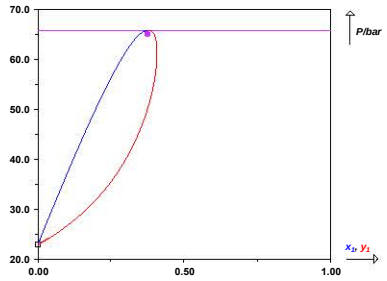

T/K = 388.66



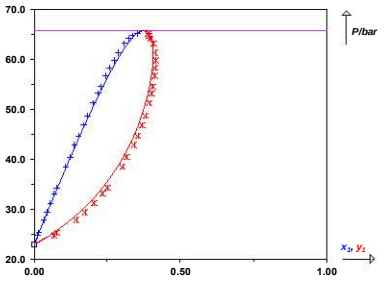

T/K = 393.15



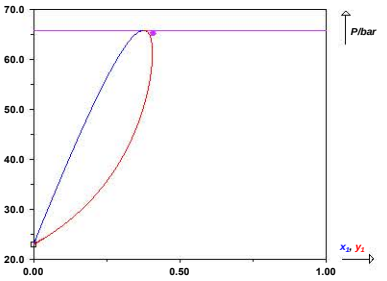
T/K = 394.57



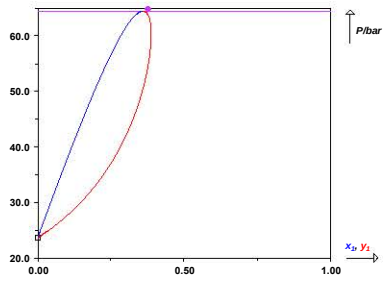

T/K = 394.60



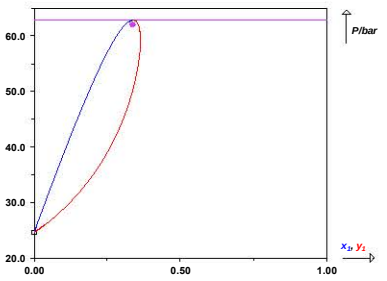

T/K = 394.68



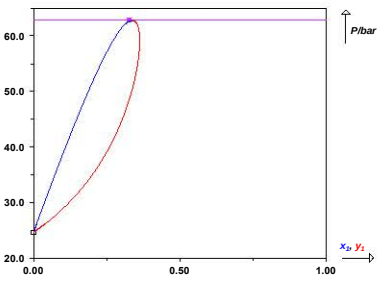

T/K = 396.48



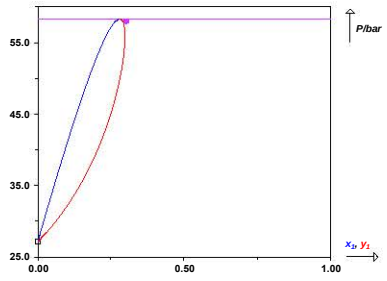

T/K = 398.71



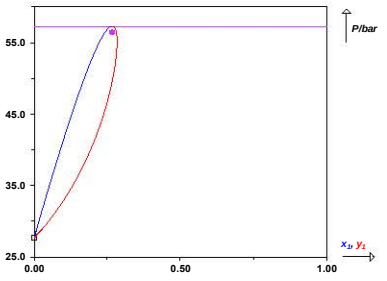

T/K = 398.76



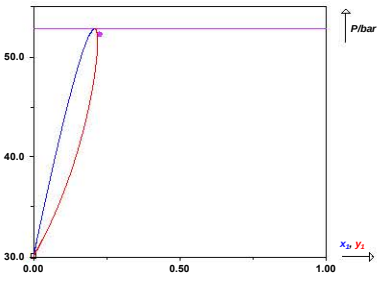

T/K = 404.39



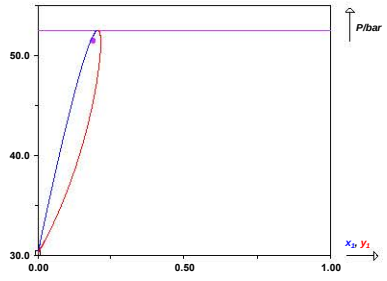

T/K = 405.58



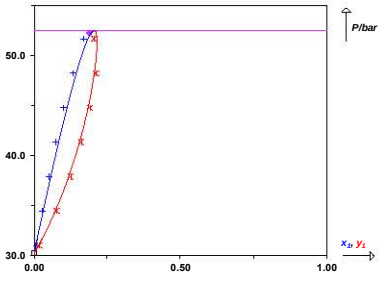

T/K = 410.60



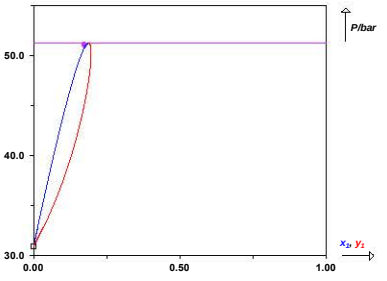

T/K = 410.90

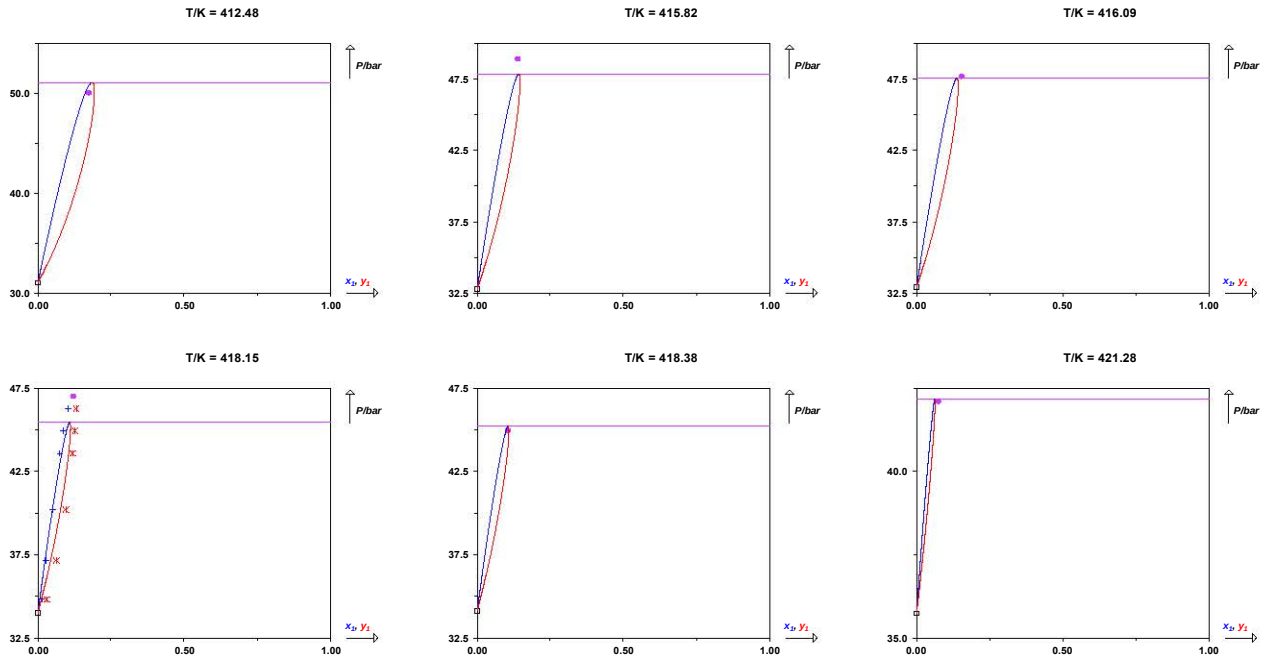



T/K = 410.93




T/K = 412.26




T/K = 412.48
P/bar
50.0
40.0
30.0
0.00
0.50
1.00
x1, y1
T/K = 415.82
P/bar
47.5
42.5
37.5
32.5
0.00
0.50
1.00
x1, y1
T/K = 416.09
P/bar
47.5
42.5
37.5
32.5
0.00
0.50
1.00
x1, y1
T/K = 418.15
P/bar
47.5
42.5
37.5
32.5
0.00
0.50
1.00
x1, y1
T/K = 418.38
P/bar
47.5
42.5
37.5
32.5
0.00
0.50
1.00
x1, y1
T/K = 421.28
P/bar
40.0
35.0
0.00
0.50
1.00
x1, y1

## n-HEXANE (1) + METHYL ETHYL KETONE (2)

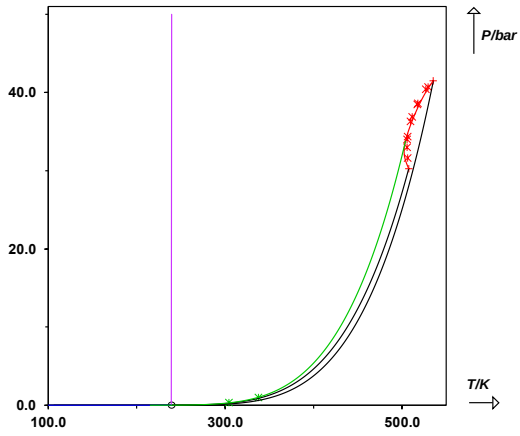
| | | |
|---|---|---|
| **CAS** | 110-54-3 | 78-93-3 |
| **InChiKey** | VLKZOEOYAKHREP-UHFFFAOYSA-N | ZWEHNKRNPOVVGH-UHFFFAOYSA-N |
| **$T_c$ / K** | 507.60 | 535.50 |
| **$P_c$ / bar** | 30.25 | 41.50 |
| **ω** | 0.3010 | 0.3230 |

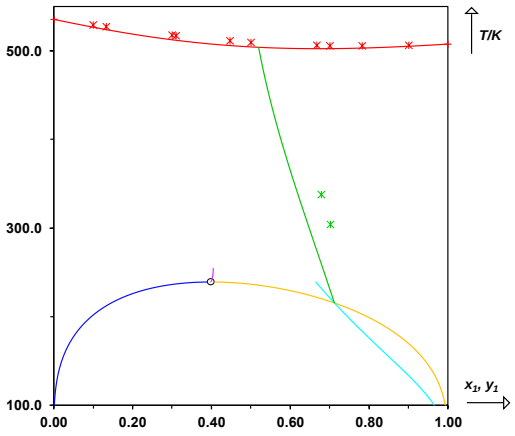
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 208
B/MPa = 238

*Deviations*
MAPE on x = 15 %
MAPE on y = 9.7 %
MAPE on $x_c$ = 21 %
MAPE on $P_c$ = 1.2 %
MAPE on $x_{az}$ = 13 %
MAPE on $P_{az}$ = 0.53 %
MAPE on $h^M$ = 13 %



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**Isothermal phase equilibrium data**

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Hanson, Donald O. - Van Winkle, Matthew, Alteration of the relative volatility of hexane-1-hexene by oxygenated and chlorinated solvents, Journal of Chemical & Engineering Data 3 (1967) 319-325. doi:10.1021/je60034a009

**T / K =** **333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.6690 | 0.0950 | 0.2820 |
| 0.6702 | 0.0980 | 0.2880 |
| 0.7587 | 0.1970 | 0.4190 |
| 0.8078 | 0.2820 | 0.4840 |
| 0.8466 | 0.3950 | 0.5500 |
| 0.8643 | 0.4790 | 0.5970 |
| 0.8758 | 0.5560 | 0.6260 |
| 0.8815 | 0.7160 | 0.6970 |
| 0.8725 | 0.8030 | 0.7480 |
| 0.8553 | 0.8720 | 0.8040 |
| 0.8343 | 0.9160 | 0.8540 |
| 0.8030 | 0.9610 | 0.9170 |

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**Isobaric phase equilibrium data**

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Lladosa, Estela - Martínez, Nelson F. - Montón, Juan B. - de la Torre, Javier, Measurements and correlation of vapour–liquid equilibria of 2-butanone and hydrocarbons binary systems at two different pressures, Fluid Phase Equilibria 1 (2011) 24-29. doi:10.1016/j.fluid.2011.05.004

**P / bar =** **0.3000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 317.76 | 0.0100 | 0.0560 |
| 313.80 | 0.0520 | 0.2180 |
| 310.48 | 0.1080 | 0.3480 |
| 308.23 | 0.1700 | 0.4340 |
| 306.78 | 0.2390 | 0.4950 |
| 305.54 | 0.3170 | 0.5390 |
| 304.94 | 0.3860 | 0.5800 |
| 304.43 | 0.4590 | 0.6080 |
| 304.08 | 0.5370 | 0.6360 |
| 303.91 | 0.6160 | 0.6650 |
| 303.83 | 0.6970 | 0.6960 |
| 303.93 | 0.7780 | 0.7330 |
| 304.38 | 0.8580 | 0.7830 |
| 305.40 | 0.9310 | 0.8680 |

Lladosa, Estela - Martínez, Nelson F. - Montón, Juan B. - de la Torre, Javier, Measurements and correlation of vapour–liquid equilibria of 2-butanone and hydrocarbons binary systems at two different pressures, Fluid Phase Equilibria 1 (2011) 24-29. doi:10.1016/j.fluid.2011.05.004

**P / bar =** **1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 352.40 | 0.0020 | 0.0090 |
| 347.18 | 0.0710 | 0.2210 |
| 344.15 | 0.1320 | 0.3330 |
| 341.97 | 0.1970 | 0.4120 |
| 340.45 | 0.2620 | 0.4650 |
| 339.36 | 0.3280 | 0.5110 |
| 338.54 | 0.3990 | 0.5500 |
| 337.95 | 0.4740 | 0.5840 |
| 337.59 | 0.5530 | 0.6190 |
| 337.38 | 0.6280 | 0.6520 |
| 337.42 | 0.7060 | 0.6910 |
| 337.64 | 0.7830 | 0.7350 |
| 338.30 | 0.8600 | 0.7920 |
| 339.60 | 0.9330 | 0.8760 |

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**Enthalpy of mixing**

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Murakami, Sachio - Amaya, Kazuo - Fujishiro, Ryoichi, Heats of Mixing for Binary Mixtures. The Energy of Hydrogen Bonding between Alcohol and Ketone Molecules, Bulletin of the Chemical Society of Japan 12 (1964) 1776-1780. doi:10.1246/bcsj.37.1776

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 946.63 | 0.2475 |
| 1245.2 | 0.4453 |
| 1267.3 | 0.5658 |
| 1162.3 | 0.6695 |
| 984.74 | 0.7602 |
| 687.47 | 0.8576 |
| 495.30 | 0.9181 |
| 354.62 | 0.9437 |

Grauer, F. - Kertes, A. S., Heats of mixing of tri-n-dodecylamine with n-octane, benzene, or chlorobenzene, Journal of Chemical & Engineering Data 4 (1973) 405-407. doi:10.1021/je60059a032

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 233.80 | 0.0500 |
| 442.30 | 0.1000 |
| 625.80 | 0.1500 |

| | |
|---|---|
| 782.50 | 0.2000 |
| 915.50 | 0.2500 |
| 1026.9 | 0.3000 |
| 1114.7 | 0.3500 |
| 1182.8 | 0.4000 |
| 1228.9 | 0.4500 |
| 1252.4 | 0.5000 |
| 1259.1 | 0.5500 |
| 1240.2 | 0.6000 |
| 1200.1 | 0.6500 |
| 1136.4 | 0.7000 |
| 1045.4 | 0.7500 |
| 925.10 | 0.8000 |
| 765.90 | 0.8500 |
| 567.50 | 0.9000 |
| 319.70 | 0.9500 |

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**Critical point**

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Kreglewski, Aleksander - Kay, Webster B., Critical constants of conformed mixtures, The Journal of Physical Chemistry 10 (1969) 3359-3366. doi:10.1021/j100844a035

| T / K | P / bar | $x_1$ |
|---|---|---|
| 506.05 | 31.65 | 0.9000 |
| 505.75 | 33.99 | 0.7000 |
| 509.65 | 36.27 | 0.5000 |
| 517.70 | 38.61 | 0.3000 |
| 529.15 | 40.69 | 0.1000 |

Kay, W.B. - Young, C.L., Gas-liquid critical properties. 2-Butanone (methyl ethyl ketone)-n-hexane system, Int. Data Ser. Sel. Data Mixtures Ser. A 2 (1975) 139-156.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 505.51 | 32.97 | 0.7829 |
| 506.13 | 34.35 | 0.6669 |
| 511.43 | 36.89 | 0.4473 |
| 517.23 | 38.47 | 0.3098 |
| 526.91 | 40.44 | 0.1331 |

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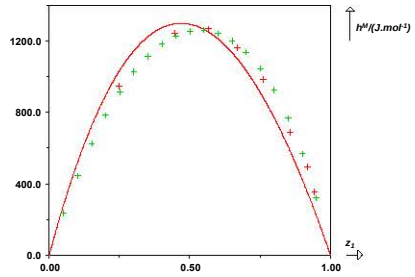
**Azeotropic point**

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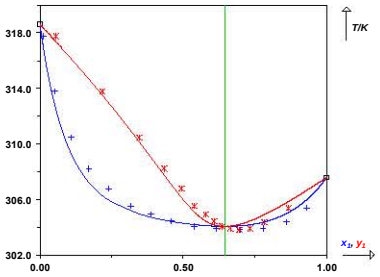
Lladosa, Estela - Martínez, Nelson F. - Montón, Juan B. - de la Torre, Javier, Measurements and correlation of vapour–liquid equilibria of 2-butanone and hydrocarbons binary systems at two different pressures, Fluid Phase Equilibria 1 (2011) 24-29. doi:10.1016/j.fluid.2011.05.004

| T / K | P / bar | $x_1$ |
|---|---|---|
| 303.90 | 0.3000 | 0.7020 |
| 337.40 | 1.013 | 0.6790 |

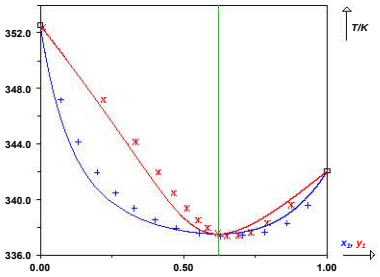
T/K = 298.15 - P/bar = 1.0132 1.0132



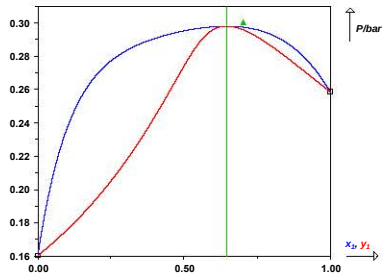

P/bar = 0.30000



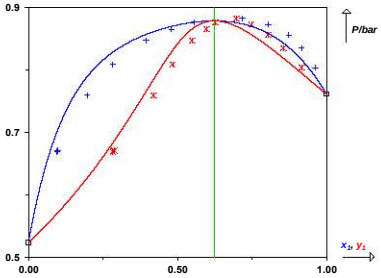

P/bar = 1.01300



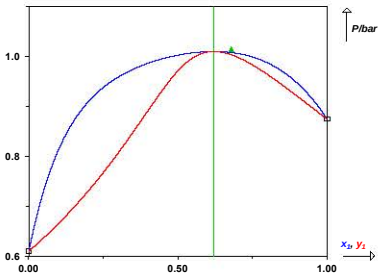

T/K = 303.90



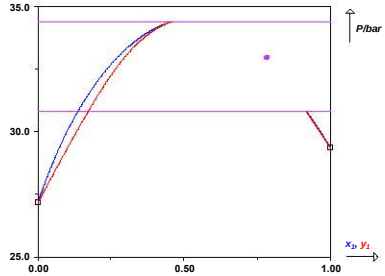

T/K = 333.15



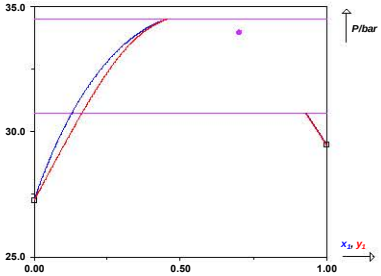

T/K = 337.40



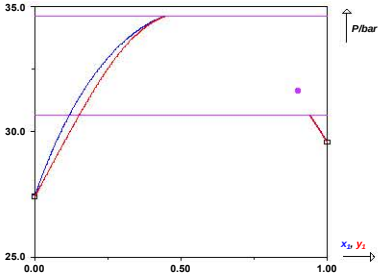

T/K = 505.51



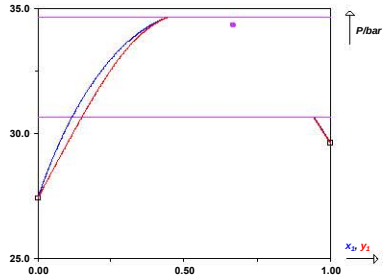

T/K = 505.75



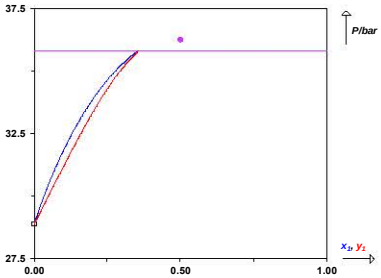

T/K = 506.05



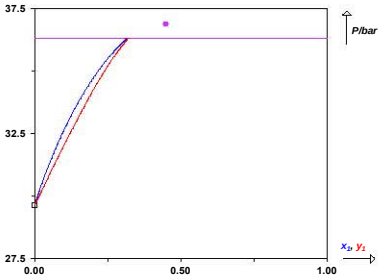

T/K = 506.13

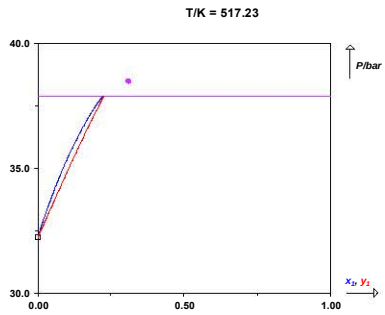


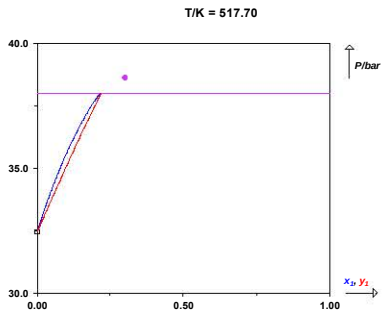

T/K = 509.65

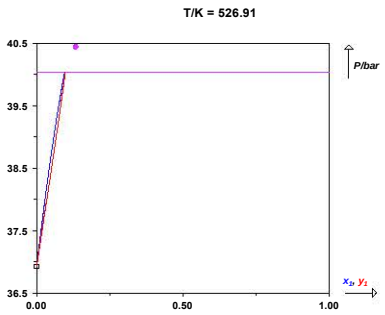


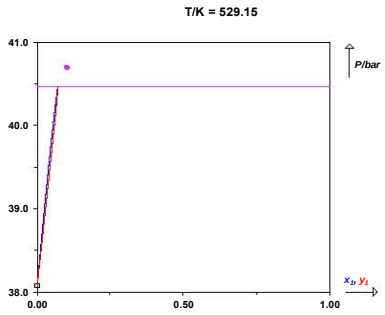

T/K = 511.43




T/K = 517.23
40.0
35.0
30.0
P/bar
0.00
0.50
1.00
x1, y1


T/K = 517.70
40.0
35.0
30.0
P/bar
0.00
0.50
1.00
x1, y1


T/K = 526.91
40.5
39.5
38.5
37.5
36.5
P/bar
0.00
0.50
1.00
x1, y1


T/K = 529.15
41.0
40.0
39.0
38.0
P/bar
0.00
0.50
1.00
x1, y1

## ACETONE (1) + BENZENE (2)

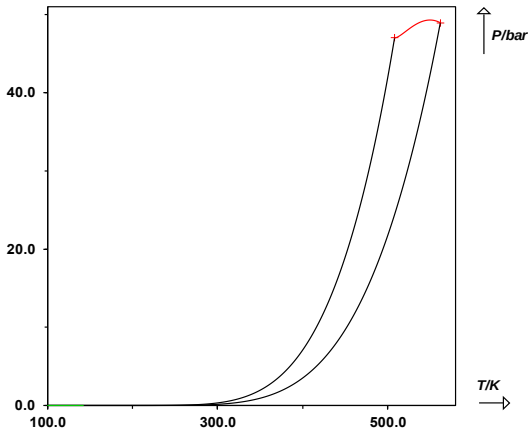
| | | |
|---|---|---|
| **CAS** | 67-64-1 | 71-43-2 |
| **InChiKey** | CSCPPACGZOOCGX-UHFFFAOYSA-N | UHOVQNZJYSORNB-UHFFFAOYSA-N |
| **$T_c$ / K** | 508.20 | 562.05 |
| **$P_c$ / bar** | 47.01 | 48.95 |
| **ω** | 0.3070 | 0.2100 |

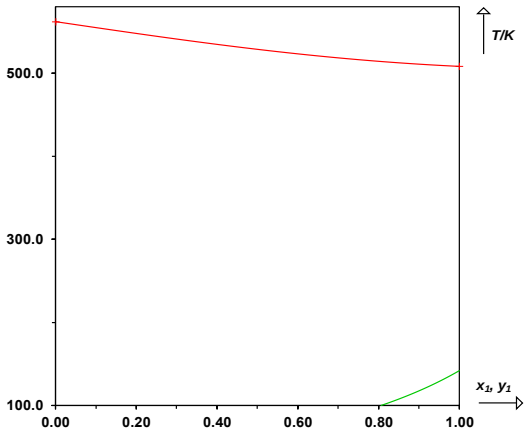
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 85.8
B/MPa = 57.9

*Deviations*
MAPE on x = 5.8 %
MAPE on y = 4.7 %
MAPE on $h^M$ = 71 %
MAPE on $c_P^M$ = 1900 %



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**Isothermal phase equilibrium data**

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Tasić, Aleksandar - Djordjević, Bojan - Grozdanić, Dušan - Afgan, Naim - Malić, Dragomir, Vapour—liquid equilibria of the systems acetone—benzene, benzene—cyclohexane and acetone—cyclohexane at 25°C, Chemical Engineering Science 2 (1978) 189-197. doi:10.1016/0009-2509(78)85053-2

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1555 | 0.0820 | 0.2480 |
| 0.1829 | 0.1850 | 0.4160 |
| 0.2084 | 0.3070 | 0.5500 |
| 0.2257 | 0.4010 | 0.6320 |
| 0.2428 | 0.5050 | 0.7030 |
| 0.2549 | 0.5900 | 0.7550 |
| 0.2709 | 0.7040 | 0.8240 |
| 0.2845 | 0.8055 | 0.8820 |
| 0.2946 | 0.8955 | 0.9360 |

Drobig, J. - Lindenau, E., A new apparatus to determine the isothermal liquid-vapor equilibrium, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 144-147.

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1419 | 0.0500 | 0.1460 |
| 0.1555 | 0.1000 | 0.2600 |
| 0.1684 | 0.1500 | 0.3530 |
| 0.1805 | 0.2000 | 0.4290 |
| 0.1920 | 0.2500 | 0.4940 |
| 0.2028 | 0.3000 | 0.5490 |
| 0.2132 | 0.3500 | 0.5980 |
| 0.2229 | 0.4000 | 0.6410 |
| 0.2323 | 0.4500 | 0.6800 |
| 0.2411 | 0.5000 | 0.7150 |
| 0.2493 | 0.5500 | 0.7470 |
| 0.2573 | 0.6000 | 0.7780 |
| 0.2648 | 0.6500 | 0.8060 |
| 0.2717 | 0.7000 | 0.8330 |
| 0.2784 | 0.7500 | 0.8590 |
| 0.2844 | 0.8000 | 0.8840 |
| 0.2900 | 0.8500 | 0.9090 |
| 0.2952 | 0.9000 | 0.9360 |
| 0.2997 | 0.9500 | 0.9650 |

Drobig, J. - Lindenau, E., A new apparatus to determine the isothermal liquid-vapor equilibrium, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 144-147.

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2200 | 0.0500 | 0.1410 |
| 0.2403 | 0.1000 | 0.2540 |
| 0.2595 | 0.1500 | 0.3460 |
| 0.2777 | 0.2000 | 0.4220 |
| 0.2949 | 0.2500 | 0.4870 |
| 0.3114 | 0.3000 | 0.5430 |
| 0.3270 | 0.3500 | 0.5930 |
| 0.3418 | 0.4000 | 0.6360 |
| 0.3558 | 0.4500 | 0.6760 |
| 0.3692 | 0.5000 | 0.7110 |
| 0.3817 | 0.5500 | 0.7440 |
| 0.3936 | 0.6000 | 0.7740 |
| 0.4048 | 0.6500 | 0.8030 |
| 0.4152 | 0.7000 | 0.8300 |
| 0.4250 | 0.7500 | 0.8560 |
| 0.4341 | 0.8000 | 0.8820 |
| 0.4425 | 0.8500 | 0.9080 |
| 0.4501 | 0.9000 | 0.9350 |
| 0.4570 | 0.9500 | 0.9650 |

Kraus, J. - Linek, J., Liquid-vapor equilibrium. XLVIII. Systems acetone-benzene, acetone-toluene, benzene-methyl ethyl ketone, methyl ethyl ketone-toluene, and methyl ethyl ketone-ethylbenzene, Collection of Czechoslovak Chemical Communications 7 (1971) 2547-2567. doi:10.1135/cccc19712547

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2814 | 0.0570 | 0.1758 |
| 0.3063 | 0.1027 | 0.2769 |
| 0.3742 | 0.2615 | 0.4921 |
| 0.3959 | 0.3240 | 0.5535 |
| 0.4124 | 0.3734 | 0.5946 |
| 0.4384 | 0.4636 | 0.6631 |
| 0.4597 | 0.5300 | 0.7085 |
| 0.4756 | 0.5892 | 0.7481 |
| 0.5087 | 0.7325 | 0.8355 |
| 0.5244 | 0.8051 | 0.8782 |
| 0.5418 | 0.8807 | 0.9238 |

Drobig, J. - Lindenau, E., A new apparatus to determine the isothermal liquid-vapor equilibrium, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 144-147.

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3293 | 0.0500 | 0.1380 |
| 0.3585 | 0.1000 | 0.2490 |
| 0.3864 | 0.1500 | 0.3400 |
| 0.4129 | 0.2000 | 0.4160 |

| | | |
|---|---|---|
| 0.4381 | 0.2500 | 0.4820 |
| 0.4621 | 0.3000 | 0.5380 |
| 0.4849 | 0.3500 | 0.5880 |
| 0.5066 | 0.4000 | 0.6320 |
| 0.5270 | 0.4500 | 0.6720 |
| 0.5465 | 0.5000 | 0.7080 |
| 0.5648 | 0.5500 | 0.7410 |
| 0.5820 | 0.6000 | 0.7710 |
| 0.5982 | 0.6500 | 0.8000 |
| 0.6133 | 0.7000 | 0.8270 |
| 0.6274 | 0.7500 | 0.8540 |
| 0.6405 | 0.8000 | 0.8800 |
| 0.6526 | 0.8500 | 0.9060 |
| 0.6637 | 0.9000 | 0.9340 |
| 0.6737 | 0.9500 | 0.9650 |

Drobig, J. - Lindenau, E., A new apparatus to determine the isothermal liquid-vapor equilibrium, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 144-147.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4773 | 0.0500 | 0.1350 |
| 0.5184 | 0.1000 | 0.2450 |
| 0.5577 | 0.1500 | 0.3350 |
| 0.5952 | 0.2000 | 0.4120 |
| 0.6309 | 0.2500 | 0.4770 |
| 0.6649 | 0.3000 | 0.5340 |
| 0.6973 | 0.3500 | 0.5840 |
| 0.7279 | 0.4000 | 0.6280 |
| 0.7569 | 0.4500 | 0.6680 |
| 0.7843 | 0.5000 | 0.7040 |
| 0.8102 | 0.5500 | 0.7370 |
| 0.8345 | 0.6000 | 0.7680 |
| 0.8571 | 0.6500 | 0.7970 |
| 0.8785 | 0.7000 | 0.8250 |
| 0.8982 | 0.7500 | 0.8510 |
| 0.9165 | 0.8000 | 0.8780 |
| 0.9333 | 0.8500 | 0.9050 |
| 0.9487 | 0.9000 | 0.9330 |
| 0.9626 | 0.9500 | 0.9650 |

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**Isobaric phase equilibrium data**

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Müller, Eckart - Stage, H, Experimentelle Vermessung von Dampf-Flüssigkeits-Phasengleichgewichten dargestellt am Beispiel des Siedeverhaltens von Fettsäuren (1961)

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 350.95 | 0.0290 | 0.0910 |
| 347.55 | 0.0830 | 0.2230 |
| 343.65 | 0.1780 | 0.3740 |
| 340.65 | 0.2750 | 0.4880 |
| 337.05 | 0.4390 | 0.6320 |
| 334.15 | 0.5920 | 0.7420 |
| 332.75 | 0.6930 | 0.8060 |
| 331.65 | 0.7860 | 0.8650 |
| 330.65 | 0.8730 | 0.9160 |
| 329.95 | 0.9420 | 0.9640 |
| 329.55 | 0.9810 | 0.9880 |

Free, K. W. - Hutchinson, H. P., Isobaric Vapor-Liquid Equilibria for the Ternary System Acetone-Benzene-Chlorobenzene., Journal of Chemical & Engineering Data 3 (1959) 193-197. doi:10.1021/je60003a001

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 349.65 | 0.0540 | 0.1550 |
| 348.05 | 0.0840 | 0.2180 |
| 344.95 | 0.1560 | 0.3380 |
| 342.25 | 0.2370 | 0.4400 |
| 341.95 | 0.2400 | 0.4440 |
| 339.55 | 0.3350 | 0.5410 |
| 337.35 | 0.4320 | 0.6230 |
| 335.55 | 0.5320 | 0.6980 |
| 333.75 | 0.6470 | 0.7740 |
| 332.75 | 0.7090 | 0.8130 |
| 332.25 | 0.7580 | 0.8450 |
| 330.85 | 0.8690 | 0.9150 |

Ishikawa, T. - Watari, R. - Kosakai, K. - Hirata, M., Vapor-liquid equilibriums of binary systems containing acetone at 760 mm of mercury. Acetone with aromatic hydrocarbons, Mem. Fac. Technol. Tokyo Metropol. Univ. (1971) 1883-1896.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 349.15 | 0.0560 | 0.1500 |
| 346.45 | 0.1060 | 0.2460 |
| 342.25 | 0.2080 | 0.3965 |
| 339.45 | 0.3180 | 0.5125 |
| 337.15 | 0.4285 | 0.6140 |
| 337.05 | 0.4360 | 0.6215 |
| 335.05 | 0.5575 | 0.7000 |
| 333.25 | 0.6730 | 0.7850 |
| 331.85 | 0.7860 | 0.8550 |
| 330.65 | 0.9030 | 0.9340 |
| 330.05 | 0.9560 | 0.9690 |

Monick, J. A. - Allen, H. D. - Marlies, C. J., Vapor-liquid equilibrium data for fatty acids and fatty methyl esters at low pressures, Oil & Soap 6 (1946) 177-182. doi:10.1007/BF02545630

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 352.35 | 0.0100 | 0.0352 |
| 349.50 | 0.0500 | 0.1496 |
| 346.75 | 0.1000 | 0.2531 |
| 342.85 | 0.2000 | 0.4030 |
| 339.90 | 0.3000 | 0.5147 |
| 337.65 | 0.4000 | 0.6030 |
| 335.80 | 0.5000 | 0.6785 |
| 334.15 | 0.6000 | 0.7464 |
| 332.75 | 0.7000 | 0.8100 |
| 331.50 | 0.8000 | 0.8737 |
| 330.40 | 0.9000 | 0.9371 |
| 329.85 | 0.9500 | 0.9687 |
| 329.42 | 0.9900 | 0.9937 |

Kojima, Kazuo - Tochigi, Katsumi - Kurihara, Kiyofumi - Nakamichi, Mikiyoshi, Isobaric vapor-liquid equilibria for acetone + chloroform + benzene and the three constituent binary systems, Journal of Chemical & Engineering Data 3 (1991) 343-345. doi:10.1021/je00003a024

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 345.38 | 0.1390 | 0.3210 |
| 343.36 | 0.1930 | 0.3990 |
| 341.03 | 0.2700 | 0.4880 |
| 338.14 | 0.3870 | 0.6010 |
| 337.31 | 0.4280 | 0.6300 |
| 336.94 | 0.4460 | 0.6470 |
| 336.54 | 0.4660 | 0.6610 |
| 335.97 | 0.4980 | 0.6830 |
| 335.06 | 0.5500 | 0.7210 |
| 334.20 | 0.6020 | 0.7530 |
| 333.86 | 0.6270 | 0.7690 |
| 333.16 | 0.6730 | 0.7980 |
| 332.39 | 0.7300 | 0.8330 |
| 332.36 | 0.7330 | 0.8340 |
| 330.90 | 0.8490 | 0.9050 |
| 330.63 | 0.8720 | 0.9190 |
| 330.49 | 0.8830 | 0.9260 |

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**Enthalpy of mixing**

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Akamatsu, Yutaka - Ogawa, Hideo - Murakami, Sachio, Molar excess enthalpies, molar excess volumes and molar isentropic compressions of mixtures of 2-propanone with heptane, benzene and trichloromethane at 298.15 K, Thermochimica Acta (1987) 141-150. doi:10.1016/0040-6031(87)88317-X

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 39.70 | 0.0500 |
| 67.90 | 0.1000 |
| 89.00 | 0.1500 |
| 105.10 | 0.2000 |
| 117.60 | 0.2500 |
| 126.70 | 0.3000 |
| 133.20 | 0.3500 |
| 135.90 | 0.4000 |
| 138.20 | 0.4500 |
| 138.40 | 0.5000 |
| 136.80 | 0.5500 |
| 132.70 | 0.6000 |
| 126.50 | 0.6500 |
| 118.00 | 0.7000 |
| 106.70 | 0.7500 |
| 92.70 | 0.8000 |
| 76.10 | 0.8500 |
| 55.00 | 0.9000 |
| 27.00 | 0.9500 |

Möbius, Hans-Heinrich, Mischungsenthalpien und Mischbarkeit von Aceton, Benzol und Wasser, Journal für Praktische Chemie 1-2 (1955) 95-104. doi:10.1002/prac.19550020108

**T / K = 303.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 53.55 | 0.0666 |
| 83.15 | 0.1215 |
| 128.41 | 0.2811 |
| 146.25 | 0.4967 |
| 112.33 | 0.7430 |
| 40.37 | 0.9285 |

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**Heat capacity of mixing**

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Yamanaka, Katsuhiko - Ogawa, Hideo - Murakami, Sachio, Excess molar isobaric heat capacities of mixtures of 2-propanone with heptane, benzene, and trichloromethane at 298.15 K, Thermochimica Acta

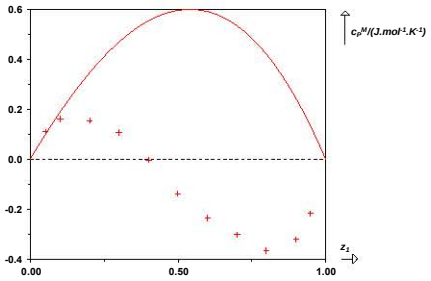
(1990) 193-201. doi:10.1016/0040-6031(90)80145-O

**T / K = 298.15**

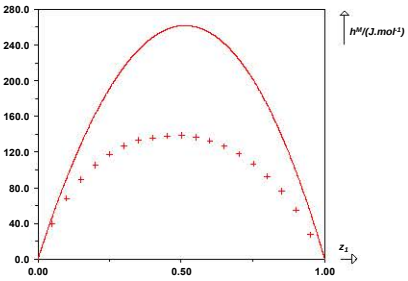
**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.1090 | 0.0500 |
| 0.1600 | 0.1000 |
| 0.1540 | 0.2000 |
| 0.1080 | 0.3000 |
| -0.0030 | 0.4000 |
| -0.1370 | 0.5000 |
| -0.2350 | 0.6000 |
| -0.3030 | 0.7000 |
| -0.3670 | 0.8000 |
| -0.3220 | 0.9000 |
| -0.2180 | 0.9500 |

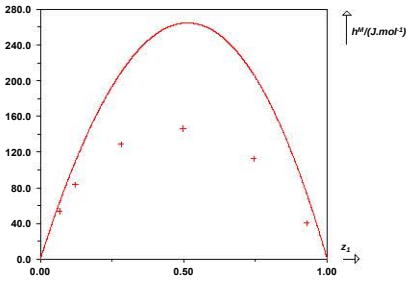
T/K = 298.15 - P/bar = 1.0132



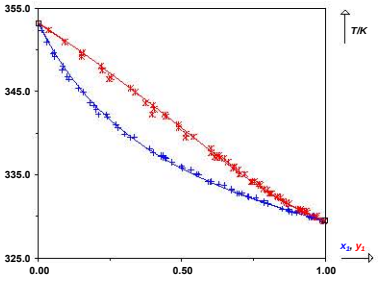

T/K = 298.15 - P/bar = 1.0132



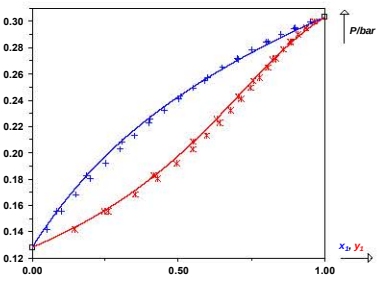

T/K = 303.15 - P/bar = 1.0132



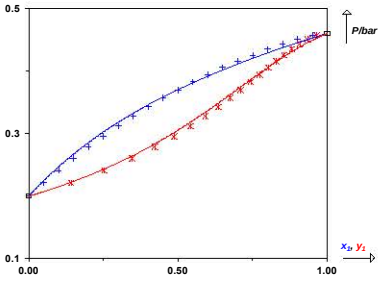

P/bar = 1.01330



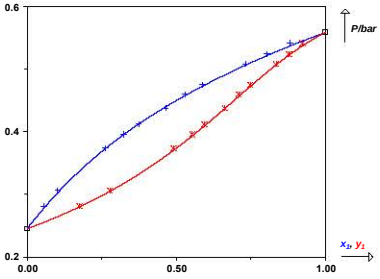

T/K = 298.15



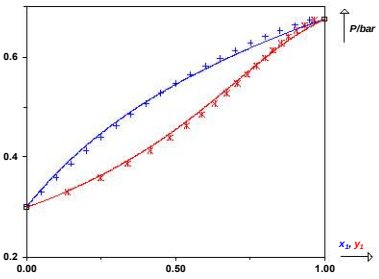

T/K = 308.15



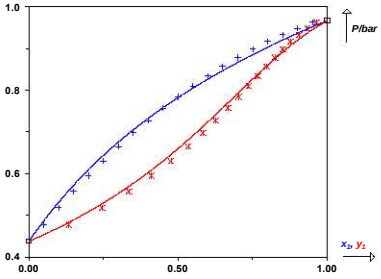

T/K = 313.15




T/K = 318.15




T/K = 328.15



## BENZENE (1) + N-METHYL-2-PYRROLIDONE (2)

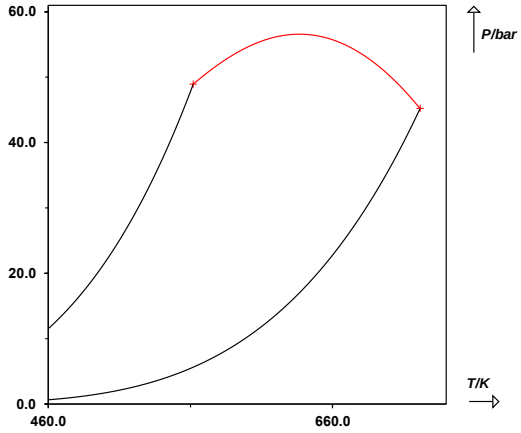
| | | |
|---|---|---|
| **CAS** | 71-43-2 | 872-50-4 |
| **InChiKey** | UHOVQNZJYSORNB-UHFFFAOYSA-N | SECXISVLQFMRJM-UHFFFAOYSA-N |
| **$T_c$ / K** | 562.05 | 721.60 |
| **$P_c$ / bar** | 48.95 | 45.20 |
| **ω** | 0.2100 | 0.3730 |

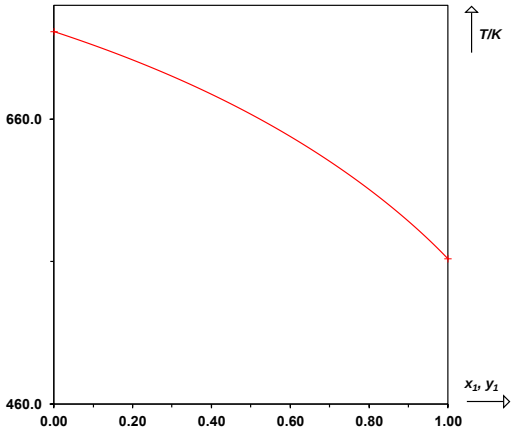
Non ideal with entropic causes

**PPR78 results**

*Parameters*
A/MPa = -30.6
B/MPa = -114

*Deviations*
MAPE on x = 7.5 %
MAPE on y = 14 %
MAPE on $h^M$ = 7.5 %



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**Isothermal phase equilibrium data**

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Linek, Jan - Wichterle, Ivan - Marsh, Kenneth N., Vapor-Liquid Equilibria for N-Methyl-2-pyrrolidone + Benzene, +Toluene, +Heptane, and +Methylcyclohexane, Journal of Chemical & Engineering Data 6 (1996) 1212-1218. doi:10.1021/je9601826

**T / K = 330.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0220 | 0.0378 | 0.8043 |
| 0.0255 | 0.0455 | 0.8420 |
| 0.0321 | 0.0615 | 0.8709 |
| 0.0343 | 0.0654 | 0.8804 |
| 0.0902 | 0.1792 | 0.9605 |
| 0.1480 | 0.2925 | 0.9778 |
| 0.2764 | 0.5407 | 0.9870 |
| 0.2944 | 0.5807 | 0.9890 |
| 0.3148 | 0.6265 | 0.9900 |
| 0.3370 | 0.6830 | 0.9890 |
| 0.3506 | 0.7190 | 0.9870 |
| 0.3548 | 0.7260 | 0.9915 |
| 0.4308 | 0.9135 | 0.9970 |
| 0.4463 | 0.9520 | 0.9940 |
| 0.4586 | 0.9850 | 0.9990 |

Linek, Jan - Wichterle, Ivan - Marsh, Kenneth N., Vapor-Liquid Equilibria for N-Methyl-2-pyrrolidone + Benzene, +Toluene, +Heptane, and +Methylcyclohexane, Journal of Chemical & Engineering Data 6 (1996) 1212-1218. doi:10.1021/je9601826

**T / K = 350.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0456 | 0.0378 | 0.7335 |
| 0.0531 | 0.0455 | 0.7680 |
| 0.0709 | 0.0654 | 0.8303 |
| 0.1639 | 0.1792 | 0.9381 |
| 0.2825 | 0.2925 | 0.9647 |
| 0.4226 | 0.4284 | 0.9830 |
| 0.5965 | 0.6020 | 0.9880 |
| 0.6299 | 0.6370 | 0.9885 |
| 0.6698 | 0.6870 | 0.9890 |
| 0.7533 | 0.7945 | 0.9940 |
| 0.8066 | 0.8655 | 0.9960 |
| 0.8453 | 0.9085 | 0.9975 |
| 0.8759 | 0.9540 | 0.9999 |
| 0.9019 | 0.9825 | 0.9999 |

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**Isobaric phase equilibrium data**

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Blanco, Beatriz - Beltrán, Sagrario - Cabezas, José Luis - Coca, José, Phase Equilibria of Binary Systems Formed by Hydrocarbons from Petroleum Fractions and the Solvents N-Methylpyrrolidone and N,N-Dimethylformamide. 1. Isobaric Vapor - Liquid Equilibria, Journal of Chemical & Engineering Data 5 (1997) 938-942. doi:10.1021/je970059u

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 448.45 | 0.0520 | 0.5300 |
| 437.85 | 0.0850 | 0.6740 |
| 426.20 | 0.1180 | 0.7900 |
| 406.65 | 0.2050 | 0.9010 |
| 398.65 | 0.2500 | 0.9310 |
| 381.60 | 0.4070 | 0.9710 |
| 378.50 | 0.4550 | 0.9770 |
| 370.40 | 0.5700 | 0.9860 |
| 365.30 | 0.6730 | 0.9920 |
| 363.45 | 0.7070 | 0.9930 |
| 360.55 | 0.7750 | 0.9950 |
| 357.30 | 0.8700 | 0.9980 |
| 355.30 | 0.9330 | 0.9990 |

Gupta, S.K. - Rawat, B.S. - Goswami, A.N. - Nanoti, S.M. - Krishna, R., Isobaric vapour—liquid equilibria of the systems: Benzene—triethylene glycol, toluene—triethylene glycol and benzene—N-methylpyrrolidone, Fluid Phase Equilibria 1 (1989) 95-102. doi:10.1016/0378-3812(89)80278-X

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 420.05 | 0.1217 | 0.8242 |
| 413.35 | 0.1514 | 0.8650 |
| 397.75 | 0.2360 | 0.9280 |
| 383.15 | 0.3660 | 0.9658 |
| 377.05 | 0.4550 | 0.9760 |
| 371.45 | 0.5493 | 0.9840 |
| 365.75 | 0.6634 | 0.9902 |
| 361.95 | 0.7471 | 0.9935 |
| 358.85 | 0.8335 | 0.9961 |
| 355.85 | 0.9173 | 0.9982 |

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**Enthalpy of mixing**

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Letcher, T.M. - Naicker, P.K., Excess molar enthalpies and excess molar volumes of mixtures containingN-methyl-2-pyrrolidinone and an aromatic hydrocarbon

atT= 298.15 K andp= 0.101325 MPa, The Journal of Chemical Thermodynamics 12 (1999) 1585-1595. doi:10.1006/jcht.1999.0555

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -237.20 | 0.1560 |
| -358.60 | 0.2390 |
| -443.00 | 0.3070 |
| -471.40 | 0.3420 |
| -540.10 | 0.4860 |
| -546.40 | 0.5160 |
| -544.10 | 0.5310 |
| -540.50 | 0.5480 |
| -533.00 | 0.5850 |
| -469.00 | 0.6880 |
| -387.10 | 0.7770 |
| -365.10 | 0.7900 |
| -163.48 | 0.1076 |
| -231.14 | 0.1607 |
| -295.81 | 0.2134 |
| -293.42 | 0.2134 |
| -390.52 | 0.3174 |
| -452.18 | 0.4197 |
| -469.33 | 0.5204 |
| -442.84 | 0.6194 |
| -374.02 | 0.7169 |
| -267.65 | 0.8127 |
| -198.96 | 0.8601 |
| -130.23 | 0.9071 |
| -94.79 | 0.9305 |

Chhikara, Yameeka - Yadav, J.S. - Sharma, Dimple - Sharma, V.K., Thermodynamic and topological investigations of molecular interactions in binary and ternary mixtures containing 1-methyl pyrrolidin-2-one at T=308.15K, The Journal of Chemical Thermodynamics 5 (2011) 737-749. doi:10.1016/j.jct.2010.12.016

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

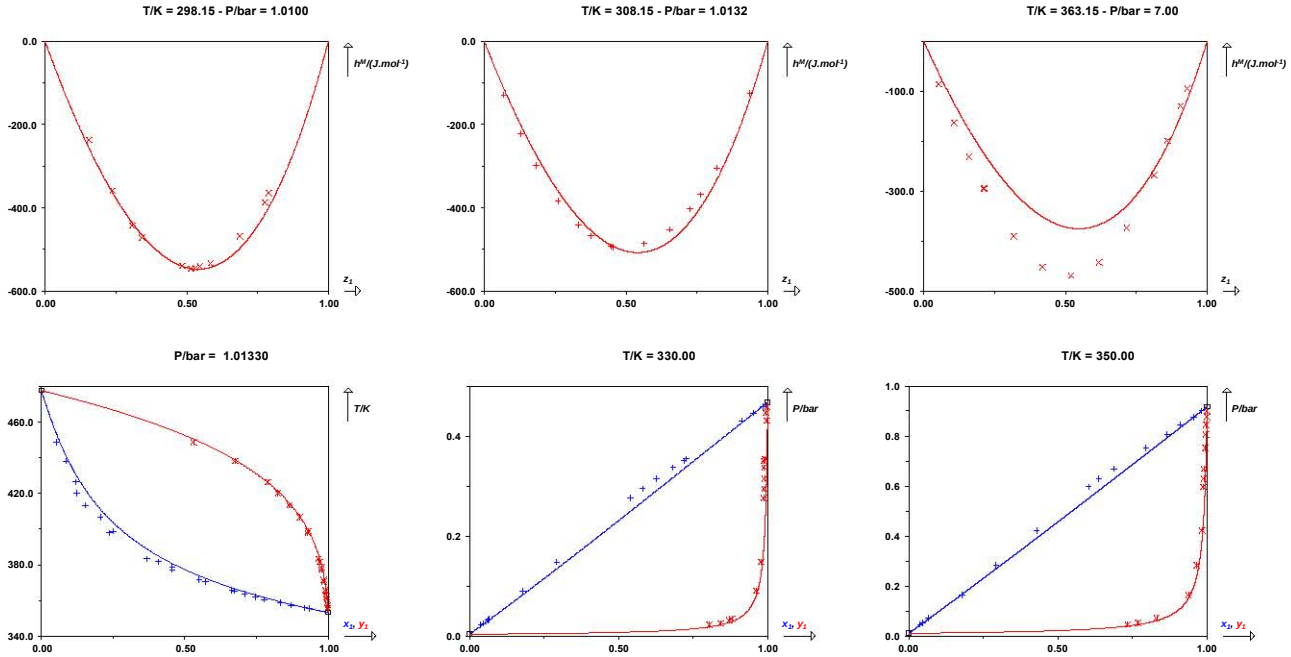
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -125.90 | 0.9375 |
| -304.40 | 0.8212 |
| -368.40 | 0.7644 |
| -402.90 | 0.7264 |
| -452.60 | 0.6538 |
| -485.80 | 0.5638 |
| -494.30 | 0.4533 |
| -492.30 | 0.4459 |
| -467.20 | 0.3757 |
| -442.10 | 0.3319 |
| -384.10 | 0.2589 |
| -298.20 | 0.1837 |
| -222.60 | 0.1281 |
| -129.30 | 0.0689 |

Gmehling, J. - Meents, B., Excess enthalpy. 1-Methyl-2-pyrrolidinone - benzene system, Int. Data Ser. Sel. Data Mixtures Ser. A 3 (1992)

**T / K = 363.15**

**P / bar = 7.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -86.27 | 0.0540 |


T/K = 298.15 - P/bar = 1.0100
T/K = 308.15 - P/bar = 1.0132
T/K = 363.15 - P/bar = 7.00
P/bar = 1.01330
T/K = 330.00
T/K = 350.00
$h^M$/(J.mol$^{-1}$)
T/K
P/bar
$z_1$
$x_1$, $y_1$

# H-NA systems (AC = 3)

## ETHYLENE (1) + DICHLOROMETHANE (2)

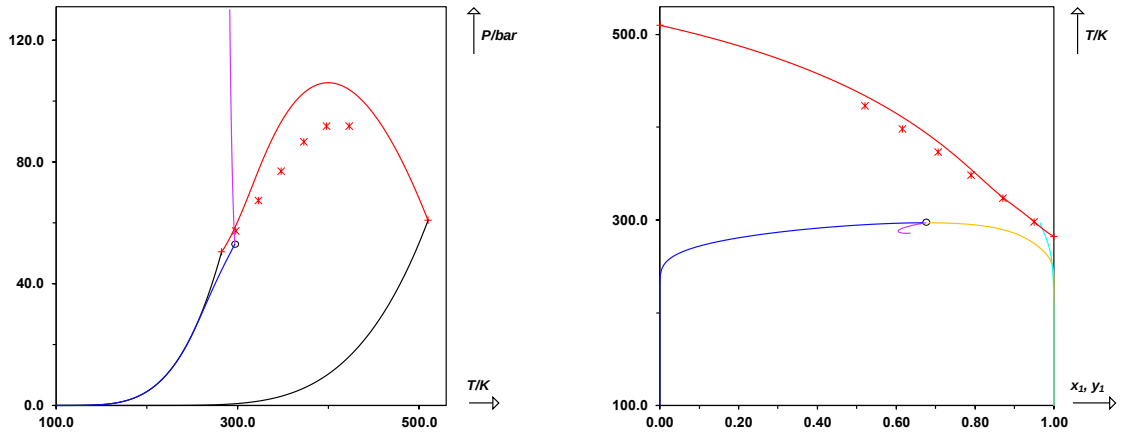
| | | |
|---|---|---|
| **CAS** | 74-85-1 | 75-09-2 |
| **InChiKey** | VGGSQFUCUMXWEO-UHFFFAOYSA-N | YMWUJEATGCHHMB-UHFFFAOYSA-N |
| **$T_c$ / K** | 282.34 | 510.00 |
| **$P_c$ / bar** | 50.41 | 60.80 |
| **ω** | 0.086 | 0.199 |

Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 364
B/MPa = 3050

*Deviations*
MAPE on x = 8.2 %
MAPE on y = 4.2 %
MAPE on $x_c$ = 5.7 %
MAPE on $P_c$ = 14 %



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**Isothermal phase equilibrium data**

---

Lebedeva, E.S. - Khodeeva, S.M., Phase equilibrium and volume relations in the system methylene chloride-ethylene, Tr. Gos. Nauchno Issled. Proektn. Inst. Azotn. Promst. Prod. Org. Sin. (1963) 79-90.

**T / K = 398.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 14.19 | 0.0350 | 0.2180 | |
| 18.24 | 0.0500 | 0.4500 | |
| 22.29 | 0.0650 | 0.5400 | |
| 30.40 | 0.1240 | 0.6250 | |
| 35.46 | 0.1500 | 0.6580 | |
| 49.14 | 0.2500 | 0.7050 | |
| 61.81 | 0.3500 | 0.7320 | |
| 72.95 | 0.4500 | 0.7400 | |
| 91.70 | 0.6150 | 0.6150 | CRIT |

Lebedeva, E.S. - Khodeeva, S.M., Phase equilibrium and volume relations in the system methylene chloride-ethylene, Tr. Gos. Nauchno Issled. Proektn. Inst. Azotn. Promst. Prod. Org. Sin. (1963) 79-90.

**T / K = 423.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 20.27 | 0.0050 | 0.1820 | |
| 24.32 | 0.0300 | 0.3080 | |
| 32.42 | 0.0720 | 0.4530 | |
| 36.48 | 0.1000 | 0.4950 | |
| 45.60 | 0.1500 | 0.5500 | |
| 60.29 | 0.2500 | 0.6000 | |
| 72.65 | 0.3500 | 0.6250 | |
| 78.22 | 0.4000 | 0.6300 | |
| 91.70 | 0.5200 | 0.5200 | CRIT |

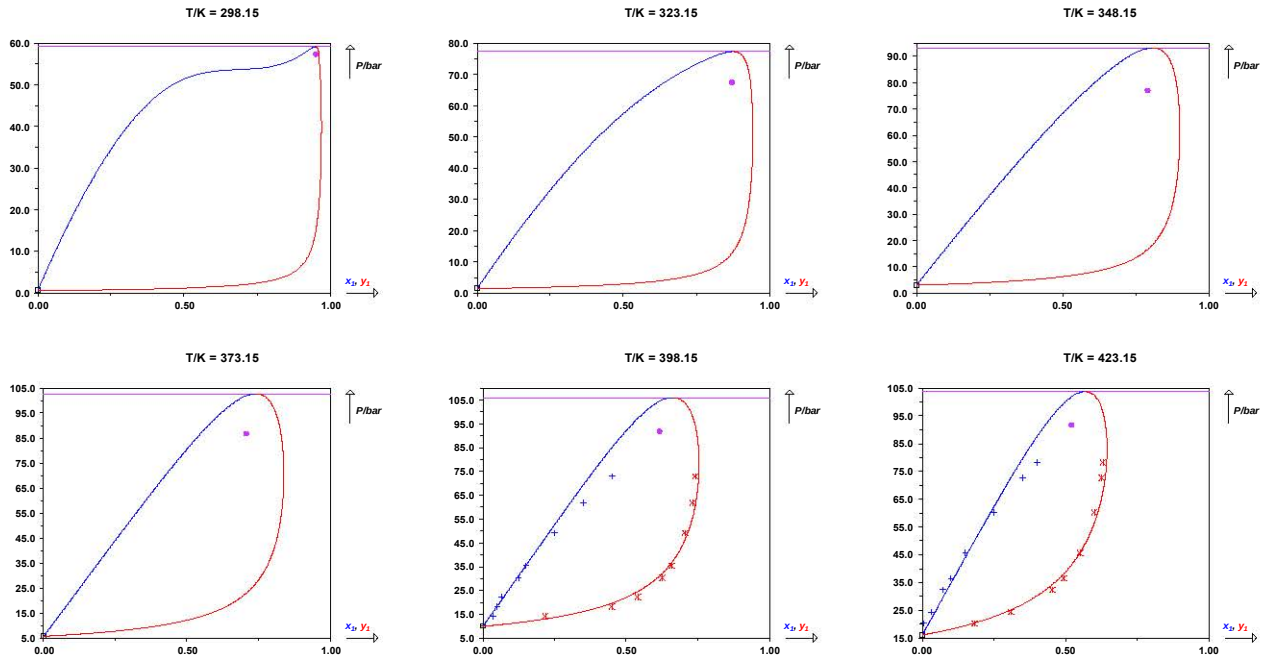
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**Critical point**

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Lebedeva, E.S. - Khodeeva, S.M., Phase equilibrium and volume relations in the system methylene chloride-ethylene, Tr. Gos. Nauchno Issled. Proektn. Inst. Azotn. Promst. Prod. Org. Sin. (1963) 79-90.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 298.15 | 57.25 | 0.9500 |
| 323.15 | 67.38 | 0.8700 |
| 348.15 | 77.01 | 0.7900 |
| 373.15 | 86.63 | 0.7060 |


T/K = 298.15
P/bar
x1, y1
T/K = 323.15
P/bar
x1, y1
T/K = 348.15
P/bar
x1, y1
T/K = 373.15
P/bar
x1, y1
T/K = 398.15
P/bar
x1, y1
T/K = 423.15
P/bar
x1, y1

## NITROGEN (1) + CHLORODIFLUOROMETHANE (2)

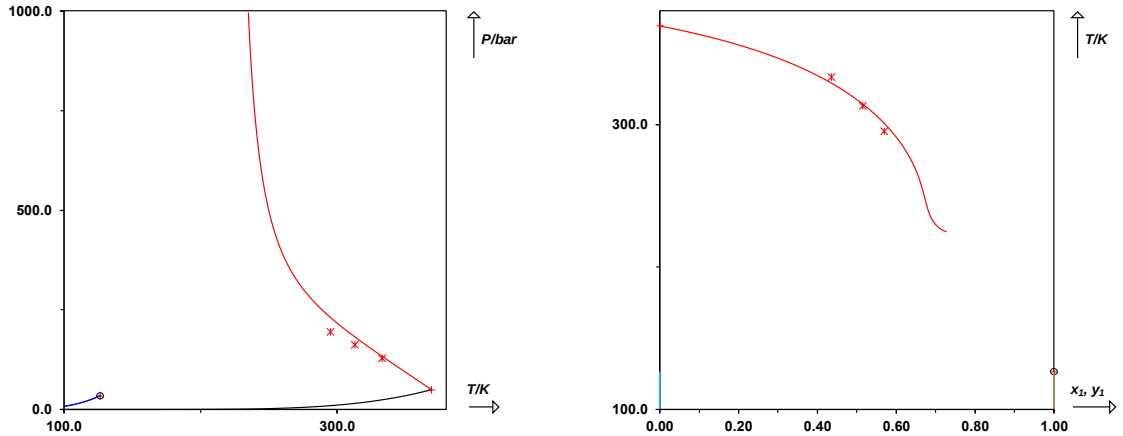
| | | |
|---|---|---|
| **CAS** | 7727-37-9 | 75-45-6 |
| **InChiKey** | MDFFNEOEWAXZRQ-UHFFFAOYSA-N | VOPWNXZWBYDODV-UHFFFAOYSA-N |
| **$T_c$ / K** | 126.20 | 369.30 |
| **$P_c$ / bar** | 34.00 | 49.71 |
| **ω** | 0.038 | 0.219 |

Unknown ideality

PPR78 results

*Parameters*
A/MPa = 211
B/MPa = 810

*Deviations*
MAPE on x = 4.4 %
MAPE on y = 5.4 %
MAPE on $x_c$ = 3.4 %
MAPE on $P_c$ = 12 %



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**Isothermal phase equilibrium data**

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Wang, Xiaoqing - Wang, Yanru - Shi, Jun - Lu, Benjamin C. Y., Isothermal vapor-liquid equilibria at elevated pressures for the systems containing nitrogen, carbon dioxide, and chlorodifluoromethane, Journal of Chemical & Engineering Data 4 (1991) 436-439. doi:10.1021/je00004a027

**T / K = 263.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.96 | 0.0130 | 0.6460 |
| 14.25 | 0.0170 | 0.7270 |
| 23.66 | 0.0320 | 0.8040 |
| 28.88 | 0.0400 | 0.8410 |
| 35.55 | 0.0520 | 0.8750 |
| 40.94 | 0.0610 | 0.8860 |
| 45.69 | 0.0730 | 0.8930 |
| 50.22 | 0.0790 | 0.8970 |

Wang, Xiaoqing - Wang, Yanru - Shi, Jun - Lu, Benjamin C. Y., Isothermal vapor-liquid equilibria at elevated pressures for the systems containing nitrogen, carbon dioxide, and chlorodifluoromethane, Journal of Chemical & Engineering Data 4 (1991) 436-439. doi:10.1021/je00004a027

**T / K = 268.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.320 | 0.0080 | 0.4780 |
| 15.54 | 0.0200 | 0.6860 |
| 20.30 | 0.0280 | 0.7370 |
| 25.97 | 0.0370 | 0.8110 |
| 29.90 | 0.0440 | 0.8350 |
| 35.98 | 0.0540 | 0.8520 |
| 40.76 | 0.0650 | 0.8630 |
| 45.72 | 0.0730 | 0.8720 |
| 51.28 | 0.0830 | 0.8780 |

Nohka, Junichi - Sarashina, Eiji - Arai, Yasuhiko - Saito, Shozaburo, Correlation Of Vapor-Liquid Equilibria For Systems Containing A Polar Component By The Bwr Equation, Journal of Chemical Engineering of Japan 1 (1973) 10-17. doi:10.1252/jcej.6.10

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 25.33 | 0.0367 | 0.7550 |
| 50.66 | 0.0842 | 0.8520 |
| 75.99 | 0.1290 | 0.8730 |
| 101.33 | 0.1770 | 0.8760 |
| 126.66 | 0.2270 | 0.8690 |
| 144.29 | 0.2650 | 0.8590 |
| 160.50 | 0.3010 | 0.8450 |
| 183.09 | 0.3500 | 0.8250 |
| 200.83 | 0.3990 | 0.8010 |
| 215.32 | 0.4470 | 0.7660 |

Wang, X. - Wang, Y.S., Vapor-liquid equilibria for nitrogen-carbon dioxide-chlorodifluoromethane at moderate pressure, Nanjing Huagong Xueyuan Xuebao (1991) 35-44.

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.160 | 0.0056 | 0.3724 |
| 11.37 | 0.0113 | 0.5419 |
| 15.97 | 0.0189 | 0.6622 |
| 20.10 | 0.0267 | 0.7243 |
| 25.88 | 0.0332 | 0.7681 |
| 30.83 | 0.0448 | 0.7965 |
| 41.26 | 0.0629 | 0.8400 |
| 50.13 | 0.0771 | 0.8566 |

Wang, Xiaoqing - Wang, Yanru - Shi, Jun - Lu, Benjamin C. Y., Isothermal vapor-liquid equilibria at elevated pressures for the systems containing nitrogen, carbon dioxide, and chlorodifluoromethane, Journal of Chemical & Engineering Data 4 (1991) 436-439. doi:10.1021/je00004a027

**T / K = 283.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.21 | 0.0060 | 0.3070 |
| 15.97 | 0.0150 | 0.5290 |
| 19.02 | 0.0210 | 0.6020 |
| 24.18 | 0.0310 | 0.6700 |
| 25.87 | 0.0330 | 0.6840 |
| 30.83 | 0.0440 | 0.7240 |
| 35.76 | 0.0520 | 0.7520 |
| 40.66 | 0.0610 | 0.7710 |
| 49.41 | 0.0760 | 0.8030 |

Wang, Xiaoqing - Wang, Yanru - Shi, Jun - Lu, Benjamin C. Y., Isothermal vapor-liquid equilibria at elevated pressures for the systems containing nitrogen, carbon dioxide, and chlorodifluoromethane, Journal of Chemical & Engineering Data 4 (1991) 436-439. doi:10.1021/je00004a027

**T / K = 288.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.390 | 0.0030 | 0.1480 |
| 11.64 | 0.0070 | 0.2940 |
| 14.56 | 0.0120 | 0.4180 |
| 19.36 | 0.0190 | 0.5400 |
| 23.37 | 0.0270 | 0.6100 |

| | | |
|---|---|---|
| 30.32 | 0.0410 | 0.6800 |
| 38.38 | 0.0560 | 0.7360 |
| 49.37 | 0.0780 | 0.7740 |

Maslennikova, V.Ya. - Goryunova, N.P. - Tsiklis, D.S., Phase equilibriums in the nitrogen-Freon 12 and nitrogen-Freon 22 systems, Russ. J. Phys. Chem. 3 (1967) 383-385.

**T / K = 295.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 25.33 | 0.0350 | 0.5900 | |
| 50.66 | 0.0850 | 0.7400 | |
| 75.99 | 0.1350 | 0.7900 | |
| 101.33 | 0.1850 | 0.8000 | |
| 126.66 | 0.2400 | 0.7900 | |
| 151.99 | 0.3150 | 0.7630 | |
| 177.32 | 0.4100 | 0.7250 | |
| 194.54 | 0.5700 | 0.5700 | CRIT |

Nohka, Junichi - Sarashina, Eiji - Arai, Yasuhiko - Saito, Shozaburo, Correlation Of Vapor-Liquid Equilibria For Systems Containing A Polar Component By The Bwr Equation, Journal of Chemical Engineering of Japan 1 (1973) 10-17. doi:10.1252/jcej.6.10

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 25.33 | 0.0268 | 0.4980 |
| 75.99 | 0.1250 | 0.7410 |
| 95.75 | 0.1640 | 0.7550 |
| 126.66 | 0.2320 | 0.7530 |
| 142.36 | 0.2790 | 0.7480 |
| 154.22 | 0.3150 | 0.7300 |
| 165.87 | 0.3470 | 0.7040 |
| 173.97 | 0.3820 | 0.6800 |
| 179.04 | 0.4090 | 0.6600 |
| 185.93 | 0.4630 | 0.6180 |

Maslennikova, V.Ya. - Goryunova, N.P. - Tsiklis, D.S., Phase equilibriums in the nitrogen-Freon 12 and nitrogen-Freon 22 systems, Russ. J. Phys. Chem. 3 (1967) 383-385.

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 25.33 | 0.0250 | 0.3650 | |
| 50.66 | 0.0850 | 0.5850 | |
| 75.99 | 0.1400 | 0.6600 | |
| 101.33 | 0.2050 | 0.6850 | |
| 126.66 | 0.2900 | 0.6730 | |
| 151.99 | 0.4200 | 0.6100 | |
| 162.12 | 0.5150 | 0.5150 | CRIT |

Nohka, Junichi - Sarashina, Eiji - Arai, Yasuhiko - Saito, Shozaburo, Correlation Of Vapor-Liquid Equilibria For Systems Containing A Polar Component By The Bwr Equation, Journal of Chemical Engineering of Japan 1 (1973) 10-17. doi:10.1252/jcej.6.10

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 30.40 | 0.0217 | 0.2580 |
| 50.66 | 0.0638 | 0.4720 |
| 75.99 | 0.1210 | 0.5610 |
| 101.33 | 0.1850 | 0.5800 |
| 130.71 | 0.2910 | 0.5400 |
| 136.38 | 0.3270 | 0.5240 |
| 139.32 | 0.3590 | 0.5070 |

Maslennikova, V.Ya. - Goryunova, N.P. - Tsiklis, D.S., Phase equilibriums in the nitrogen-Freon 12 and nitrogen-Freon 22 systems, Russ. J. Phys. Chem. 3 (1967) 383-385.

**T / K = 333.15**

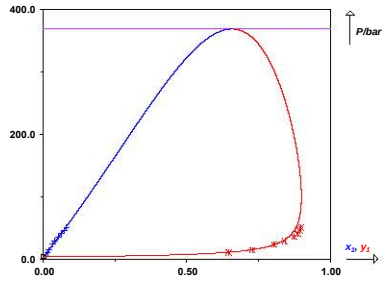
| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 25.33 | 0.0030 | 0.0450 | |
| 50.66 | 0.0670 | 0.3900 | |
| 75.99 | 0.1400 | 0.5200 | |
| 101.33 | 0.2300 | 0.5450 | |
| 126.66 | 0.3900 | 0.4800 | |
| 128.68 | 0.4350 | 0.4350 | CRIT |

Nohka, Junichi - Sarashina, Eiji - Arai, Yasuhiko - Saito, Shozaburo, Correlation Of Vapor-Liquid Equilibria For Systems Containing A Polar Component By The Bwr Equation, Journal of Chemical Engineering of Japan 1 (1973) 10-17. doi:10.1252/jcej.6.10

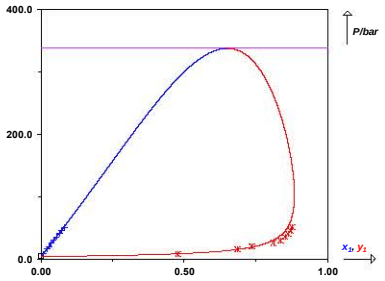
**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 43.87 | 0.0261 | 0.1400 |
| 49.65 | 0.0429 | 0.1980 |
| 64.34 | 0.0820 | 0.2780 |
| 73.97 | 0.1140 | 0.3080 |
| 82.58 | 0.1450 | 0.3160 |
| 91.19 | 0.1980 | 0.2810 |

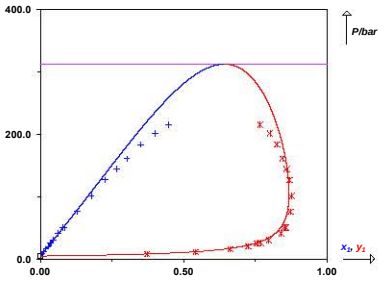
T/K = 263.20



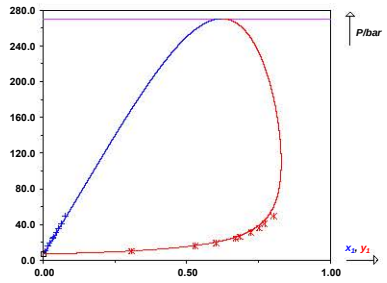

T/K = 268.20



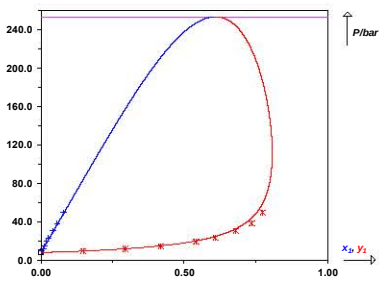

T/K = 273.15



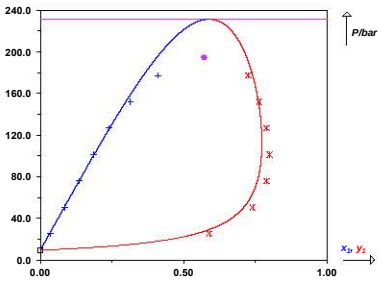

T/K = 283.20



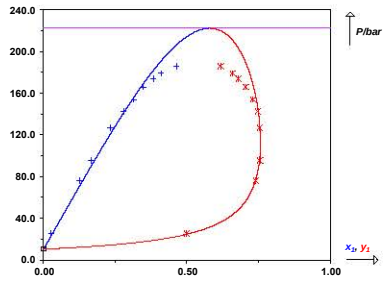

T/K = 288.20



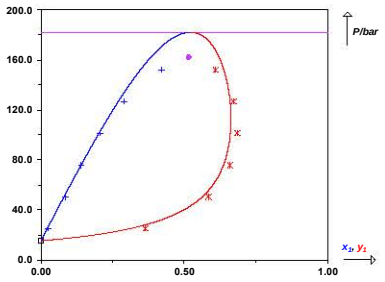

T/K = 295.15



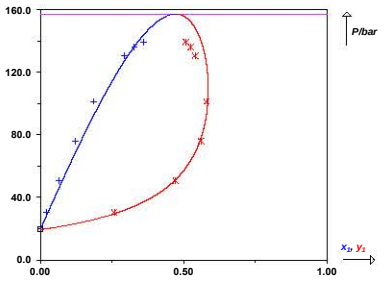

T/K = 298.15



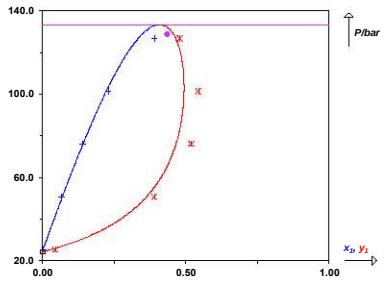

T/K = 313.15



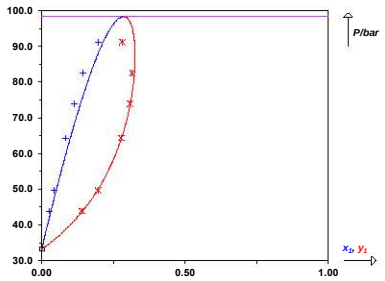

T/K = 323.15




T/K = 333.15




T/K = 348.15



## CHLOROFORM (1) + BENZENE (2)

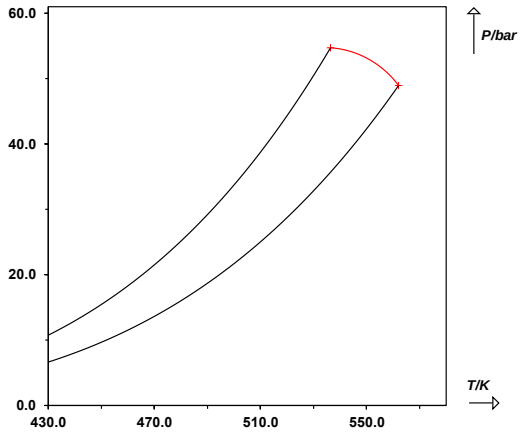
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 71-43-2 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | UHOVQNZJYSORNB-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.4 | 562.05 |
| **$P_c$ / bar** | 54.72 | 48.95 |
| **ω** | 0.222 | 0.21 |

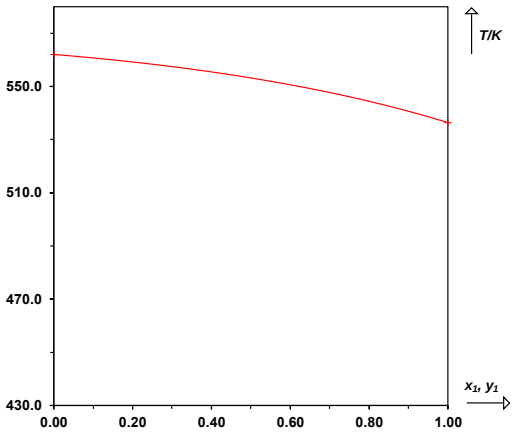
Ideal

**PPR78 results**

*Parameters*
A/MPa = -51.6
B/MPa = -60.9

*Deviations*
MAPE on x = 6.1 %
MAPE on y = 5.8 %
MAPE on $h^M$ = 41 %
MAPE on $c_P^M$ = 94 %



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**Isothermal phase equilibrium data**

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Fu, H. - Mo, X. - Han, S. - Li, H., Study on Isothermal Vapor-Liquid Equilibrium for Ethanol - Benzene, Chloroform - Benzene and Ethanol - Chloroform Binary Systems, Shiyou Xuebao Shiyou Jiagong 1 (1995) 87-92.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4377 | 0.0168 | 0.0246 |
| 0.4483 | 0.0504 | 0.0774 |
| 0.4652 | 0.1193 | 0.1797 |
| 0.4781 | 0.1701 | 0.2499 |
| 0.4972 | 0.2343 | 0.3367 |
| 0.5193 | 0.3057 | 0.4401 |
| 0.5440 | 0.3774 | 0.5214 |
| 0.5559 | 0.4128 | 0.5658 |
| 0.5781 | 0.4689 | 0.6205 |
| 0.5974 | 0.5181 | 0.6726 |
| 0.6187 | 0.5679 | 0.7218 |
| 0.6664 | 0.6789 | 0.8093 |
| 0.6946 | 0.7396 | 0.8546 |
| 0.7322 | 0.8180 | 0.9088 |
| 0.7702 | 0.8975 | 0.9513 |
| 0.7985 | 0.9546 | 0.9801 |
| 0.8113 | 0.9819 | 0.9930 |

Fu, H. - Mo, X. - Han, S. - Li, H., Study on Isothermal Vapor-Liquid Equilibrium for Ethanol - Benzene, Chloroform - Benzene and Ethanol - Chloroform Binary Systems, Shiyou Xuebao Shiyou Jiagong 1 (1995) 87-92.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5278 | 0.0136 | 0.0218 |
| 0.5418 | 0.0617 | 0.0951 |
| 0.5606 | 0.1220 | 0.1855 |
| 0.5778 | 0.1761 | 0.2615 |
| 0.6127 | 0.2734 | 0.3841 |
| 0.6472 | 0.3602 | 0.4881 |
| 0.6726 | 0.4177 | 0.5579 |
| 0.7040 | 0.4900 | 0.6321 |
| 0.7322 | 0.5489 | 0.6913 |
| 0.7509 | 0.5871 | 0.7268 |
| 0.7747 | 0.6339 | 0.7678 |
| 0.7993 | 0.6800 | 0.8065 |
| 0.8271 | 0.7314 | 0.8452 |
| 0.8663 | 0.8028 | 0.8949 |
| 0.8988 | 0.8604 | 0.9300 |
| 0.9230 | 0.9051 | 0.9540 |
| 0.9482 | 0.9478 | 0.9762 |

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**Isobaric phase equilibrium data**

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Nagata, Isamu, Vapor-Liquid Equilibrium at Atmospheric Pressure for the Ternary System, Methyl Acetate-Chloroform-Benzene., Journal of Chemical & Engineering Data 3 (1962) 360-366. doi:10.1021/je60014a012

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 352.35 | 0.0600 | 0.0890 |
| 352.15 | 0.0680 | 0.1000 |
| 351.55 | 0.1160 | 0.1670 |
| 351.05 | 0.1330 | 0.1900 |
| 350.05 | 0.1930 | 0.2700 |
| 349.35 | 0.2290 | 0.3160 |
| 348.85 | 0.2660 | 0.3610 |
| 347.85 | 0.3180 | 0.4290 |
| 347.55 | 0.3330 | 0.4430 |
| 346.45 | 0.3880 | 0.5080 |
| 345.35 | 0.4430 | 0.5700 |
| 344.75 | 0.4670 | 0.6010 |
| 343.95 | 0.5170 | 0.6520 |
| 342.85 | 0.5700 | 0.7020 |
| 341.45 | 0.6370 | 0.7620 |
| 340.15 | 0.7000 | 0.8140 |
| 338.55 | 0.7830 | 0.8750 |
| 337.25 | 0.8530 | 0.9220 |
| 335.75 | 0.9340 | 0.9680 |

Kojima, Kazuo - Tochigi, Katsumi - Kurihara, Kiyofumi - Nakamichi, Mikiyoshi, Isobaric vapor-liquid equilibria for acetone + chloroform + benzene and the three constituent binary systems, Journal of Chemical & Engineering Data 3 (1991) 343-345. doi:10.1021/je00003a024

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 350.92 | 0.1420 | 0.2030 |
| 350.15 | 0.1850 | 0.2620 |
| 348.64 | 0.2690 | 0.3730 |
| 347.21 | 0.3470 | 0.4680 |
| 346.42 | 0.3840 | 0.5130 |
| 345.31 | 0.4490 | 0.5830 |
| 344.28 | 0.4960 | 0.6340 |
| 343.75 | 0.5240 | 0.6660 |
| 342.43 | 0.5900 | 0.7300 |

| | | |
|---|---|---|
| 340.93 | 0.6590 | 0.7910 |
| 340.33 | 0.6930 | 0.8170 |
| 338.82 | 0.7680 | 0.8720 |
| 337.05 | 0.8570 | 0.9280 |
| 335.53 | 0.9350 | 0.9690 |

Chen, Geng-Hua - Wang, Qi - Ma, Zhong-Min - Yan, Xin-Huan - Han, Shi-Jun, Phase equilibria at superatmospheric pressures for systems containing halohydrocarbon, aromatic hydrocarbon, and alcohol, Journal of Chemical & Engineering Data 2 (1995) 361-366. doi:10.1021/je00018a003

**P / bar = 2.050**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 377.46 | 0.0399 | 0.0627 |
| 376.83 | 0.0709 | 0.1037 |
| 376.20 | 0.1113 | 0.1619 |
| 375.30 | 0.1544 | 0.2153 |
| 374.33 | 0.2093 | 0.2798 |
| 373.13 | 0.2579 | 0.3494 |
| 372.10 | 0.3094 | 0.4061 |
| 370.92 | 0.3707 | 0.4939 |
| 369.92 | 0.4141 | 0.5381 |
| 368.82 | 0.4621 | 0.5897 |
| 367.51 | 0.5303 | 0.6613 |
| 366.33 | 0.5781 | 0.7067 |
| 365.47 | 0.6141 | 0.7376 |
| 363.84 | 0.6819 | 0.7923 |
| 362.48 | 0.7440 | 0.8405 |
| 361.28 | 0.8091 | 0.8886 |
| 360.10 | 0.8667 | 0.9313 |
| 359.55 | 0.8973 | 0.9516 |
| 358.92 | 0.9248 | 0.9614 |
| 358.32 | 0.9521 | 0.9763 |

Chen, Geng-Hua - Wang, Qi - Ma, Zhong-Min - Yan, Xin-Huan - Han, Shi-Jun, Phase equilibria at superatmospheric pressures for systems containing halohydrocarbon, aromatic hydrocarbon, and alcohol, Journal of Chemical & Engineering Data 2 (1995) 361-366. doi:10.1021/je00018a003

**P / bar = 3.030**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 392.40 | 0.0457 | 0.0723 |
| 391.87 | 0.0847 | 0.1225 |
| 391.18 | 0.1259 | 0.1768 |
| 390.34 | 0.1879 | 0.2588 |
| 388.87 | 0.2553 | 0.3436 |
| 387.56 | 0.3207 | 0.4201 |
| 387.06 | 0.3349 | 0.4406 |
| 385.94 | 0.4070 | 0.5215 |
| 383.87 | 0.4851 | 0.6043 |
| 382.90 | 0.5279 | 0.6495 |
| 381.53 | 0.5961 | 0.7151 |
| 380.03 | 0.6555 | 0.7642 |
| 378.80 | 0.7115 | 0.8109 |
| 377.69 | 0.7515 | 0.8503 |
| 376.91 | 0.7961 | 0.8817 |
| 375.06 | 0.8715 | 0.9303 |
| 374.33 | 0.9063 | 0.9527 |
| 373.36 | 0.9380 | 0.9701 |
| 372.65 | 0.9620 | 0.9847 |
| 372.27 | 0.9880 | 0.9957 |

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**Enthalpy of mixing**

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Baud, E., Thermal analysis of binary mixtures, Bull. Soc. Chim. Fr. (1915) 329-345.

**T / K = 290.65**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -63.22 | 0.0670 |
| -192.59 | 0.2300 |
| -267.95 | 0.3400 |
| -360.06 | 0.5840 |
| -305.64 | 0.7370 |
| -200.97 | 0.8500 |

Hirobe, H., Thermochemical studies, J. Fac. Sci. Univ. Tokyo Sect. 1 4 (1926) 155-222.

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -196.78 | 0.1461 |
| -324.48 | 0.3115 |
| -401.51 | 0.4584 |
| -424.54 | 0.5601 |
| -369.28 | 0.7572 |
| -238.65 | 0.8681 |

Nagata, Isamu - Tamura, Kazuhiro - Tokuriki, Shinji, Excess enthalpies and complex formation of acetonitrile with acetone, chloroform, and benzene, Thermochimica Acta 3 (1981) 315-331. doi:10.1016/0040-6031(81)80110-4

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -55.40 | 0.0452 |

| | |
|---|---|
| -106.20 | 0.0873 |
| -197.40 | 0.1701 |
| -234.20 | 0.2061 |
| -275.20 | 0.2455 |
| -321.20 | 0.3030 |
| -357.10 | 0.3590 |
| -383.70 | 0.4122 |
| -407.40 | 0.4902 |
| -415.20 | 0.5584 |
| -413.80 | 0.5620 |
| -404.70 | 0.6191 |
| -385.20 | 0.6729 |
| -354.70 | 0.7236 |
| -321.40 | 0.7675 |
| -276.00 | 0.8144 |
| -216.80 | 0.8642 |
| -185.10 | 0.8870 |
| -151.90 | 0.9105 |
| -116.40 | 0.9319 |
| -79.50 | 0.9547 |
| -40.60 | 0.9770 |

Rastogi, R.P. - Nath, Jagan - Misra, R.R., Thermodynamics of weak interactions in liquid mixtures of chloroform and aromatic hydrocarbons, The Journal of Chemical Thermodynamics 3 (1971) 307-317. doi:10.1016/S0021-9614(71)80047-2

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -184.00 | 0.1533 |
| -267.00 | 0.2340 |
| -292.00 | 0.2604 |
| -360.00 | 0.3371 |
| -400.00 | 0.4286 |
| -430.00 | 0.5200 |
| -421.00 | 0.6009 |
| -418.00 | 0.6238 |
| -407.00 | 0.6302 |
| -398.00 | 0.6693 |
| -318.00 | 0.7801 |
| -308.00 | 0.7836 |
| -309.00 | 0.7940 |

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**Heat capacity of mixing**

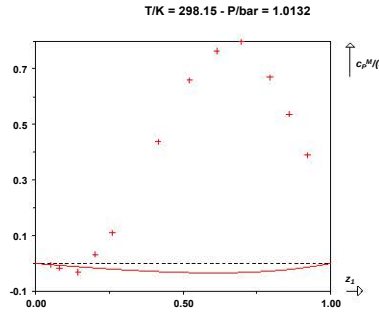
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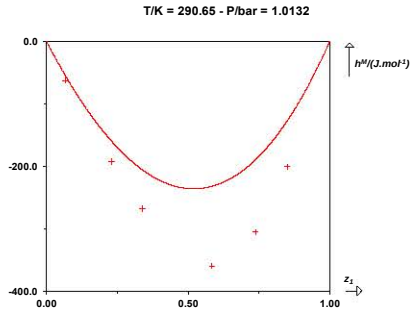
Grolier, Jean-Pierre E. - Roux-Desgranges, Genevieve - Kooner, Zorawar S. - Smith, John F. - Hepler, Loren G., Thermal and volumetric properties of chloroform+benzene mixtures and the ideal associated solution model of complex formation, Journal of Solution Chemistry 9 (1987) 745-752. doi:10.1007/BF00652577

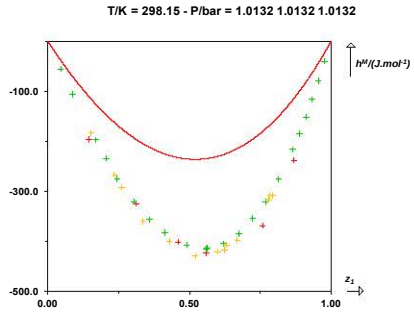
**T / K =** **298.15**

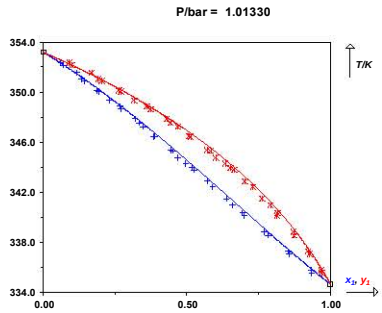
**P / bar =** **UNKNOWN (1.0132)**

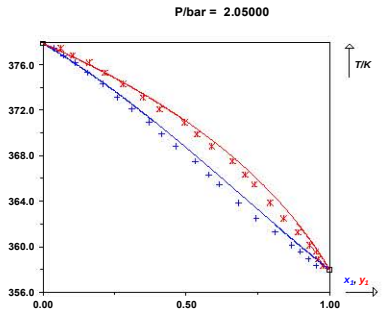
| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.0046 | 0.0524 |
| -0.0163 | 0.0806 |
| -0.0306 | 0.1445 |
| 0.0319 | 0.2031 |
| 0.1080 | 0.2597 |
| 0.4378 | 0.4162 |
| 0.6590 | 0.5220 |
| 0.7643 | 0.6145 |
| 0.7984 | 0.6981 |
| 0.6698 | 0.7949 |
| 0.5365 | 0.8598 |
| 0.3904 | 0.9228 |

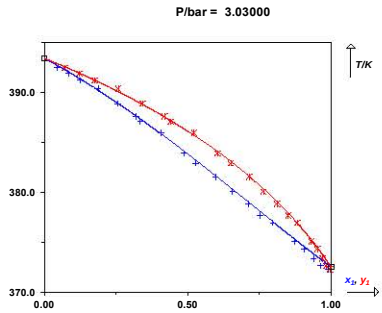

T/K = 298.15 - P/bar = 1.0132
$c_P^M$/(J.mol$^{-1}$.K$^{-1}$)
$z_1$

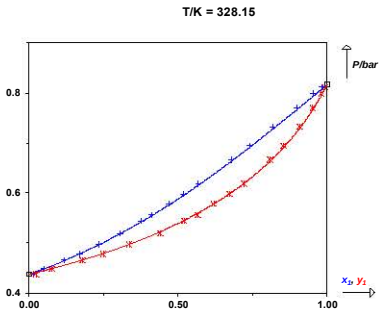

T/K = 290.65 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
$z_1$

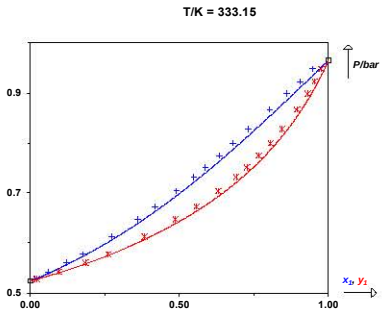

T/K = 298.15 - P/bar = 1.0132 1.0132 1.0132
$h^M$/(J.mol$^{-1}$)
$z_1$


P/bar = 1.01330
T/K
$x_1$, $y_1$


P/bar = 2.05000
T/K
$x_1$, $y_1$


P/bar = 3.03000
T/K
$x_1$, $y_1$


T/K = 328.15
P/bar
$x_1$, $y_1$


T/K = 333.15
P/bar
$x_1$, $y_1$

## CHLOROFORM (1) + 1,2-DICHLOROETHANE (2)

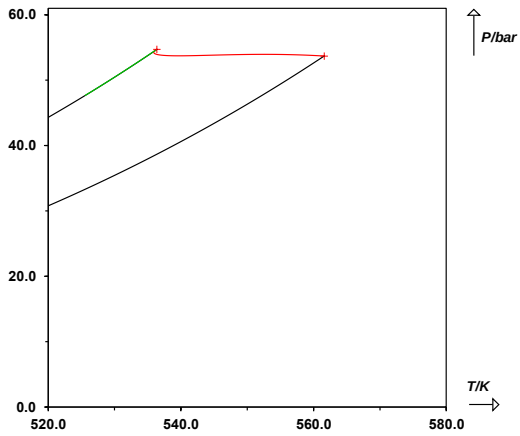
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 107-06-2 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | WSLDOOZREJYCGB-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.40 | 561.60 |
| **$P_c$ / bar** | 54.72 | 53.70 |
| **ω** | 0.222 | 0.287 |

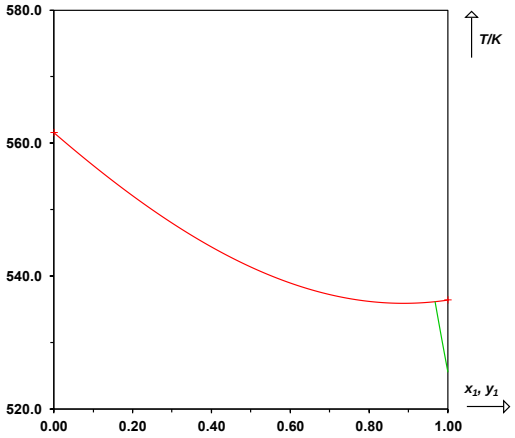
Ideal

**PPR78 results**

*Parameters*
A/MPa = 29.7
B/MPa = -44

*Deviations*
MAPE on x = 2.9 %
MAPE on y = 3.8 %
MAPE on $h^M$ = 9.3 %



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**Isobaric phase equilibrium data**

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Al-Hayan, M.N.M - Newsham, D.M.T, Isobaric vapour–liquid equilibria for mixtures containing halogenated hydrocarbons at atmospheric pressure: I. Binary mixtures of trichloromethane+ 1, 2-dichloroethane, 1, 2-dichloroethane+ 1, 1, 2, 2-tetrachloroethane, trichloromethane+ 1, 1, 2, 2-tetrachloroethane and n-heptane+ 1, 1, 2, 2-tetrachloroethane, Fluid Phase Equilibria 1 (1999) 91-100. doi:10.1016/S0378-3812(99)00297-6

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 353.90 | 0.0814 | 0.1626 |
| 350.80 | 0.1826 | 0.3239 |
| 349.40 | 0.2352 | 0.3952 |
| 346.70 | 0.3395 | 0.5186 |
| 344.40 | 0.4392 | 0.6192 |
| 342.80 | 0.5171 | 0.6882 |
| 340.00 | 0.6567 | 0.7953 |
| 337.20 | 0.8116 | 0.8956 |

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**Enthalpy of mixing**

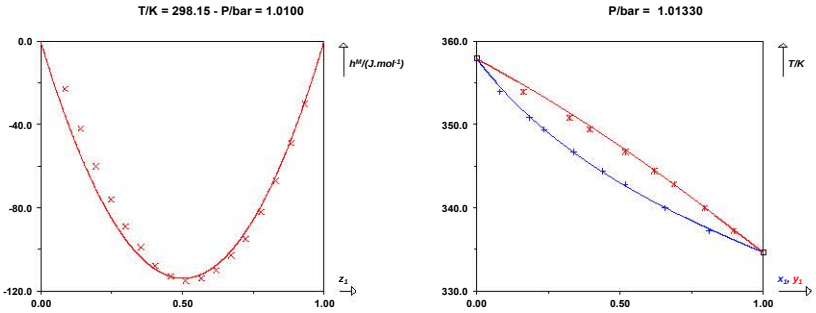
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Munoz Embid, J. - Roux, A.H. - Grolier, J.P.E., Excess enthalpy. Trichloromethane - 1,2-dichloroethane system, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1990) 59-78.

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -23.00 | 0.0869 |
| -42.00 | 0.1406 |
| -60.00 | 0.1947 |
| -76.00 | 0.2489 |
| -89.00 | 0.3008 |
| -99.00 | 0.3540 |
| -108.00 | 0.4058 |
| -113.00 | 0.4595 |
| -115.00 | 0.5130 |
| -114.00 | 0.5664 |
| -110.00 | 0.6207 |
| -103.00 | 0.6738 |
| -95.00 | 0.7240 |
| -82.00 | 0.7789 |
| -67.00 | 0.8304 |
| -49.00 | 0.8853 |
| -30.00 | 0.9328 |


T/K = 298.15 - P/bar = 1.0100
0.0
-40.0
-80.0
-120.0
0.00
0.50
1.00
$h^{M}/(J.mol^{-1})$
$z_1$
P/bar = 1.01330
360.0
350.0
340.0
330.0
0.00
0.50
1.00
T/K
$x_1, y_1$

## CHLOROFORM (1) + CARBON TETRACHLORIDE (2)

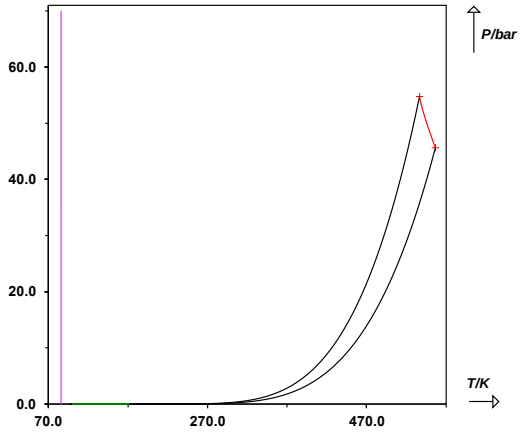
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 56-23-5 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | VZGDMQKNWNREIO-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.40 | 556.35 |
| **$P_c$ / bar** | 54.72 | 45.60 |
| **ω** | 0.222 | 0.193 |

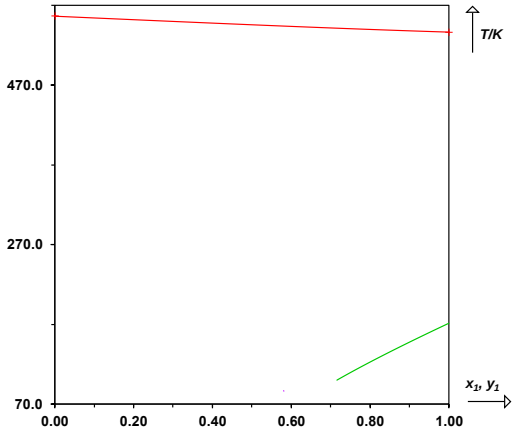
Ideal

**PPR78 results**

*Parameters*
A/MPa = 33.5
B/MPa = 62.2

*Deviations*
MAPE on x = 7.6 %
MAPE on y = 7.8 %
MAPE on $h^M$ = 4.2 %



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**Isothermal phase equilibrium data**

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Góral, M. - Oracz, P. - Warycha, S., Vapour—liquid equilibria. IV. The ternary system carbon tetrachloride—methanol—chloroform at 293.15 K, Fluid Phase Equilibria 1 (1988) 77-93. doi:10.1016/0378-3812(88)80104-3

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1281 | 0.0542 | 0.1040 |
| 0.1358 | 0.1181 | 0.2099 |
| 0.1426 | 0.1780 | 0.2962 |
| 0.1491 | 0.2378 | 0.3726 |
| 0.1549 | 0.2949 | 0.4384 |
| 0.1610 | 0.3576 | 0.5040 |
| 0.1665 | 0.4161 | 0.5602 |
| 0.1716 | 0.4724 | 0.6107 |
| 0.1767 | 0.5329 | 0.6616 |
| 0.1813 | 0.5883 | 0.7058 |
| 0.1869 | 0.6587 | 0.7594 |
| 0.1916 | 0.7198 | 0.8041 |
| 0.1951 | 0.7630 | 0.8350 |
| 0.2004 | 0.8400 | 0.8890 |
| 0.2053 | 0.9125 | 0.9393 |
| 0.2086 | 0.9617 | 0.9733 |

Rulewicz, G. - Schuberth, H. - Leibnitz, E., Untersuchungen über das Dampf-Flüssigkeits-Phasengleichgewicht des Systems Methylenchlorid/Chloroform/Tetrachlorkohlenstoff bei 45°C unter Verwendung einer gaschromatographischen Analysenmethode, Journal für Praktische Chemie 3-4 (1968) 122-136. doi:10.1002/prac.19680370303

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3530 | 0.0250 | 0.0460 |
| 0.3610 | 0.0500 | 0.0880 |
| 0.3766 | 0.1000 | 0.1690 |
| 0.3920 | 0.1500 | 0.2440 |
| 0.4060 | 0.2000 | 0.3120 |
| 0.4192 | 0.2500 | 0.3740 |
| 0.4324 | 0.3000 | 0.4320 |
| 0.4448 | 0.3500 | 0.4900 |
| 0.4564 | 0.4000 | 0.5390 |
| 0.4684 | 0.4500 | 0.5870 |
| 0.4796 | 0.5000 | 0.6300 |
| 0.4910 | 0.5500 | 0.6740 |
| 0.5021 | 0.6000 | 0.7140 |
| 0.5125 | 0.6500 | 0.7550 |
| 0.5226 | 0.7000 | 0.7920 |
| 0.5320 | 0.7500 | 0.8290 |
| 0.5410 | 0.8000 | 0.8640 |
| 0.5502 | 0.8500 | 0.8990 |
| 0.5596 | 0.9000 | 0.9330 |
| 0.5630 | 0.9200 | 0.9470 |
| 0.5689 | 0.9500 | 0.9650 |
| 0.5724 | 0.9700 | 0.9790 |

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**Isobaric phase equilibrium data**

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Krauze, R. - Serwinski, M., Liquid-vapor equilibrium in he system chloroform-carbon tetrachloride, Zesz. Nauk. Politech. Lodz. Chem. (1973) 53-63.

**P / bar = 0.9959**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 346.85 | 0.0950 | 0.1600 |
| 345.15 | 0.1710 | 0.2690 |
| 344.65 | 0.2030 | 0.3070 |
| 342.75 | 0.2970 | 0.4170 |
| 340.35 | 0.4480 | 0.5690 |
| 338.05 | 0.6170 | 0.7190 |
| 336.15 | 0.7650 | 0.8330 |
| 335.25 | 0.8510 | 0.9000 |

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**Enthalpy of mixing**

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Siddiqi, M.A. - Lucas, K., Excess enthalpy of the system chloroform + carbon tetrachloride and a thermodynamic evaluation of its state dependence, Fluid Phase Equilibria 1 (1984) 87-98. doi:10.1016/0378-3812(84)85023-2

**T / K = 283.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 134.90 | 0.1750 |
| 190.30 | 0.2850 |
| 223.30 | 0.3920 |
| 229.80 | 0.4440 |
| 233.00 | 0.4950 |
| 232.50 | 0.5450 |
| 224.40 | 0.5940 |
| 199.70 | 0.6900 |
| 182.40 | 0.7370 |
| 133.60 | 0.8270 |

Siddiqi, M.A. - Lucas, K., Excess enthalpy of the system chloroform + carbon tetrachloride and a

thermodynamic evaluation of its state dependence, Fluid Phase Equilibria 1 (1984) 87-98. doi:10.1016/0378-3812(84)85023-2

**T / K = 303.15**

**P / bar = UNKNOWN (1.0132)**

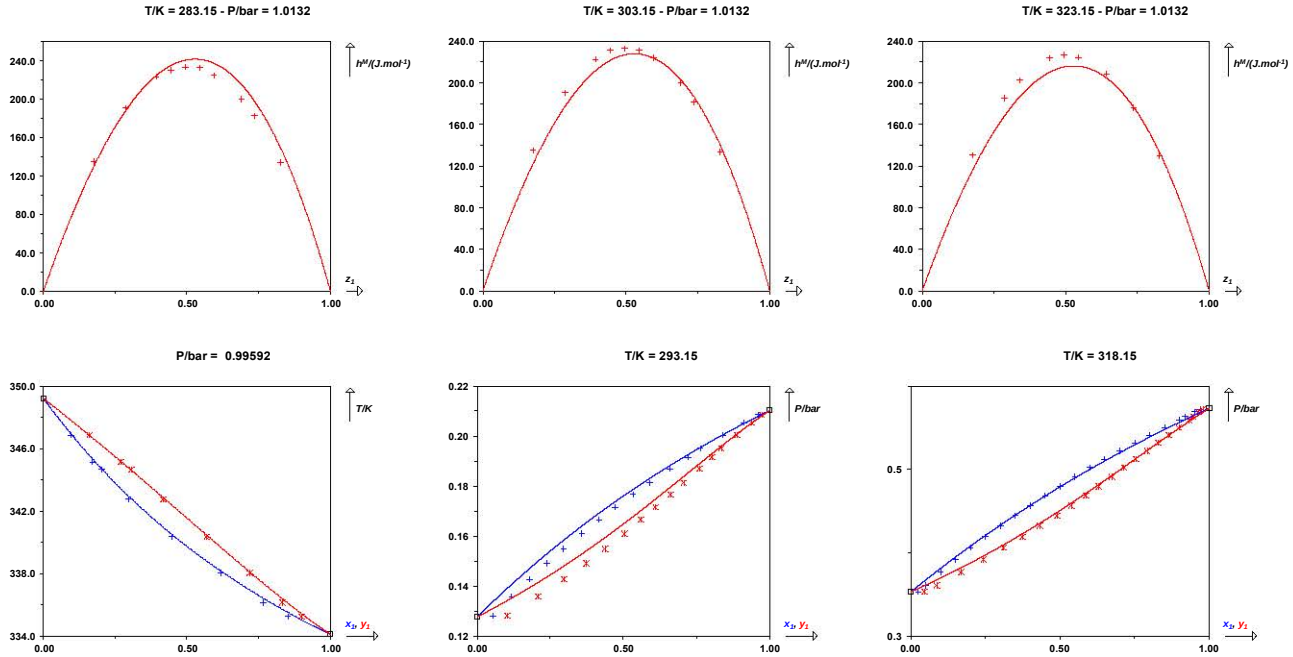
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 135.20 | 0.1750 |
| 190.50 | 0.2850 |
| 222.70 | 0.3920 |
| 230.90 | 0.4440 |
| 233.00 | 0.4950 |
| 230.90 | 0.5450 |
| 223.90 | 0.5940 |
| 199.70 | 0.6900 |
| 181.20 | 0.7370 |
| 133.60 | 0.8270 |

Siddiqi, M.A. - Lucas, K., Excess enthalpy of the system chloroform + carbon tetrachloride and a thermodynamic evaluation of its state dependence, Fluid Phase Equilibria 1 (1984) 87-98. doi:10.1016/0378-3812(84)85023-2

**T / K = 323.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 130.70 | 0.1750 |
| 185.10 | 0.2850 |
| 202.70 | 0.3390 |
| 223.70 | 0.4440 |
| 226.60 | 0.4950 |
| 224.60 | 0.5450 |
| 208.70 | 0.6420 |
| 175.80 | 0.7370 |
| 129.50 | 0.8270 |


T/K = 283.15 - P/bar = 1.0132
T/K = 303.15 - P/bar = 1.0132
T/K = 323.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
$z_1$
P/bar = 0.99592
T/K = 293.15
T/K = 318.15
P/bar
$x_1$, $y_1$

## 1,1,1-TRIFLUOROETHANE (1) + 2,3,3,3-TETRAFLUOROPROPENE (2)

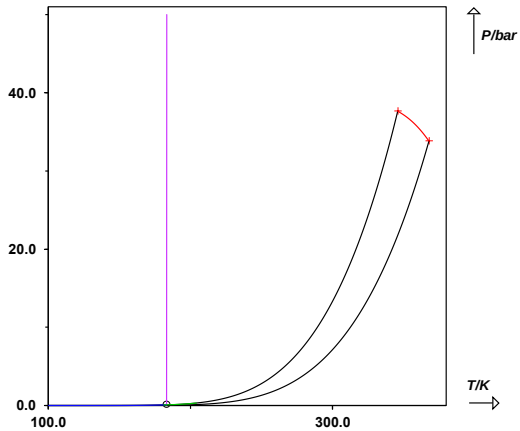
| | | |
|---|---|---|
| **CAS** | 420-46-2 | 754-12-1 |
| **InChiKey** | UJPMYEOUBPIPHQ-UHFFFAOYSA-N | FXRLMCRCYDHQFW-UHFFFAOYSA-N |
| **$T_c$ / K** | 345.88 | 367.85 |
| **$P_c$ / bar** | 37.64 | 33.82 |
| **ω** | 0.261 | 0.282 |

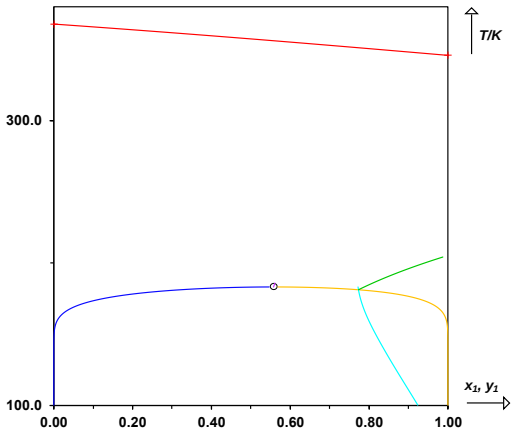
Ideal

**PPR78 results**

*Parameters*
A/MPa = 15.3
B/MPa = 103

*Deviations*
MAPE on x = 2.2 %
MAPE on y = 2.8 %



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**Isothermal phase equilibrium data**

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Hu, Peng - Chen, Long-Xiang - Chen, Ze-Shao, Vapor–liquid equilibria for the 1,1,1,2-tetrafluoroethane (HFC-134a)+1,1,1,2,3,3,3-heptafluoropropane (HFC-227ea) and 1,1,1-trifluoroethane (HFC-143a)+2,3,3,3-tetrafluoroprop-1-ene (HFO-1234yf) systems, Fluid Phase Equilibria (2013) 293-297. doi:10.1016/j.fluid.2013.09.056

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.726 | 0.0809 | 0.1338 |
| 5.246 | 0.2022 | 0.3134 |
| 5.913 | 0.3656 | 0.4991 |
| 6.423 | 0.4954 | 0.6266 |
| 7.167 | 0.6858 | 0.7875 |
| 7.533 | 0.7799 | 0.8551 |
| 7.747 | 0.8390 | 0.8975 |

Hu, Peng - Chen, Long-Xiang - Chen, Ze-Shao, Vapor–liquid equilibria for the 1,1,1,2-tetrafluoroethane (HFC-134a)+1,1,1,2,3,3,3-heptafluoropropane (HFC-227ea) and 1,1,1-trifluoroethane (HFC-143a)+2,3,3,3-tetrafluoroprop-1-ene (HFO-1234yf) systems, Fluid Phase Equilibria (2013) 293-297. doi:10.1016/j.fluid.2013.09.056

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.356 | 0.0809 | 0.1299 |
| 7.024 | 0.2022 | 0.3029 |
| 7.873 | 0.3656 | 0.4905 |
| 8.536 | 0.4954 | 0.6172 |
| 9.500 | 0.6858 | 0.7802 |
| 9.963 | 0.7799 | 0.8497 |
| 10.25 | 0.8390 | 0.8938 |

Hu, Peng - Chen, Long-Xiang - Chen, Ze-Shao, Vapor–liquid equilibria for the 1,1,1,2-tetrafluoroethane (HFC-134a)+1,1,1,2,3,3,3-heptafluoropropane (HFC-227ea) and 1,1,1-trifluoroethane (HFC-143a)+2,3,3,3-tetrafluoroprop-1-ene (HFO-1234yf) systems, Fluid Phase Equilibria (2013) 293-297. doi:10.1016/j.fluid.2013.09.056

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.428 | 0.0809 | 0.1258 |
| 9.215 | 0.2022 | 0.2933 |
| 10.28 | 0.3656 | 0.4812 |
| 11.11 | 0.4954 | 0.6071 |
| 12.33 | 0.6858 | 0.7718 |
| 12.93 | 0.7799 | 0.8438 |
| 13.24 | 0.8390 | 0.8880 |

Hu, Peng - Chen, Long-Xiang - Chen, Ze-Shao, Vapor–liquid equilibria for the 1,1,1,2-tetrafluoroethane (HFC-134a)+1,1,1,2,3,3,3-heptafluoropropane (HFC-227ea) and 1,1,1-trifluoroethane (HFC-143a)+2,3,3,3-tetrafluoroprop-1-ene (HFO-1234yf) systems, Fluid Phase Equilibria (2013) 293-297. doi:10.1016/j.fluid.2013.09.056

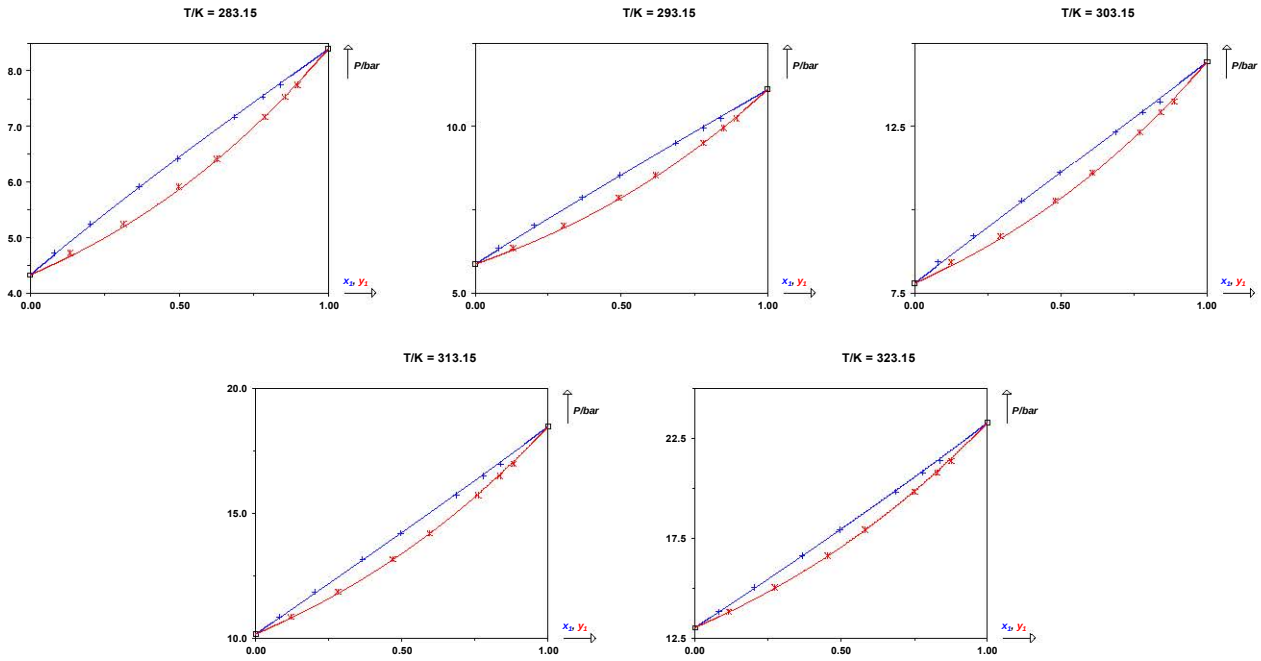
**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.84 | 0.0809 | 0.1204 |
| 11.85 | 0.2022 | 0.2821 |
| 13.16 | 0.3656 | 0.4684 |
| 14.20 | 0.4954 | 0.5958 |
| 15.72 | 0.6858 | 0.7617 |
| 16.49 | 0.7799 | 0.8365 |
| 16.96 | 0.8390 | 0.8825 |

Hu, Peng - Chen, Long-Xiang - Chen, Ze-Shao, Vapor–liquid equilibria for the 1,1,1,2-tetrafluoroethane (HFC-134a)+1,1,1,2,3,3,3-heptafluoropropane (HFC-227ea) and 1,1,1-trifluoroethane (HFC-143a)+2,3,3,3-tetrafluoroprop-1-ene (HFO-1234yf) systems, Fluid Phase Equilibria (2013) 293-297. doi:10.1016/j.fluid.2013.09.056

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.82 | 0.0809 | 0.1158 |
| 15.03 | 0.2022 | 0.2722 |
| 16.63 | 0.3656 | 0.4540 |
| 17.93 | 0.4954 | 0.5820 |
| 19.79 | 0.6858 | 0.7518 |
| 20.76 | 0.7799 | 0.8287 |
| 21.37 | 0.8390 | 0.8770 |


T/K = 283.15
P/bar
8.0
7.0
6.0
5.0
4.0
0.00
0.50
1.00
x1, y1
T/K = 293.15
P/bar
10.0
5.0
0.00
0.50
1.00
x1, y1
T/K = 303.15
P/bar
12.5
7.5
0.00
0.50
1.00
x1, y1
T/K = 313.15
P/bar
20.0
15.0
10.0
0.00
0.50
1.00
x1, y1
T/K = 323.15
P/bar
22.5
17.5
12.5
0.00
0.50
1.00
x1, y1

## ETHYL FLUORIDE (1) + 1,1,1,2-TETRAFLUOROETHANE (2)

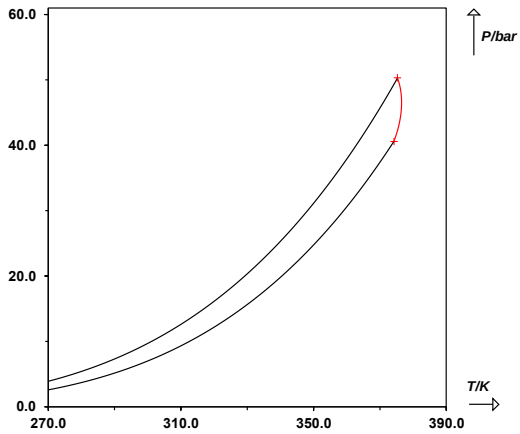
| | | |
|---|---|---|
| **CAS** | 353-36-6 | 811-97-2 |
| **InChiKey** | UHCBBWUQDAVSMS-UHFFFAOYSA-N | LVGUZGTVOIAKKC-UHFFFAOYSA-N |
| **$T_c$ / K** | 375.31 | 374.18 |
| **$P_c$ / bar** | 50.28 | 40.56 |
| **ω** | 0.218 | 0.327 |

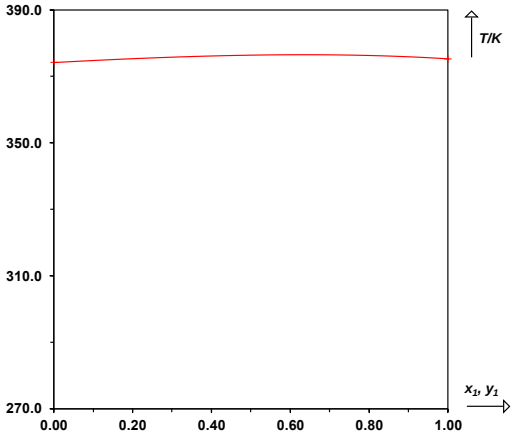
Ideal

**PPR78 results**

*Parameters*
A/MPa = -20.3
B/MPa = 14.4

*Deviations*
MAPE on x = 1.9 %
MAPE on y = 2.9 %



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**Isothermal phase equilibrium data**

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Kostrzewa, Dorota - Dobrzyńska-Inger, Agnieszka - Rój, Edward, Experimental data on xanthohumol solubility in supercritical carbon dioxide, Fluid Phase Equilibria (2013) 445-450. doi:10.1016/j.fluid.2013.10.001

**T / K = 253.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.457 | 0.2034 | 0.2596 |
| 1.532 | 0.3015 | 0.3787 |
| 1.599 | 0.4080 | 0.5022 |
| 1.680 | 0.5038 | 0.6099 |
| 1.763 | 0.6025 | 0.7109 |
| 1.868 | 0.7059 | 0.8012 |
| 1.938 | 0.8084 | 0.8762 |

Kostrzewa, Dorota - Dobrzyńska-Inger, Agnieszka - Rój, Edward, Experimental data on xanthohumol solubility in supercritical carbon dioxide, Fluid Phase Equilibria (2013) 445-450. doi:10.1016/j.fluid.2013.10.001

**T / K = 263.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.112 | 0.1179 | 0.1406 |
| 2.173 | 0.1914 | 0.2412 |
| 2.260 | 0.2944 | 0.3604 |
| 2.349 | 0.3870 | 0.4733 |
| 2.442 | 0.4824 | 0.5810 |
| 2.568 | 0.5901 | 0.6864 |
| 2.711 | 0.6974 | 0.7852 |
| 2.832 | 0.8092 | 0.8764 |

Kostrzewa, Dorota - Dobrzyńska-Inger, Agnieszka - Rój, Edward, Experimental data on xanthohumol solubility in supercritical carbon dioxide, Fluid Phase Equilibria (2013) 445-450. doi:10.1016/j.fluid.2013.10.001

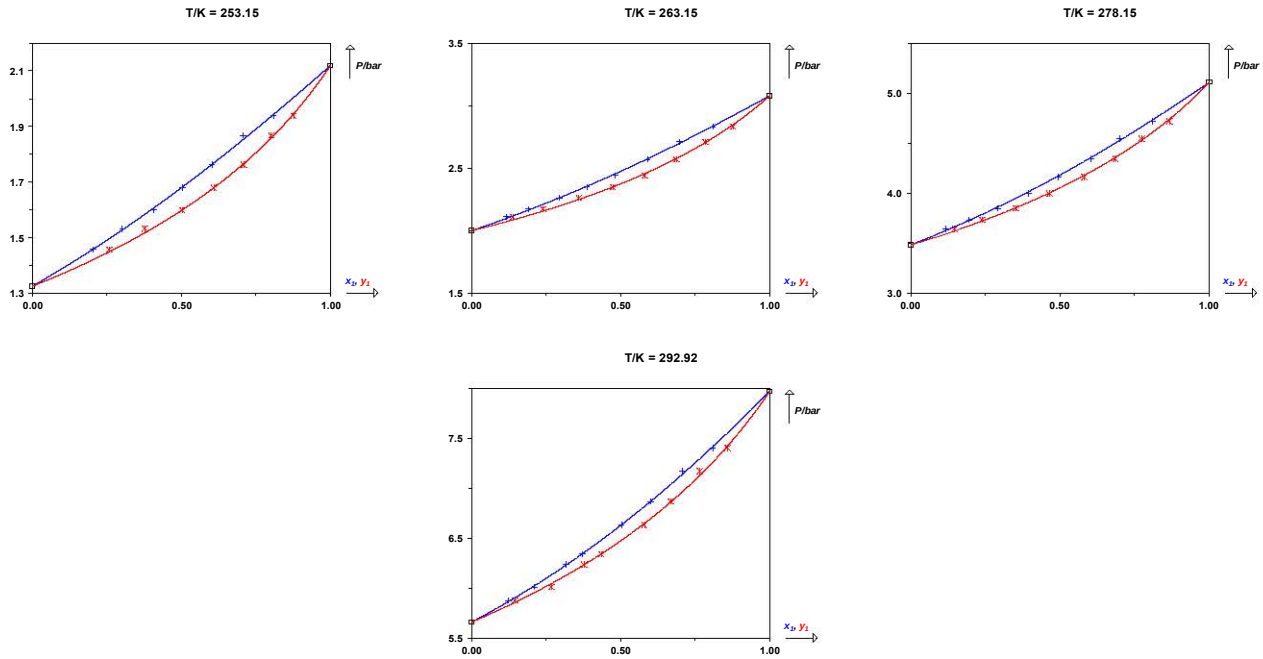
**T / K = 278.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.643 | 0.1161 | 0.1470 |
| 3.732 | 0.1955 | 0.2402 |
| 3.847 | 0.2924 | 0.3520 |
| 3.996 | 0.3954 | 0.4650 |
| 4.160 | 0.4948 | 0.5818 |
| 4.343 | 0.6037 | 0.6854 |
| 4.544 | 0.7010 | 0.7746 |
| 4.719 | 0.8098 | 0.8668 |

Kostrzewa, Dorota - Dobrzyńska-Inger, Agnieszka - Rój, Edward, Experimental data on xanthohumol solubility in supercritical carbon dioxide, Fluid Phase Equilibria (2013) 445-450. doi:10.1016/j.fluid.2013.10.001

**T / K = 292.92**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.877 | 0.1229 | 0.1466 |
| 6.010 | 0.2105 | 0.2681 |
| 6.235 | 0.3172 | 0.3780 |
| 6.339 | 0.3710 | 0.4354 |
| 6.634 | 0.5032 | 0.5808 |
| 6.866 | 0.5991 | 0.6690 |
| 7.168 | 0.7068 | 0.7658 |
| 7.402 | 0.8084 | 0.8586 |


T/K = 253.15
P/bar
2.1
1.9
1.7
1.5
1.3
0.00
0.50
1.00
$x_1, y_1$
T/K = 263.15
P/bar
3.5
2.5
1.5
0.00
0.50
1.00
$x_1, y_1$
T/K = 278.15
P/bar
5.0
4.0
3.0
0.00
0.50
1.00
$x_1, y_1$
T/K = 292.92
P/bar
7.5
6.5
5.5
0.00
0.50
1.00
$x_1, y_1$

## PROPYLENE (1) + CHLORODIFLUOROMETHANE (2)

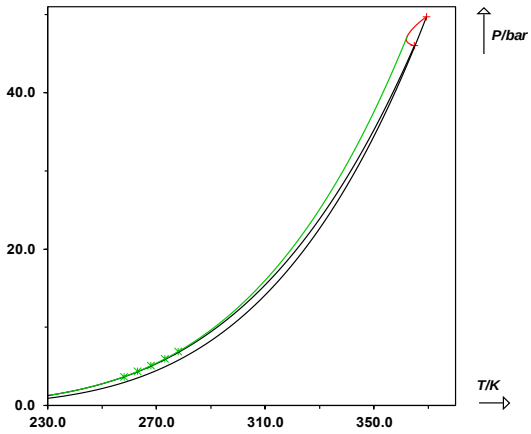
| | | |
|---|---|---|
| **CAS** | 115-07-1 | 75-45-6 |
| **InChiKey** | QQONPFPTGQHPMA-UHFFFAOYSA-N | VOPWNXZWBYDODV-UHFFFAOYSA-N |
| **$T_c$ / K** | 364.85 | 369.3 |
| **$P_c$ / bar** | 46 | 49.71 |
| **ω** | 0.138 | 0.219 |

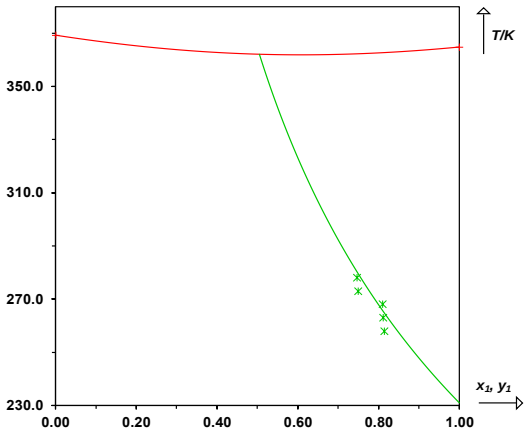
Ideal

**PPR78 results**

*Parameters*
A/MPa = 83.2
B/MPa = 28.7

*Deviations*
MAPE on x = 6.5 %
MAPE on y = 5.9 %
MAPE on $x_{az}$ = 5.5 %
MAPE on $P_{az}$ = 0.084 %



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**Isothermal phase equilibrium data**

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Kleiber, Michael, Vapor-liquid equilibria of binary refrigerant mixtures containing propylene or R134a, Fluid Phase Equilibria (1994) 149-194. doi:10.1016/0378-3812(94)80046-4

**T / K = 258.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.218 | 0.1517 | 0.2167 | |
| 3.487 | 0.3830 | 0.4460 | |
| 3.631 | 0.6070 | 0.6383 | |
| 3.649 | 0.6633 | 0.6831 | |
| 3.669 | 0.7465 | 0.7562 | |
| 3.670 | 0.8133 | 0.8138 | |
| 3.670 | 0.8141 | 0.8141 | AZEO |

Kleiber, Michael, Vapor-liquid equilibria of binary refrigerant mixtures containing propylene or R134a, Fluid Phase Equilibria (1994) 149-194. doi:10.1016/0378-3812(94)80046-4

**T / K = 263.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.841 | 0.1527 | 0.2138 | |
| 4.143 | 0.3797 | 0.4407 | |
| 4.303 | 0.6066 | 0.6329 | |
| 4.321 | 0.6618 | 0.6807 | |
| 4.340 | 0.7480 | 0.7539 | |
| 4.339 | 0.8119 | 0.8119 | AZEO |
| 4.339 | 0.8139 | 0.8126 | |

Kleiber, Michael, Vapor-liquid equilibria of binary refrigerant mixtures containing propylene or R134a, Fluid Phase Equilibria (1994) 149-194. doi:10.1016/0378-3812(94)80046-4

**T / K = 268.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 4.545 | 0.1517 | 0.2085 | |
| 4.884 | 0.3782 | 0.4363 | |
| 5.061 | 0.6073 | 0.6309 | |
| 5.078 | 0.6600 | 0.6768 | |
| 5.095 | 0.7473 | 0.7517 | |
| 5.094 | 0.8098 | 0.8098 | AZEO |
| 5.094 | 0.8142 | 0.8113 | |

Kleiber, Michael, Vapor-liquid equilibria of binary refrigerant mixtures containing propylene or R134a, Fluid Phase Equilibria (1994) 149-194. doi:10.1016/0378-3812(94)80046-4

**T / K = 273.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.347 | 0.1486 | 0.1989 | |
| 5.726 | 0.3793 | 0.4222 | |
| 5.916 | 0.6052 | 0.6271 | |
| 5.950 | 0.7472 | 0.7491 | |
| 5.950 | 0.7500 | 0.7500 | AZEO |
| 5.942 | 0.8131 | 0.8098 | |

Kleiber, Michael, Vapor-liquid equilibria of binary refrigerant mixtures containing propylene or R134a, Fluid Phase Equilibria (1994) 149-194. doi:10.1016/0378-3812(94)80046-4

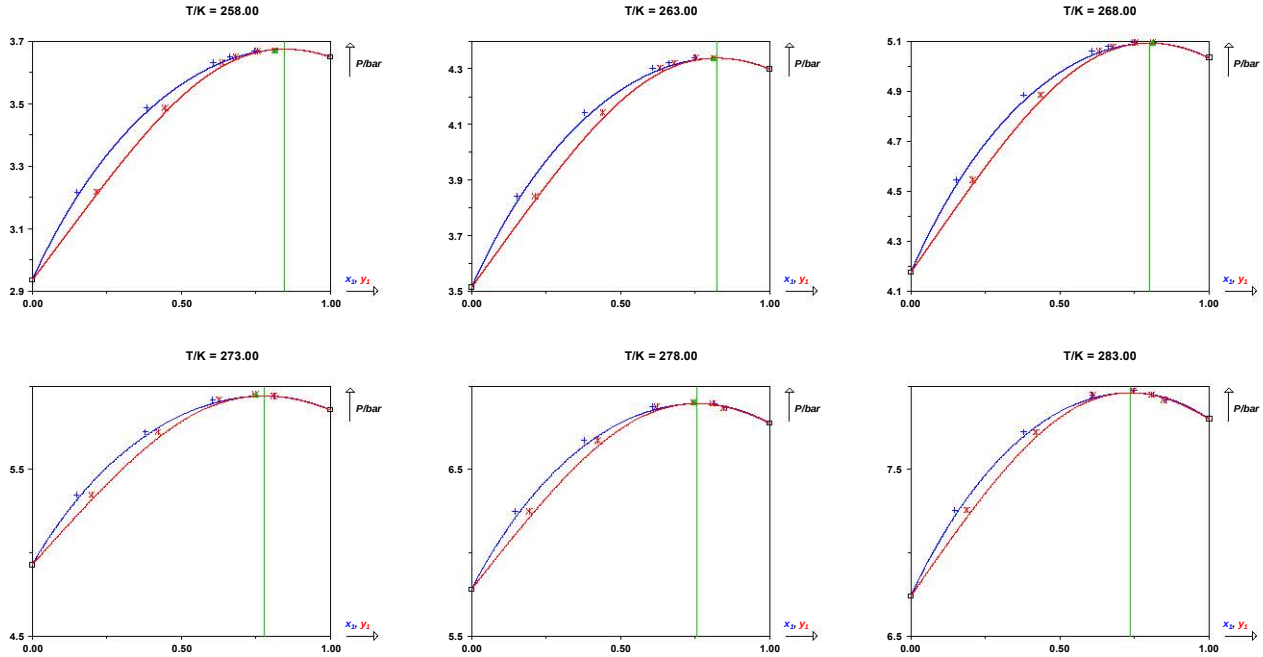
**T / K = 278.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 6.250 | 0.1450 | 0.1933 | |
| 6.675 | 0.3765 | 0.4233 | |
| 6.877 | 0.6060 | 0.6219 | |
| 6.903 | 0.7461 | 0.7461 | AZEO |
| 6.903 | 0.7472 | 0.7465 | |
| 6.895 | 0.8146 | 0.8084 | |
| 6.868 | 0.8543 | 0.8468 | |

Kleiber, Michael, Vapor-liquid equilibria of binary refrigerant mixtures containing propylene or R134a, Fluid Phase Equilibria (1994) 149-194. doi:10.1016/0378-3812(94)80046-4

**T / K = 283.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.257 | 0.1468 | 0.1870 |
| 7.725 | 0.3778 | 0.4197 |
| 7.947 | 0.6074 | 0.6106 |
| 7.972 | 0.7487 | 0.7448 |
| 7.949 | 0.8129 | 0.8070 |
| 7.918 | 0.8553 | 0.8469 |


T/K = 258.00
P/bar
x1, y1
T/K = 263.00
P/bar
x1, y1
T/K = 268.00
P/bar
x1, y1
T/K = 273.00
P/bar
x1, y1
T/K = 278.00
P/bar
x1, y1
T/K = 283.00
P/bar
x1, y1

## DIFLUOROMETHANE (1) + PROPANE (2)

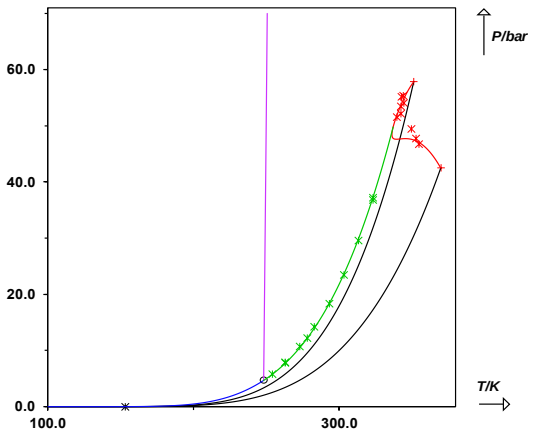
| | | |
|---|---|---|
| **CAS** | 75-10-5 | 74-98-6 |
| **InChiKey** | RWRIWBAIICGTTQ-UHFFFAOYSA-N | ATUOYWHBWRKTHZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 351.255 | 369.83 |
| **$P_c$ / bar** | 57.84 | 42.48 |
| **ω** | 0.277 | 0.152 |

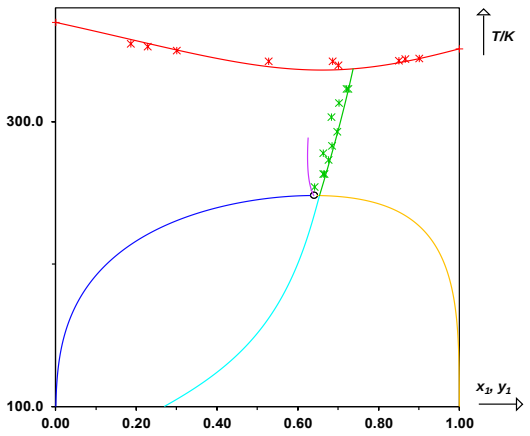
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 496
B/MPa = 687

*Deviations*
MAPE on x = 8.4 %
MAPE on y = 4.2 %
MAPE on $x_c$ = 13 %
MAPE on $P_c$ = 0.83 %
MAPE on $x_{az}$ = 2.2 %
MAPE on $P_{az}$ = 0.72 %



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**Isothermal phase equilibrium data**

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Bobbo, S. - Fedele, L. - Camporese, R. - Stryjek, R., VLE measurements and modeling for the strongly positive azeotropic R32+propane system, Fluid Phase Equilibria 1-2 (2002) 175-183. doi:10.1016/S0378-3812(01)00798-1

**T / K = 248.13**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 4.130 | 0.1577 | 0.5375 | |
| 4.628 | 0.4204 | 0.6158 | |
| 4.658 | 0.5850 | 0.6301 | |
| 4.659 | 0.5892 | 0.6308 | |
| 4.659 | 0.6707 | 0.6386 | |
| 4.661 | 0.6732 | 0.6394 | |
| 4.659 | 0.6911 | 0.6430 | |
| 4.657 | 0.7061 | 0.6437 | |
| 4.536 | 0.8510 | 0.6866 | |
| 4.248 | 0.9248 | 0.7583 | |

Bobbo, S. - Fedele, L. - Camporese, R. - Stryjek, R., VLE measurements and modeling for the strongly positive azeotropic R32+propane system, Fluid Phase Equilibria 1-2 (2002) 175-183. doi:10.1016/S0378-3812(01)00798-1

**T / K = 254.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.432 | 0.0377 | 0.2676 | |
| 3.908 | 0.0589 | 0.3594 | |
| 4.486 | 0.0993 | 0.4522 | |
| 5.015 | 0.1589 | 0.5227 | |
| 5.393 | 0.2358 | 0.5705 | |
| 5.527 | 0.2872 | 0.5872 | |
| 5.648 | 0.3763 | 0.6064 | |
| 5.743 | 0.5354 | 0.6287 | |
| 5.751 | 0.5668 | 0.6329 | |
| 5.752 | 0.6407 | 0.6410 | |
| 5.750 | 0.6416 | 0.6416 | AZEO |
| 5.746 | 0.7184 | 0.6539 | |
| 5.735 | 0.7485 | 0.6602 | |
| 5.556 | 0.8616 | 0.7084 | |
| 5.434 | 0.8921 | 0.7348 | |
| 4.934 | 0.9562 | 0.8394 | |

Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

**T / K = 263.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 4.343 | 0.0360 | 0.2040 | |
| 5.382 | 0.0890 | 0.3650 | |
| 6.558 | 0.1740 | 0.5030 | |
| 7.012 | 0.2230 | 0.5490 | |
| 7.322 | 0.2930 | 0.5870 | |
| 7.538 | 0.3690 | 0.6150 | |
| 7.663 | 0.4530 | 0.6380 | |
| 7.748 | 0.5540 | 0.6520 | |
| 7.776 | 0.6590 | 0.6620 | |
| 7.776 | 0.6635 | 0.6635 | AZEO |
| 7.746 | 0.7320 | 0.6750 | |
| 7.729 | 0.7880 | 0.6800 | |
| 7.516 | 0.8670 | 0.7170 | |
| 7.303 | 0.9100 | 0.7570 | |

Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.946 | 0.0370 | 0.1850 | |
| 7.086 | 0.0840 | 0.3350 | |
| 8.154 | 0.1420 | 0.4460 | |
| 9.317 | 0.2330 | 0.5290 | |
| 9.775 | 0.3040 | 0.5770 | |
| 10.13 | 0.3700 | 0.6050 | |
| 10.34 | 0.4420 | 0.6270 | |
| 10.50 | 0.5430 | 0.6520 | |
| 10.54 | 0.5840 | 0.6590 | |
| 10.55 | 0.6420 | 0.6670 | |
| 10.67 | 0.6760 | 0.6760 | AZEO |
| 10.52 | 0.7200 | 0.6810 | |
| 10.48 | 0.7780 | 0.7020 | |
| 10.21 | 0.8650 | 0.7380 | |
| 9.906 | 0.9100 | 0.7860 | |

Coquelet, Christophe - Chareton, Albert - Valtz, Alain - Baba-Ahmed, Abdelatif - Richon, Dominique, Vapor–Liquid Equilibrium Data for the Azeotropic Difluoromethane + Propane System at Temperatures from 294.83 to 343.26 K and Pressures up to 5.4 MPa, Journal of Chemical & Engineering Data 2 (2003) 317-323. doi:10.1021/je020115d

**T / K = 278.10**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.270 | 0.0430 | 0.2360 |

| | | | |
|---|---|---|---|
| 9.360 | 0.1240 | 0.4190 | |
| 11.09 | 0.2620 | 0.5260 | |
| 11.89 | 0.4240 | 0.5960 | |
| 12.01 | 0.4740 | 0.6100 | |
| 12.09 | 0.5160 | 0.6220 | |
| 12.15 | 0.5630 | 0.6340 | |
| 12.18 | 0.5830 | 0.6390 | |
| 12.20 | 0.6080 | 0.6460 | |
| 12.21 | 0.6280 | 0.6510 | |
| 12.21 | 0.6630 | 0.6630 | AZEO |
| 12.22 | 0.6730 | 0.6640 | |
| 12.21 | 0.6800 | 0.6660 | |
| 12.14 | 0.7560 | 0.6930 | |
| 12.05 | 0.7910 | 0.7110 | |
| 11.31 | 0.9090 | 0.8050 | |
| 10.23 | 0.9750 | 0.9210 | |

Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 7.695 | 0.0350 | 0.1680 | |
| 8.164 | 0.0500 | 0.2160 | |
| 9.214 | 0.0840 | 0.3090 | |
| 10.12 | 0.1150 | 0.3740 | |
| 11.65 | 0.1940 | 0.4750 | |
| 12.71 | 0.3020 | 0.5560 | |
| 13.34 | 0.4000 | 0.6040 | |
| 13.61 | 0.4590 | 0.6220 | |
| 13.96 | 0.5700 | 0.6540 | |
| 14.02 | 0.6540 | 0.6750 | |
| 14.22 | 0.6850 | 0.6850 | AZEO |
| 13.99 | 0.7240 | 0.6980 | |
| 13.52 | 0.8650 | 0.7560 | |
| 13.15 | 0.9100 | 0.8030 | |

Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 10.67 | 0.0650 | 0.2320 | |
| 12.27 | 0.1130 | 0.3360 | |
| 14.33 | 0.1860 | 0.4390 | |
| 16.20 | 0.3020 | 0.5320 | |
| 17.32 | 0.4010 | 0.5880 | |
| 17.62 | 0.4470 | 0.6080 | |
| 18.10 | 0.5650 | 0.6510 | |
| 18.24 | 0.6410 | 0.6750 | |
| 18.33 | 0.6980 | 0.6980 | AZEO |
| 18.22 | 0.7290 | 0.7140 | |
| 17.59 | 0.8630 | 0.7850 | |
| 17.09 | 0.9080 | 0.8300 | |

Coquelet, Christophe - Chareton, Albert - Valtz, Alain - Baba-Ahmed, Abdelatif - Richon, Dominique, Vapor–Liquid Equilibrium Data for the Azeotropic Difluoromethane + Propane System at Temperatures from 294.83 to 343.26 K and Pressures up to 5.4 MPa, Journal of Chemical & Engineering Data 2 (2003) 317-323. doi:10.1021/je020115d

**T / K = 303.23**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 12.55 | 0.0270 | 0.1260 | |
| 14.92 | 0.0730 | 0.2580 | |
| 18.24 | 0.1650 | 0.4040 | |
| 20.76 | 0.2870 | 0.5030 | |
| 22.62 | 0.4560 | 0.5900 | |
| 23.11 | 0.5350 | 0.6150 | |
| 23.17 | 0.5640 | 0.6300 | |
| 23.36 | 0.6460 | 0.6650 | |
| 23.42 | 0.6830 | 0.6830 | AZEO |
| 23.40 | 0.6940 | 0.6890 | |
| 23.45 | 0.7050 | 0.6950 | |
| 23.18 | 0.7940 | 0.7470 | |
| 22.26 | 0.8900 | 0.8240 | |
| 20.94 | 0.9530 | 0.9160 | |

Coquelet, Christophe - Chareton, Albert - Valtz, Alain - Baba-Ahmed, Abdelatif - Richon, Dominique, Vapor–Liquid Equilibrium Data for the Azeotropic Difluoromethane + Propane System at Temperatures from 294.83 to 343.26 K and Pressures up to 5.4 MPa, Journal of Chemical & Engineering Data 2 (2003) 317-323. doi:10.1021/je020115d

**T / K = 313.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 14.96 | 0.0170 | 0.0750 |
| 16.08 | 0.0340 | 0.1330 |
| 23.44 | 0.1980 | 0.4120 |
| 25.40 | 0.2720 | 0.4750 |
| 27.20 | 0.3670 | 0.5300 |
| 28.44 | 0.4680 | 0.5830 |
| 29.31 | 0.5820 | 0.6390 |

| | | | |
|---|---|---|---|
| 29.40 | 0.6050 | 0.6490 | |
| 29.52 | 0.6220 | 0.6580 | |
| 29.61 | 0.7020 | 0.7020 | AZEO |
| 29.64 | 0.7100 | 0.7050 | |
| 29.23 | 0.7990 | 0.7610 | |
| 28.80 | 0.8440 | 0.7970 | |
| 26.85 | 0.9470 | 0.9010 | |

Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 19.47 | 0.0390 | 0.1120 | |
| 22.12 | 0.0930 | 0.2270 | |
| 26.21 | 0.1670 | 0.3440 | |
| 28.86 | 0.2280 | 0.4010 | |
| 32.43 | 0.3420 | 0.4870 | |
| 34.30 | 0.4350 | 0.5480 | |
| 35.69 | 0.5190 | 0.5950 | |
| 36.59 | 0.6310 | 0.6630 | |
| 36.74 | 0.7200 | 0.7200 | AZEO |
| 36.59 | 0.7790 | 0.7630 | |
| 35.55 | 0.8690 | 0.8310 | |
| 34.83 | 0.9020 | 0.8660 | |

Coquelet, Christophe - Chareton, Albert - Valtz, Alain - Baba-Ahmed, Abdelatif - Richon, Dominique, Vapor–Liquid Equilibrium Data for the Azeotropic Difluoromethane + Propane System at Temperatures from 294.83 to 343.26 K and Pressures up to 5.4 MPa, Journal of Chemical & Engineering Data 2 (2003) 317-323. doi:10.1021/je020115d

**T / K = 343.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 31.39 | 0.0650 | 0.1460 |
| 34.99 | 0.1130 | 0.2260 |
| 39.64 | 0.1880 | 0.3100 |
| 42.22 | 0.2370 | 0.3450 |

Coquelet, Christophe - Chareton, Albert - Valtz, Alain - Baba-Ahmed, Abdelatif - Richon, Dominique, Vapor–Liquid Equilibrium Data for the Azeotropic Difluoromethane + Propane System at Temperatures from 294.83 to 343.26 K and Pressures up to 5.4 MPa, Journal of Chemical & Engineering Data 2 (2003) 317-323. doi:10.1021/je020115d

**T / K = 343.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 44.42 | 0.2820 | 0.3750 |
| 47.02 | 0.3450 | 0.4200 |
| 50.09 | 0.4320 | 0.4720 |
| 50.77 | 0.4570 | 0.4800 |
| 54.51 | 0.8580 | 0.8490 |
| 54.13 | 0.8760 | 0.8660 |
| 53.08 | 0.9110 | 0.9010 |
| 52.59 | 0.9240 | 0.9150 |
| 52.01 | 0.9390 | 0.9300 |
| 50.49 | 0.9720 | 0.9650 |
| 49.40 | 0.9920 | 0.9890 |

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**Critical point**

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Li, Jun - Rodrigues, Miguel - Paiva, Alexandre - Matos, Henrique A. - Azevedo, Edmundo Gomes de, Binary solid–liquid–gas equilibrium of the tripalmitin/CO2 and ubiquinone/CO2 systems, Fluid Phase Equilibria 1-2 (2006) 196-204. doi:10.1016/j.fluid.2005.12.017

| T / K | P / bar | $x_1$ |
|---|---|---|
| 354.78 | 46.68 | 0.1862 |
| 352.81 | 47.73 | 0.2275 |
| 349.80 | 49.43 | 0.3006 |
| 342.24 | 53.40 | 0.6859 |
| 343.01 | 55.16 | 0.8500 |

Higashi, Yukihiro, Experimental determination of the critical locus for the difluoromethane (R32) and propane (R290) system, Fluid Phase Equilibria 1 (2004) 99-103. doi:10.1016/j.fluid.2004.02.004

| T / K | P / bar | $x_1$ |
|---|---|---|
| 339.63 | 51.59 | 0.7000 |
| 344.56 | 54.06 | 0.9000 |

Coquelet, Christophe - Chareton, Albert - Valtz, Alain - Baba-Ahmed, Abdelatif - Richon, Dominique, Vapor–Liquid Equilibrium Data for the Azeotropic Difluoromethane + Propane System at Temperatures from 294.83 to 343.26 K and Pressures up to 5.4 MPa, Journal of Chemical & Engineering Data 2 (2003) 317-323. doi:10.1021/je020115d

| T / K | P / bar | $x_1$ |
|---|---|---|
| 342.50 | 52.10 | 0.5270 |
| 344.00 | 55.32 | 0.8660 |

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**Azeotropic point**

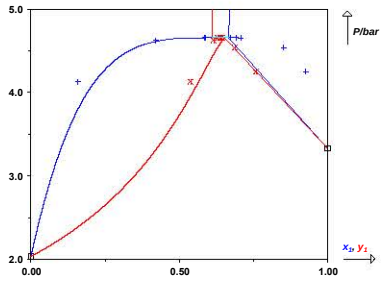
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Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a

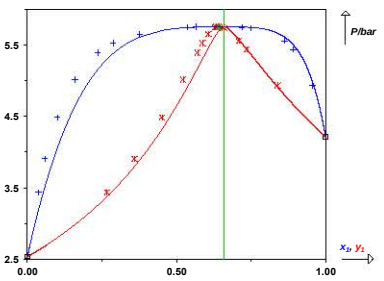
temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

| T / K | P / bar | $x_1$ |
|---|---|---|
| 263.15 | 7.870 | 0.6660 |
| 323.15 | 37.21 | 0.7250 |

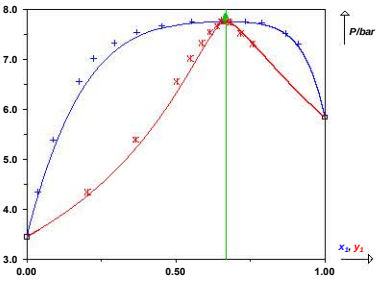
T/K = 248.13



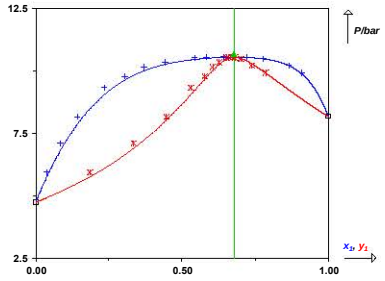

T/K = 254.15



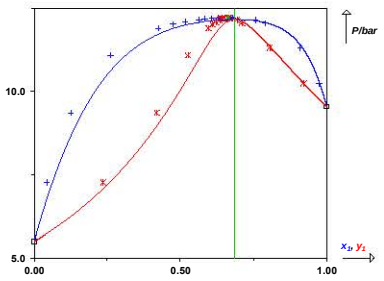

T/K = 263.15



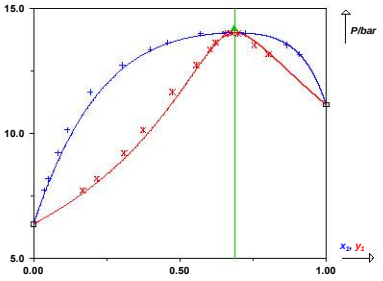

T/K = 273.15



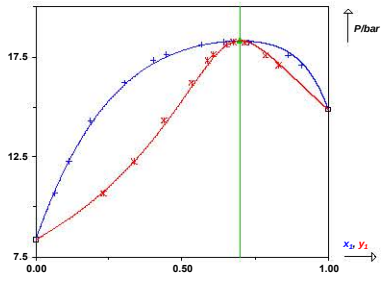

T/K = 278.10



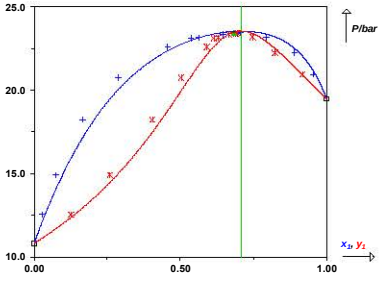

T/K = 283.15



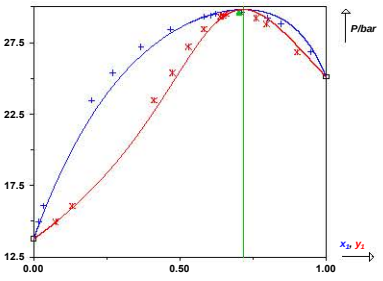

T/K = 293.15



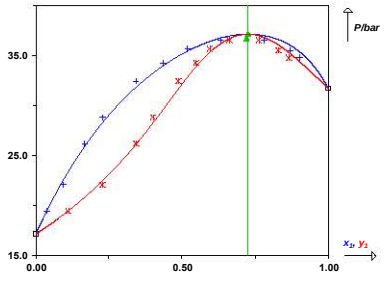

T/K = 303.23



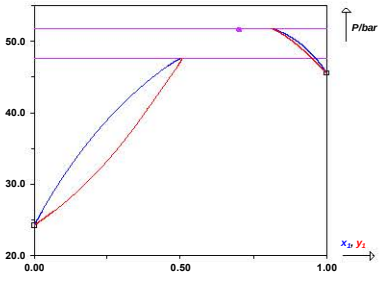

T/K = 313.26



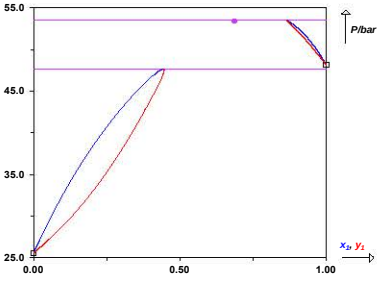

T/K = 323.15



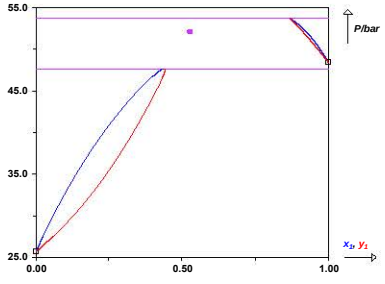

T/K = 339.63



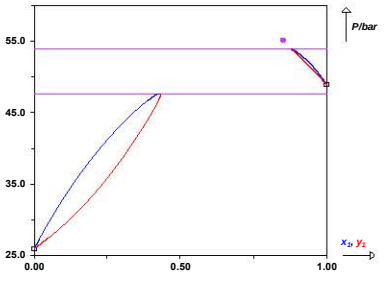

T/K = 342.24



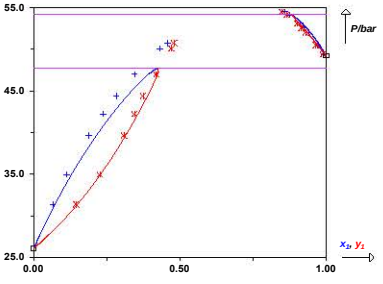

T/K = 342.50

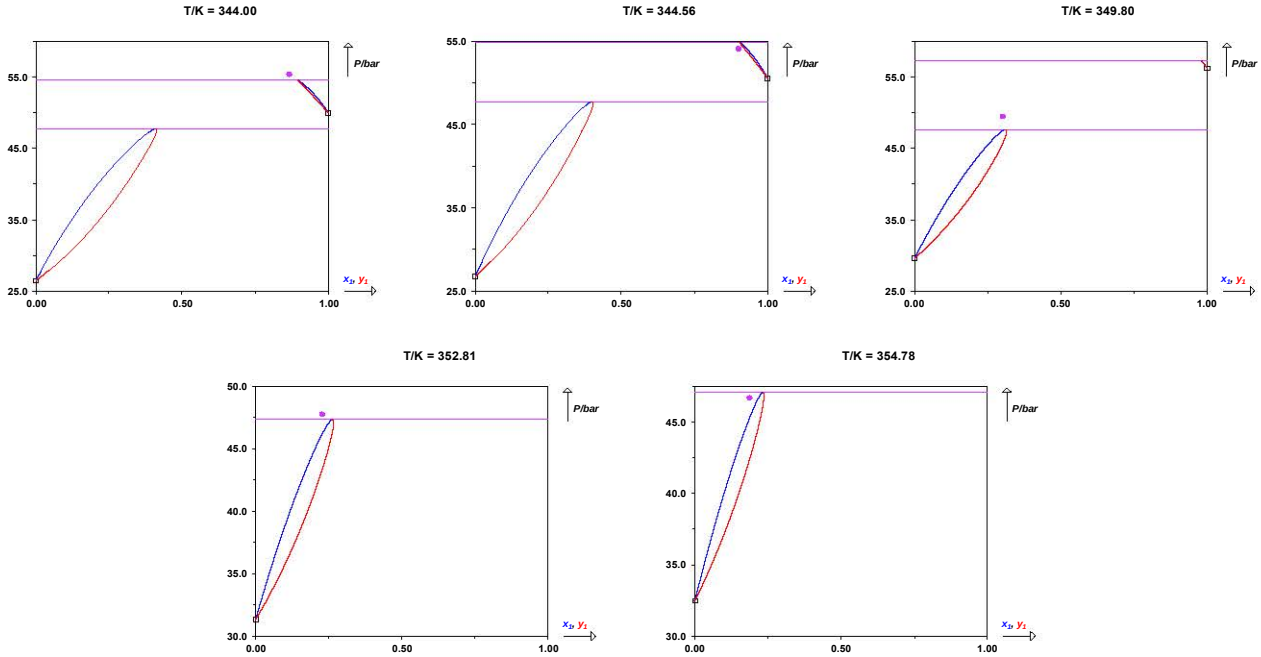



T/K = 343.01




T/K = 343.26




T/K = 344.00
P/bar
55.0
45.0
35.0
25.0
0.00
0.50
1.00
x1, y1
T/K = 344.56
P/bar
55.0
45.0
35.0
25.0
0.00
0.50
1.00
x1, y1
T/K = 349.80
P/bar
55.0
45.0
35.0
25.0
0.00
0.50
1.00
x1, y1
T/K = 352.81
P/bar
50.0
45.0
40.0
35.0
30.0
0.00
0.50
1.00
x1, y1
T/K = 354.78
P/bar
45.0
40.0
35.0
30.0
0.00
0.50
1.00
x1, y1

## TRIFLUOROMETHANE (1) + ETHANE (2)

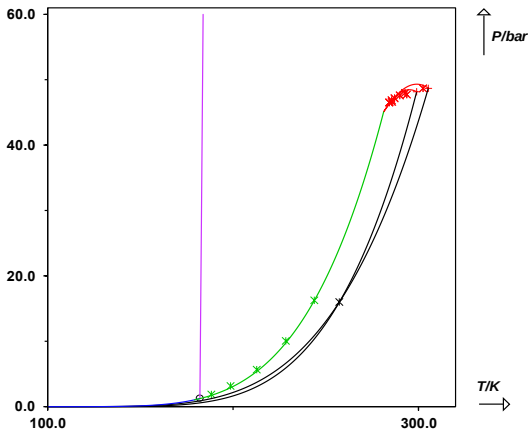
| | | |
|---|---|---|
| **CAS** | 75-46-7 | 74-84-0 |
| **InChiKey** | XPDWGBQVDMORPB-UHFFFAOYSA-N | OTMSDBZUPAUEDD-UHFFFAOYSA-N |
| **$T_c$ / K** | 299.01 | 305.32 |
| **$P_c$ / bar** | 48.162 | 48.72 |
| **ω** | 0.264 | 0.099 |

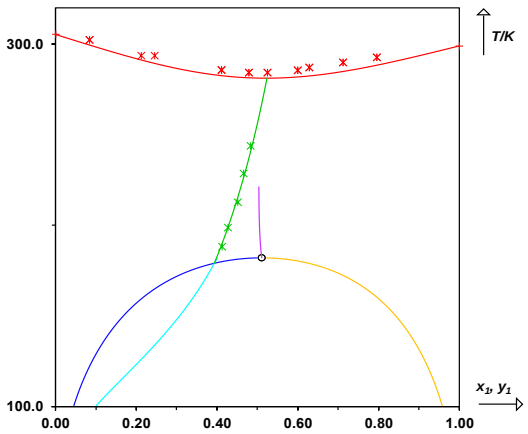
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 495
B/MPa = 334

*Deviations*
MAPE on x = 14 %
MAPE on y = 3.7 %
MAPE on $x_c$ = 27 %
MAPE on $P_c$ = 0.94 %
MAPE on $x_{az}$ = 0.49 %
MAPE on $P_{az}$ = 4.8 %



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**Isothermal phase equilibrium data**

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Zhang, Yu - Gong, Maoqiong - Zhu, Hongbo - Wu, Jianfeng, Vapor−Liquid Equilibrium Data for the Ethane + Trifluoromethane System at Temperatures from (188.31 to 243.76) K, Journal of Chemical & Engineering Data 4 (2006) 1411-1414. doi:10.1021/je0601107

**T / K = 188.31**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 1.798 | 0.8561 | 0.4660 | |
| 1.899 | 0.7226 | 0.4301 | |
| 1.914 | 0.6064 | 0.4205 | |
| 1.915 | 0.4977 | 0.4171 | |
| 1.908 | 0.4126 | 0.4126 | AZEO |
| 1.914 | 0.3779 | 0.4128 | |
| 1.892 | 0.2032 | 0.3931 | |

Zhang, Yu - Gong, Maoqiong - Zhu, Hongbo - Wu, Jianfeng, Vapor−Liquid Equilibrium Data for the Ethane + Trifluoromethane System at Temperatures from (188.31 to 243.76) K, Journal of Chemical & Engineering Data 4 (2006) 1411-1414. doi:10.1021/je0601107

**T / K = 198.66**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 2.735 | 0.9059 | 0.5532 | |
| 3.064 | 0.7283 | 0.4637 | |
| 3.121 | 0.6038 | 0.4437 | |
| 3.130 | 0.4937 | 0.4339 | |
| 3.134 | 0.4272 | 0.4272 | AZEO |
| 3.125 | 0.3758 | 0.4232 | |
| 3.053 | 0.2043 | 0.3872 | |

Zhang, Yu - Gong, Maoqiong - Zhu, Hongbo - Wu, Jianfeng, Vapor−Liquid Equilibrium Data for the Ethane + Trifluoromethane System at Temperatures from (188.31 to 243.76) K, Journal of Chemical & Engineering Data 4 (2006) 1411-1414. doi:10.1021/je0601107

**T / K = 212.84**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 4.691 | 0.9129 | 0.6474 | |
| 5.461 | 0.7532 | 0.5209 | |
| 5.644 | 0.6075 | 0.4833 | |
| 5.685 | 0.4886 | 0.4578 | |
| 5.689 | 0.4506 | 0.4506 | AZEO |
| 5.689 | 0.4495 | 0.4502 | |
| 5.687 | 0.4312 | 0.4449 | |
| 5.665 | 0.3880 | 0.4356 | |
| 5.446 | 0.1964 | 0.3726 | |

Zhang, Yu - Gong, Maoqiong - Zhu, Hongbo - Wu, Jianfeng, Vapor−Liquid Equilibrium Data for the Ethane + Trifluoromethane System at Temperatures from (188.31 to 243.76) K, Journal of Chemical & Engineering Data 4 (2006) 1411-1414. doi:10.1021/je0601107

**T / K = 228.50**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 8.641 | 0.8792 | 0.6576 | |
| 9.688 | 0.7142 | 0.5470 | |
| 9.954 | 0.5742 | 0.4963 | |
| 10.00 | 0.4991 | 0.4749 | |
| 10.01 | 0.4753 | 0.4683 | |
| 10.03 | 0.4663 | 0.4663 | AZEO |
| 10.01 | 0.4615 | 0.4651 | |
| 9.984 | 0.3836 | 0.4414 | |
| 9.408 | 0.1834 | 0.3540 | |

Zhang, Yu - Gong, Maoqiong - Zhu, Hongbo - Wu, Jianfeng, Vapor−Liquid Equilibrium Data for the Ethane + Trifluoromethane System at Temperatures from (188.31 to 243.76) K, Journal of Chemical & Engineering Data 4 (2006) 1411-1414. doi:10.1021/je0601107

**T / K = 243.76**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 13.90 | 0.8818 | 0.7213 | |
| 15.48 | 0.7383 | 0.6029 | |
| 16.10 | 0.5951 | 0.5279 | |
| 16.19 | 0.5044 | 0.4957 | |
| 16.21 | 0.4931 | 0.4900 | |
| 16.26 | 0.4830 | 0.4830 | AZEO |
| 16.20 | 0.4805 | 0.4853 | |
| 16.10 | 0.3881 | 0.4463 | |
| 14.85 | 0.1745 | 0.3270 | |

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**Critical point**

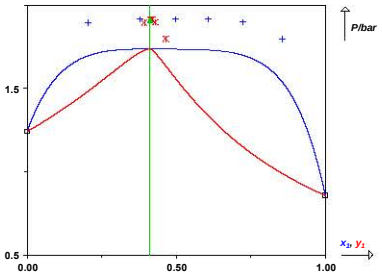
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Kordikowski, Andreas - Poliakoff, Martyn, Acoustic probing of phase equilibria in near-critical fluids, Fluid Phase Equilibria (1998) 493-499. doi:10.1016/S0378-3812(98)00296-9

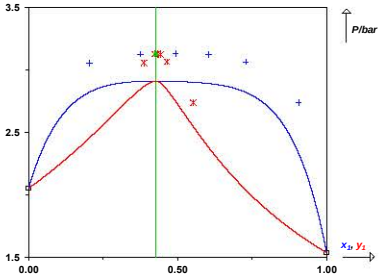
| T / K | P / bar | $x_1$ |
|---|---|---|
| 302.35 | 48.70 | 0.0840 |
| 293.55 | 47.70 | 0.2450 |
| 285.85 | 46.60 | 0.4110 |
| 284.20 | 46.54 | 0.4790 |
| 285.45 | 46.88 | 0.6000 |
| 287.05 | 47.16 | 0.6290 |

| | | |
|---|---|---|
| 289.85 | 47.64 | 0.7120 |
| 292.75 | 48.00 | 0.7950 |

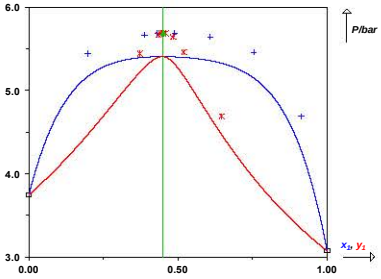
T/K = 188.31



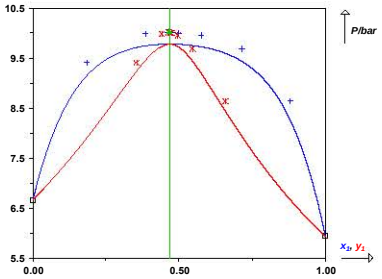

T/K = 198.66



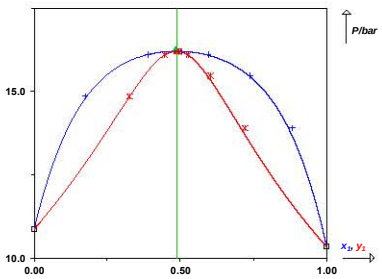

T/K = 212.84



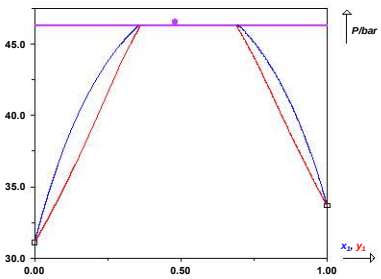

T/K = 228.50



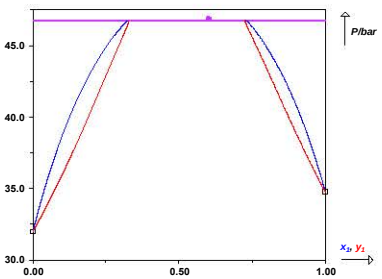

T/K = 243.76



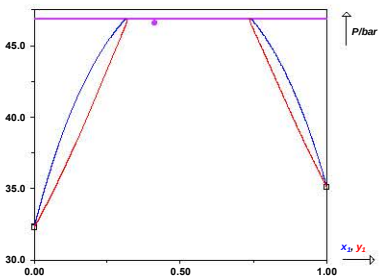

T/K = 284.20



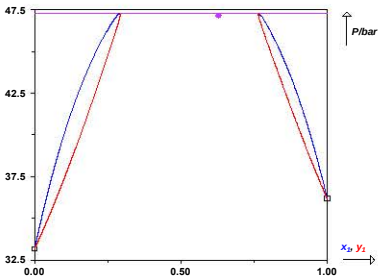

T/K = 285.45



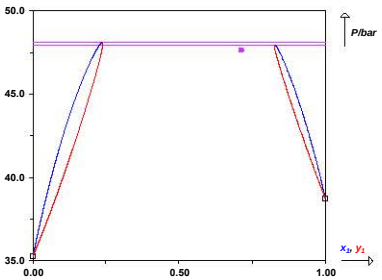

T/K = 285.85



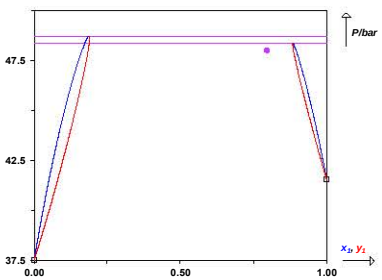

T/K = 287.05



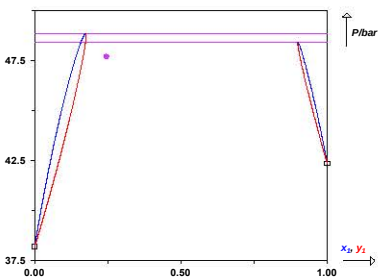

T/K = 289.85



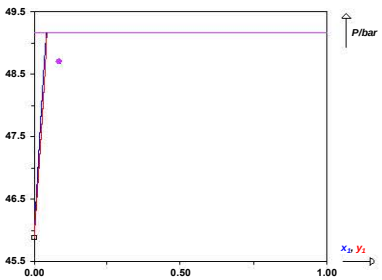

T/K = 292.75




T/K = 293.55




T/K = 302.35



## CARBON TETRAFLUORIDE (1) + CHLORODIFLUOROMETHANE (2)

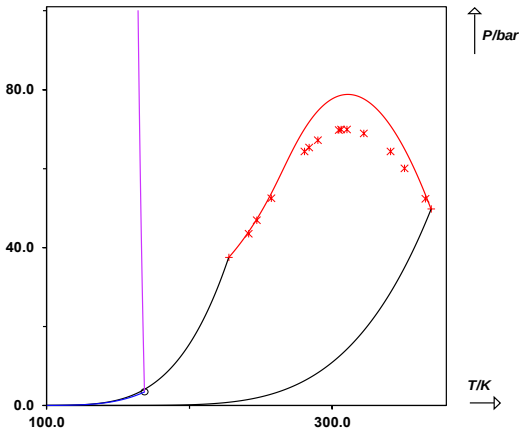
| | | |
|---|---|---|
| **CAS** | 75-73-0 | 75-45-6 |
| **InChiKey** | TXEYQDLBPFQVAA-UHFFFAOYSA-N | VOPWNXZWBYDODV-UHFFFAOYSA-N |
| **$T_c$ / K** | 227.51 | 369.3 |
| **$P_c$ / bar** | 37.45 | 49.71 |
| **ω** | 0.179 | 0.219 |

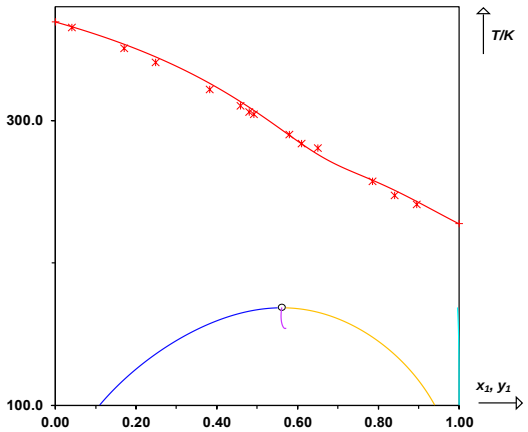
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 320
B/MPa = 250

*Deviations*
MAPE on x = 17 %
MAPE on y = 14 %
MAPE on $x_c$ = 5.3 %
MAPE on $P_c$ = 8.1 %



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**Isothermal phase equilibrium data**

---

Baginskii, V.A. - Zakharov, N.D. - Lapardin, N.I., Study and calculation of the liquid-vapor phase equilibrium of mixtures of refrigerants, Issled. Teplofiz. Svoistv Rab. Veshchestv i Protsessov Teploobmena v Kholod. Tekhn., L. (1989) 9-15.

**T / K = 180.44**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.840 | 0.0921 | 0.9933 |
| 6.080 | 0.3269 | 0.9975 |
| 6.480 | 0.5830 | 0.9969 |
| 6.650 | 0.7121 | 0.9971 |

Baginskii, V.A. - Zakharov, N.D. - Lapardin, N.I., Study and calculation of the liquid-vapor phase equilibrium of mixtures of refrigerants, Issled. Teplofiz. Svoistv Rab. Veshchestv i Protsessov Teploobmena v Kholod. Tekhn., L. (1989) 9-15.

**T / K = 214.50**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.100 | 0.0116 | 0.7929 |
| 11.51 | 0.1435 | 0.9571 |
| 17.83 | 0.3600 | 0.9643 |
| 19.57 | 0.5340 | 0.9628 |
| 21.23 | 0.8264 | 0.9771 |
| 22.40 | 0.9070 | 0.9835 |

Baginskii, V.A. - Zakharov, N.D. - Lapardin, N.I., Study and calculation of the liquid-vapor phase equilibrium of mixtures of refrigerants, Issled. Teplofiz. Svoistv Rab. Veshchestv i Protsessov Teploobmena v Kholod. Tekhn., L. (1989) 9-15.

**T / K = 232.98**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.060 | 0.0046 | 0.4487 |
| 4.710 | 0.0264 | 0.7632 |
| 8.330 | 0.0563 | 0.8530 |
| 14.88 | 0.1233 | 0.9152 |
| 24.98 | 0.3168 | 0.9411 |
| 28.64 | 0.4631 | 0.9460 |
| 30.49 | 0.6000 | 0.9460 |
| 31.41 | 0.6476 | 0.9460 |
| 31.55 | 0.6559 | 0.9485 |
| 32.32 | 0.7078 | 0.9601 |
| 32.93 | 0.7413 | 0.9776 |
| 34.24 | 0.7930 | 0.9878 |
| 35.34 | 0.8485 | 0.9678 |

Baginskii, V.A. - Zakharov, N.D. - Lapardin, N.I., Study and calculation of the liquid-vapor phase equilibrium of mixtures of refrigerants, Issled. Teplofiz. Svoistv Rab. Veshchestv i Protsessov Teploobmena v Kholod. Tekhn., L. (1989) 9-15.

**T / K = 250.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.830 | 0.0082 | 0.3882 |
| 7.530 | 0.0300 | 0.6790 |
| 12.66 | 0.0653 | 0.7933 |
| 20.48 | 0.1341 | 0.8623 |
| 28.02 | 0.2183 | 0.8866 |
| 37.55 | 0.3965 | 0.8985 |
| 38.32 | 0.4095 | 0.8976 |
| 41.77 | 0.5148 | 0.8966 |
| 43.17 | 0.5737 | 0.8973 |

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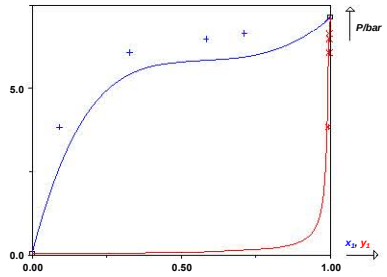
**Critical point**

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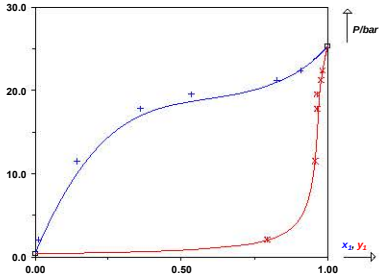
Lavrenchenko, G.K. - Valyakin, V.N., Liquid-liquid, liquid-liquid-vapor, and liquid-vapor equilibria in binary Freon and Freon-hydrocarbon mixtures based on tetrafluoromethane (R14), Teplofiz. Svoistva Veshchestv Mater. 22 (1985) 10-18.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 365.32 | 52.37 | 0.0405 |
| 350.69 | 60.06 | 0.1700 |
| 340.71 | 64.32 | 0.2485 |
| 322.01 | 68.96 | 0.3815 |
| 310.48 | 69.91 | 0.4580 |
| 306.18 | 69.83 | 0.4800 |
| 304.47 | 69.73 | 0.4920 |
| 290.05 | 67.17 | 0.5800 |
| 283.93 | 65.39 | 0.6095 |
| 280.74 | 64.32 | 0.6505 |
| 257.18 | 52.45 | 0.7855 |
| 247.37 | 46.85 | 0.8405 |
| 241.31 | 43.48 | 0.8945 |

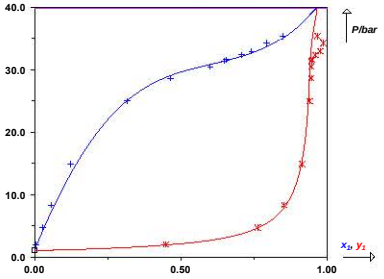
T/K = 180.44



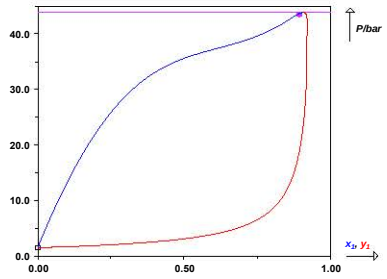

T/K = 214.50



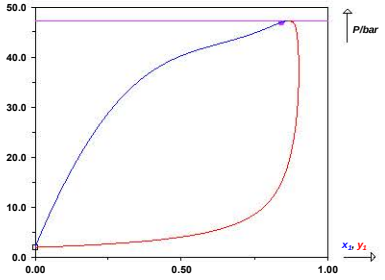

T/K = 232.98



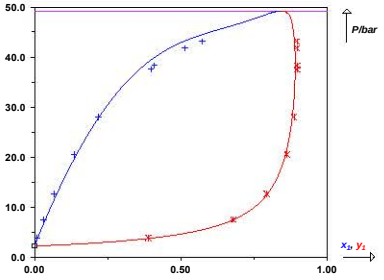

T/K = 241.31



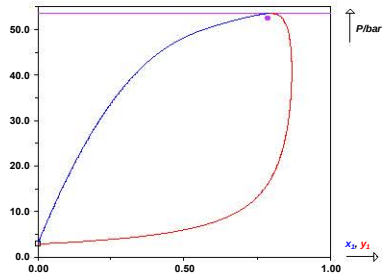

T/K = 247.37



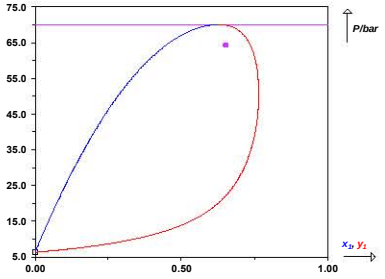

T/K = 250.65



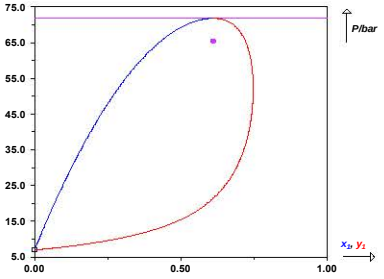

T/K = 257.18



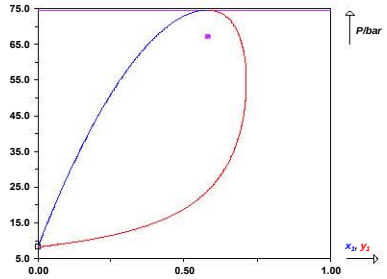

T/K = 280.74



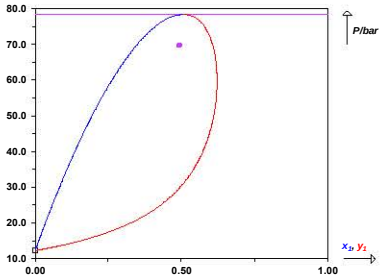

T/K = 283.93



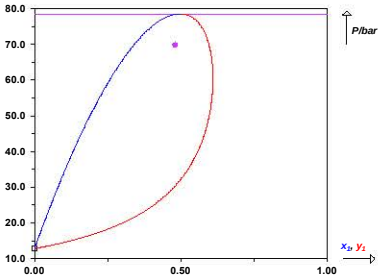

T/K = 290.05

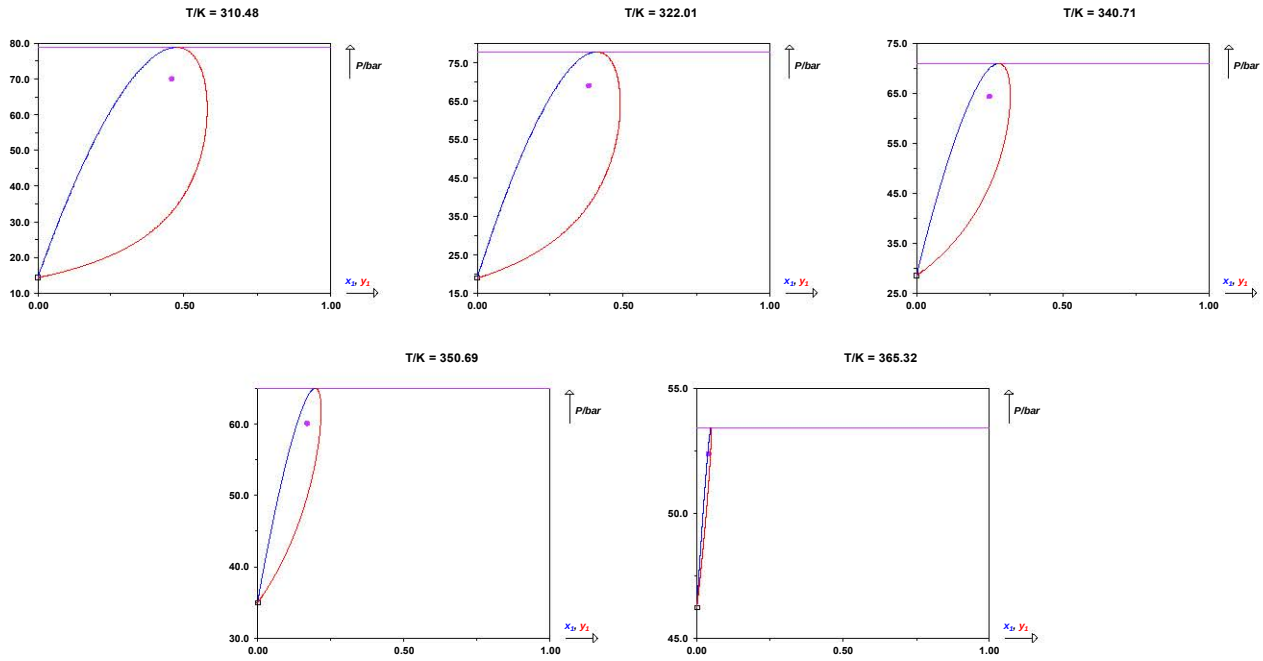



T/K = 304.47




T/K = 306.18




T/K = 310.48
P/bar
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.00
0.50
1.00
x1, y1
T/K = 322.01
P/bar
75.0
65.0
55.0
45.0
35.0
25.0
15.0
0.00
0.50
1.00
x1, y1
T/K = 340.71
P/bar
75.0
65.0
55.0
45.0
35.0
25.0
0.00
0.50
1.00
x1, y1
T/K = 350.69
P/bar
60.0
50.0
40.0
30.0
0.00
0.50
1.00
x1, y1
T/K = 365.32
P/bar
55.0
50.0
45.0
0.00
0.50
1.00
x1, y1

## PENTAFLUOROETHANE (1) + PROPANE (2)

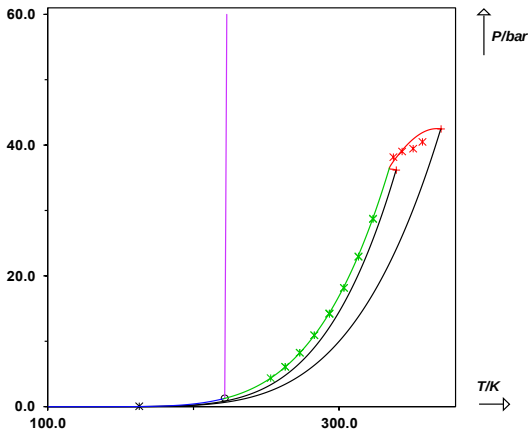
| | | |
|---|---|---|
| **CAS** | 354-33-6 | 74-98-6 |
| **InChiKey** | GTLACDSXYULKMZ-UHFFFAOYSA-N | ATUOYWHBWRKTHZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 339.17 | 369.83 |
| **$P_c$ / bar** | 36.20 | 42.48 |
| **ω** | 0.305 | 0.152 |

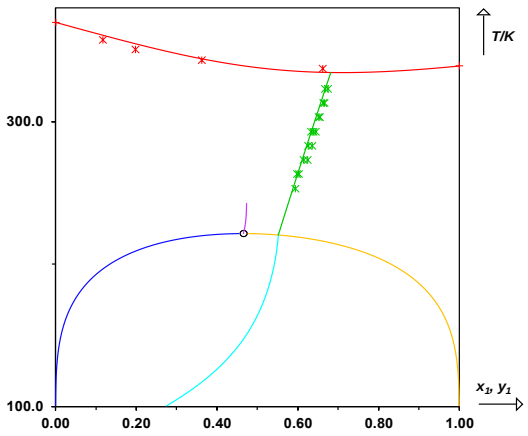
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 294
B/MPa = 488

*Deviations*
MAPE on x = 2.9 %
MAPE on y = 2 %
MAPE on $x_c$ = 15 %
MAPE on $P_c$ = 2.6 %
MAPE on $x_{az}$ = 1.3 %
MAPE on $P_{az}$ = 0.28 %



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**Isothermal phase equilibrium data**

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Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

**T / K = 253.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.022 | 0.0450 | 0.2010 | |
| 3.168 | 0.0630 | 0.2520 | |
| 3.625 | 0.1410 | 0.3870 | |
| 3.886 | 0.1920 | 0.4470 | |
| 4.097 | 0.2770 | 0.4880 | |
| 4.301 | 0.4050 | 0.5370 | |
| 4.351 | 0.5130 | 0.5670 | |
| 4.349 | 0.5940 | 0.5940 | AZEO |
| 4.348 | 0.6860 | 0.6300 | |
| 4.267 | 0.7690 | 0.6750 | |
| 4.196 | 0.8070 | 0.7020 | |
| 3.965 | 0.8970 | 0.7950 | |

Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

**T / K = 263.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 4.175 | 0.0460 | 0.1910 | |
| 4.376 | 0.0600 | 0.2280 | |
| 4.681 | 0.0910 | 0.2970 | |
| 4.985 | 0.1270 | 0.3530 | |
| 5.312 | 0.1780 | 0.4130 | |
| 5.827 | 0.3160 | 0.4980 | |
| 5.944 | 0.3840 | 0.5280 | |
| 6.053 | 0.5150 | 0.5710 | |
| 6.092 | 0.6030 | 0.6030 | AZEO |
| 6.095 | 0.6180 | 0.6120 | |
| 5.946 | 0.7720 | 0.6910 | |
| 5.864 | 0.8180 | 0.7260 | |
| 5.555 | 0.8970 | 0.8130 | |

Hou, Shu-Xin - Duan, Yuan-Yuan, Isothermal vapor–liquid equilibria for the pentafluoroethane+propane and pentafluoroethane+1,1,1,2,3,3,3-heptafluoropropane systems, Fluid Phase Equilibria 1-2 (2010) 121-126. doi:10.1016/j.fluid.2009.09.008

**T / K = 263.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 4.322 | 0.0538 | 0.2184 | |
| 5.314 | 0.1763 | 0.4182 | |
| 5.757 | 0.2804 | 0.4918 | |
| 5.969 | 0.3819 | 0.5182 | |
| 6.054 | 0.4810 | 0.5537 | |
| 6.065 | 0.5878 | 0.6052 | |
| 6.107 | 0.5979 | 0.5979 | AZEO |
| 6.066 | 0.6635 | 0.6333 | |
| 5.806 | 0.8549 | 0.7418 | |
| 5.376 | 0.9360 | 0.8568 | |

Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.630 | 0.0450 | 0.1750 | |
| 5.888 | 0.0600 | 0.2100 | |
| 6.215 | 0.0880 | 0.2680 | |
| 6.674 | 0.1300 | 0.3370 | |
| 7.184 | 0.1860 | 0.3980 | |
| 7.603 | 0.2730 | 0.4600 | |
| 8.166 | 0.4780 | 0.5570 | |
| 8.203 | 0.5130 | 0.5640 | |
| 8.261 | 0.5710 | 0.5940 | |
| 8.253 | 0.6140 | 0.6140 | AZEO |
| 8.228 | 0.6810 | 0.6450 | |
| 8.094 | 0.7710 | 0.7030 | |
| 7.976 | 0.8170 | 0.7410 | |
| 7.594 | 0.8980 | 0.8270 | |

Bobbo, S. - Fedele, L. - Camporese, R. - Stryjek, R., Hydrogen-bonding of HFCs with dimethyl ether: evaluation by isothermal VLE measurements, Fluid Phase Equilibria 1-2 (2002) 153-160. doi:10.1016/S0378-3812(01)00813-5

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.189 | 0.0208 | 0.0913 |
| 5.811 | 0.0564 | 0.2039 |
| 6.410 | 0.1013 | 0.2941 |
| 7.197 | 0.1941 | 0.4028 |
| 7.670 | 0.2896 | 0.4676 |
| 8.064 | 0.4395 | 0.5403 |
| 8.183 | 0.7081 | 0.6652 |
| 8.153 | 0.7324 | 0.6796 |
| 8.037 | 0.7899 | 0.7188 |
| 7.632 | 0.8906 | 0.8146 |

Lim, Jong Sung - Park, Ji Young - Lee, Kab-Soo - Kim, Jae-Duck - Lee, Byung Gwon, Measurement of Vapor–Liquid Equilibria for the Binary Mixture of Pentafluoroethane (HFC-125) + Propane (R-290), Journal of Chemical & Engineering Data 4 (2004) 750-755. doi:10.1021/je030156p

| **T / K =** | **273.15** | | |
|---|---|---|---|
| P / bar | $x_1$ | $y_1$ | |
| 6.920 | 0.1660 | 0.3670 | |
| 7.682 | 0.3080 | 0.4750 | |
| 8.208 | 0.5060 | 0.5720 | |
| 8.271 | 0.6247 | 0.6247 | AZEO |
| 8.284 | 0.6790 | 0.6280 | |
| 7.864 | 0.8540 | 0.7630 | |

Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

| **T / K =** | **283.15** | | |
|---|---|---|---|
| P / bar | $x_1$ | $y_1$ | |
| 7.202 | 0.0340 | 0.1230 | |
| 7.446 | 0.0460 | 0.1570 | |
| 7.962 | 0.0740 | 0.2240 | |
| 8.828 | 0.1300 | 0.3150 | |
| 9.244 | 0.1710 | 0.3670 | |
| 9.857 | 0.2470 | 0.4300 | |
| 10.48 | 0.3830 | 0.5090 | |
| 10.80 | 0.4760 | 0.5530 | |
| 10.87 | 0.5090 | 0.5670 | |
| 10.95 | 0.5710 | 0.6020 | |
| 10.96 | 0.6250 | 0.6250 | AZEO |
| 10.92 | 0.6970 | 0.6660 | |
| 10.78 | 0.7660 | 0.7150 | |
| 10.61 | 0.8190 | 0.7550 | |
| 10.17 | 0.8980 | 0.8360 | |

Lim, Jong Sung - Park, Ji Young - Lee, Kab-Soo - Kim, Jae-Duck - Lee, Byung Gwon, Measurement of Vapor–Liquid Equilibria for the Binary Mixture of Pentafluoroethane (HFC-125) + Propane (R-290), Journal of Chemical & Engineering Data 4 (2004) 750-755. doi:10.1021/je030156p

| **T / K =** | **283.15** | | |
|---|---|---|---|
| P / bar | $x_1$ | $y_1$ | |
| 8.904 | 0.1380 | 0.3280 | |
| 10.20 | 0.3090 | 0.4700 | |
| 10.89 | 0.5420 | 0.5830 | |
| 10.92 | 0.6352 | 0.6352 | AZEO |
| 10.87 | 0.7170 | 0.6680 | |
| 10.49 | 0.8300 | 0.7670 | |

Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

| **T / K =** | **293.15** | | |
|---|---|---|---|
| P / bar | $x_1$ | $y_1$ | |
| 9.299 | 0.0310 | 0.1020 | |
| 9.692 | 0.0520 | 0.1560 | |
| 10.23 | 0.0740 | 0.2060 | |
| 11.29 | 0.1340 | 0.3000 | |
| 12.68 | 0.2510 | 0.4170 | |
| 13.53 | 0.3780 | 0.4990 | |
| 14.01 | 0.4780 | 0.5510 | |
| 14.24 | 0.5700 | 0.6010 | |
| 14.24 | 0.6380 | 0.6380 | AZEO |
| 14.32 | 0.6490 | 0.6460 | |
| 14.22 | 0.7010 | 0.6800 | |
| 14.05 | 0.7730 | 0.7320 | |
| 13.84 | 0.8190 | 0.7680 | |
| 13.30 | 0.8990 | 0.8510 | |

Hou, Shu-Xin - Duan, Yuan-Yuan, Isothermal vapor–liquid equilibria for the pentafluoroethane+propane and pentafluoroethane+1,1,1,2,3,3,3-heptafluoropropane systems, Fluid Phase Equilibria 1-2 (2010) 121-126. doi:10.1016/j.fluid.2009.09.008

| **T / K =** | **293.15** | | |
|---|---|---|---|
| P / bar | $x_1$ | $y_1$ | |
| 9.515 | 0.0425 | 0.1278 | |
| 10.34 | 0.0757 | 0.2022 | |
| 12.17 | 0.1973 | 0.3749 | |
| 13.02 | 0.2843 | 0.4427 | |
| 14.25 | 0.6063 | 0.6229 | |
| 14.25 | 0.6328 | 0.6328 | AZEO |
| 14.27 | 0.6513 | 0.6520 | |
| 14.16 | 0.7419 | 0.7122 | |
| 13.60 | 0.8646 | 0.8211 | |
| 12.81 | 0.9519 | 0.9237 | |

Lim, Jong Sung - Park, Ji Young - Lee, Kab-Soo - Kim, Jae-Duck - Lee, Byung Gwon, Measurement of Vapor–Liquid Equilibria for the Binary Mixture of Pentafluoroethane (HFC-125) + Propane (R-290), Journal of Chemical & Engineering Data 4 (2004) 750-755. doi:10.1021/je030156p

| **T / K =** | **293.15** | |
|---|---|---|
| P / bar | $x_1$ | $y_1$ |
| 11.20 | 0.1450 | 0.3100 |
| 13.28 | 0.3290 | 0.4730 |
| 14.08 | 0.5110 | 0.5660 |

| | | | |
|---|---|---|---|
| 14.19 | 0.6440 | 0.6440 | AZEO |
| 14.20 | 0.6740 | 0.6560 | |
| 13.70 | 0.8310 | 0.7740 | |

Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

**T / K =** **303.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 11.86 | 0.0310 | 0.0940 | |
| 12.65 | 0.0560 | 0.1530 | |
| 14.18 | 0.1330 | 0.2790 | |
| 14.97 | 0.1740 | 0.3260 | |
| 15.96 | 0.2470 | 0.4000 | |
| 17.13 | 0.3680 | 0.4800 | |
| 17.85 | 0.4760 | 0.5430 | |
| 18.18 | 0.5690 | 0.5980 | |
| 18.27 | 0.6470 | 0.6500 | |
| 18.20 | 0.6510 | 0.6510 | AZEO |
| 18.20 | 0.7170 | 0.7010 | |
| 17.99 | 0.7750 | 0.7440 | |
| 17.74 | 0.8200 | 0.7810 | |
| 17.09 | 0.8990 | 0.8640 | |

Bobbo, S. - Fedele, L. - Camporese, R. - Stryjek, R., Hydrogen-bonding of HFCs with dimethyl ether: evaluation by isothermal VLE measurements, Fluid Phase Equilibria 1-2 (2002) 153-160. doi:10.1016/S0378-3812(01)00813-5

**T / K =** **303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 12.01 | 0.0349 | 0.1091 |
| 13.46 | 0.0876 | 0.2208 |
| 15.07 | 0.1707 | 0.3306 |
| 16.55 | 0.2887 | 0.4313 |
| 17.48 | 0.4069 | 0.5060 |
| 17.99 | 0.5034 | 0.5647 |
| 18.08 | 0.5384 | 0.5838 |
| 18.13 | 0.5568 | 0.5945 |
| 18.17 | 0.5752 | 0.6053 |
| 18.18 | 0.5850 | 0.6097 |
| 18.23 | 0.6718 | 0.6644 |
| 17.98 | 0.7783 | 0.7421 |
| 17.40 | 0.8680 | 0.8241 |
| 16.51 | 0.9480 | 0.9169 |

Lim, Jong Sung - Park, Ji Young - Lee, Kab-Soo - Kim, Jae-Duck - Lee, Byung Gwon, Measurement of Vapor−Liquid Equilibria for the Binary Mixture of Pentafluoroethane (HFC-125) + Propane (R-290), Journal of Chemical & Engineering Data 4 (2004) 750-755. doi:10.1021/je030156p

**T / K =** **303.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 14.32 | 0.1400 | 0.2910 | |
| 16.78 | 0.3290 | 0.4570 | |
| 17.97 | 0.5180 | 0.5700 | |
| 18.14 | 0.6545 | 0.6545 | AZEO |
| 18.13 | 0.6960 | 0.6850 | |
| 17.57 | 0.8320 | 0.7860 | |

Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

**T / K =** **313.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 15.38 | 0.0460 | 0.1170 | |
| 15.87 | 0.0610 | 0.1500 | |
| 17.52 | 0.1180 | 0.2440 | |
| 18.27 | 0.1540 | 0.2870 | |
| 19.71 | 0.2330 | 0.3640 | |
| 20.26 | 0.2710 | 0.3960 | |
| 21.43 | 0.3630 | 0.4640 | |
| 22.44 | 0.4680 | 0.5300 | |
| 22.65 | 0.5060 | 0.5540 | |
| 22.94 | 0.5670 | 0.5980 | |
| 23.00 | 0.6630 | 0.6630 | AZEO |
| 23.02 | 0.7000 | 0.6900 | |
| 22.94 | 0.7250 | 0.7090 | |
| 22.78 | 0.7810 | 0.7580 | |
| 22.47 | 0.8230 | 0.7930 | |
| 21.70 | 0.9030 | 0.8780 | |

Lim, Jong Sung - Park, Ji Young - Lee, Kab-Soo - Kim, Jae-Duck - Lee, Byung Gwon, Measurement of Vapor−Liquid Equilibria for the Binary Mixture of Pentafluoroethane (HFC-125) + Propane (R-290), Journal of Chemical & Engineering Data 4 (2004) 750-755. doi:10.1021/je030156p

**T / K =** **313.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 17.89 | 0.1440 | 0.2800 | |
| 21.13 | 0.3380 | 0.4490 | |
| 22.67 | 0.5220 | 0.5700 | |
| 22.92 | 0.6664 | 0.6664 | AZEO |
| 22.92 | 0.7030 | 0.6950 | |
| 22.40 | 0.8130 | 0.7820 | |

Kim, Ju Hyok - Kim, Min Soo - Kim, Youngil, Vapor–liquid equilibria for pentafluoroethane + propane and difluoromethane + propane systems over a temperature range from 253.15 to 323.15 K, Fluid Phase Equilibria 2 (2003) 273-287. doi:10.1016/S0378-3812(03)00237-1

| **T / K =** | **323.15** | | |
|---|---|---|---|
| P / bar | $x_1$ | $y_1$ | |
| 19.47 | 0.0550 | 0.1250 | |
| 22.34 | 0.1490 | 0.2630 | |
| 24.26 | 0.2250 | 0.3380 | |
| 26.32 | 0.3480 | 0.4400 | |
| 27.79 | 0.4660 | 0.5220 | |
| 28.53 | 0.5640 | 0.5920 | |
| 28.72 | 0.6740 | 0.6740 | AZEO |
| 28.73 | 0.7020 | 0.6990 | |
| 28.47 | 0.7820 | 0.7700 | |
| 28.08 | 0.8230 | 0.8040 | |
| 27.22 | 0.8990 | 0.8820 | |

Hou, Shu-Xin - Duan, Yuan-Yuan, Isothermal vapor–liquid equilibria for the pentafluoroethane+propane and pentafluoroethane+1,1,1,2,3,3,3-heptafluoropropane systems, Fluid Phase Equilibria 1-2 (2010) 121-126. doi:10.1016/j.fluid.2009.09.008

| **T / K =** | **323.15** | | |
|---|---|---|---|
| P / bar | $x_1$ | $y_1$ | |
| 21.93 | 0.1333 | 0.2427 | |
| 25.28 | 0.2762 | 0.3827 | |
| 27.26 | 0.4170 | 0.4809 | |
| 28.59 | 0.5823 | 0.6064 | |
| 28.77 | 0.6378 | 0.6484 | |
| 28.77 | 0.6674 | 0.6674 | AZEO |
| 28.81 | 0.6833 | 0.6835 | |
| 28.75 | 0.7264 | 0.7179 | |
| 28.50 | 0.7871 | 0.7692 | |
| 27.93 | 0.8555 | 0.8337 | |
| 27.24 | 0.9072 | 0.8873 | |

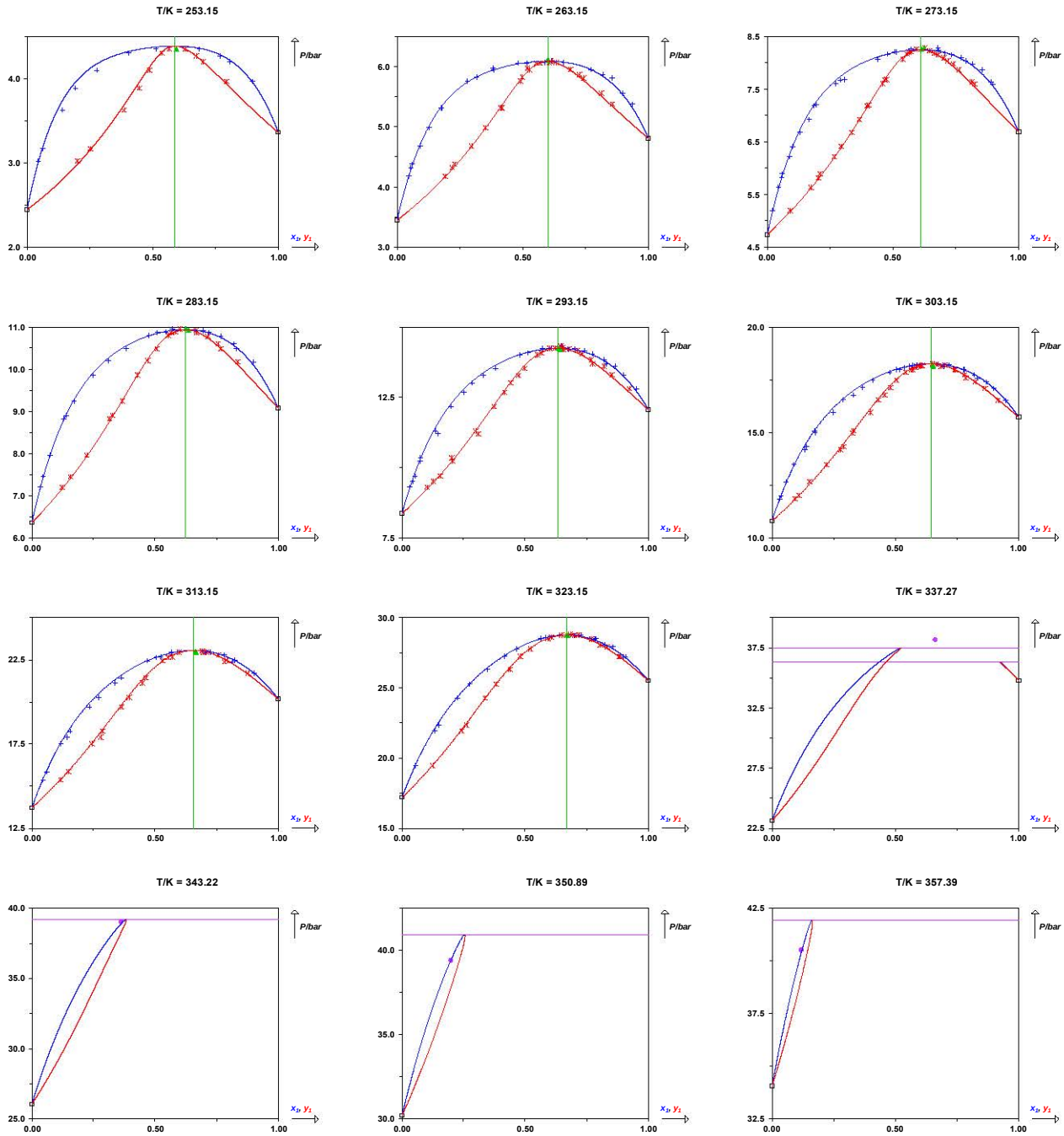
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**Data to represent in the T-P plane**

---

| T / K | P / bar | $x_1$ | |
|---|---|---|---|
| 357.40 | 40.51 | 0.1174 | CRIT (1) |
| 350.90 | 39.41 | 0.1974 | CRIT (1) |
| 343.20 | 39.02 | 0.3615 | CRIT (1) |
| 337.30 | 38.17 | 0.6609 | CRIT (1) |

(1) Li, Jun - Rodrigues, Miguel - Paiva, Alexandre - Matos, Henrique A. - Azevedo, Edmundo Gomes de, Binary solid–liquid–gas equilibrium of the tripalmitin/CO2 and ubiquinone/CO2 systems, Fluid Phase Equilibria 1-2 (2006) 196-204. doi:10.1016/j.fluid.2005.12.017


T/K = 253.15
T/K = 263.15
T/K = 273.15
T/K = 283.15
T/K = 293.15
T/K = 303.15
T/K = 313.15
T/K = 323.15
T/K = 337.27
T/K = 343.22
T/K = 350.89
T/K = 357.39
P/bar
x1, y1

## CARBON TETRAFLUORIDE (1) + TRIFLUOROMETHANE (2)

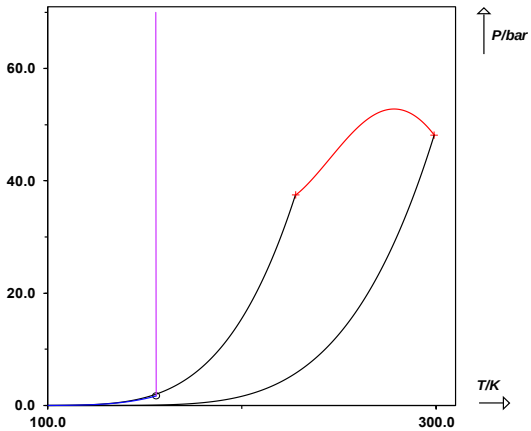
| | | |
|---|---|---|
| **CAS** | 75-73-0 | 75-46-7 |
| **InChiKey** | TXEYQDLBPFQVAA-UHFFFAOYSA-N | XPDWGBQVDMORPB-UHFFFAOYSA-N |
| **$T_c$ / K** | 227.51 | 299.01 |
| **$P_c$ / bar** | 37.45 | 48.162 |
| **ω** | 0.179 | 0.264 |

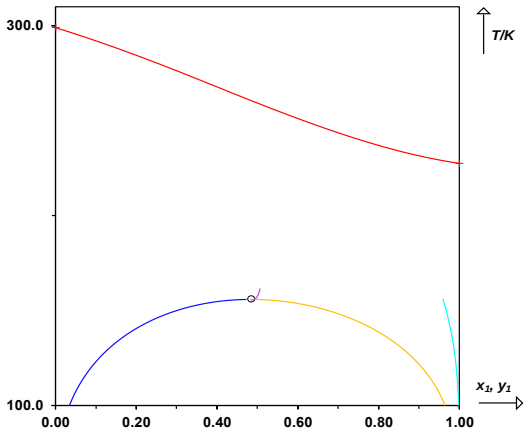
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 284
B/MPa = 349

*Deviations*
MAPE on x = 12 %
MAPE on y = 16 %



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**Isothermal phase equilibrium data**

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Baginskii, V.A. - Zakharov, N.D. - Lapardin, N.I., Study and calculation of the liquid-vapor phase equilibrium of mixtures of refrigerants, Issled. Teplofiz. Svoistv Rab. Veshchestv i Protsessov Teploobmena v Kholod. Tekhn., L. (1989) 9-15.

**T / K = 145.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2448 | 0.0273 | 0.8773 |
| 0.3978 | 0.0728 | 0.9287 |
| 0.5081 | 0.1016 | 0.9493 |
| 0.6419 | 0.1657 | 0.9579 |
| 0.7632 | 0.2560 | 0.9662 |
| 0.8322 | 0.3303 | 0.9722 |
| 0.8550 | 0.4066 | 0.9706 |
| 0.9211 | 0.6128 | 0.9743 |
| 0.9411 | 0.6466 | 0.9804 |
| 0.9680 | 0.8189 | 0.9834 |
| 0.9804 | 0.9808 | 0.9851 |

Kubic, William L. - Stein, Fred P., An experimental and correlative study of the vapor-liquid equilibria of the tetrafluoromethane-chlorotrifluoromethane system, Fluid Phase Equilibria 3-4 (1981) 289-304. doi:10.1016/0378-3812(80)80062-8

**T / K = 172.04**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.7364 | 0.0200 | 0.5860 |
| 1.298 | 0.0519 | 0.7736 |
| 2.612 | 0.1557 | 0.8908 |
| 3.034 | 0.2154 | 0.9191 |
| 3.227 | 0.2397 | 0.9136 |
| 3.660 | 0.3492 | 0.9275 |
| 3.993 | 0.4822 | 0.9355 |
| 4.029 | 0.5054 | 0.9388 |
| 4.033 | 0.5078 | 0.9390 |
| 4.229 | 0.6282 | 0.9448 |
| 4.326 | 0.7241 | 0.9496 |
| 4.462 | 0.8024 | 0.9564 |
| 4.579 | 0.8705 | 0.9635 |
| 4.702 | 0.9267 | 0.9737 |

Kubic, William L. - Stein, Fred P., An experimental and correlative study of the vapor-liquid equilibria of the tetrafluoromethane-chlorotrifluoromethane system, Fluid Phase Equilibria 3-4 (1981) 289-304. doi:10.1016/0378-3812(80)80062-8

**T / K = 199.82**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.846 | 0.0032 | 0.1056 |
| 2.031 | 0.0070 | 0.1860 |
| 2.217 | 0.0127 | 0.2629 |
| 2.576 | 0.0203 | 0.3485 |
| 3.235 | 0.0362 | 0.4786 |
| 3.936 | 0.0557 | 0.5754 |
| 5.127 | 0.0924 | 0.6759 |
| 6.445 | 0.1350 | 0.7472 |
| 8.729 | 0.2424 | 0.8209 |
| 10.77 | 0.3956 | 0.8563 |
| 11.82 | 0.5103 | 0.8772 |
| 12.32 | 0.5721 | 0.8846 |
| 12.31 | 0.5794 | 0.8843 |
| 13.46 | 0.7462 | 0.9125 |
| 14.06 | 0.8194 | 0.9287 |
| 14.71 | 0.9068 | 0.9547 |
| 14.76 | 0.9190 | 0.9548 |
| 15.09 | 0.9484 | 0.9710 |

Kubic, William L. - Stein, Fred P., An experimental and correlative study of the vapor-liquid equilibria of the tetrafluoromethane-chlorotrifluoromethane system, Fluid Phase Equilibria 3-4 (1981) 289-304. doi:10.1016/0378-3812(80)80062-8

**T / K = 224.82**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.196 | 0.0140 | 0.1542 |
| 8.940 | 0.0562 | 0.4025 |
| 9.524 | 0.0674 | 0.4384 |
| 13.21 | 0.1356 | 0.5955 |
| 17.90 | 0.2508 | 0.7036 |
| 20.80 | 0.3461 | 0.7445 |
| 22.88 | 0.4354 | 0.7755 |
| 25.89 | 0.5613 | 0.8079 |
| 27.89 | 0.6729 | 0.8367 |
| 29.71 | 0.7593 | 0.8640 |
| 29.79 | 0.7612 | 0.8646 |
| 30.31 | 0.8026 | 0.8779 |
| 32.91 | 0.9128 | 0.9346 |
| 33.76 | 0.9664 | 0.9699 |

Kubic, William L. - Stein, Fred P., An experimental and correlative study of the vapor-liquid equilibria of the tetrafluoromethane-chlorotrifluoromethane system, Fluid Phase Equilibria 3-4 (1981) 289-304. doi:10.1016/0378-3812(80)80062-8

**T / K = 250.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.830 | 0.0082 | 0.3882 |
| 7.530 | 0.0300 | 0.6790 |
| 12.66 | 0.0653 | 0.7933 |
| 20.48 | 0.1341 | 0.8623 |

| | | |
|---|---|---|
| 28.02 | 0.2183 | 0.8866 |
| 37.55 | 0.3965 | 0.8985 |
| 38.32 | 0.4095 | 0.8976 |
| 41.77 | 0.5148 | 0.8966 |
| 43.17 | 0.5737 | 0.8973 |

Kubic, William L. - Stein, Fred P., An experimental and correlative study of the vapor-liquid equilibria of the tetrafluoromethane-chlorotrifluoromethane system, Fluid Phase Equilibria 3-4 (1981) 289-304. doi:10.1016/0378-3812(80)80062-8

**T / K = 255.37**

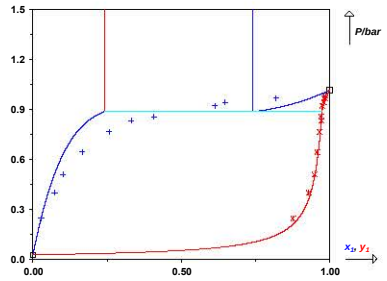
| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 19.53 | 0.0509 | 0.2006 |
| 22.30 | 0.0741 | 0.2851 |
| 25.48 | 0.1130 | 0.3634 |
| 29.06 | 0.1571 | 0.4293 |
| 37.99 | 0.2850 | 0.5353 |
| 40.29 | 0.3294 | 0.5545 |
| 43.16 | 0.3821 | 0.5744 |
| 46.64 | 0.4189 | 0.5829 |
| 48.52 | 0.4773 | 0.5356 |

Kubic, William L. - Stein, Fred P., An experimental and correlative study of the vapor-liquid equilibria of the tetrafluoromethane-chlorotrifluoromethane system, Fluid Phase Equilibria 3-4 (1981) 289-304. doi:10.1016/0378-3812(80)80062-8

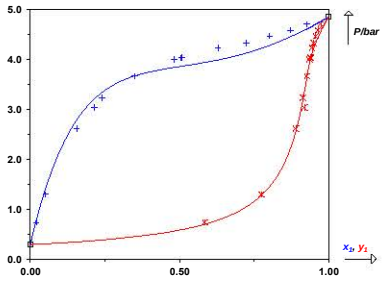
**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 35.82 | 0.0244 | 0.0649 |
| 39.06 | 0.0506 | 0.1195 |
| 41.17 | 0.0714 | 0.1464 |
| 41.32 | 0.0706 | 0.1490 |
| 43.57 | 0.0933 | 0.1748 |
| 43.63 | 0.0944 | 0.1749 |
| 46.82 | 0.1302 | 0.2039 |
| 46.44 | 0.1209 | 0.2011 |
| 48.45 | 0.1428 | 0.2162 |
| 50.95 | 0.1690 | 0.2282 |
| 51.61 | 0.1805 | 0.2254 |
| 51.95 | 0.1927 | 0.2229 |

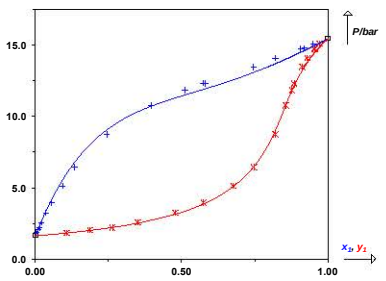
T/K = 145.15



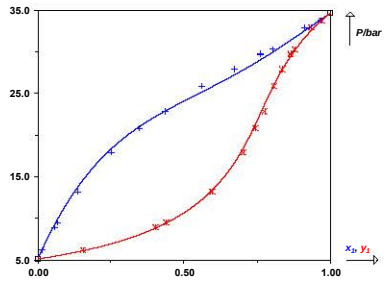

T/K = 172.04



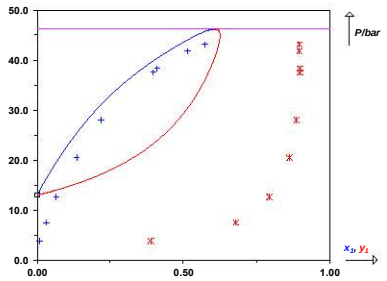

T/K = 199.82



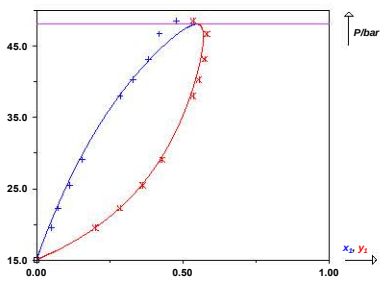

T/K = 224.82



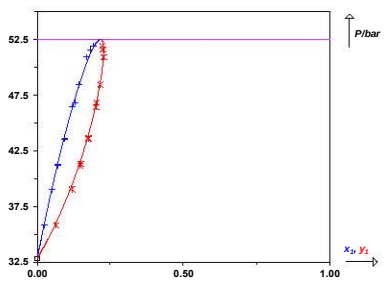

T/K = 250.65




T/K = 255.37




T/K = 283.15



## HEXAFLUOROETHANE (1) + 1,1,1,2-TETRAFLUOROETHANE (2)

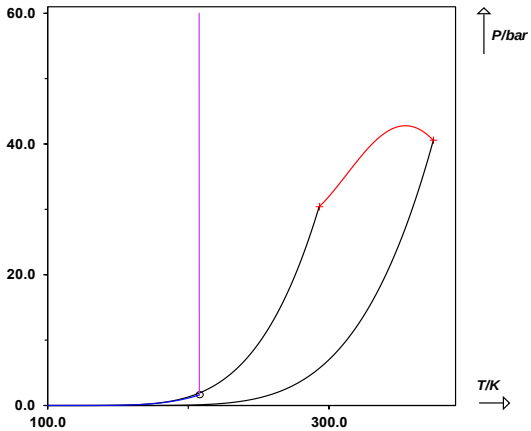
| | | |
|---|---|---|
| **CAS** | 76-16-4 | 811-97-2 |
| **InChiKey** | WMIYKQLTONQJES-UHFFFAOYSA-N | LVGUZGTVOIAKKC-UHFFFAOYSA-N |
| **$T_c$ / K** | 293.03 | 374.18 |
| **$P_c$ / bar** | 30.43 | 40.56 |
| **ω** | 0.255 | 0.327 |

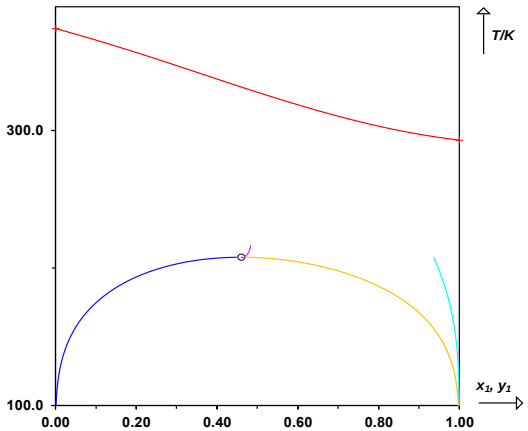
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 241
B/MPa = 368

*Deviations*
MAPE on x = 4.1 %
MAPE on y = 1.7 %



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**Isothermal phase equilibrium data**

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Kleiber, Michael, Vapor-liquid equilibria of binary refrigerant mixtures containing propylene or R134a, Fluid Phase Equilibria (1994) 149-194. doi:10.1016/0378-3812(94)80046-4

**T / K = 251.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.852 | 0.7714 | 0.9083 |
| 8.463 | 0.6780 | 0.8884 |
| 7.790 | 0.5325 | 0.8635 |
| 6.521 | 0.3186 | 0.8217 |
| 5.745 | 0.2381 | 0.7880 |
| 4.761 | 0.1618 | 0.7400 |
| 3.155 | 0.0770 | 0.6039 |
| 1.859 | 0.0238 | 0.3324 |

Madani, Hakim - Valtz, Alain - Coquelet, Christophe - Meniai, Abdeslam Hassen - Richon, Dominique, Vapor–liquid equilibrium data for the (hexafluoroethane +1,1,1,2-tetrafluoroethane) system at temperatures from 263 to 353K and pressures up to 4.16MPa, Fluid Phase Equilibria 1-2 (2008) 68-73. doi:10.1016/j.fluid.2008.04.002

**T / K = 263.43**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.001 | 0.0560 | 0.4898 |
| 5.860 | 0.1223 | 0.6537 |
| 6.998 | 0.1767 | 0.7137 |
| 7.748 | 0.2188 | 0.7443 |
| 8.806 | 0.2900 | 0.7808 |
| 10.13 | 0.4202 | 0.8195 |
| 11.54 | 0.6053 | 0.8581 |
| 13.19 | 0.8567 | 0.9232 |

Madani, Hakim - Valtz, Alain - Coquelet, Christophe - Meniai, Abdeslam Hassen - Richon, Dominique, Vapor–liquid equilibrium data for the (hexafluoroethane +1,1,1,2-tetrafluoroethane) system at temperatures from 263 to 353K and pressures up to 4.16MPa, Fluid Phase Equilibria 1-2 (2008) 68-73. doi:10.1016/j.fluid.2008.04.002

**T / K = 273.32**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.832 | 0.0412 | 0.3794 |
| 8.305 | 0.1504 | 0.6378 |
| 10.31 | 0.2384 | 0.7140 |
| 12.32 | 0.3618 | 0.7700 |
| 14.53 | 0.5636 | 0.8245 |
| 15.95 | 0.7148 | 0.8641 |
| 17.25 | 0.8552 | 0.9143 |

Madani, Hakim - Valtz, Alain - Coquelet, Christophe - Meniai, Abdeslam Hassen - Richon, Dominique, Vapor–liquid equilibrium data for the (hexafluoroethane +1,1,1,2-tetrafluoroethane) system at temperatures from 263 to 353K and pressures up to 4.16MPa, Fluid Phase Equilibria 1-2 (2008) 68-73. doi:10.1016/j.fluid.2008.04.002

**T / K = 288.30**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.927 | 0.0582 | 0.3649 |
| 10.71 | 0.1234 | 0.5243 |
| 12.83 | 0.1849 | 0.6041 |
| 15.42 | 0.2792 | 0.6749 |
| 17.83 | 0.3922 | 0.7277 |
| 20.31 | 0.5424 | 0.7781 |
| 22.26 | 0.6718 | 0.8195 |
| 24.78 | 0.8376 | 0.8890 |
| 25.69 | 0.8993 | 0.9243 |

Madani, Hakim - Valtz, Alain - Coquelet, Christophe - Meniai, Abdeslam Hassen - Richon, Dominique, Vapor–liquid equilibrium data for the (hexafluoroethane +1,1,1,2-tetrafluoroethane) system at temperatures from 263 to 353K and pressures up to 4.16MPa, Fluid Phase Equilibria 1-2 (2008) 68-73. doi:10.1016/j.fluid.2008.04.002

**T / K = 293.29**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.385 | 0.0471 | 0.2989 |
| 11.73 | 0.1173 | 0.4891 |
| 13.25 | 0.1552 | 0.5471 |
| 14.48 | 0.1898 | 0.5856 |
| 16.67 | 0.2622 | 0.6415 |
| 18.69 | 0.3413 | 0.6854 |
| 20.70 | 0.4375 | 0.7253 |
| 22.68 | 0.5468 | 0.7614 |
| 24.54 | 0.6523 | 0.7971 |
| 26.79 | 0.7804 | 0.8495 |
| 27.67 | 0.8298 | 0.8738 |
| 28.32 | 0.8668 | 0.8953 |

Madani, Hakim - Valtz, Alain - Coquelet, Christophe - Meniai, Abdeslam Hassen - Richon, Dominique, Vapor–liquid equilibrium data for the (hexafluoroethane +1,1,1,2-tetrafluoroethane) system at temperatures from 263 to 353K and pressures up to 4.16MPa, Fluid Phase Equilibria 1-2 (2008) 68-73. doi:10.1016/j.fluid.2008.04.002

**T / K = 313.31**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.36 | 0.0446 | 0.2135 |

| | | |
|---|---|---|
| 16.91 | 0.1005 | 0.3644 |
| 19.48 | 0.1479 | 0.4431 |
| 23.79 | 0.2412 | 0.5373 |
| 26.63 | 0.3152 | 0.5835 |
| 29.44 | 0.4011 | 0.6238 |
| 32.30 | 0.4949 | 0.6561 |
| 34.30 | 0.5686 | 0.6741 |

Madani, Hakim - Valtz, Alain - Coquelet, Christophe - Meniai, Abdeslam Hassen - Richon, Dominique, Vapor–liquid equilibrium data for the (hexafluoroethane +1,1,1,2-tetrafluoroethane) system at temperatures from 263 to 353K and pressures up to 4.16MPa, Fluid Phase Equilibria 1-2 (2008) 68-73. doi:10.1016/j.fluid.2008.04.002

**T / K = 333.32**

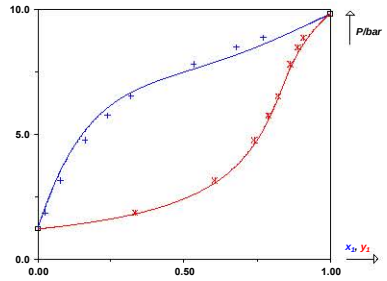
| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 19.10 | 0.0261 | 0.0985 |
| 22.33 | 0.0655 | 0.2073 |
| 25.54 | 0.1091 | 0.2924 |
| 31.58 | 0.2044 | 0.4028 |
| 35.24 | 0.2730 | 0.4450 |
| 38.55 | 0.3498 | 0.4676 |
| 39.96 | 0.3913 | 0.4615 |

Madani, Hakim - Valtz, Alain - Coquelet, Christophe - Meniai, Abdeslam Hassen - Richon, Dominique, Vapor–liquid equilibrium data for the (hexafluoroethane +1,1,1,2-tetrafluoroethane) system at temperatures from 263 to 353K and pressures up to 4.16MPa, Fluid Phase Equilibria 1-2 (2008) 68-73. doi:10.1016/j.fluid.2008.04.002

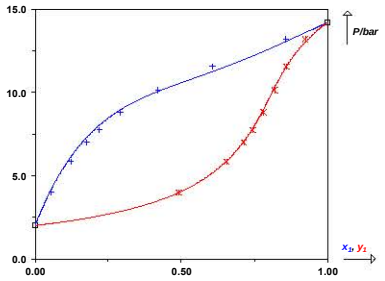
**T / K = 353.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 28.75 | 0.0254 | 0.0652 |
| 30.82 | 0.0467 | 0.1105 |
| 33.27 | 0.0746 | 0.1558 |
| 34.30 | 0.0864 | 0.1731 |
| 37.01 | 0.1205 | 0.2109 |
| 38.32 | 0.1382 | 0.2254 |
| 39.78 | 0.1598 | 0.2377 |
| 40.29 | 0.1681 | 0.2417 |
| 41.61 | 0.1945 | 0.2560 |

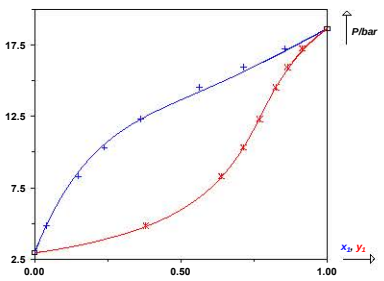
T/K = 251.00



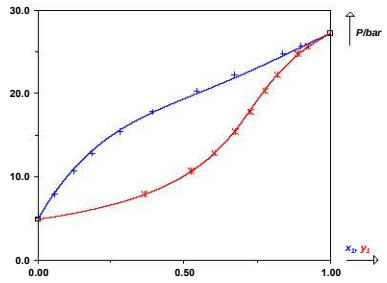

T/K = 263.43



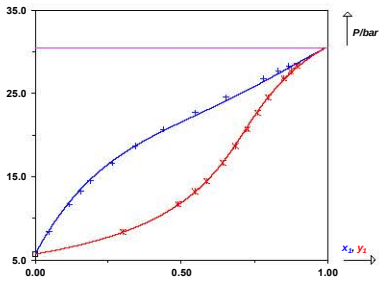

T/K = 273.32



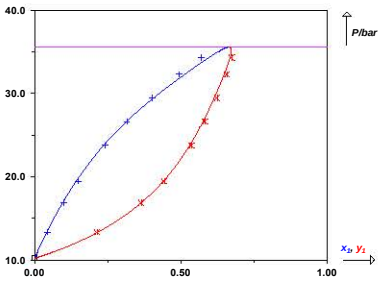

T/K = 288.30



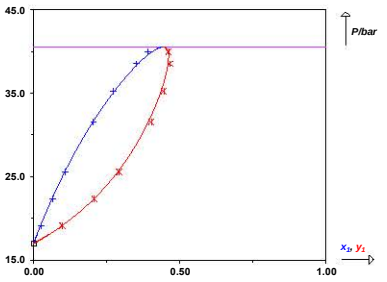

T/K = 293.29



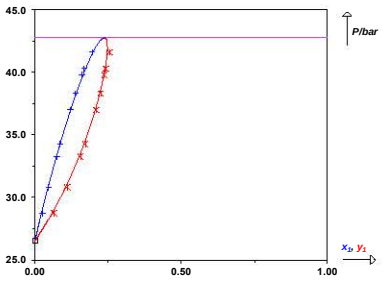

T/K = 313.31




T/K = 333.32




T/K = 353.20



## DECAFLUOROBUTANE (1) + 1,1,1,3,3-PENTAFLUOROBUTANE (2)

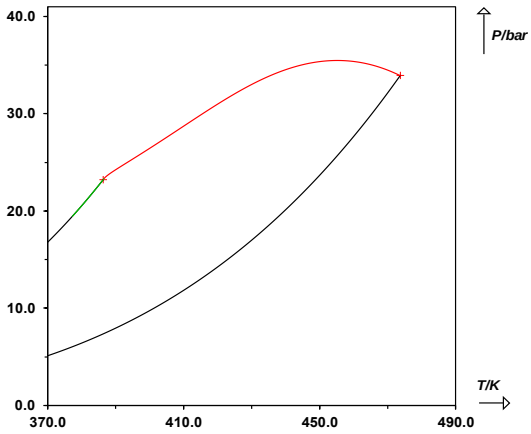
| | | |
|---|---|---|
| **CAS** | 355-25-9 | 406-58-6 |
| **InChiKey** | KAVGMUDTWQVPDF-UHFFFAOYSA-N | WZLFPVPRZGTCKP-UHFFFAOYSA-N |
| **$T_c$ / K** | 386.35 | 473.70 |
| **$P_c$ / bar** | 23.23 | 33.92 |
| **ω** | 0.366 | 0.257 |

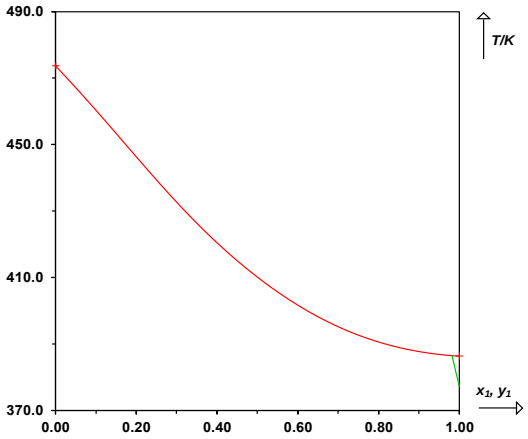
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 166
B/MPa = -38.2

*Deviations*
MAPE on x = 9.2 %
MAPE on y = 20 %



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**Isothermal phase equilibrium data**

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Perrotin-Brunel, Helene - van Roosmalen, Maaike J. E. - Kroon, Maaike C. - van Spronsen, Jaap - Witkamp, Geert-Jan - Peters, Cor J., Solubility of Cannabinol in Supercritical Carbon Dioxide, Journal of Chemical & Engineering Data 9 (2010) 3704-3707. doi:10.1021/je100245n

**T / K = 333.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.864 | 0.1082 | 0.4780 |
| 4.303 | 0.1487 | 0.5396 |
| 4.802 | 0.2070 | 0.6000 |
| 5.203 | 0.2690 | 0.6310 |
| 5.691 | 0.3682 | 0.6870 |
| 6.125 | 0.4720 | 0.7310 |
| 6.515 | 0.6100 | 0.7780 |

Perrotin-Brunel, Helene - van Roosmalen, Maaike J. E. - Kroon, Maaike C. - van Spronsen, Jaap - Witkamp, Geert-Jan - Peters, Cor J., Solubility of Cannabinol in Supercritical Carbon Dioxide, Journal of Chemical & Engineering Data 9 (2010) 3704-3707. doi:10.1021/je100245n

**T / K = 353.34**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.096 | 0.0566 | 0.2760 |
| 5.470 | 0.0736 | 0.3320 |
| 6.204 | 0.1130 | 0.4239 |
| 6.970 | 0.1630 | 0.4940 |
| 7.972 | 0.2450 | 0.5740 |
| 8.948 | 0.3590 | 0.6455 |
| 9.360 | 0.4240 | 0.6726 |
| 10.06 | 0.5430 | 0.7250 |

Perrotin-Brunel, Helene - van Roosmalen, Maaike J. E. - Kroon, Maaike C. - van Spronsen, Jaap - Witkamp, Geert-Jan - Peters, Cor J., Solubility of Cannabinol in Supercritical Carbon Dioxide, Journal of Chemical & Engineering Data 9 (2010) 3704-3707. doi:10.1021/je100245n

**T / K = 373.71**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.822 | 0.0526 | 0.2000 |
| 10.05 | 0.1370 | 0.3653 |
| 11.26 | 0.2028 | 0.4705 |
| 13.10 | 0.3294 | 0.5737 |
| 13.96 | 0.4050 | 0.6120 |
| 15.03 | 0.5150 | 0.6690 |
| 15.90 | 0.6160 | 0.7260 |
| 16.82 | 0.7420 | 0.7990 |

Perrotin-Brunel, Helene - van Roosmalen, Maaike J. E. - Kroon, Maaike C. - van Spronsen, Jaap - Witkamp, Geert-Jan - Peters, Cor J., Solubility of Cannabinol in Supercritical Carbon Dioxide, Journal of Chemical & Engineering Data 9 (2010) 3704-3707. doi:10.1021/je100245n

**T / K = 393.64**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.61 | 0.0257 | 0.0816 |
| 12.08 | 0.0698 | 0.2040 |
| 16.93 | 0.2365 | 0.4420 |
| 18.12 | 0.2949 | 0.4880 |
| 18.64 | 0.3188 | 0.5046 |
| 19.51 | 0.3693 | 0.5351 |
| 20.10 | 0.4062 | 0.5590 |
| 20.77 | 0.4477 | 0.5830 |
| 21.60 | 0.5048 | 0.6170 |
| 22.47 | 0.5660 | 0.6494 |
| 23.56 | 0.6490 | 0.7020 |
| 24.48 | 0.7242 | 0.7331 |

Perrotin-Brunel, Helene - van Roosmalen, Maaike J. E. - Kroon, Maaike C. - van Spronsen, Jaap - Witkamp, Geert-Jan - Peters, Cor J., Solubility of Cannabinol in Supercritical Carbon Dioxide, Journal of Chemical & Engineering Data 9 (2010) 3704-3707. doi:10.1021/je100245n

**T / K = 413.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.56 | 0.0257 | 0.0761 |
| 16.41 | 0.0420 | 0.1170 |
| 17.32 | 0.0615 | 0.1520 |
| 18.36 | 0.0853 | 0.2030 |
| 19.23 | 0.1062 | 0.2350 |
| 20.49 | 0.1409 | 0.2860 |
| 21.71 | 0.1748 | 0.3236 |
| 23.02 | 0.2182 | 0.3660 |
| 23.56 | 0.2367 | 0.3756 |
| 24.72 | 0.2755 | 0.4060 |
| 25.46 | 0.3057 | 0.4260 |
| 26.94 | 0.3671 | 0.4538 |
| 27.78 | 0.4049 | 0.4350 |

Perrotin-Brunel, Helene - van Roosmalen, Maaike J. E. - Kroon, Maaike C. - van Spronsen, Jaap - Witkamp, Geert-Jan - Peters, Cor J., Solubility of Cannabinol in Supercritical Carbon Dioxide, Journal of Chemical & Engineering Data 9 (2010) 3704-3707. doi:10.1021/je100245n

**T / K = 433.61**

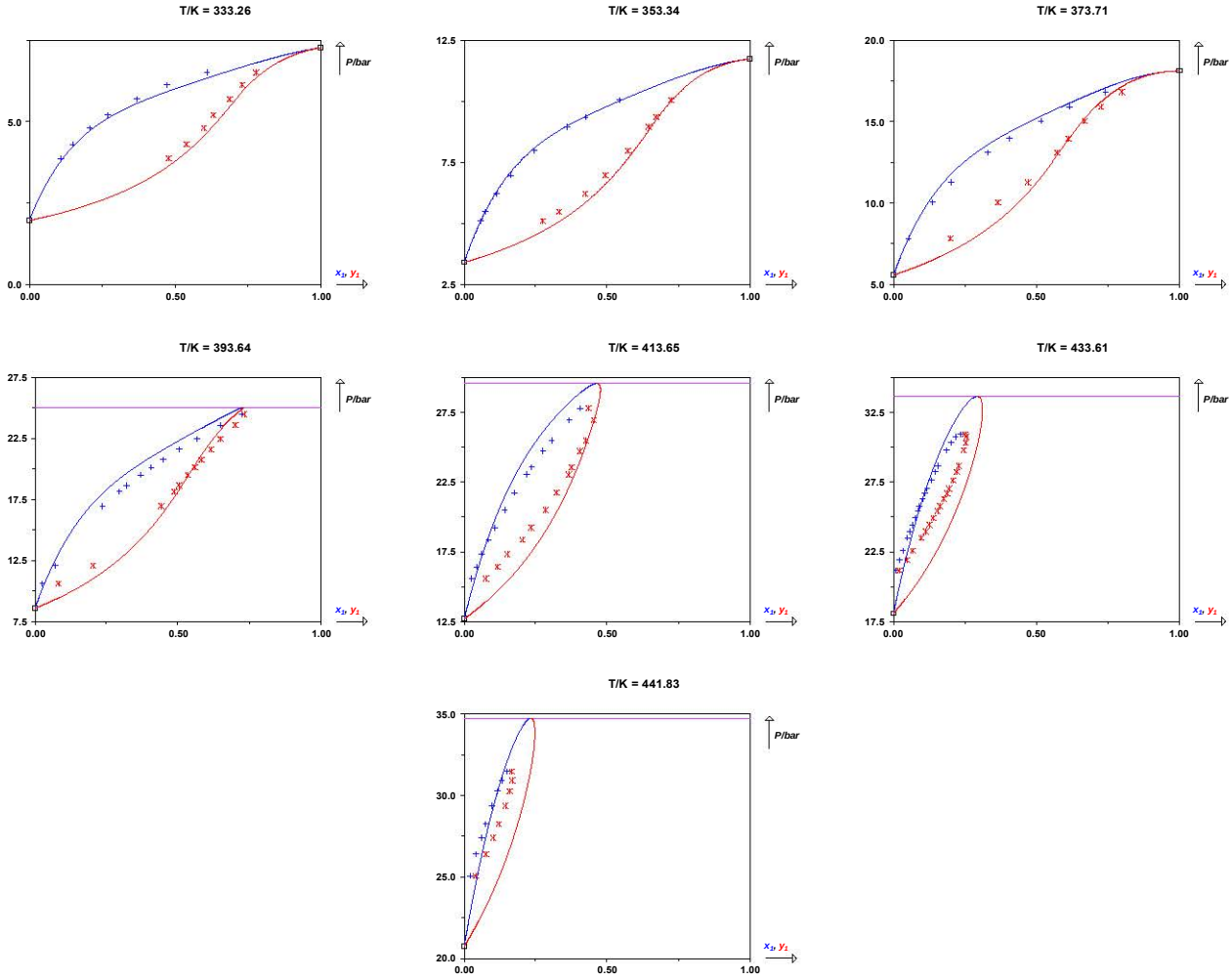
| P / bar | $x_1$ | $y_1$ |
|---|---|---|

| | | |
|---|---|---|
| 21.16 | 0.0089 | 0.0211 |
| 21.89 | 0.0216 | 0.0479 |
| 22.58 | 0.0326 | 0.0675 |
| 23.49 | 0.0483 | 0.0976 |
| 23.95 | 0.0566 | 0.1137 |
| 24.43 | 0.0654 | 0.1260 |
| 24.93 | 0.0749 | 0.1394 |
| 25.43 | 0.0847 | 0.1540 |
| 25.75 | 0.0913 | 0.1620 |
| 26.26 | 0.1017 | 0.1766 |
| 26.69 | 0.1109 | 0.1884 |
| 27.02 | 0.1181 | 0.1952 |
| 27.62 | 0.1317 | 0.2089 |
| 28.23 | 0.1461 | 0.2224 |
| 28.66 | 0.1559 | 0.2290 |
| 29.77 | 0.1852 | 0.2462 |
| 30.31 | 0.2012 | 0.2530 |
| 30.71 | 0.2162 | 0.2564 |
| 30.93 | 0.2352 | 0.2500 |

Perrotin-Brunel, Helene - van Roosmalen, Maaike J. E. - Kroon, Maaike C. - van Spronsen, Jaap - Witkamp, Geert-Jan - Peters, Cor J., Solubility of Cannabinol in Supercritical Carbon Dioxide, Journal of Chemical & Engineering Data 9 (2010) 3704-3707. doi:10.1021/je100245n

**T / K = 441.83**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 25.06 | 0.0203 | 0.0402 |
| 26.40 | 0.0419 | 0.0768 |
| 27.42 | 0.0595 | 0.1019 |
| 28.26 | 0.0748 | 0.1213 |
| 29.36 | 0.0962 | 0.1438 |
| 30.28 | 0.1157 | 0.1595 |
| 30.93 | 0.1313 | 0.1678 |
| 31.49 | 0.1484 | 0.1664 |


T/K = 333.26
P/bar
5.0
0.0
0.00
0.50
1.00
x1, y1
T/K = 353.34
P/bar
12.5
7.5
2.5
0.00
0.50
1.00
x1, y1
T/K = 373.71
P/bar
20.0
15.0
10.0
5.0
0.00
0.50
1.00
x1, y1
T/K = 393.64
P/bar
27.5
22.5
17.5
12.5
7.5
0.00
0.50
1.00
x1, y1
T/K = 413.65
P/bar
27.5
22.5
17.5
12.5
0.00
0.50
1.00
x1, y1
T/K = 433.61
P/bar
32.5
27.5
22.5
17.5
0.00
0.50
1.00
x1, y1
T/K = 441.83
P/bar
35.0
30.0
25.0
20.0
0.00
0.50
1.00
x1, y1

## CHLORODIFLUOROMETHANE (1) + DICHLORODIFLUOROMETHANE (2)

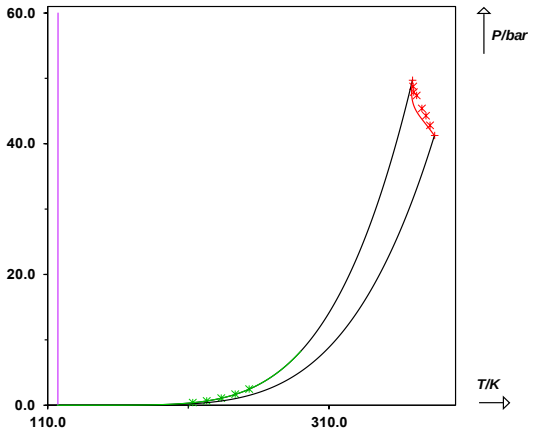
| | | |
|---|---|---|
| **CAS** | 75-45-6 | 75-71-8 |
| **InChiKey** | VOPWNXZWBYDODV-UHFFFAOYSA-N | PXBRQCKWGAHEHS-UHFFFAOYSA-N |
| **$T_c$ / K** | 369.30 | 384.95 |
| **$P_c$ / bar** | 49.71 | 41.25 |
| **ω** | 0.219 | 0.180 |

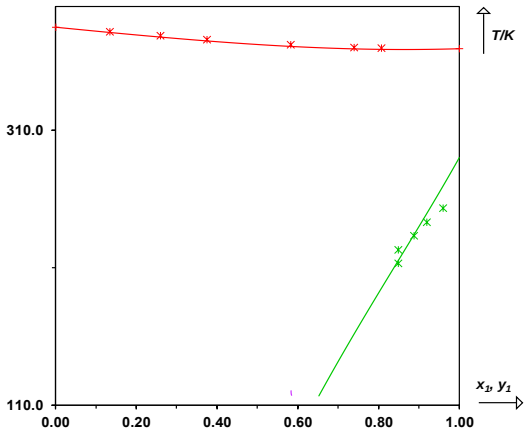
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 108
B/MPa = 167

*Deviations*
MAPE on x = 6.3 %
MAPE on y = 6.6 %
MAPE on $x_c$ = 20 %
MAPE on $P_c$ = 3.8 %
MAPE on $x_{az}$ = 12 %
MAPE on $P_{az}$ = 1.6 %
MAPE on $h^M$ = 6.9 %



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**Isothermal phase equilibrium data**

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Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 213.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2650 | 0.0686 | 0.2054 | |
| 0.2890 | 0.1345 | 0.3156 | |
| 0.3100 | 0.1979 | 0.3925 | |
| 0.3270 | 0.2590 | 0.4467 | |
| 0.3480 | 0.3747 | 0.5276 | |
| 0.3740 | 0.4825 | 0.5956 | |
| 0.3890 | 0.5830 | 0.6524 | |
| 0.4000 | 0.6772 | 0.7087 | |
| 0.4060 | 0.7654 | 0.7782 | |
| 0.4070 | 0.8075 | 0.8116 | |
| 0.4080 | 0.8483 | 0.8483 | AZEO |
| 0.4070 | 0.8879 | 0.8762 | |
| 0.4040 | 0.9264 | 0.9111 | |
| 0.3980 | 0.9637 | 0.9489 | |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 223.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.4490 | 0.0686 | 0.1979 | |
| 0.4880 | 0.1345 | 0.3214 | |
| 0.5230 | 0.1979 | 0.4013 | |
| 0.5520 | 0.2590 | 0.4573 | |
| 0.5970 | 0.3747 | 0.5366 | |
| 0.6300 | 0.4825 | 0.6043 | |
| 0.6550 | 0.5830 | 0.6625 | |
| 0.6720 | 0.6772 | 0.7229 | |
| 0.6820 | 0.7654 | 0.7866 | |
| 0.6850 | 0.8075 | 0.8207 | |
| 0.6860 | 0.8483 | 0.8483 | AZEO |
| 0.6850 | 0.8879 | 0.8770 | |
| 0.6820 | 0.9264 | 0.9111 | |
| 0.6760 | 0.9637 | 0.9489 | |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 233.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.7071 | 0.0685 | 0.1892 | |
| 0.7649 | 0.1345 | 0.3121 | |
| 0.8149 | 0.1979 | 0.3936 | |
| 0.8591 | 0.2590 | 0.4530 | |
| 0.9277 | 0.3747 | 0.5296 | |
| 0.9797 | 0.4824 | 0.5966 | |
| 1.017 | 0.5830 | 0.6680 | |
| 1.042 | 0.6772 | 0.7246 | |
| 1.060 | 0.7654 | 0.7917 | |
| 1.065 | 0.8075 | 0.8240 | |
| 1.068 | 0.8483 | 0.8548 | |
| 1.069 | 0.8879 | 0.8879 | AZEO |
| 1.067 | 0.9264 | 0.9211 | |
| 1.063 | 0.9637 | 0.9512 | |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 243.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 1.096 | 0.0685 | 0.1879 | |
| 1.178 | 0.1345 | 0.3098 | |
| 1.245 | 0.1979 | 0.3847 | |
| 1.305 | 0.2590 | 0.4392 | |
| 1.406 | 0.3747 | 0.5255 | |
| 1.487 | 0.4824 | 0.5985 | |
| 1.551 | 0.5830 | 0.6680 | |
| 1.599 | 0.6772 | 0.7343 | |
| 1.630 | 0.7654 | 0.7967 | |
| 1.641 | 0.8075 | 0.8289 | |
| 1.648 | 0.8483 | 0.8651 | |
| 1.651 | 0.9188 | 0.9188 | AZEO |
| 1.649 | 0.9637 | 0.9534 | |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 253.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.626 | 0.0685 | 0.1728 |
| 1.734 | 0.1345 | 0.2899 |
| 1.836 | 0.1979 | 0.3714 |
| 1.927 | 0.2590 | 0.4328 |
| 2.084 | 0.3747 | 0.5245 |
| 2.209 | 0.4824 | 0.5966 |
| 2.307 | 0.5830 | 0.6698 |
| 2.377 | 0.6772 | 0.7351 |

| | | | |
|---|---|---|---|
| 2.425 | 0.7654 | 0.7933 | |
| 2.453 | 0.8483 | 0.8563 | |
| 2.465 | 0.9600 | 0.9600 | AZEO |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 263.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.362 | 0.0685 | 0.1589 |
| 2.519 | 0.1345 | 0.2757 |
| 2.663 | 0.1979 | 0.3590 |
| 2.790 | 0.2590 | 0.4198 |
| 3.006 | 0.3747 | 0.5154 |
| 3.179 | 0.4824 | 0.5937 |
| 3.315 | 0.5830 | 0.6680 |
| 3.413 | 0.6772 | 0.7334 |
| 3.481 | 0.7654 | 0.7967 |
| 3.521 | 0.8483 | 0.8627 |
| 3.542 | 0.9264 | 0.9332 |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.368 | 0.0685 | 0.1525 |
| 3.601 | 0.1345 | 0.2602 |
| 3.789 | 0.1979 | 0.3409 |
| 3.947 | 0.2590 | 0.4046 |
| 4.211 | 0.3747 | 0.5093 |
| 4.425 | 0.4824 | 0.5927 |
| 4.604 | 0.5830 | 0.6680 |
| 4.754 | 0.6772 | 0.7360 |
| 4.867 | 0.7654 | 0.7967 |
| 4.943 | 0.8483 | 0.8667 |
| 4.972 | 0.9264 | 0.9324 |

Feng, Y. - Li, C. - Shou, Z., Vapor-Liquid Equilibrium for Freon-22 and Freon-12 Vapor Phase Fugacity from a Generalized Virial Equation, Zhejiang Daxue Xuebao 5 (1985) 58-67.

**T / K = 278.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.114 | 0.1173 | 0.2012 |
| 4.519 | 0.2262 | 0.3463 |
| 4.641 | 0.2641 | 0.3898 |
| 4.904 | 0.3510 | 0.4820 |
| 5.137 | 0.4372 | 0.5567 |
| 5.259 | 0.4904 | 0.5945 |
| 5.431 | 0.5768 | 0.6610 |
| 5.573 | 0.6706 | 0.7352 |
| 5.695 | 0.7729 | 0.8105 |
| 5.755 | 0.8287 | 0.8549 |
| 5.776 | 0.8541 | 0.8751 |
| 5.796 | 0.8725 | 0.8884 |
| 5.816 | 0.8970 | 0.9086 |
| 5.826 | 0.9230 | 0.9305 |
| 5.852 | 0.9483 | 0.9527 |
| 5.857 | 0.9774 | 0.9780 |
| 5.846 | 0.9786 | 0.9788 |
| 5.836 | 0.9904 | 0.9902 |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.593 | 0.0685 | 0.1422 |
| 4.899 | 0.1345 | 0.2506 |
| 5.164 | 0.1979 | 0.3317 |
| 5.387 | 0.2590 | 0.3936 |
| 5.761 | 0.3747 | 0.5000 |
| 6.065 | 0.4824 | 0.5840 |
| 6.316 | 0.5830 | 0.6607 |
| 6.514 | 0.6772 | 0.7334 |
| 6.655 | 0.7654 | 0.7992 |
| 6.745 | 0.8483 | 0.8659 |
| 6.792 | 0.9264 | 0.9309 |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.082 | 0.0685 | 0.1254 |
| 6.477 | 0.1345 | 0.2361 |
| 6.833 | 0.1979 | 0.3168 |
| 7.144 | 0.2590 | 0.3825 |
| 7.647 | 0.3747 | 0.4908 |
| 8.044 | 0.4824 | 0.5811 |
| 8.366 | 0.5830 | 0.6607 |
| 8.621 | 0.6772 | 0.7317 |
| 8.811 | 0.7654 | 0.8000 |
| 8.946 | 0.8483 | 0.8659 |
| 9.037 | 0.9264 | 0.9339 |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.952 | 0.0685 | 0.1241 |
| 8.439 | 0.1345 | 0.2324 |
| 8.895 | 0.1979 | 0.3156 |
| 9.311 | 0.2590 | 0.3836 |
| 9.978 | 0.3747 | 0.4866 |
| 10.49 | 0.4824 | 0.5733 |
| 10.91 | 0.5830 | 0.6560 |
| 11.24 | 0.6772 | 0.7299 |
| 11.49 | 0.7654 | 0.8000 |
| 11.69 | 0.8483 | 0.8691 |
| 11.83 | 0.9264 | 0.9347 |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.21 | 0.0685 | 0.1228 |
| 10.77 | 0.1345 | 0.2190 |
| 11.30 | 0.1979 | 0.2981 |
| 11.80 | 0.2590 | 0.3669 |
| 12.66 | 0.3747 | 0.4793 |
| 13.35 | 0.4824 | 0.5723 |
| 13.89 | 0.5830 | 0.6560 |
| 14.31 | 0.6772 | 0.7299 |
| 14.66 | 0.7654 | 0.8017 |
| 14.93 | 0.8483 | 0.8699 |
| 15.14 | 0.9264 | 0.9332 |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.30 | 0.0686 | 0.1137 |
| 14.01 | 0.1345 | 0.2128 |
| 14.67 | 0.1979 | 0.2911 |
| 15.27 | 0.2590 | 0.3568 |
| 16.36 | 0.3747 | 0.4678 |
| 17.27 | 0.4825 | 0.5605 |
| 18.01 | 0.5830 | 0.6505 |
| 18.61 | 0.6772 | 0.7299 |
| 19.09 | 0.7654 | 0.8001 |
| 19.48 | 0.8483 | 0.8699 |
| 19.79 | 0.9264 | 0.9355 |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 16.63 | 0.0686 | 0.1110 |
| 17.49 | 0.1345 | 0.2029 |
| 18.28 | 0.1979 | 0.2852 |
| 19.01 | 0.2590 | 0.3534 |
| 20.33 | 0.3747 | 0.4636 |
| 21.49 | 0.4825 | 0.5595 |
| 22.45 | 0.5830 | 0.6505 |
| 23.24 | 0.6772 | 0.7334 |
| 23.85 | 0.7654 | 0.8042 |
| 24.33 | 0.8483 | 0.8691 |
| 24.72 | 0.9264 | 0.9355 |

Kriebel, M., Liquid-vapor phase equilibriums of the binary system difluoromonochloromethane (R 22)-difluorodichloromethane (R 12), Kaeltetechnik 1 (1967) 8-14.

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.45 | 0.0686 | 0.1202 |
| 21.50 | 0.1345 | 0.2190 |
| 22.47 | 0.1979 | 0.2958 |
| 23.37 | 0.2590 | 0.3579 |
| 24.95 | 0.3747 | 0.4636 |
| 26.35 | 0.4825 | 0.5654 |
| 27.52 | 0.5830 | 0.6561 |
| 28.46 | 0.6772 | 0.7334 |
| 29.24 | 0.7654 | 0.8034 |
| 29.89 | 0.8483 | 0.8675 |
| 30.44 | 0.9264 | 0.9332 |

Nishiumi, H. - Kohmatsu, S. - Yokoyama, T. - Konda, A., Phase Behavior of the Binary Refrigerant Mixtures HCF22 - CFC12 and HCF22 - HCFC123, Fluid Phase Equilib. (1995) 131-143. doi:10.1016/0378-3812(94)02644-G

**T / K = 369.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 32.35 | 0.0540 | 0.0730 |
| 34.30 | 0.1210 | 0.1550 |
| 36.57 | 0.2120 | 0.2550 |

| | | |
|---|---|---|
| 39.19 | 0.3310 | 0.3740 |

Nishiumi, H. - Kohmatsu, S. - Yokoyama, T. - Konda, A., Phase Behavior of the Binary Refrigerant Mixtures HCF22 - CFC12 and HCF22 - HCFC123, Fluid Phase Equilib. (1995) 131-143. doi:10.1016/0378-3812(94)02644-G

**T / K = 369.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 41.95 | 0.4480 | 0.4830 |
| 45.08 | 0.6110 | 0.6310 |
| 46.76 | 0.7240 | 0.7330 |
| 48.28 | 0.8580 | 0.8610 |

Nishiumi, H. - Kohmatsu, S. - Yokoyama, T. - Konda, A., Phase Behavior of the Binary Refrigerant Mixtures HCF22 - CFC12 and HCF22 - HCFC123, Fluid Phase Equilib. (1995) 131-143. doi:10.1016/0378-3812(94)02644-G

**T / K = 370.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 34.55 | 0.1180 | 0.1480 | |
| 37.09 | 0.2160 | 0.2550 | |
| 39.42 | 0.3140 | 0.3570 | |
| 41.09 | 0.4000 | 0.4370 | |
| 42.36 | 0.4570 | 0.4900 | |
| 43.39 | 0.4940 | 0.5250 | |
| 44.67 | 0.5480 | 0.5730 | |
| 45.41 | 0.6020 | 0.6220 | |
| 46.07 | 0.6330 | 0.6500 | |
| 46.60 | 0.6670 | 0.6790 | |
| 47.06 | 0.6940 | 0.7030 | |
| 47.29 | 0.7110 | 0.7200 | |
| 47.66 | 0.7260 | 0.7330 | |
| 47.65 | 0.7280 | 0.7380 | |
| 47.87 | 0.7380 | 0.7410 | |
| 47.87 | 0.7395 | 0.7395 | CRIT |

Nishiumi, H. - Kohmatsu, S. - Yokoyama, T. - Konda, A., Phase Behavior of the Binary Refrigerant Mixtures HCF22 - CFC12 and HCF22 - HCFC123, Fluid Phase Equilib. (1995) 131-143. doi:10.1016/0378-3812(94)02644-G

**T / K = 372.12**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 33.33 | 0.0230 | 0.0310 |
| 33.53 | 0.0340 | 0.0460 |
| 34.07 | 0.0480 | 0.0630 |
| 34.42 | 0.0520 | 0.0830 |
| 34.52 | 0.0680 | 0.0880 |
| 35.11 | 0.0910 | 0.1160 |
| 35.28 | 0.0960 | 0.1210 |
| 35.35 | 0.0980 | 0.1250 |
| 35.52 | 0.1070 | 0.1340 |
| 35.92 | 0.1240 | 0.1540 |
| 36.08 | 0.1270 | 0.1570 |
| 36.48 | 0.1410 | 0.1730 |
| 36.72 | 0.1490 | 0.1820 |
| 36.92 | 0.1580 | 0.1920 |
| 37.27 | 0.1710 | 0.2070 |
| 37.70 | 0.1840 | 0.2200 |
| 38.05 | 0.1950 | 0.2320 |
| 38.63 | 0.2200 | 0.2590 |
| 38.88 | 0.2340 | 0.2720 |
| 39.17 | 0.2420 | 0.2800 |
| 39.96 | 0.2790 | 0.3160 |
| 40.40 | 0.2980 | 0.3350 |
| 41.16 | 0.3270 | 0.3630 |
| 41.46 | 0.3460 | 0.3810 |
| 41.84 | 0.3680 | 0.4040 |
| 42.35 | 0.3890 | 0.4210 |
| 43.13 | 0.4180 | 0.4490 |
| 43.73 | 0.4470 | 0.4740 |
| 44.12 | 0.4630 | 0.4900 |
| 44.65 | 0.4930 | 0.5170 |
| 45.19 | 0.5210 | 0.5410 |
| 45.54 | 0.5350 | 0.5530 |
| 45.98 | 0.5570 | 0.5720 |
| 46.28 | 0.5720 | 0.5840 |
| 46.48 | 0.5850 | 0.5960 |
| 46.68 | 0.5950 | 0.6020 |

Nishiumi, H. - Kohmatsu, S. - Yokoyama, T. - Konda, A., Phase Behavior of the Binary Refrigerant Mixtures HCF22 - CFC12 and HCF22 - HCFC123, Fluid Phase Equilib. (1995) 131-143. doi:10.1016/0378-3812(94)02644-G

**T / K = 374.14**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.27 | 0.0320 | 0.0440 |
| 36.40 | 0.1070 | 0.1350 |
| 36.98 | 0.1330 | 0.1620 |
| 38.53 | 0.1930 | 0.2270 |
| 39.52 | 0.2260 | 0.2610 |
| 39.98 | 0.2470 | 0.2780 |
| 40.85 | 0.2940 | 0.3300 |
| 41.26 | 0.3130 | 0.3500 |
| 41.67 | 0.3310 | 0.3670 |
| 42.16 | 0.3440 | 0.3790 |
| 42.98 | 0.3770 | 0.4040 |

| | | |
|---|---|---|
| 43.80 | 0.4080 | 0.4370 |
| 44.05 | 0.4170 | 0.4420 |
| 44.36 | 0.4340 | 0.4600 |
| 44.66 | 0.4430 | 0.4660 |
| 45.11 | 0.4630 | 0.4830 |
| 45.28 | 0.4770 | 0.4980 |
| 45.45 | 0.4820 | 0.5000 |
| 45.74 | 0.5000 | 0.5180 |
| 378.76 | 44.30 | 0.2594 |
| 375.91 | 45.40 | 0.3747 |
| 372.32 | 47.40 | 0.5830 |
| 369.87 | 48.80 | 0.8075 |

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**Enthalpy of mixing**

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Geller, Z.I. - Chaikovskii, V.F. - Egorov, A.V., Heats of mixing of Freons, Teplofiz. Svoist. Zhidk. (1973) 148-152.

**T / K = 222.00**

**P / bar = 0.6500**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 461.00 | 0.2430 |
| 463.00 | 0.2430 |
| 499.00 | 0.3150 |
| 502.00 | 0.3150 |
| 525.00 | 0.4180 |
| 526.00 | 0.4180 |
| 538.00 | 0.5030 |
| 535.00 | 0.5030 |
| 476.00 | 0.7080 |
| 475.00 | 0.7080 |

Geller, Z.I. - Chaikovskii, V.F. - Egorov, A.V., Heats of mixing of Freons 112 and 115 with Freon 22, Kholod. Tekh. 8 (1971) 29-30.

**T / K = 253.00**

**P / bar = UNKNOWN (4.8659)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 464.00 | 0.2600 |
| 504.20 | 0.3310 |
| 539.20 | 0.5220 |
| 478.30 | 0.7260 |

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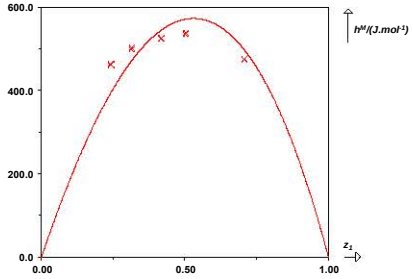
**Critical point**

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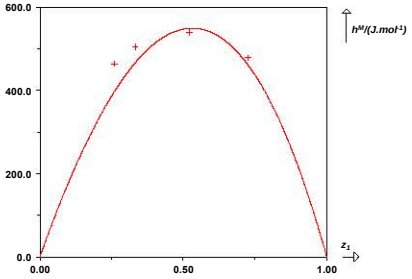
Higashi, Y. - Okazaki, S. - Takaishi, Y. - Uematsu, M. - Watanabe, K., Measurements of the vapor-liquid coexistence curve for the binary R12 + R22 system in the critical region, J. Chem. Eng. Data 1 (1984) 31-36. doi:10.1021/je00035a012

| T / K | P / bar | $x_1$ |
|---|---|---|
| 381.68 | 42.80 | 0.1345 |

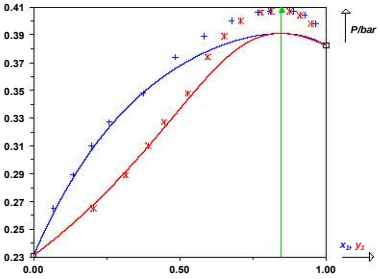
T/K = 222.00 - P/bar = 0.6500



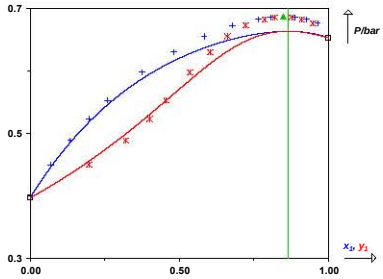

T/K = 253.00 - P/bar = 4.8659



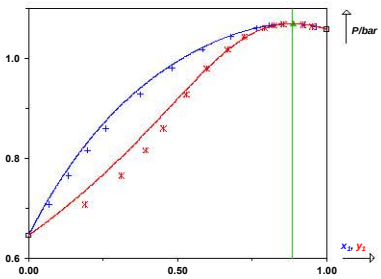

T/K = 213.15



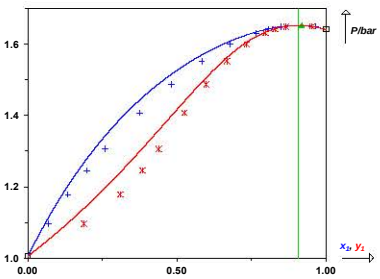

T/K = 223.15



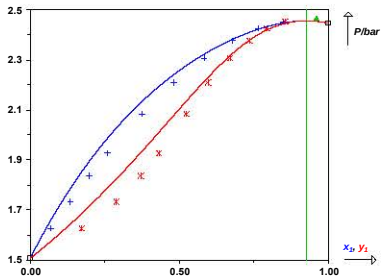

T/K = 233.15



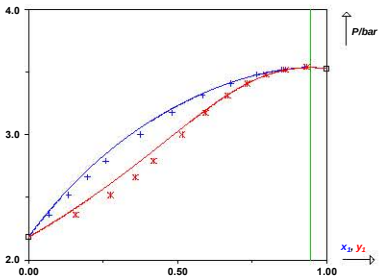

T/K = 243.15



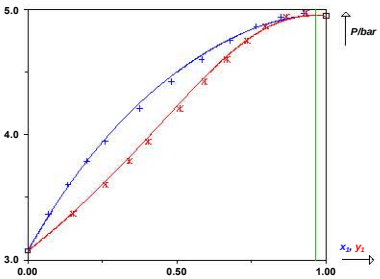

T/K = 253.15



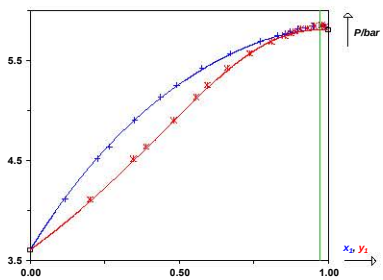

T/K = 263.15



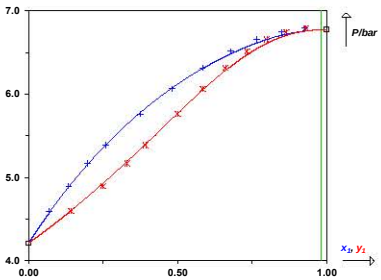

T/K = 273.15



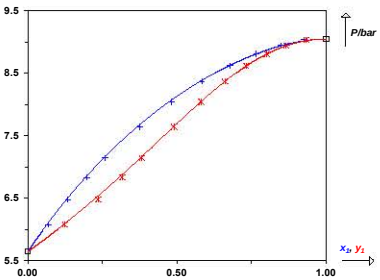

T/K = 278.15



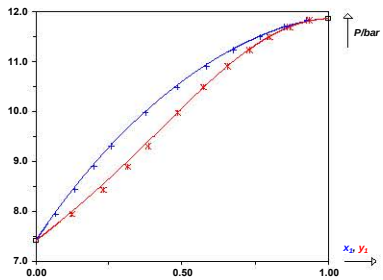

T/K = 283.15



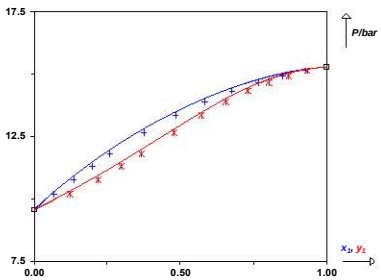

T/K = 293.15



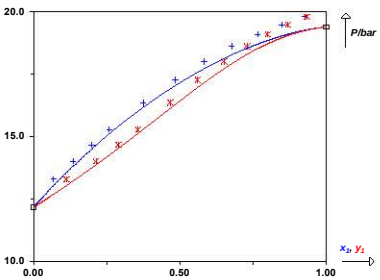

T/K = 303.15



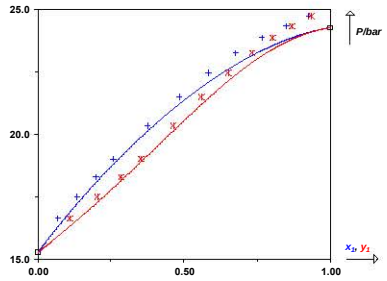

T/K = 313.15



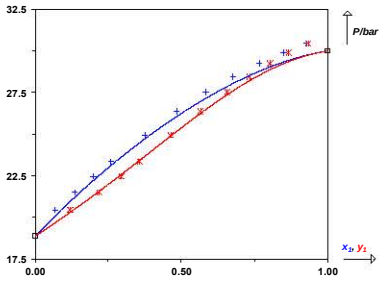

T/K = 323.15



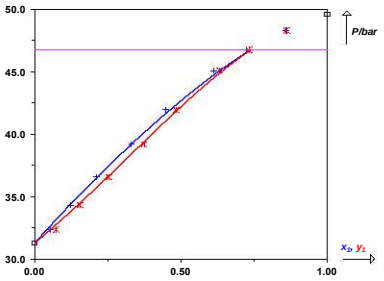
T/K = 333.15



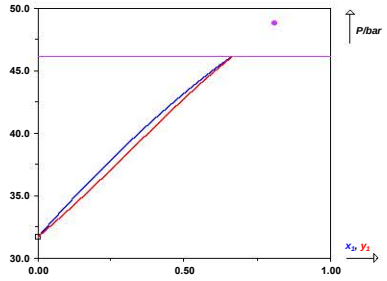

T/K = 343.15



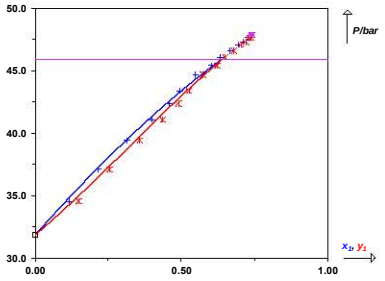

T/K = 369.15



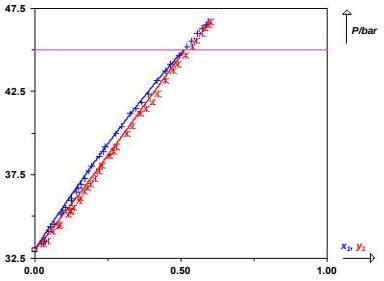

T/K = 369.87



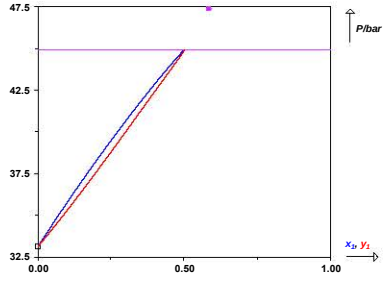

T/K = 370.15



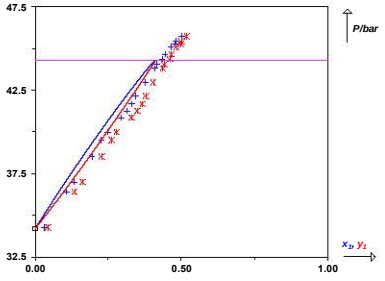

T/K = 372.12



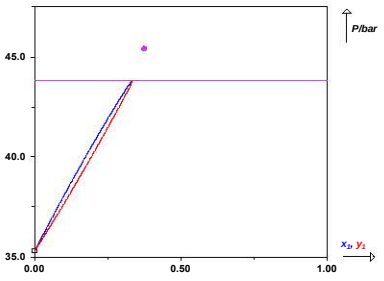

T/K = 372.32



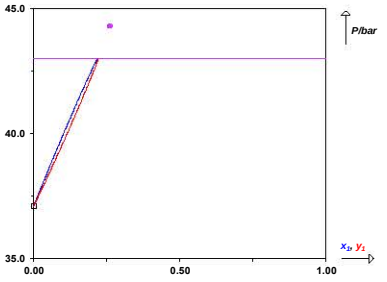

T/K = 374.14



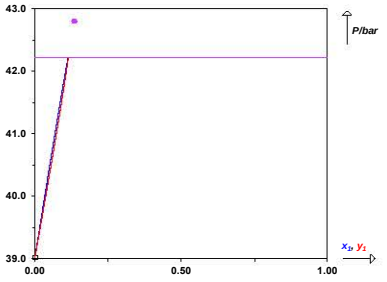

T/K = 375.91




T/K = 378.76




T/K = 381.68



## DICHLOROMETHANE (1) + CARBON TETRACHLORIDE (2)

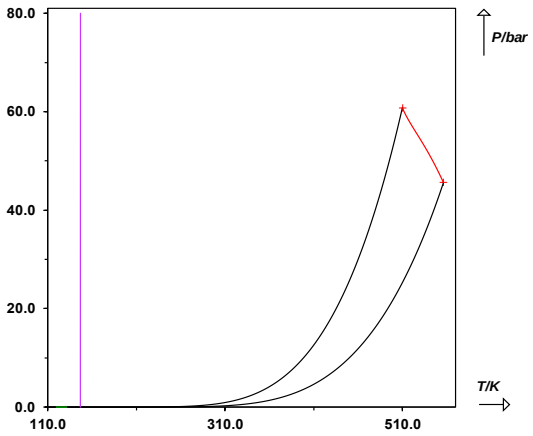
| | | |
|---|---|---|
| **CAS** | 75-09-2 | 56-23-5 |
| **InChiKey** | YMWUJEATGCHHMB-UHFFFAOYSA-N | VZGDMQKNWNREIO-UHFFFAOYSA-N |
| **$T_c$ / K** | 510.00 | 556.35 |
| **$P_c$ / bar** | 60.80 | 45.60 |
| **ω** | 0.199 | 0.193 |

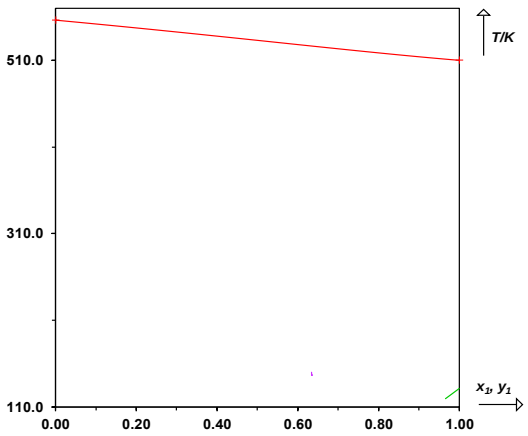
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 91.4
B/MPa = 182

*Deviations*
MAPE on x = 3.2 %
MAPE on y = 3.4 %
MAPE on $h^M$ = 8.6 %



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**Isothermal phase equilibrium data**

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Azpiazu, Y. - Royo, F. - Gutiérrez Losa, C., Vapour pressures of (tetrachloromethane + α,ω-dichloroalkane), The Journal of Chemical Thermodynamics 6 (1984) 561-565. doi:10.1016/0021-9614(84)90007-7

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2606 | 0.0820 | 0.3250 |
| 0.2890 | 0.1240 | 0.4140 |
| 0.2934 | 0.1350 | 0.4350 |
| 0.3236 | 0.1740 | 0.5020 |
| 0.3350 | 0.1930 | 0.5300 |
| 0.3650 | 0.2380 | 0.5820 |
| 0.4318 | 0.3410 | 0.6940 |
| 0.5073 | 0.4900 | 0.7840 |
| 0.5318 | 0.5590 | 0.8170 |
| 0.5403 | 0.5740 | 0.8240 |
| 0.5846 | 0.6600 | 0.8650 |
| 0.5995 | 0.6920 | 0.8790 |
| 0.5980 | 0.6960 | 0.8810 |
| 0.6260 | 0.7470 | 0.9030 |
| 0.6669 | 0.8500 | 0.9360 |
| 0.6740 | 0.8890 | 0.9510 |
| 0.6874 | 0.9280 | 0.9620 |

Rulewicz, G. - Schuberth, H. - Leibnitz, E., Untersuchungen über das Dampf-Flüssigkeits-Phasengleichgewicht des Systems Methylenchlorid/Chloroform/Tetrachlorkohlenstoff bei 45°C unter Verwendung einer gaschromatographischen Analysenmethode, Journal für Praktische Chemie 3-4 (1968) 122-136. doi:10.1002/prac.19680370303

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3806 | 0.0250 | 0.1170 |
| 0.4140 | 0.0500 | 0.2110 |
| 0.4773 | 0.1000 | 0.3520 |
| 0.5386 | 0.1500 | 0.4540 |
| 0.5926 | 0.2000 | 0.5340 |
| 0.6425 | 0.2500 | 0.5940 |
| 0.6906 | 0.3000 | 0.6430 |
| 0.7359 | 0.3500 | 0.6850 |
| 0.7799 | 0.4000 | 0.7220 |
| 0.8215 | 0.4500 | 0.7530 |
| 0.8597 | 0.5000 | 0.7800 |
| 0.8977 | 0.5500 | 0.8070 |
| 0.9339 | 0.6000 | 0.8300 |
| 0.9686 | 0.6500 | 0.8510 |
| 1.004 | 0.7000 | 0.8720 |
| 1.039 | 0.7500 | 0.8930 |
| 1.074 | 0.8000 | 0.9160 |
| 1.108 | 0.8500 | 0.9380 |
| 1.144 | 0.9000 | 0.9590 |
| 1.157 | 0.9200 | 0.9670 |
| 1.179 | 0.9500 | 0.9790 |
| 1.193 | 0.9700 | 0.9870 |

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**Enthalpy of mixing**

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Ortega, Juan, Measurements and Analysis of Excess Enthalpies of Alkyl Acetates + 1-Chloroalkanes Using the Unifac Model, Berichte der Bunsengesellschaft für physikalische Chemie 10 (1988) 1146-1149. doi:10.1002/bbpc.198800288

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 137.00 | 0.0533 |
| 270.00 | 0.1165 |
| 397.00 | 0.1948 |
| 510.00 | 0.2884 |
| 567.00 | 0.3603 |
| 602.00 | 0.4369 |
| 608.00 | 0.4987 |
| 594.00 | 0.5621 |
| 548.00 | 0.6372 |
| 481.00 | 0.7060 |
| 360.00 | 0.7955 |
| 277.00 | 0.8477 |
| 135.00 | 0.9276 |

Siddiqi, M.A. - Lucas, K., The excess enthalpy of (tetrachloromethane + carbon disulphide) and (tetrachloromethane + dichloromethane) over a range of temperatures and pressures, The Journal of Chemical Thermodynamics 12 (1983) 1181-1187. doi:10.1016/0021-9614(83)90009-5

**T / K = 298.15**

**P / bar = 150.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 402.80 | 0.2010 |
| 445.90 | 0.2320 |
| 534.70 | 0.3340 |
| 583.80 | 0.4300 |
| 605.40 | 0.5180 |
| 586.60 | 0.6010 |

| | |
|---|---|
| 558.10 | 0.6620 |
| 492.40 | 0.7510 |
| 291.20 | 0.8830 |

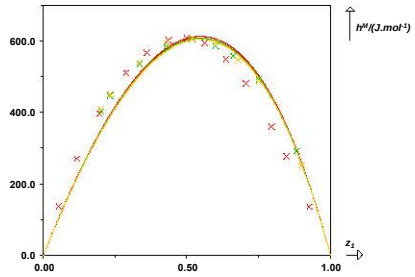
Siddiqi, M.A. - Lucas, K., The excess enthalpy of (tetrachloromethane + carbon disulphide) and (tetrachloromethane + dichloromethane) over a range of temperatures and pressures, The Journal of Chemical Thermodynamics 12 (1983) 1181-1187. doi:10.1016/0021-9614(83)90009-5

| **T / K =** | **298.15** |
|---|---|
| **P / bar =** | **300.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 409.00 | 0.2010 |
| 450.00 | 0.2320 |
| 538.60 | 0.3340 |
| 592.20 | 0.4300 |
| 606.00 | 0.5180 |
| 595.00 | 0.6010 |
| 545.60 | 0.6780 |
| 486.30 | 0.7510 |
| 250.90 | 0.9000 |

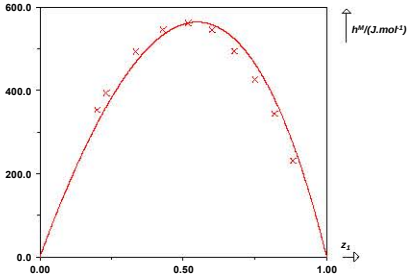
Siddiqi, M.A. - Lucas, K., The excess enthalpy of (tetrachloromethane + carbon disulphide) and (tetrachloromethane + dichloromethane) over a range of temperatures and pressures, The Journal of Chemical Thermodynamics 12 (1983) 1181-1187. doi:10.1016/0021-9614(83)90009-5

| **T / K =** | **323.15** |
|---|---|
| **P / bar =** | **2.000** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 353.50 | 0.2010 |
| 394.00 | 0.2320 |
| 492.80 | 0.3340 |
| 545.80 | 0.4300 |
| 561.80 | 0.5180 |
| 545.90 | 0.6010 |
| 493.90 | 0.6780 |
| 426.20 | 0.7510 |
| 343.60 | 0.8190 |
| 231.60 | 0.8830 |

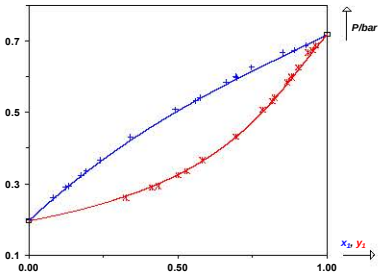
T/K = 298.15 - P/bar = 1.0100 150.00 300.00



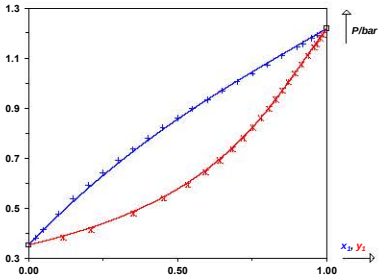

T/K = 323.15 - P/bar = 2.00




T/K = 303.15




T/K = 318.15



## CHLORODIFLUOROMETHANE (1) + CHLOROPENTAFLUOROETHANE (2)

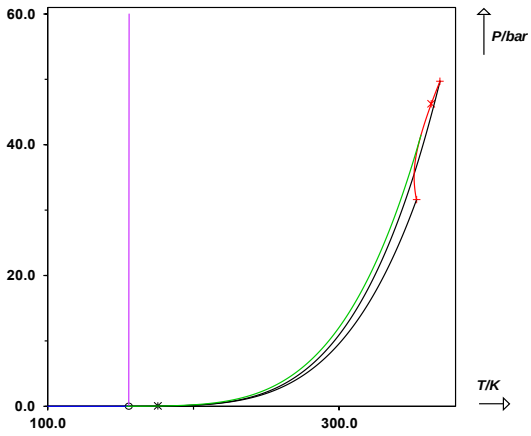
| | | |
|---|---|---|
| **CAS** | 75-45-6 | 76-15-3 |
| **InChiKey** | VOPWNXZWBYDODV-UHFFFAOYSA-N | RFCAUADVODFSLZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 369.3 | 353.15 |
| **$P_c$ / bar** | 49.71 | 31.57 |
| **ω** | 0.219 | 0.251 |

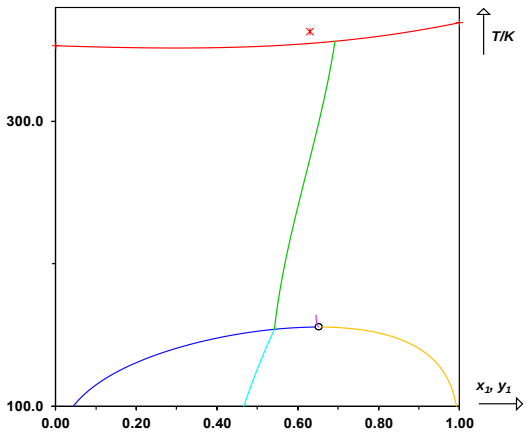
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 161
B/MPa = 246

*Deviations*
MAPE on $x_c$ = 54 %
MAPE on $P_c$ = 0.32 %
MAPE on $h^M$ = 5.7 %



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**Enthalpy of mixing**

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Geller, Z.I. - Chaikovskii, V.F. - Egorov, A.V., Heats of mixing of Freons 112 and 115 with Freon 22, Kholod. Tekh. 8 (1971) 29-30.

**T / K = 223.00**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 648.40 | 0.2650 |
| 743.30 | 0.3190 |
| 842.40 | 0.3870 |
| 865.30 | 0.4740 |
| 868.90 | 0.5010 |
| 846.40 | 0.6050 |
| 722.80 | 0.6800 |
| 643.40 | 0.7480 |

Geller, Z.I. - Chaikovskii, V.F. - Egorov, A.V., Heats of mixing of Freons 112 and 115 with Freon 22, Kholod. Tekh. 8 (1971) 29-30.

**T / K = 243.00**

**P / bar = UNKNOWN (3.2591)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 672.90 | 0.2670 |
| 769.10 | 0.3230 |
| 869.90 | 0.3900 |
| 894.50 | 0.4760 |
| 898.00 | 0.5090 |
| 873.50 | 0.6020 |
| 753.60 | 0.6850 |
| 668.40 | 0.7510 |

Geller, Z.I. - Chaikovskii, V.F. - Egorov, A.V., Heats of mixing of Freons 112 and 115 with Freon 22, Kholod. Tekh. 8 (1971) 29-30.

**T / K = 263.00**

**P / bar = UNKNOWN (7.0444)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 696.00 | 0.2750 |
| 798.20 | 0.3310 |
| 902.00 | 0.4060 |
| 926.90 | 0.4840 |
| 930.50 | 0.5170 |
| 905.40 | 0.6100 |
| 774.00 | 0.6930 |
| 693.10 | 0.7590 |

Geller, Z.I. - Chaikovskii, V.F. - Egorov, A.V., Heats of mixing of Freons 112 and 115 with Freon 22, Kholod. Tekh. 8 (1971) 29-30.

**T / K = 283.00**

**P / bar = UNKNOWN (13.4928)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 720.80 | 0.2800 |
| 725.40 | 0.3390 |
| 933.20 | 0.4130 |
| 967.10 | 0.4920 |
| 964.30 | 0.5250 |
| 941.40 | 0.6170 |
| 801.90 | 0.7000 |
| 713.60 | 0.7670 |

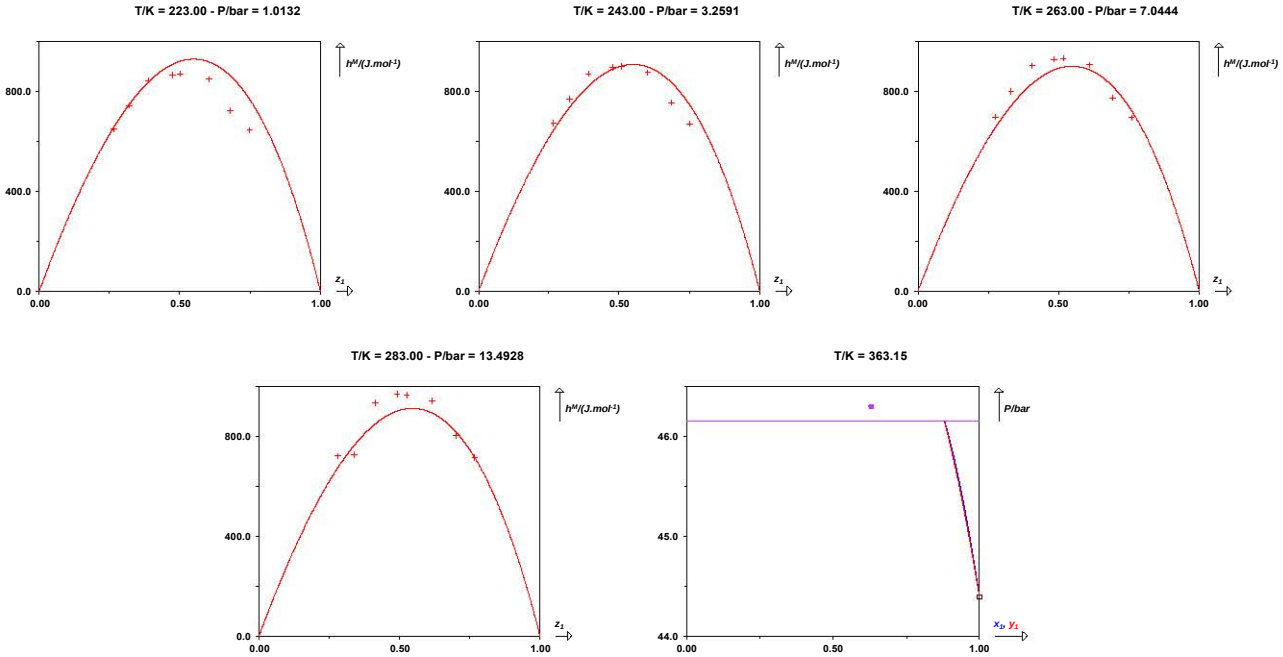
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**Critical point**

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Thies, Mark C. - Paulaitis, Michael E., Vapor-liquid equilibrium for 1-naphthol-methanol and naphthalene-methanol mixtures at elevated temperatures and pressures, Journal of Chemical & Engineering Data 1 (1986) 23-25. doi:10.1021/je00043a007

| T / K | P / bar | $x_1$ |
|---|---|---|
| 363.15 | 46.30 | 0.6300 |


T/K = 223.00 - P/bar = 1.0132
T/K = 243.00 - P/bar = 3.2591
T/K = 263.00 - P/bar = 7.0444
T/K = 283.00 - P/bar = 13.4928
T/K = 363.15
hᴹ/(J.mol⁻¹)
P/bar
z₁
x₁, y₁
800.0
400.0
0.0
46.0
45.0
44.0
0.00
0.50
1.00

## CHLOROFORM (1) + n-HEXANE (2)

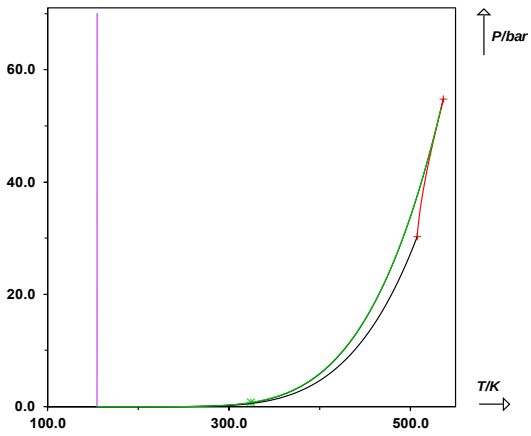
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 110-54-3 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | VLKZOEOYAKHREP-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.40 | 507.60 |
| **$P_c$ / bar** | 54.72 | 30.25 |
| **ω** | 0.222 | 0.301 |

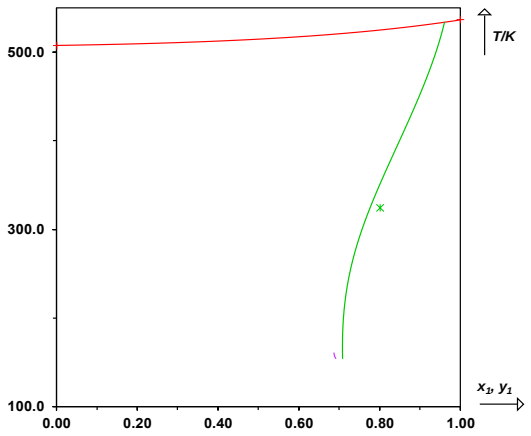
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 115
B/MPa = 167

*Deviations*
MAPE on x = 4.5 %
MAPE on y = 4.0 %
MAPE on $x_{az}$ = 7.6 %
MAPE on $P_{az}$ = 0.57 %
MAPE on $h^M$ = 18 %
MAPE on $c_P^M$ = 64 %



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**Isothermal phase equilibrium data**

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Bissell, T.G - Williamson, A.G, Vapour pressures and excess Gibbs energies of n-hexane and of n-heptane + carbon tetrachloride and + chloroform at 298.15 K, The Journal of Chemical Thermodynamics 2 (1975) 131-136. doi:10.1016/0021-9614(75)90260-8

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2273 | 0.1312 | 0.2230 |
| 0.2439 | 0.2441 | 0.3579 |
| 0.2555 | 0.3455 | 0.4538 |
| 0.2609 | 0.4052 | 0.5030 |
| 0.2637 | 0.4442 | 0.5331 |
| 0.2675 | 0.5022 | 0.5755 |
| 0.2692 | 0.5345 | 0.5984 |
| 0.2720 | 0.6013 | 0.6445 |
| 0.2732 | 0.6169 | 0.6552 |
| 0.2745 | 0.7015 | 0.7140 |
| 0.2747 | 0.7898 | 0.7799 |
| 0.2714 | 0.8937 | 0.8717 |

Kudryavtseva, L.S. - Susarev, M.P., Liquid-vapor equilibrium in systems chloroform-hexane and acetone-chloroform, J. Appl. Chem. USSR 6 (1963) 1231-1237.

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3294 | 0.1005 | 0.1680 |
| 0.3545 | 0.2005 | 0.3050 |
| 0.3730 | 0.2885 | 0.3920 |
| 0.3878 | 0.3954 | 0.4870 |
| 0.4006 | 0.4977 | 0.5710 |
| 0.4084 | 0.5993 | 0.6440 |
| 0.4141 | 0.6981 | 0.7140 |
| 0.4134 | 0.8000 | 0.7910 |
| 0.4081 | 0.9009 | 0.8800 |

Kudryavtseva, L.S. - Susarev, M.P., Liquid-vapor equilibrium in systems chloroform-hexane and acetone-chloroform, J. Appl. Chem. USSR 6 (1963) 1231-1237.

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4866 | 0.1015 | 0.1630 |
| 0.5218 | 0.2025 | 0.3010 |
| 0.5458 | 0.2895 | 0.3920 |
| 0.5666 | 0.3959 | 0.4840 |
| 0.5860 | 0.4982 | 0.5710 |
| 0.5952 | 0.5979 | 0.6400 |
| 0.6028 | 0.6986 | 0.7150 |
| 0.6046 | 0.8000 | 0.7930 |
| 0.5992 | 0.9006 | 0.8820 |

Kudryavtseva, L.S. - Susarev, M.P., Liquid-vapor equilibrium in systems chloroform-hexane and acetone-chloroform, J. Appl. Chem. USSR 6 (1963) 1231-1237.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.6925 | 0.1035 | 0.1610 |
| 0.7361 | 0.2035 | 0.2960 |
| 0.7667 | 0.2905 | 0.3850 |
| 0.7941 | 0.3964 | 0.4840 |
| 0.8230 | 0.4992 | 0.5690 |
| 0.8367 | 0.5965 | 0.6400 |
| 0.8467 | 0.6991 | 0.7200 |
| 0.8491 | 0.8000 | 0.7940 |
| 0.8415 | 0.9003 | 0.8830 |

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**Isobaric phase equilibrium data**

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Brzostowski, W. - Verhoeye, L., Thermodynamic properties of mixtures of hexane and chloroform, Rocz. Chem. (1968) 507-515.

**P / bar = 0.7519**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 330.55 | 0.1000 | 0.1590 |
| 329.10 | 0.2000 | 0.2890 |
| 327.80 | 0.3000 | 0.4000 |
| 326.70 | 0.4000 | 0.4960 |
| 325.75 | 0.5000 | 0.5810 |
| 325.10 | 0.6000 | 0.6580 |
| 324.65 | 0.7000 | 0.7290 |
| 324.40 | 0.8000 | 0.8010 |
| 324.50 | 0.9000 | 0.8860 |

Kudryavtseva, L.S. - Susarev, M.P., Liquid-vapor equilibrium in systems chloroform-hexane and acetone-chloroform, J. Appl. Chem. USSR 6 (1963) 1231-1237.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 339.68 | 0.1055 | 0.1590 |
| 337.93 | 0.2055 | 0.2920 |
| 336.65 | 0.2915 | 0.3830 |
| 335.47 | 0.3969 | 0.4840 |
| 334.55 | 0.4997 | 0.5660 |
| 334.02 | 0.5937 | 0.6410 |

| | | |
|---|---|---|
| 333.62 | 0.6998 | 0.7200 |
| 333.56 | 0.8000 | 0.7960 |
| 333.80 | 0.9001 | 0.8840 |

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**Enthalpy of mixing**

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Belousov, V.P. - Starodubtsev, A.M. - Balyakina, T.D. - Obukhova, M.E., Enthalpies of mixing and intermolecular interactions in binary mixtures of n-decane with chloroform and tributyl phosphate and of tributyl phosphate with diethylene glycol, Trudy po Khimii i Khimicheskoi Tekhnologii 4 (1975) 85-90.

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 153.10 | 0.0809 |
| 355.20 | 0.1687 |
| 473.90 | 0.2533 |
| 605.80 | 0.3343 |
| 687.30 | 0.4071 |
| 726.60 | 0.4714 |
| 746.10 | 0.5334 |
| 739.70 | 0.5826 |
| 722.60 | 0.6253 |
| 697.80 | 0.6623 |
| 657.30 | 0.7066 |
| 602.20 | 0.7526 |
| 527.40 | 0.7996 |
| 440.30 | 0.8406 |
| 338.60 | 0.8856 |
| 225.50 | 0.9287 |
| 113.40 | 0.9674 |

Bissell, T.G. - Okafor, G.E. - Williamson, A.G., Enthalpies and volumes of mixing of alkanes with carbon tetrachloride, chloroform, and methylene chloride at 25 °C, The Journal of Chemical Thermodynamics 3 (1971) 393-399. doi:10.1016/S0021-9614(71)80056-3

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 276.00 | 0.1060 |
| 468.00 | 0.1920 |
| 605.00 | 0.2810 |
| 718.00 | 0.4100 |
| 750.00 | 0.4960 |
| 761.00 | 0.4990 |
| 738.00 | 0.6030 |
| 670.00 | 0.6980 |
| 527.00 | 0.7950 |
| 287.00 | 0.9070 |

Sharma, B.R. - Pundeer, G.S. - Singh, P.P., Thermodynamics of weak interactions: excess enthalpies and excess Gibbs free energies of mixing, Thermochimica Acta 2 (1975) 105-114. doi:10.1016/0040-6031(75)80013-X

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 67.03 | 0.0598 |
| 132.90 | 0.1102 |
| 228.25 | 0.1803 |
| 450.38 | 0.3499 |
| 518.17 | 0.4201 |
| 586.04 | 0.5800 |
| 572.11 | 0.6297 |
| 471.96 | 0.7502 |
| 405.06 | 0.8001 |
| 344.82 | 0.8398 |
| 249.78 | 0.8903 |
| 162.15 | 0.9299 |

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**Heat capacity of mixing**

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Fenclova, D. - Dohnal, V. - Perez-Casas, S. - Frigolet, C. - Costas, M., Excess heat capacities, excess enthalpies, and excess volumes of trichloromethane + some oxygenated solvents or + the corresponding homomorphic hydrocarbons at 298.15 K, ELDATA Int. Electron. J. Phys. Chem. Data 3 (1995) 217-237.

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -1.010 | 0.1051 |
| -1.690 | 0.2211 |
| -2.010 | 0.3138 |
| -2.230 | 0.4089 |
| -2.230 | 0.5147 |
| -2.080 | 0.6083 |
| -1.800 | 0.7069 |
| -1.410 | 0.8033 |
| -0.7500 | 0.9049 |

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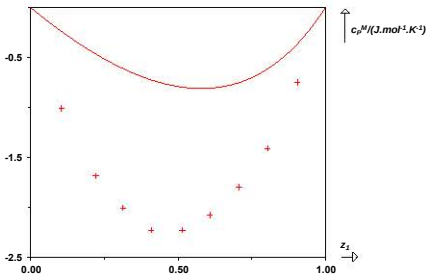
**Azeotropic point**

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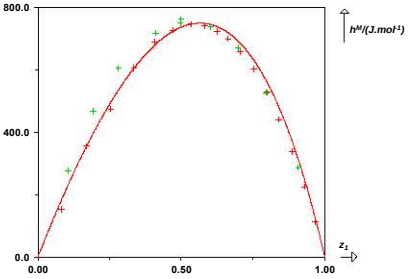
Brzostowski, W. - Verhoeye, L., Thermodynamic properties of mixtures of hexane and chloroform, Rocz. Chem. (1968) 507-515.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 324.40 | 0.7519 | 0.8015 |

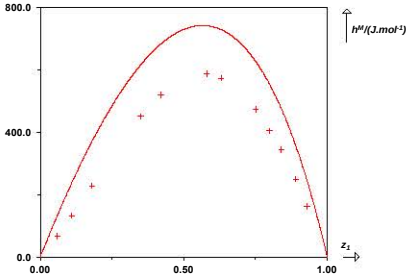
T/K = 298.15 - P/bar = 1.0132



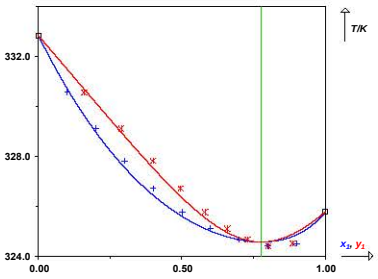

T/K = 298.15 - P/bar = 1.0132 1.0132



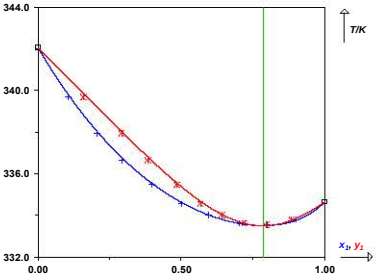

T/K = 308.15 - P/bar = 1.0132



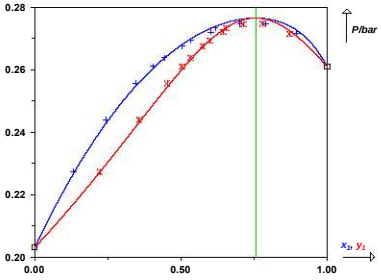

P/bar = 0.75194



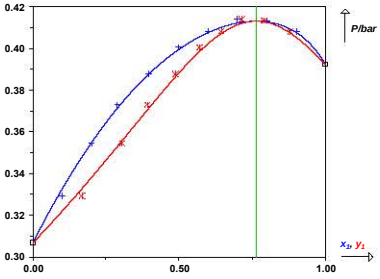

P/bar = 1.01330



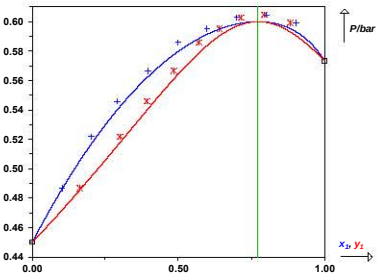

T/K = 298.15



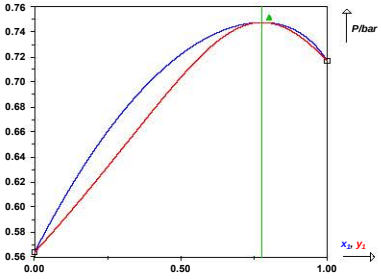

T/K = 308.15



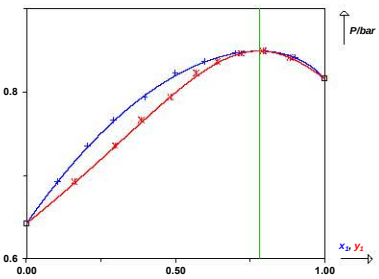

T/K = 318.15




T/K = 324.40




T/K = 328.15



## CHLOROFORM (1) + n-HEPTANE (2)

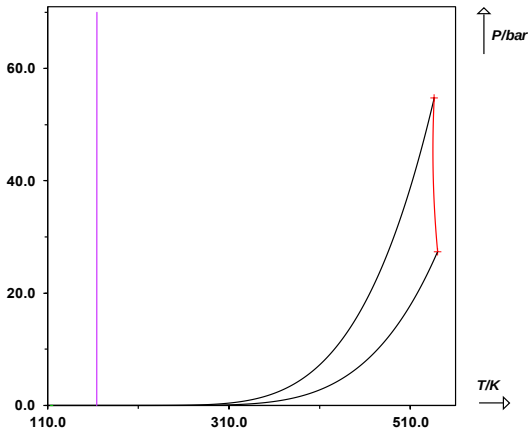
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 142-82-5 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | IMNFDUFMRHMDMM-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.40 | 540.20 |
| **$P_c$ / bar** | 54.72 | 27.40 |
| **ω** | 0.222 | 0.349 |

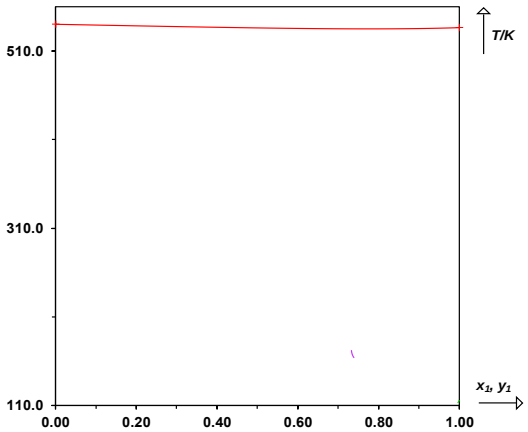
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 90.8
B/MPa = 171

*Deviations*
MAPE on x = 5.3 %
MAPE on y = 3.9 %
MAPE on $h^M$ = 9.2 %
MAPE on $c_P^M$ = 17 %



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**Isothermal phase equilibrium data**

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Bissell, T.G - Williamson, A.G, Vapour pressures and excess Gibbs energies of n-hexane and of n-heptane + carbon tetrachloride and + chloroform at 298.15 K, The Journal of Chemical Thermodynamics 2 (1975) 131-136. doi:10.1016/0021-9614(75)90260-8

**T / K =** **298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0966 | 0.1142 | 0.4391 |
| 0.1250 | 0.2181 | 0.6103 |
| 0.1459 | 0.3047 | 0.6971 |
| 0.1673 | 0.4045 | 0.7666 |
| 0.1854 | 0.5011 | 0.8165 |
| 0.1859 | 0.5019 | 0.8168 |
| 0.2027 | 0.6003 | 0.8574 |
| 0.2035 | 0.6058 | 0.8594 |
| 0.2199 | 0.7105 | 0.8962 |
| 0.2320 | 0.7922 | 0.9233 |
| 0.2455 | 0.8872 | 0.9556 |

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**Enthalpy of mixing**

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Abello, L., Enthalpies d'excès des systèmes binaires constitués d'hydrocarbures benzéniques et du chloroforme ou du methylchloroforme - I. — Résultats expérimentaux, J. Chim. Phys. Phys. Chim. Biol. 9 (1973) 1355-1359. doi:10.1051/jcp/1973701355

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 449.50 | 0.1870 |
| 604.00 | 0.2780 |
| 737.50 | 0.4080 |
| 803.20 | 0.5520 |
| 736.60 | 0.6750 |
| 648.40 | 0.7510 |
| 364.60 | 0.8905 |

Belousov, V.P. - Starodubtsev, A.M. - Balyakina, T.D. - Obukhova, M.E., Enthalpies of mixing and intermolecular interactions in binary mixtures of n-decane with chloroform and tributyl phosphate and of tributyl phosphate with diethylene glycol, Trudy po Khimii i Khimicheskoi Tekhnologii 4 (1975) 85-90.

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 208.20 | 0.0931 |
| 403.40 | 0.1870 |
| 568.20 | 0.2771 |
| 681.60 | 0.3584 |
| 760.80 | 0.4338 |
| 798.90 | 0.4987 |
| 806.70 | 0.5559 |
| 793.20 | 0.6043 |
| 767.30 | 0.6472 |
| 730.40 | 0.6830 |
| 714.60 | 0.6948 |
| 661.40 | 0.7362 |
| 592.10 | 0.7784 |
| 517.90 | 0.8208 |
| 428.40 | 0.8631 |
| 327.60 | 0.8997 |
| 217.00 | 0.9381 |
| 109.10 | 0.9706 |

Bissell, T.G. - Okafor, G.E. - Williamson, A.G., Enthalpies and volumes of mixing of alkanes with carbon tetrachloride, chloroform, and methylene chloride at 25 °C, The Journal of Chemical Thermodynamics 3 (1971) 393-399. doi:10.1016/S0021-9614(71)80056-3

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 280.00 | 0.1080 |
| 421.00 | 0.1720 |
| 563.00 | 0.2490 |
| 743.00 | 0.3980 |
| 797.00 | 0.4940 |
| 792.00 | 0.5950 |
| 708.00 | 0.7020 |
| 570.00 | 0.7970 |
| 481.00 | 0.8420 |
| 328.00 | 0.9020 |

Shatas, Joseph P. - Abbott, Michael M. - Van Ness, Hendrick C., Excess thermodynamic functions for ternary systems. II. Chloroform-ethanol-n-heptane at 50°C, Journal of Chemical & Engineering Data 4 (1975) 406-409. doi:10.1021/je60067a020

**T / K =** **323.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 39.90 | 0.0148 |
| 81.00 | 0.0303 |
| 149.30 | 0.0573 |
| 251.60 | 0.1005 |

| | |
|---|---|
| 326.80 | 0.1348 |
| 444.30 | 0.1948 |
| 538.20 | 0.2501 |
| 632.60 | 0.3181 |
| 702.90 | 0.3873 |
| 763.90 | 0.4835 |
| 772.80 | 0.5403 |
| 765.60 | 0.5854 |
| 757.90 | 0.6074 |
| 721.30 | 0.6710 |
| 702.10 | 0.6906 |
| 663.10 | 0.7253 |
| 620.60 | 0.7557 |
| 567.60 | 0.7889 |
| 481.90 | 0.8335 |
| 391.90 | 0.8733 |
| 292.90 | 0.9109 |
| 252.00 | 0.9250 |
| 187.40 | 0.9461 |
| 131.10 | 0.9633 |
| 80.40 | 0.9780 |
| 46.10 | 0.9876 |
| 11.30 | 0.9970 |

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**Heat capacity of mixing**

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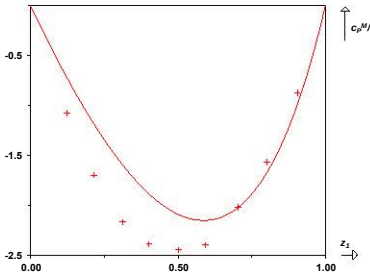
Fenclova, D. - Dohnal, V. - Perez-Casas, S. - Frigolet, C. - Costas, M., Excess heat capacities, excess enthalpies, and excess volumes of trichloromethane + some oxygenated solvents or + the corresponding homomorphic hydrocarbons at 298.15 K, ELDATA Int. Electron. J. Phys. Chem. Data 3 (1995) 217-237.

**T / K =** **298.15**

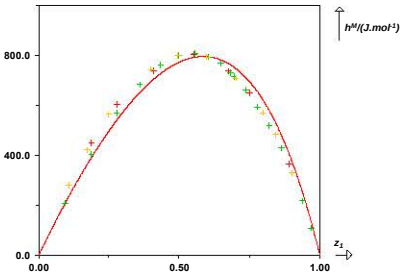
**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / $J.mol^{-1}.K^{-1}$ | $x_1$ |
|---|---|
| -1.080 | 0.1233 |
| -1.700 | 0.2139 |
| -2.170 | 0.3126 |
| -2.390 | 0.4023 |
| -2.450 | 0.5009 |
| -2.400 | 0.5923 |
| -2.020 | 0.7026 |
| -1.570 | 0.8030 |
| -0.8800 | 0.9048 |

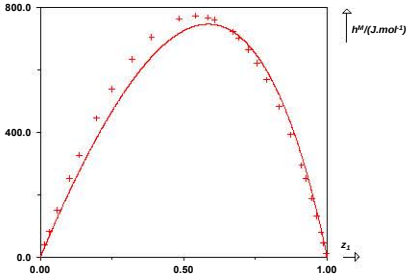
T/K = 298.15 - P/bar = 1.0132



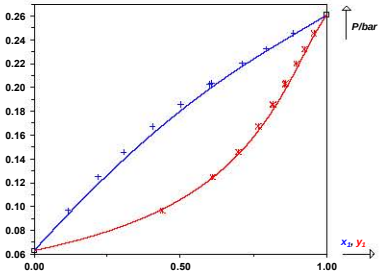

T/K = 298.15 - P/bar = 1.0132 1.0132 1.0132




T/K = 323.15 - P/bar = 1.0132




T/K = 298.15



## DICHLOROMETHANE (1) + n-PENTANE (2)

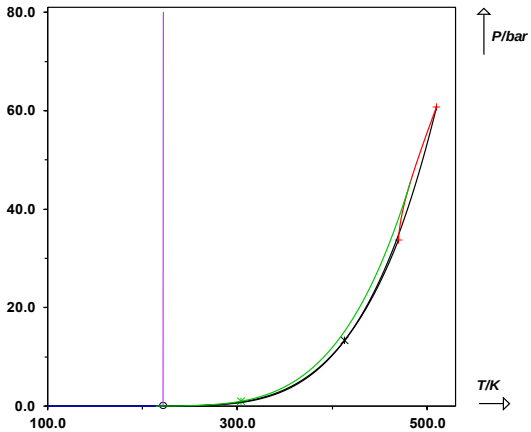
| | | |
|---|---|---|
| **CAS** | 75-09-2 | 109-66-0 |
| **InChiKey** | YMWUJEATGCHHMB-UHFFFAOYSA-N | OFBQJSOFQDEBGM-UHFFFAOYSA-N |
| **$T_c$ / K** | 510 | 469.7 |
| **$P_c$ / bar** | 60.8 | 33.7 |
| **ω** | 0.199 | 0.252 |

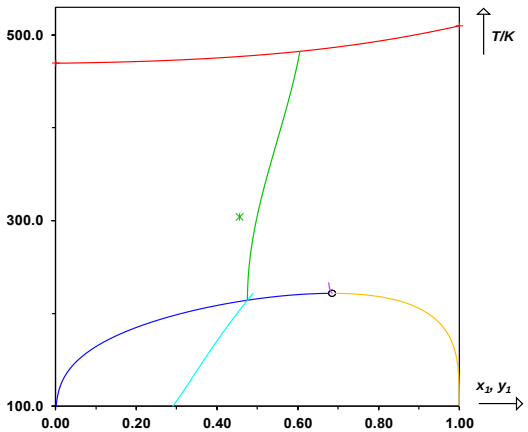
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 224
B/MPa = 380

*Deviations*
MAPE on x = 14 %
MAPE on y = 8.3 %
MAPE on $x_{az}$ = 8.9 %
MAPE on $P_{az}$ = 0.28 %
MAPE on $h^M$ = 4.4 %



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**Isothermal phase equilibrium data**

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Wang, Kun - Ying, Xu-gen - Xia, Ming-Si - Xia, Jian-Zhong - Hu, Ying, Isobaric vapor-liquid equilibria for 6-methyl-5-hepten-2-one + bis(3-methyl-2-butenyl) ether, bis(3-methyl-2-butenyl) ether + 3,3-dimethyl-2-propen-1-ol, 3,3-dimethyl-2-propen-1-ol + 6-methyl-5-hepten-2-one, and 6-methyl-5-hepten-2-one + 6-methyl-3-isopropenyl-5-hepten-2-one binary systems, Journal of Chemical & Engineering Data 1 (1989) 126-130. doi:10.1021/je00055a034

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.6330 | 0.9631 | 0.8977 |
| 0.6706 | 0.9356 | 0.8408 |
| 0.7073 | 0.8910 | 0.7620 |
| 0.7445 | 0.8394 | 0.6837 |
| 0.7701 | 0.7485 | 0.6130 |
| 0.7901 | 0.6774 | 0.5667 |
| 0.8078 | 0.5792 | 0.5102 |
| 0.8198 | 0.4439 | 0.4407 |
| 0.8131 | 0.3636 | 0.3937 |
| 0.8118 | 0.3493 | 0.3831 |
| 0.7825 | 0.2226 | 0.2954 |
| 0.7611 | 0.1552 | 0.2349 |

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**Isobaric phase equilibrium data**

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Tenn, F. G. - Missen, R. W., A study of the condensation of binary vapors of miscible liquids: Part I: The equilibrium relations, The Canadian Journal of Chemical Engineering 1 (1963) 12-14. doi:10.1002/cjce.5450410105

**P / bar = 0.9999**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 312.03 | 0.9940 | 0.9800 |
| 311.89 | 0.9910 | 0.9720 |
| 311.47 | 0.9850 | 0.9540 |
| 311.15 | 0.9800 | 0.9390 |
| 310.63 | 0.9720 | 0.9180 |
| 310.17 | 0.9620 | 0.8940 |
| 309.63 | 0.9500 | 0.8650 |
| 308.89 | 0.9300 | 0.8300 |
| 308.01 | 0.9030 | 0.7980 |
| 307.15 | 0.8720 | 0.7640 |
| 306.17 | 0.8250 | 0.7250 |
| 305.35 | 0.7700 | 0.6800 |
| 304.65 | 0.7010 | 0.6290 |
| 304.09 | 0.6160 | 0.5670 |
| 303.81 | 0.3780 | 0.4080 |
| 303.83 | 0.3740 | 0.4060 |
| 303.95 | 0.3460 | 0.3890 |
| 304.13 | 0.3060 | 0.3600 |
| 304.35 | 0.2650 | 0.3310 |
| 304.73 | 0.2180 | 0.2990 |
| 305.97 | 0.1120 | 0.1810 |
| 306.81 | 0.0710 | 0.1210 |
| 307.07 | 0.0550 | 0.1030 |
| 308.01 | 0.0170 | 0.0410 |

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**Enthalpy of mixing**

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Postigo, Miguel A. - Zurita, José L. - Soria, María L. G. De - Katz, Miguel, Excess thermodynamic properties of n-pentane + dichloromethane system at 298.15 K, Canadian Journal of Chemistry 10 (1986) 1966-1968. doi:10.1139/v86-325

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 424.00 | 0.9479 |
| 701.00 | 0.8973 |
| 1026.0 | 0.8014 |
| 1251.0 | 0.7328 |
| 1443.0 | 0.6130 |
| 1380.0 | 0.4968 |
| 1164.0 | 0.3614 |
| 774.00 | 0.2009 |
| 444.00 | 0.1035 |

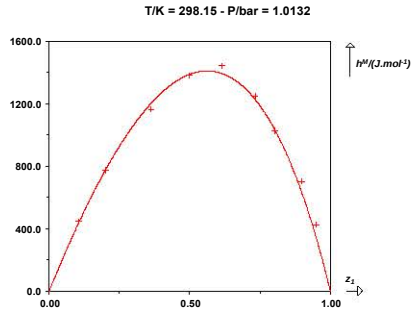
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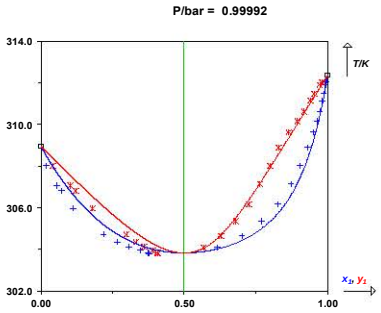
**Azeotropic point**

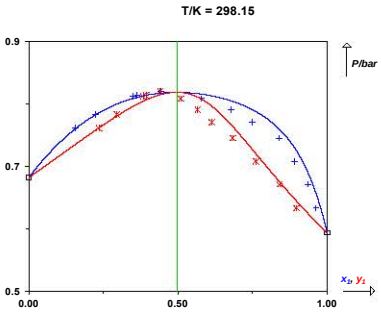
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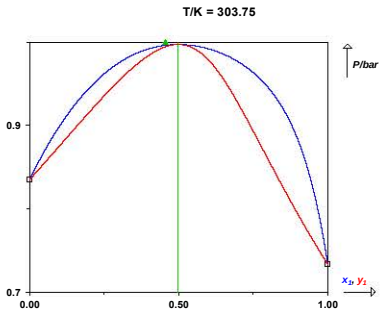
Tenn, F. G. - Missen, R. W., A study of the condensation of binary vapors of miscible liquids: Part I: The equilibrium relations, The Canadian Journal of Chemical Engineering 1 (1963) 12-14. doi:10.1002/cjce.5450410105

| T / K | P / bar | $x_1$ |
|---|---|---|
| 303.75 | 0.9999 | 0.4550 |


T/K = 298.15 - P/bar = 1.0132
1600.0
1200.0
800.0
400.0
0.0
0.00
0.50
1.00
$h^M$/(J.mol$^{-1}$)
$z_1$


P/bar = 0.99992
314.0
310.0
306.0
302.0
0.00
0.50
1.00
T/K
$x_1$, $y_1$


T/K = 298.15
0.9
0.7
0.5
0.00
0.50
1.00
P/bar
$x_1$, $y_1$


T/K = 303.75
0.9
0.7
0.00
0.50
1.00
P/bar
$x_1$, $y_1$

# H-H and E-E systems (AC = 4)

## CARBON DIOXIDE (1) + DIMETHYL ETHER (2)

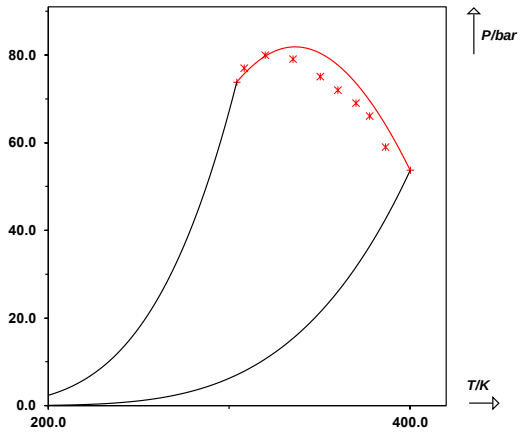
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 115-10-6 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | LCGLNKUTAGEVQW-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 400.10 |
| **$P_c$ / bar** | 73.83 | 53.70 |
| **ω** | 0.224 | 0.2 |

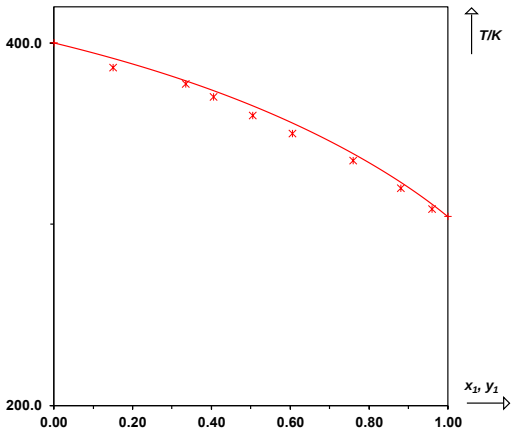
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = -42.2
B/MPa = -55.9

*Deviations*
MAPE on x = 4 %
MAPE on y = 4.8 %
MAPE on $x_c$ = 13 %
MAPE on $P_c$ = 5.2 %



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**Isothermal phase equilibrium data**

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Tsang, Charles Y. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide/dimethyl ether, Journal of Chemical & Engineering Data 2 (1981) 155-159. doi:10.1021/je00024a018

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.100 | 0.0763 | 0.3613 |
| 5.200 | 0.1270 | 0.5024 |
| 10.90 | 0.3658 | 0.7959 |
| 12.40 | 0.4286 | 0.8346 |
| 14.50 | 0.4877 | 0.8699 |
| 17.30 | 0.5722 | 0.9004 |
| 20.70 | 0.6631 | 0.9300 |
| 24.10 | 0.7445 | 0.9527 |
| 27.60 | 0.8325 | 0.9694 |
| 31.00 | 0.9149 | 0.9833 |

Tsang, Charles Y. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide/dimethyl ether, Journal of Chemical & Engineering Data 2 (1981) 155-159. doi:10.1021/je00024a018

**T / K = 288.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.80 | 0.3016 | 0.6943 |
| 17.40 | 0.3955 | 0.7793 |
| 20.70 | 0.4708 | 0.8277 |
| 25.50 | 0.5729 | 0.8733 |
| 31.00 | 0.6788 | 0.9097 |
| 35.90 | 0.7572 | 0.9345 |
| 39.30 | 0.8140 | 0.9490 |

Jonasson, Ari - Persson, Ole - Fredenslund, Aage, High Pressure Solubility of Carbon Dioxide and Carbon Monoxide in Dimethyl Ether, Journal of Chemical & Engineering Data 1 (1995) 296-300. doi:10.1021/je00017a066

**T / K = 288.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.000 | 0.0149 | 0.1733 |
| 6.000 | 0.0541 | 0.3061 |
| 7.200 | 0.1019 | 0.4312 |
| 8.600 | 0.1518 | 0.5242 |
| 10.20 | 0.2022 | 0.6047 |
| 12.40 | 0.2663 | 0.6794 |
| 14.80 | 0.3240 | 0.7365 |
| 17.70 | 0.4030 | 0.7888 |
| 21.00 | 0.4782 | 0.8322 |
| 24.60 | 0.5526 | 0.8639 |
| 28.40 | 0.6284 | 0.8937 |
| 32.70 | 0.7079 | 0.9161 |
| 37.30 | 0.7822 | 0.9391 |
| 41.20 | 0.8501 | 0.9580 |

Laursen, T. - Rasmussen, P. - Andersen, S.I., VLE and VLLE Measurements of Dimethyl Ether Containing Systems, J. Chem. Eng. Data 2 (2002) 198-202. doi:10.1021/je010154+

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 16.60 | 0.2597 | 0.6857 |
| 25.60 | 0.4546 | 0.8179 |
| 34.60 | 0.6164 | 0.8875 |
| 41.20 | 0.7261 | 0.9190 |
| 49.80 | 0.8478 | 0.9542 |

Laursen, T. - Rasmussen, P. - Andersen, S.I., VLE and VLLE Measurements of Dimethyl Ether Containing Systems, J. Chem. Eng. Data 2 (2002) 198-202. doi:10.1021/je010154+

**T / K = 308.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.00 | 0.1023 | 0.4052 |
| 17.70 | 0.1954 | 0.5821 |
| 19.30 | 0.2272 | 0.5908 |
| 25.70 | 0.3443 | 0.7292 |
| 31.10 | 0.4289 | 0.7874 |
| 38.80 | 0.5491 | 0.8476 |
| 45.80 | 0.6515 | 0.8791 |
| 50.80 | 0.7154 | 0.8986 |
| 57.30 | 0.7939 | 0.9221 |

Tsang, Charles Y. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide/dimethyl ether, Journal of Chemical & Engineering Data 2 (1981) 155-159. doi:10.1021/je00024a018

**T / K = 308.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.000 | 0.0291 | 0.1354 |
| 11.70 | 0.0891 | 0.3421 |
| 15.90 | 0.1840 | 0.4987 |
| 18.60 | 0.2433 | 0.5743 |
| 22.10 | 0.3102 | 0.6528 |
| 24.50 | 0.3535 | 0.6856 |
| 27.60 | 0.4055 | 0.7320 |
| 30.70 | 0.4568 | 0.7702 |
| 37.90 | 0.5695 | 0.8241 |
| 41.40 | 0.6141 | 0.8488 |
| 44.80 | 0.6597 | 0.8670 |

| | | |
|---|---|---|
| 48.30 | 0.7006 | 0.8857 |
| 51.70 | 0.7427 | 0.8962 |
| 60.00 | 0.8375 | 0.9257 |
| 62.60 | 0.8611 | 0.9329 |

Jonasson, Ari - Persson, Ole - Fredenslund, Aage, High Pressure Solubility of Carbon Dioxide and Carbon Monoxide in Dimethyl Ether, Journal of Chemical & Engineering Data 1 (1995) 296-300. doi:10.1021/je00017a066

**T / K = 308.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.700 | 0.0212 | 0.1230 |
| 10.60 | 0.0689 | 0.2783 |
| 12.40 | 0.1094 | 0.3828 |
| 14.60 | 0.1569 | 0.4773 |
| 17.00 | 0.2067 | 0.5468 |
| 19.60 | 0.2583 | 0.6103 |
| 22.30 | 0.3061 | 0.6633 |
| 25.00 | 0.3575 | 0.7035 |
| 28.00 | 0.4050 | 0.7465 |
| 34.30 | 0.5055 | 0.8171 |
| 37.60 | 0.5602 | 0.8417 |
| 42.80 | 0.6266 | 0.8710 |
| 45.20 | 0.6582 | 0.8808 |
| 48.00 | 0.6934 | 0.8839 |
| 51.10 | 0.7291 | 0.8922 |
| 53.90 | 0.7596 | 0.9149 |
| 56.60 | 0.7917 | 0.9186 |
| 61.20 | 0.8395 | 0.9271 |
| 62.50 | 0.8516 | 0.9294 |
| 63.30 | 0.8577 | 0.9335 |

Laursen, T. - Rasmussen, P. - Andersen, S.I., VLE and VLLE Measurements of Dimethyl Ether Containing Systems, J. Chem. Eng. Data 2 (2002) 198-202. doi:10.1021/je010154+

**T / K = 320.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 14.50 | 0.0708 | 0.2862 |
| 18.70 | 0.1412 | 0.4432 |
| 25.60 | 0.2590 | 0.5992 |
| 34.30 | 0.3880 | 0.7106 |
| 40.40 | 0.4768 | 0.7651 |
| 50.30 | 0.5932 | 0.8218 |
| 55.90 | 0.6536 | 0.8476 |
| 64.10 | 0.7414 | 0.8684 |
| 69.70 | 0.7869 | 0.8769 |
| 73.20 | 0.8140 | 0.8886 |

Tsang, Charles Y. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide/dimethyl ether, Journal of Chemical & Engineering Data 2 (1981) 155-159. doi:10.1021/je00024a018

**T / K = 335.17**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 17.90 | 0.0448 | 0.1563 | |
| 20.00 | 0.0756 | 0.2404 | |
| 23.60 | 0.1254 | 0.3588 | |
| 28.30 | 0.1930 | 0.4663 | |
| 32.50 | 0.2499 | 0.5298 | |
| 38.60 | 0.3286 | 0.6033 | |
| 48.30 | 0.4361 | 0.6780 | |
| 55.90 | 0.5216 | 0.7126 | |
| 65.40 | 0.6130 | 0.7525 | |
| 72.40 | 0.6845 | 0.7710 | |
| 75.80 | 0.7126 | 0.7720 | |
| 79.30 | 0.7364 | 0.7701 | |
| 79.00 | 0.7600 | 0.7600 | CRIT |

Tsang, Charles Y. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide/dimethyl ether, Journal of Chemical & Engineering Data 2 (1981) 155-159. doi:10.1021/je00024a018

**T / K = 350.20**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 21.70 | 0.0112 | 0.0340 | |
| 23.40 | 0.0312 | 0.0895 | |
| 25.50 | 0.0553 | 0.1611 | |
| 27.60 | 0.0797 | 0.2143 | |
| 31.40 | 0.1231 | 0.3074 | |
| 35.70 | 0.1722 | 0.3879 | |
| 41.50 | 0.2410 | 0.4652 | |
| 46.50 | 0.2955 | 0.5065 | |
| 57.90 | 0.4137 | 0.5916 | |
| 62.40 | 0.4508 | 0.6110 | |
| 66.90 | 0.4900 | 0.6272 | |
| 69.10 | 0.5168 | 0.6342 | |
| 75.00 | 0.6050 | 0.6050 | CRIT |

Tsang, Charles Y. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide/dimethyl ether, Journal of Chemical & Engineering Data 2 (1981) 155-159. doi:10.1021/je00024a018

**T / K = 360.07**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 26.10 | 0.0104 | 0.0313 |
| 27.90 | 0.0296 | 0.0809 |
| 29.90 | 0.0502 | 0.1336 |
| 32.50 | 0.0787 | 0.1952 |

| | | | |
|---|---|---|---|
| 35.30 | 0.1082 | 0.2528 | |
| 45.20 | 0.2135 | 0.3942 | |
| 49.30 | 0.2531 | 0.4320 | |
| 52.50 | 0.2850 | 0.4570 | |
| 56.90 | 0.3269 | 0.4878 | |
| 60.90 | 0.3652 | 0.5040 | |
| 65.50 | 0.4093 | 0.5273 | |
| 69.00 | 0.4434 | 0.5351 | |
| 71.10 | 0.4734 | 0.5283 | |
| 72.00 | 0.5050 | 0.5050 | CRIT |

Tsang, Charles Y. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide/dimethyl ether, Journal of Chemical & Engineering Data 2 (1981) 155-159. doi:10.1021/je00024a018

**T / K = 370.13**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 31.90 | 0.0134 | 0.0317 | |
| 33.80 | 0.0317 | 0.0774 | |
| 36.40 | 0.0564 | 0.1304 | |
| 40.30 | 0.0923 | 0.1975 | |
| 43.40 | 0.1226 | 0.2462 | |
| 53.70 | 0.2268 | 0.3611 | |
| 55.20 | 0.2376 | 0.3724 | |
| 56.80 | 0.2546 | 0.3835 | |
| 66.10 | 0.3460 | 0.4276 | |
| 69.00 | 0.4050 | 0.4050 | CRIT |

Tsang, Charles Y. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide/dimethyl ether, Journal of Chemical & Engineering Data 2 (1981) 155-159. doi:10.1021/je00024a018

**T / K = 377.57**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 35.90 | 0.0101 | 0.0187 | |
| 41.00 | 0.0523 | 0.1109 | |
| 42.70 | 0.0679 | 0.1358 | |
| 45.50 | 0.0932 | 0.1798 | |
| 48.30 | 0.1177 | 0.2127 | |
| 51.00 | 0.1436 | 0.2429 | |
| 53.80 | 0.1692 | 0.2729 | |
| 56.90 | 0.1996 | 0.2972 | |
| 60.00 | 0.2311 | 0.3164 | |
| 63.70 | 0.2765 | 0.3288 | |
| 66.00 | 0.3350 | 0.3350 | CRIT |

Tsang, Charles Y. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide/dimethyl ether, Journal of Chemical & Engineering Data 2 (1981) 155-159. doi:10.1021/je00024a018

**T / K = 386.56**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 41.90 | 0.0060 | 0.0102 | |
| 42.90 | 0.0146 | 0.0273 | |
| 44.10 | 0.0251 | 0.0457 | |
| 47.30 | 0.0508 | 0.0832 | |
| 49.30 | 0.0684 | 0.1122 | |
| 51.70 | 0.0888 | 0.1388 | |
| 53.80 | 0.1064 | 0.1589 | |
| 55.90 | 0.1243 | 0.1744 | |
| 59.00 | 0.1500 | 0.1500 | CRIT |

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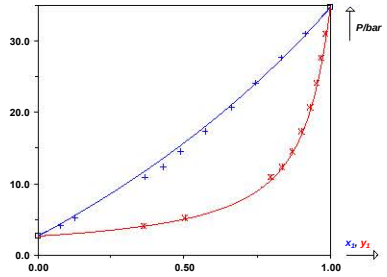
**Critical point**

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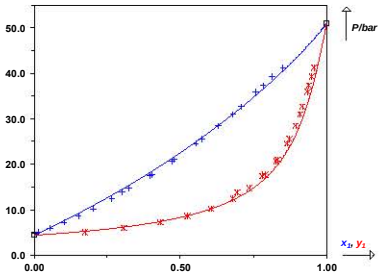
Tsang, Charles Y. - Streett, William B., Vapor-liquid equilibrium in the system carbon dioxide/dimethyl ether, Journal of Chemical & Engineering Data 2 (1981) 155-159. doi:10.1021/je00024a018

| T / K | P / bar | $x_1$ |
|---|---|---|
| 308.45 | 77.00 | 0.9600 |
| 320.06 | 80.00 | 0.8800 |

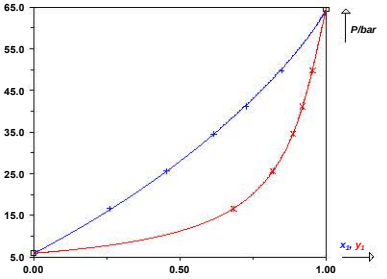
T/K = 273.15



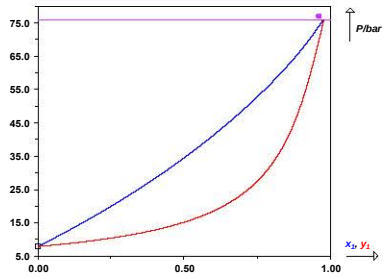

T/K = 288.20



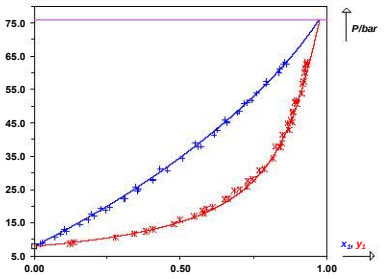

T/K = 298.15



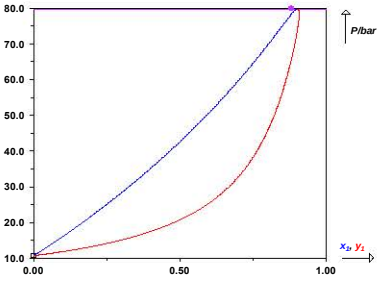

T/K = 308.45



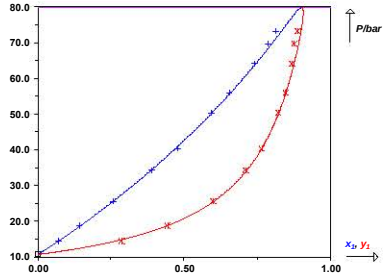

T/K = 308.65



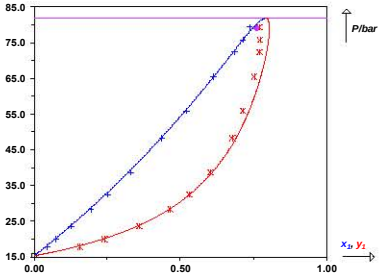

T/K = 320.06



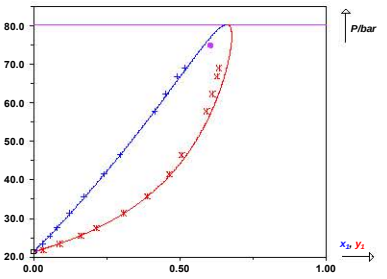

T/K = 320.15



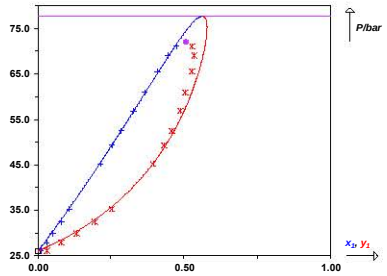

T/K = 335.17



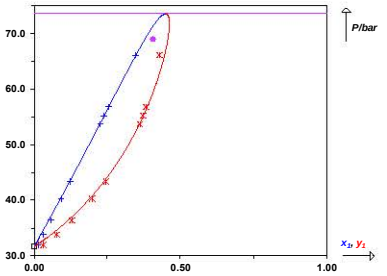

T/K = 350.20



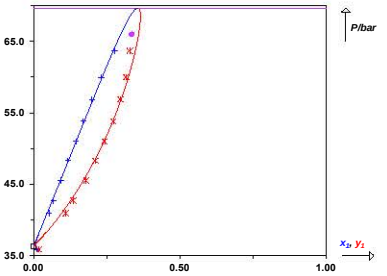

T/K = 360.07



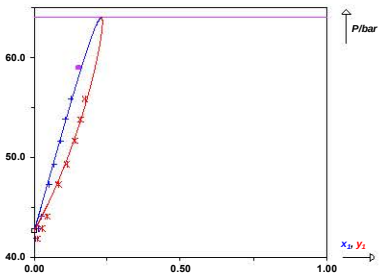

T/K = 370.13




T/K = 377.57




T/K = 386.56



## CARBON DIOXIDE (1) + HYDROGEN SULFIDE (2)

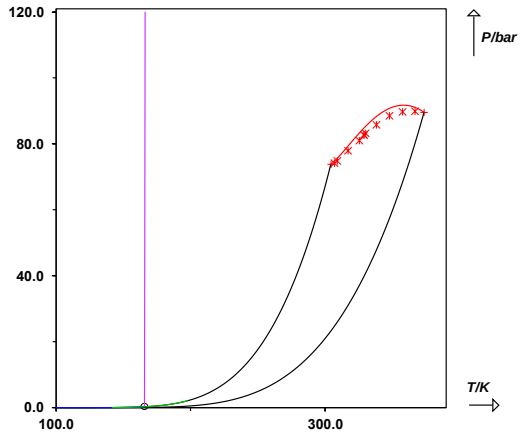
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 04/06/7783 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | RWSOTUBLDIXVET-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 373.53 |
| **$P_c$ / bar** | 73.83 | 89.63 |
| **ω** | 0.224 | 0.094 |

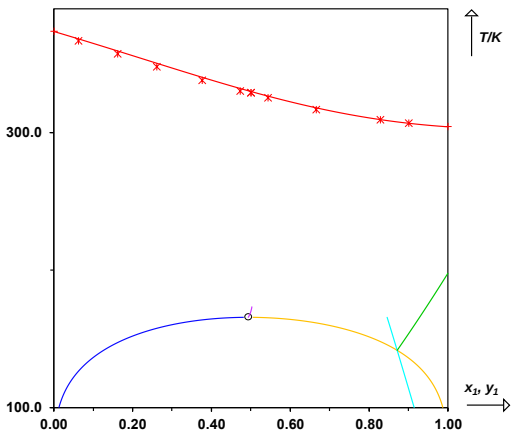
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 408
B/MPa = 600

*Deviations*
MAPE on x = 5.2 %
MAPE on y = 2.9 %
MAPE on $x_c$ = 5.3 %
MAPE on $P_c$ = 2.1 %



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**Isothermal phase equilibrium data**

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Chapoy, Antonin - Coquelet, Christophe - Liu, Haifan - Valtz, Alain - Tohidi, Bahman, Vapour–liquid equilibrium data for the hydrogen sulphide (H2S)+carbon dioxide (CO2) system at temperatures from 258 to 313K, Fluid Phase Equilibria (2013) 223-228. doi:10.1016/j.fluid.2013.07.050

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.75 | 0.0541 | 0.2346 |
| 17.22 | 0.1260 | 0.4006 |
| 22.46 | 0.2920 | 0.5878 |
| 24.84 | 0.3959 | 0.6506 |
| 28.99 | 0.5897 | 0.7522 |

Ferrell, J.K. - Rousseau, R.W. - Bass, D.G., The solubility of acid gases in methanol (1979) 1-40.

**T / K = 293.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.27 | 0.0200 | 0.1310 |
| 25.33 | 0.0900 | 0.3150 |
| 30.40 | 0.1790 | 0.4500 |
| 35.46 | 0.2850 | 0.5430 |
| 40.53 | 0.4200 | 0.6300 |
| 45.60 | 0.5630 | 0.7100 |
| 50.66 | 0.7390 | 0.8110 |
| 52.69 | 0.8200 | 0.8700 |

Chapoy, Antonin - Coquelet, Christophe - Liu, Haifan - Valtz, Alain - Tohidi, Bahman, Vapour–liquid equilibrium data for the hydrogen sulphide (H2S)+carbon dioxide (CO2) system at temperatures from 258 to 313K, Fluid Phase Equilibria (2013) 223-228. doi:10.1016/j.fluid.2013.07.050

**T / K = 313.02**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.34 | 0.0489 | 0.1482 |
| 39.14 | 0.0983 | 0.2483 |
| 44.72 | 0.1655 | 0.3560 |
| 54.75 | 0.3028 | 0.5008 |

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**Isobaric phase equilibrium data**

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Sobocinski, D. P. - Kurata, Fred, Heterogeneous phase equilibria of the hydrogen sulfide–carbon dioxide system, AIChE Journal 4 (1959) 545-551. doi:10.1002/aic.690050425

**P / bar = 6.895**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 224.82 | 0.7180 | 0.8980 |
| 227.59 | 0.4990 | 0.7960 |
| 233.15 | 0.2860 | 0.6710 |
| 238.71 | 0.1500 | 0.5500 |
| 244.26 | 0.0850 | 0.4280 |
| 249.82 | 0.0440 | 0.3000 |
| 255.37 | 0.0160 | 0.1600 |

Sobocinski, D. P. - Kurata, Fred, Heterogeneous phase equilibria of the hydrogen sulfide–carbon dioxide system, AIChE Journal 4 (1959) 545-551. doi:10.1002/aic.690050425

**P / bar = 13.79**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 243.15 | 0.8590 | 0.9250 |
| 244.26 | 0.7650 | 0.8800 |
| 249.82 | 0.4530 | 0.7410 |
| 255.37 | 0.2800 | 0.6310 |
| 260.93 | 0.1780 | 0.5250 |
| 266.48 | 0.1130 | 0.4100 |
| 272.04 | 0.0690 | 0.2770 |
| 277.59 | 0.0330 | 0.1450 |
| 280.37 | 0.0170 | 0.0780 |

Sobocinski, D. P. - Kurata, Fred, Heterogeneous phase equilibria of the hydrogen sulfide–carbon dioxide system, AIChE Journal 4 (1959) 545-551. doi:10.1002/aic.690050425

**P / bar = 20.68**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 294.26 | 0.0220 | 0.1060 |
| 288.71 | 0.0520 | 0.2300 |
| 283.15 | 0.0930 | 0.3490 |
| 277.59 | 0.1500 | 0.4600 |
| 272.04 | 0.2480 | 0.5640 |
| 266.48 | 0.3700 | 0.6600 |
| 260.93 | 0.5510 | 0.7590 |
| 258.15 | 0.6990 | 0.8250 |
| 256.48 | 0.8050 | 0.8810 |

Bierlein, James A. - Kay, Webster B., Phase-Equilibrium Properties of System Carbon Dioxide-Hydrogen Sulfide, Industrial & Engineering Chemistry 3 (1953) 618-624. doi:10.1021/ie50519a043

**P / bar = 40.53**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 303.15 | 0.2320 | 0.4670 |
| 298.15 | 0.3130 | 0.5460 |
| 293.15 | 0.4200 | 0.6300 |
| 288.15 | 0.5630 | 0.7200 |

| | | |
|---|---|---|
| 283.15 | 0.7560 | 0.8350 |
| 282.15 | 0.7970 | 0.8620 |
| 281.15 | 0.8520 | 0.8990 |
| 280.15 | 0.9160 | 0.9420 |

Bierlein, James A. - Kay, Webster B., Phase-Equilibrium Properties of System Carbon Dioxide-Hydrogen Sulfide, Industrial & Engineering Chemistry 3 (1953) 618-624. doi:10.1021/ie50519a043

**P / bar = 40.53**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 323.15 | 0.0350 | 0.1240 |
| 318.15 | 0.0740 | 0.2160 |
| 313.15 | 0.1170 | 0.3000 |
| 308.15 | 0.1680 | 0.3820 |

Bierlein, James A. - Kay, Webster B., Phase-Equilibrium Properties of System Carbon Dioxide-Hydrogen Sulfide, Industrial & Engineering Chemistry 3 (1953) 618-624. doi:10.1021/ie50519a043

**P / bar = 50.66**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 303.15 | 0.4380 | 0.6140 |
| 298.15 | 0.5720 | 0.7010 |
| 293.15 | 0.7390 | 0.8110 |
| 290.15 | 0.8740 | 0.9080 |
| 289.15 | 0.9320 | 0.9500 |

Bierlein, James A. - Kay, Webster B., Phase-Equilibrium Properties of System Carbon Dioxide-Hydrogen Sulfide, Industrial & Engineering Chemistry 3 (1953) 618-624. doi:10.1021/ie50519a043

**P / bar = 50.66**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 338.15 | 0.0100 | 0.0450 |
| 333.15 | 0.0480 | 0.1320 |
| 328.15 | 0.0890 | 0.2160 |
| 323.15 | 0.1350 | 0.2950 |
| 318.15 | 0.1900 | 0.3740 |
| 313.15 | 0.2550 | 0.4550 |
| 308.15 | 0.3360 | 0.5340 |

Bierlein, James A. - Kay, Webster B., Phase-Equilibrium Properties of System Carbon Dioxide-Hydrogen Sulfide, Industrial & Engineering Chemistry 3 (1953) 618-624. doi:10.1021/ie50519a043

**P / bar = 60.80**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 303.15 | 0.6870 | 0.7590 |
| 298.15 | 0.8730 | 0.9010 |
| 297.15 | 0.9220 | 0.9380 |

Bierlein, James A. - Kay, Webster B., Phase-Equilibrium Properties of System Carbon Dioxide-Hydrogen Sulfide, Industrial & Engineering Chemistry 3 (1953) 618-624. doi:10.1021/ie50519a043

**P / bar = 60.80**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 348.15 | 0.0090 | 0.0350 |
| 343.15 | 0.0500 | 0.1220 |
| 338.15 | 0.0920 | 0.1940 |
| 333.15 | 0.1370 | 0.2710 |
| 328.15 | 0.1900 | 0.3450 |
| 323.15 | 0.2560 | 0.4230 |
| 318.15 | 0.3300 | 0.4960 |
| 313.15 | 0.4250 | 0.5830 |
| 308.15 | 0.5400 | 0.6620 |

Bierlein, James A. - Kay, Webster B., Phase-Equilibrium Properties of System Carbon Dioxide-Hydrogen Sulfide, Industrial & Engineering Chemistry 3 (1953) 618-624. doi:10.1021/ie50519a043

**P / bar = 81.06**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 363.15 | 0.0250 | 0.0500 |
| 358.15 | 0.0700 | 0.1270 |
| 353.15 | 0.1160 | 0.1760 |
| 348.15 | 0.1670 | 0.2400 |
| 343.15 | 0.2250 | 0.3080 |
| 338.15 | 0.2920 | 0.3730 |
| 333.15 | 0.3660 | 0.4380 |
| 328.15 | 0.4560 | 0.5080 |

Sobocinski, D. P. - Kurata, Fred, Heterogeneous phase equilibria of the hydrogen sulfide–carbon dioxide system, AIChE Journal 4 (1959) 545-551. doi:10.1002/aic.690050425

**P / bar = 82.74**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 363.71 | 0.0380 | 0.0610 |
| 360.93 | 0.0620 | 0.0990 |
| 355.37 | 0.1120 | 0.1700 |
| 349.82 | 0.1650 | 0.2400 |
| 344.26 | 0.2260 | 0.3160 |
| 338.71 | 0.3040 | 0.3900 |
| 333.15 | 0.4050 | 0.4550 |
| 330.37 | 0.4650 | 0.4850 |

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**Critical point**

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Bierlein, James A. - Kay, Webster B., Phase-Equilibrium Properties of System Carbon Dioxide-Hydrogen Sulfide, Industrial & Engineering Chemistry 3 (1953) 618-624. doi:10.1021/ie50519a043

| T / K | P / bar | $x_1$ |
|---|---|---|
| 366.65 | 89.97 | 0.0630 |
| 357.31 | 89.77 | 0.1614 |
| 347.63 | 88.52 | 0.2608 |
| 337.89 | 85.86 | 0.3759 |
| 330.13 | 83.21 | 0.4728 |
| 316.87 | 77.85 | 0.6659 |
| 309.11 | 74.83 | 0.8292 |
| 306.68 | 74.16 | 0.9009 |

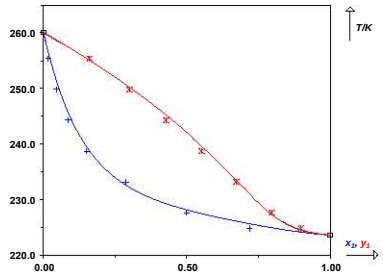
Sobocinski, D. P. - Kurata, Fred, Heterogeneous phase equilibria of the hydrogen sulfide–carbon dioxide system, AIChE Journal 4 (1959) 545-551. doi:10.1002/aic.690050425

| T / K | P / bar | $x_1$ |
|---|---|---|
| 328.82 | 82.74 | 0.5000 |

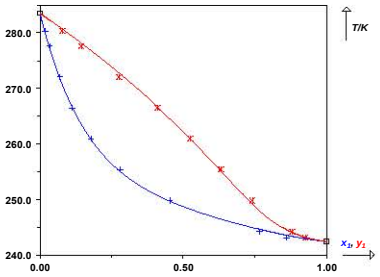
Bierlein, James A. - Kay, Webster B., Phase-Equilibrium Properties of System Carbon Dioxide-Hydrogen Sulfide, Industrial & Engineering Chemistry 3 (1953) 618-624. doi:10.1021/ie50519a043

| T / K | P / bar | $x_1$ |
|---|---|---|
| 325.23 | 81.06 | 0.5440 |

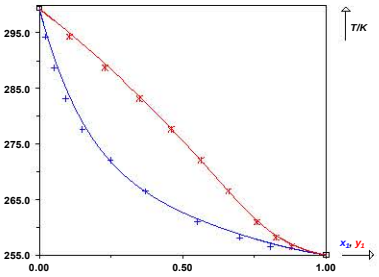
P/bar = 6.89480



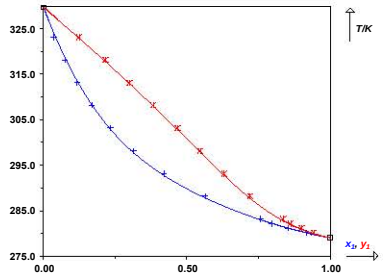

P/bar = 13.79000



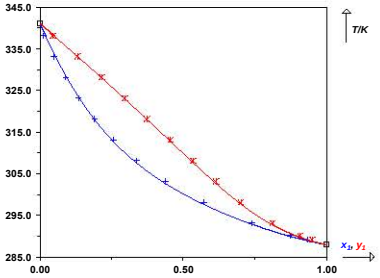

P/bar = 20.68400



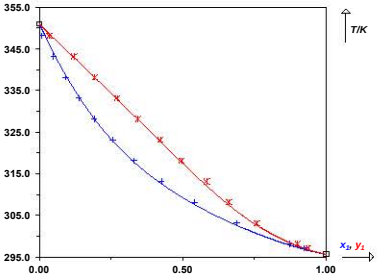

P/bar = 40.53000



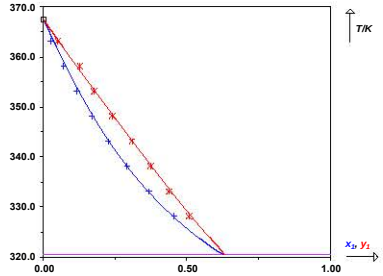

P/bar = 50.66200



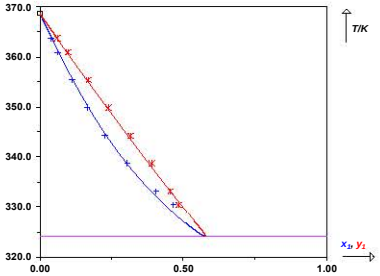

P/bar = 60.79500



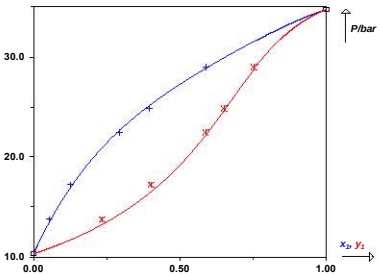

P/bar = 81.06000



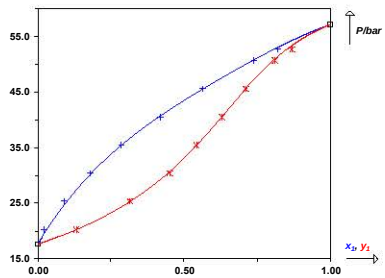

P/bar = 82.73800



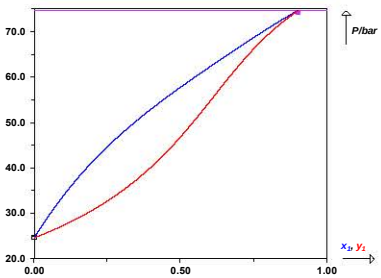

T/K = 273.15



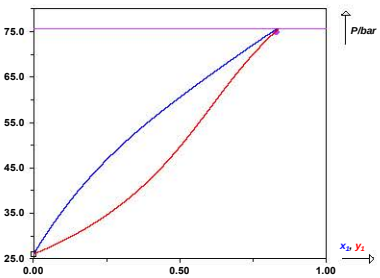

T/K = 293.00



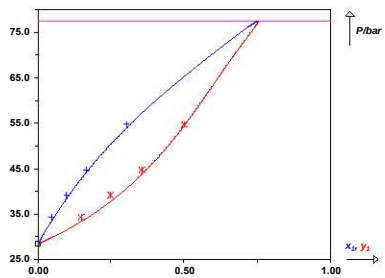

T/K = 306.68



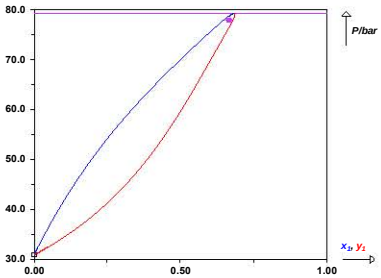

T/K = 309.11



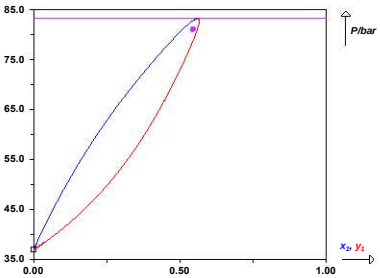

T/K = 313.02

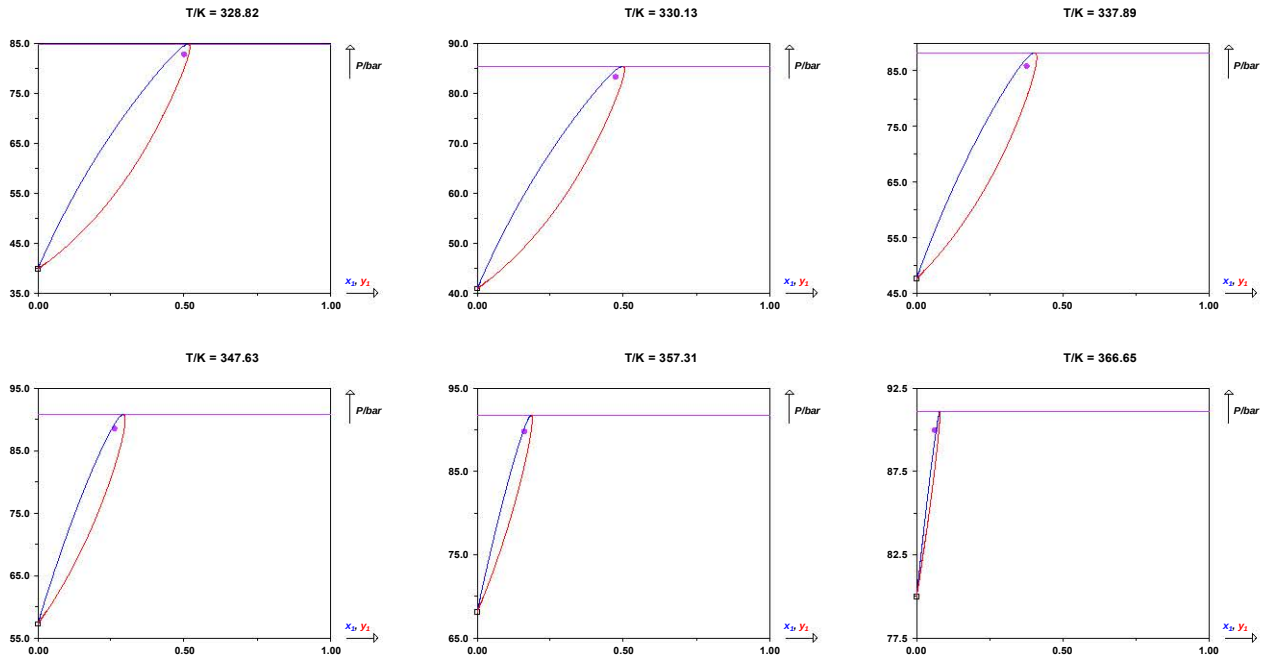



T/K = 316.87




T/K = 325.23




T/K = 328.82
P/bar
85.0
75.0
65.0
55.0
45.0
35.0
0.00
0.50
1.00
$x_1, y_1$
T/K = 330.13
P/bar
90.0
80.0
70.0
60.0
50.0
40.0
0.00
0.50
1.00
$x_1, y_1$
T/K = 337.89
P/bar
85.0
75.0
65.0
55.0
45.0
0.00
0.50
1.00
$x_1, y_1$
T/K = 347.63
P/bar
95.0
85.0
75.0
65.0
55.0
0.00
0.50
1.00
$x_1, y_1$
T/K = 357.31
P/bar
95.0
85.0
75.0
65.0
0.00
0.50
1.00
$x_1, y_1$
T/K = 366.65
P/bar
92.5
87.5
82.5
77.5
0.00
0.50
1.00
$x_1, y_1$

## CARBON DIOXIDE (1) + ETHYL ACETATE (2)

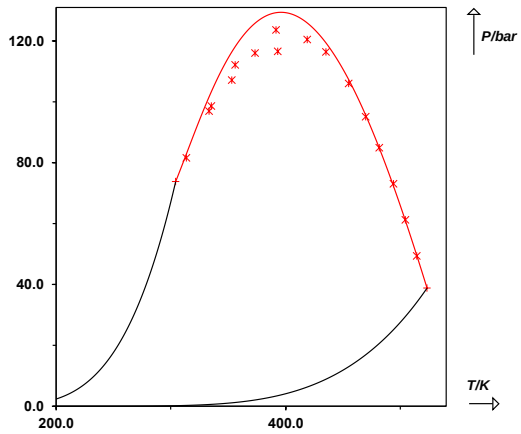
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 141-78-6 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | XEKOWRVHYACXOJ-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 523.30 |
| **$P_c$ / bar** | 73.83 | 38.80 |
| **ω** | 0.224 | 0.366 |

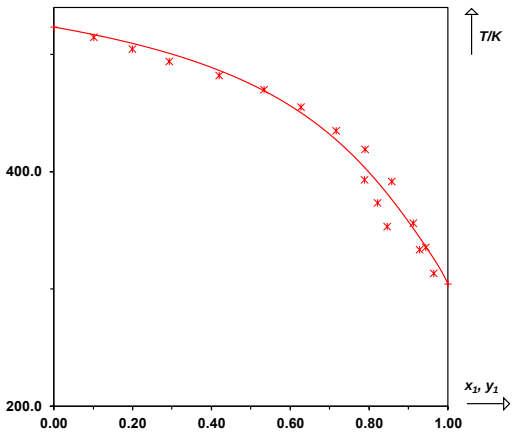
Unknown ideality

PPR78 results

*Parameters*
A/MPa = -4.39
B/MPa = 23.8

*Deviations*
MAPE on x = 32 %
MAPE on y = 23 %
MAPE on $x_c$ = 13 %
MAPE on $P_c$ = 3.7 %
MAPE on $h^M$ = 16 %



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**Isothermal phase equilibrium data**

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da Silva, Marta Vázquez - Barbosa, Domingos - Ferreira, Palmira O - Mendonça, João, High pressure phase equilibrium data for the systems carbon dioxide/ethyl acetate and carbon dioxide/isoamyl acetate at 295.2, 303.2 and 313.2 K, Fluid Phase Equilibria 1-2 (2000) 19-33. doi:10.1016/S0378-3812(00)00439-8

**T / K = 295.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 19.50 | 0.7270 | 0.9970 |
| 20.80 | 0.7410 | 0.9960 |
| 24.40 | 0.7780 | 0.9980 |
| 29.50 | 0.8170 | 0.9960 |
| 32.80 | 0.8510 | 0.9980 |

Wagner, Zdeněk - Pavlíček, Jan, Vapour-liquid equilibrium in the carbon dioxide—ethyl acetate system at high pressure, Fluid Phase Equilibria (1994) 119-126. doi:10.1016/0378-3812(94)85010-0

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.47 | 0.4500 | 0.9878 |
| 20.66 | 0.4464 | 0.9849 |
| 29.64 | 0.5733 | 0.9900 |
| 30.53 | 0.5815 | 0.9894 |
| 39.07 | 0.6727 | 0.9898 |
| 39.29 | 0.6739 | 0.9897 |
| 49.64 | 0.7605 | 0.9915 |
| 52.25 | 0.7771 | 0.9911 |
| 58.00 | 0.8159 | 0.9884 |
| 61.73 | 0.8401 | 0.9922 |
| 66.00 | 0.8634 | 0.9915 |
| 73.55 | 0.9052 | 0.9893 |
| 77.61 | 0.9238 | 0.9900 |
| 80.24 | 0.9347 | 0.9903 |
| 83.69 | 0.9473 | 0.9889 |
| 89.07 | 0.9684 | 0.9866 |
| 90.20 | 0.9752 | 0.9826 |

Tian, Yi-Ling - Zhu, Hu-Gang - Xue, Yuan - Liu, Zhi-Hua - Yin, Liang, Vapor−Liquid Equilibria of the Carbon Dioxide + Ethyl Propanoate and Carbon Dioxide + Ethyl Acetate Systems at Pressure from 2.96 MPa to 11.79 MPa and Temperature from 313 K to 393 K, Journal of Chemical & Engineering Data 6 (2004) 1554-1559. doi:10.1021/je034224j

**T / K = 353.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 39.60 | 0.5532 | 0.9802 |
| 50.60 | 0.5767 | 0.9783 |
| 62.70 | 0.6075 | 0.9739 |
| 74.70 | 0.6270 | 0.9678 |
| 84.70 | 0.6668 | 0.9661 |
| 94.70 | 0.7587 | 0.9560 |

Tian, Yi-Ling - Zhu, Hu-Gang - Xue, Yuan - Liu, Zhi-Hua - Yin, Liang, Vapor−Liquid Equilibria of the Carbon Dioxide + Ethyl Propanoate and Carbon Dioxide + Ethyl Acetate Systems at Pressure from 2.96 MPa to 11.79 MPa and Temperature from 313 K to 393 K, Journal of Chemical & Engineering Data 6 (2004) 1554-1559. doi:10.1021/je034224j

**T / K = 373.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 56.90 | 0.4697 | 0.9641 |
| 64.60 | 0.5001 | 0.9612 |
| 79.60 | 0.5505 | 0.9555 |
| 94.70 | 0.6046 | 0.9440 |
| 105.70 | 0.6715 | 0.9239 |
| 113.70 | 0.7259 | 0.9135 |

Tian, Yi-Ling - Zhu, Hu-Gang - Xue, Yuan - Liu, Zhi-Hua - Yin, Liang, Vapor−Liquid Equilibria of the Carbon Dioxide + Ethyl Propanoate and Carbon Dioxide + Ethyl Acetate Systems at Pressure from 2.96 MPa to 11.79 MPa and Temperature from 313 K to 393 K, Journal of Chemical & Engineering Data 6 (2004) 1554-1559. doi:10.1021/je034224j

**T / K = 393.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 50.60 | 0.4550 | 0.9516 |
| 54.60 | 0.4831 | 0.9419 |
| 69.70 | 0.5129 | 0.9321 |
| 84.80 | 0.5450 | 0.9173 |
| 99.70 | 0.5744 | 0.8956 |
| 114.70 | 0.6237 | 0.8568 |
| 119.70 | 0.6629 | 0.8466 |

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**Enthalpy of mixing**

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Zahran, Fouad - Pando, Concepción - Renuncio, Juan A.R. - Cabañas, Albertina, Excess molar enthalpies for mixtures of supercritical CO2 and ethyl acetate and their role in supercritical fluid applications, The Journal of Chemical Thermodynamics (2012) 59-64. doi:10.1016/j.jct.2012.02.034

**T / K = 313.15**

**P / bar = 90.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -453.00 | 0.0870 |

| | |
|---|---|
| -947.00 | 0.1720 |
| -1361.0 | 0.2560 |
| -1924.0 | 0.3810 |
| -2196.0 | 0.4620 |
| -2524.0 | 0.5420 |
| -2861.0 | 0.6600 |
| -3042.0 | 0.7370 |
| -2983.0 | 0.8140 |
| -2660.0 | 0.8890 |
| -2262.0 | 0.9260 |
| -1584.0 | 0.9630 |

Zahran, Fouad - Pando, Concepción - Renuncio, Juan A.R. - Cabañas, Albertina, Excess molar enthalpies for mixtures of supercritical CO2 and ethyl acetate and their role in supercritical fluid applications, The Journal of Chemical Thermodynamics (2012) 59-64. doi:10.1016/j.jct.2012.02.034

**T / K = 313.15**

**P / bar = 120.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -419.00 | 0.1230 |
| -776.00 | 0.2350 |
| -1015.0 | 0.3380 |
| -1166.0 | 0.4320 |
| -1288.0 | 0.5190 |
| -1368.0 | 0.5990 |
| -1403.0 | 0.6730 |
| -1349.0 | 0.7420 |
| -1265.0 | 0.8060 |
| -1099.0 | 0.8660 |
| -669.00 | 0.9490 |
| -371.00 | 0.9750 |

Zahran, Fouad - Pando, Concepción - Renuncio, Juan A.R. - Cabañas, Albertina, Excess molar enthalpies for mixtures of supercritical CO2 and ethyl acetate and their role in supercritical fluid applications, The Journal of Chemical Thermodynamics (2012) 59-64. doi:10.1016/j.jct.2012.02.034

**T / K = 313.15**

**P / bar = 150.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -362.00 | 0.1320 |
| -632.00 | 0.2500 |
| -871.00 | 0.3560 |
| -1013.0 | 0.4520 |
| -1148.0 | 0.5390 |
| -1194.0 | 0.6180 |
| -1151.0 | 0.7240 |
| -1023.0 | 0.7880 |
| -948.00 | 0.8180 |
| -762.00 | 0.8750 |
| -518.00 | 0.9270 |
| -375.00 | 0.9530 |

Zahran, Fouad - Pando, Concepción - Renuncio, Juan A.R. - Cabañas, Albertina, Excess molar enthalpies for mixtures of supercritical CO2 and ethyl acetate and their role in supercritical fluid applications, The Journal of Chemical Thermodynamics (2012) 59-64. doi:10.1016/j.jct.2012.02.034

**T / K = 313.15**

**P / bar = 180.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -258.00 | 0.0710 |
| -424.00 | 0.1370 |
| -693.00 | 0.2590 |
| -843.00 | 0.3670 |
| -938.00 | 0.4630 |
| -990.00 | 0.5500 |
| -1005.0 | 0.6290 |
| -942.00 | 0.7000 |
| -754.00 | 0.8250 |
| -607.00 | 0.8800 |
| -414.00 | 0.9310 |
| -312.00 | 0.9550 |

Zahran, Fouad - Pando, Concepción - Renuncio, Juan A.R. - Cabañas, Albertina, Excess molar enthalpies for mixtures of supercritical CO2 and ethyl acetate and their role in supercritical fluid applications, The Journal of Chemical Thermodynamics (2012) 59-64. doi:10.1016/j.jct.2012.02.034

**T / K = 323.15**

**P / bar = 90.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -881.00 | 0.0870 |
| -1586.0 | 0.1720 |
| -2202.0 | 0.2560 |
| -3338.0 | 0.4210 |
| -3724.0 | 0.5020 |
| -4136.0 | 0.5820 |
| -4455.0 | 0.6600 |
| -4489.0 | 0.7370 |
| -4313.0 | 0.8140 |
| -3349.0 | 0.8890 |
| -2290.0 | 0.9260 |
| -1153.0 | 0.9630 |

Zahran, Fouad - Pando, Concepción - Renuncio, Juan A.R. - Cabañas, Albertina, Excess molar enthalpies for mixtures of supercritical CO2 and ethyl acetate and their role in supercritical fluid applications, The Journal of Chemical Thermodynamics (2012) 59-64. doi:10.1016/j.jct.2012.02.034

**T / K = 323.15**

**P / bar = 120.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -640.00 | 0.1230 |
| -1136.0 | 0.2350 |
| -1486.0 | 0.3380 |
| -1737.0 | 0.4320 |
| -1986.0 | 0.5590 |
| -2047.0 | 0.6360 |
| -2044.0 | 0.7420 |
| -1902.0 | 0.8060 |
| -1691.0 | 0.8660 |
| -1373.0 | 0.9220 |
| -1133.0 | 0.9490 |
| -651.00 | 0.9750 |

Zahran, Fouad - Pando, Concepción - Renuncio, Juan A.R. - Cabañas, Albertina, Excess molar enthalpies for mixtures of supercritical CO2 and ethyl acetate and their role in supercritical fluid applications, The Journal of Chemical Thermodynamics (2012) 59-64. doi:10.1016/j.jct.2012.02.034

**T / K = 323.15**

**P / bar = 150.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -454.00 | 0.1320 |
| -730.00 | 0.2500 |
| -987.00 | 0.3690 |
| -1141.0 | 0.4520 |
| -1281.0 | 0.5390 |
| -1357.0 | 0.6550 |
| -1341.0 | 0.7240 |
| -1315.0 | 0.7570 |
| -1192.0 | 0.8800 |
| -1046.0 | 0.8750 |
| -734.00 | 0.9270 |
| -553.00 | 0.9530 |

Zahran, Fouad - Pando, Concepción - Renuncio, Juan A.R. - Cabañas, Albertina, Excess molar enthalpies for mixtures of supercritical CO2 and ethyl acetate and their role in supercritical fluid applications, The Journal of Chemical Thermodynamics (2012) 59-64. doi:10.1016/j.jct.2012.02.034

**T / K = 323.15**

**P / bar = 180.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -282.00 | 0.0710 |
| -456.00 | 0.1370 |
| -713.00 | 0.2590 |
| -899.00 | 0.3670 |
| -1008.0 | 0.4630 |
| -1090.0 | 0.5500 |
| -1147.0 | 0.6290 |
| -1117.0 | 0.7000 |
| -1005.0 | 0.7960 |
| -843.00 | 0.8530 |
| -768.00 | 0.8800 |
| -518.00 | 0.9310 |
| -387.00 | 0.9550 |

Zahran, Fouad - Pando, Concepción - Renuncio, Juan A.R. - Cabañas, Albertina, Excess molar enthalpies for mixtures of supercritical CO2 and ethyl acetate and their role in supercritical fluid applications, The Journal of Chemical Thermodynamics (2012) 59-64. doi:10.1016/j.jct.2012.02.034

**T / K = 333.15**

**P / bar = 90.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -863.00 | 0.0870 |
| -1798.0 | 0.1720 |
| -2551.0 | 0.2570 |
| -3119.0 | 0.3390 |
| -3609.0 | 0.4210 |
| -4148.0 | 0.5420 |
| -4356.0 | 0.6600 |
| -4407.0 | 0.7370 |
| -4150.0 | 0.8140 |
| -3388.0 | 0.8890 |
| -2228.0 | 0.9260 |
| -1077.0 | 0.9630 |

Zahran, Fouad - Pando, Concepción - Renuncio, Juan A.R. - Cabañas, Albertina, Excess molar enthalpies for mixtures of supercritical CO2 and ethyl acetate and their role in supercritical fluid applications, The Journal of Chemical Thermodynamics (2012) 59-64. doi:10.1016/j.jct.2012.02.034

**T / K = 333.15**

**P / bar = 150.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -565.00 | 0.1320 |
| -949.00 | 0.2500 |
| -1244.0 | 0.3560 |
| -1433.0 | 0.4520 |

| | |
|---|---|
| -1560.0 | 0.5390 |
| -1656.0 | 0.6180 |
| -1705.0 | 0.6900 |
| -1679.0 | 0.7570 |
| -1574.0 | 0.8180 |
| -1337.0 | 0.8750 |
| -942.00 | 0.9270 |
| -756.00 | 0.9530 |

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**Critical point**

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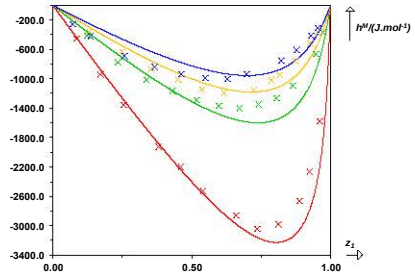
Byun, Hun-Soo - Choi, Min-Yong - Lim, Jong-Sung, High-pressure phase behavior and modeling of binary mixtures for alkyl acetate in supercritical carbon dioxide, The Journal of Supercritical Fluids 3 (2006) 323-332. doi:10.1016/j.supflu.2005.10.007

| T / K | P / bar | $x_1$ |
|---|---|---|
| 313.20 | 81.60 | 0.9640 |
| 333.20 | 97.00 | 0.9280 |
| 353.20 | 107.10 | 0.8460 |
| 373.20 | 116.10 | 0.8210 |
| 393.20 | 116.60 | 0.7880 |

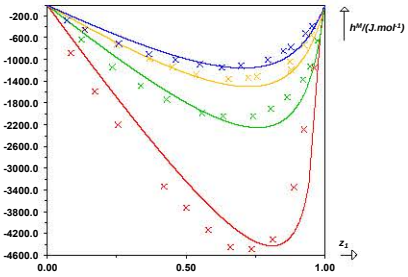
Juntarachat, Niramol - Privat, Romain - Coniglio, Lucie - Jaubert, Jean-Noël, Development of a Predictive Equation of State for CO2 + Ethyl Ester Mixtures Based on Critical Points Measurements, Journal of Chemical & Engineering Data 10 (2014) 3205-3219. doi:10.1021/je5002494

| T / K | P / bar | $x_1$ |
|---|---|---|
| 514.36 | 49.33 | 0.1011 |
| 504.49 | 61.30 | 0.1988 |
| 493.95 | 73.12 | 0.2934 |
| 481.81 | 84.88 | 0.4198 |
| 469.78 | 95.14 | 0.5328 |
| 455.01 | 106.10 | 0.6271 |
| 434.98 | 116.36 | 0.7158 |
| 418.78 | 120.54 | 0.7902 |
| 391.38 | 123.62 | 0.8577 |
| 356.13 | 112.08 | 0.9115 |
| 335.14 | 98.59 | 0.9443 |

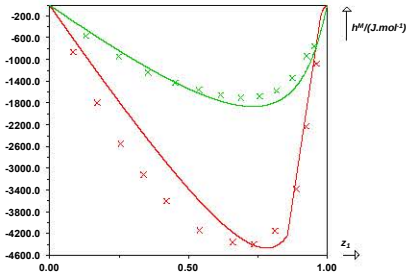
T/K = 313.15 - P/bar = 90.00 120.00 150.00 180.00



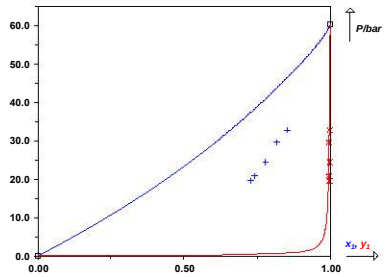

T/K = 323.15 - P/bar = 90.00 120.00 150.00 180.00



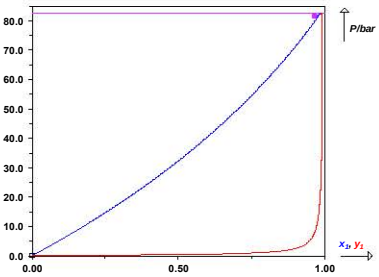

T/K = 333.15 - P/bar = 90.00 150.00



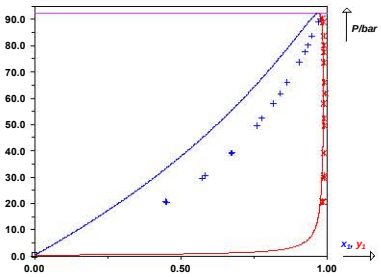

T/K = 295.20



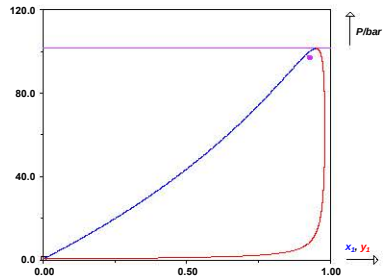

T/K = 313.20



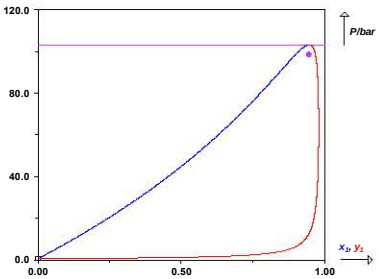

T/K = 323.15



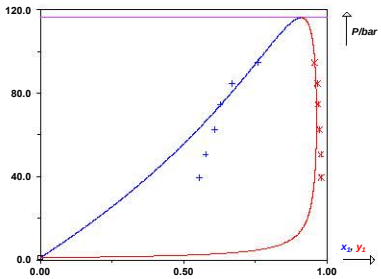

T/K = 333.20



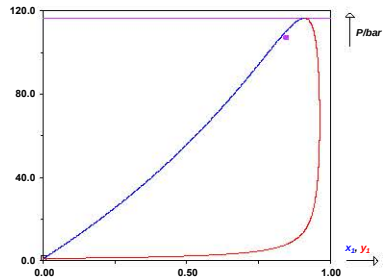

T/K = 335.14



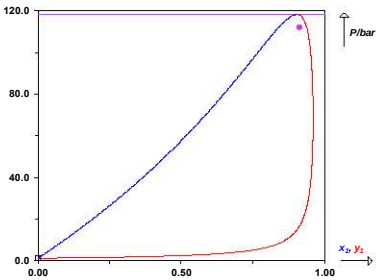

T/K = 353.00



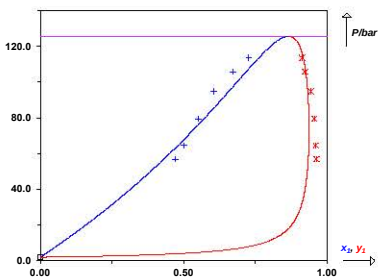

T/K = 353.20



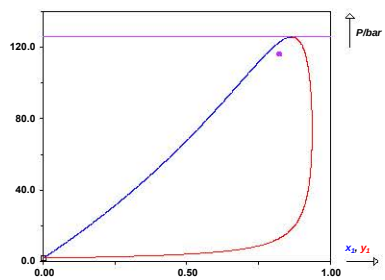

T/K = 356.13



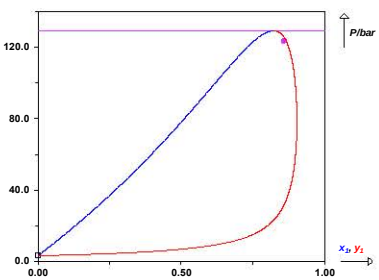

T/K = 373.00



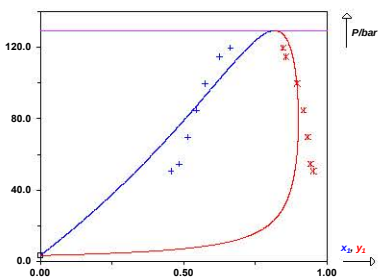

T/K = 373.20

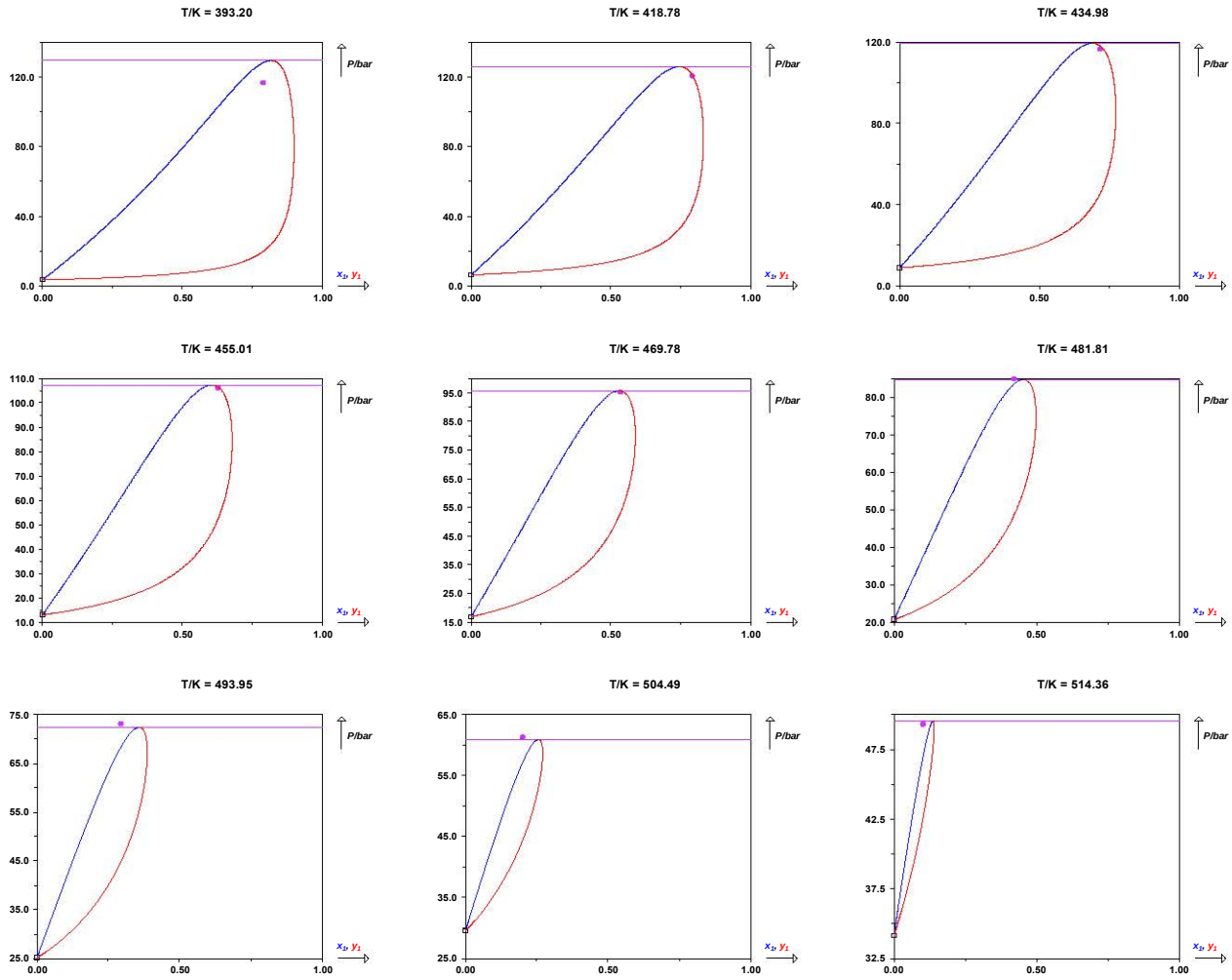



T/K = 391.38




T/K = 393.00




T/K = 393.20
T/K = 418.78
T/K = 434.98
T/K = 455.01
T/K = 469.78
T/K = 481.81
T/K = 493.95
T/K = 504.49
T/K = 514.36
P/bar
x1, y1

## CARBON DIOXIDE (1) + CARBON DISULFIDE (2)

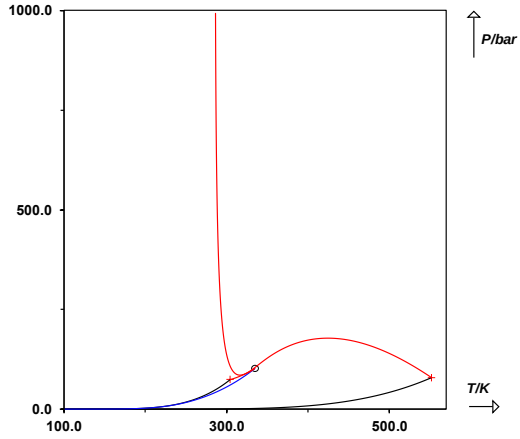
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 75-15-0 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | QGJOPFRUJISHPQ-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 552.00 |
| **$P_c$ / bar** | 73.83 | 79.00 |
| **ω** | 0.224 | 0.111 |

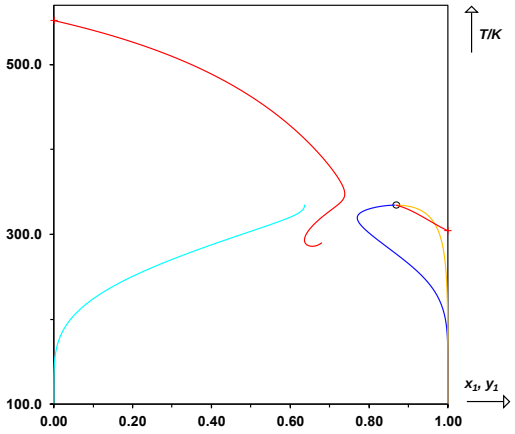
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 607
B/MPa = 1360

*Deviations*
MAPE on x = 14 %
MAPE on y = 6.8 %
MAPE on $h^M$ = 16 %



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**Isothermal phase equilibrium data**

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Reiff, W.-E. - Roth, H. - Lucas, K., Phase equilibria in the binary system carbon disulfide-carbon dioxide, Fluid Phase Equilibria 3 (1992) 323-338. doi:10.1016/0378-3812(92)80016-3

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.740 | 0.0260 | 0.9593 |
| 10.32 | 0.0518 | 0.9797 |
| 20.14 | 0.1182 | 0.9862 |
| 25.71 | 0.1761 | 0.9878 |
| 28.07 | 0.2100 | 0.9861 |
| 30.08 | 0.2630 | 0.9883 |
| 31.22 | 0.8711 | 0.9892 |
| 31.68 | 0.8967 | 0.9910 |
| 32.22 | 0.9237 | 0.9919 |

Reiff, W.-E. - Roth, H. - Lucas, K., Phase equilibria in the binary system carbon disulfide-carbon dioxide, Fluid Phase Equilibria 3 (1992) 323-338. doi:10.1016/0378-3812(92)80016-3

**T / K = 280.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.740 | 0.0301 | 0.9557 |
| 11.78 | 0.0604 | 0.9723 |
| 20.11 | 0.1135 | 0.9806 |
| 27.07 | 0.1683 | 0.9830 |
| 31.08 | 0.2189 | 0.9845 |
| 33.14 | 0.2523 | 0.9850 |
| 34.65 | 0.3042 | 0.9853 |
| 35.90 | 0.3674 | 0.9859 |
| 37.02 | 0.8846 | 0.9889 |
| 37.61 | 0.9123 | 0.9899 |
| 38.45 | 0.9367 | 0.9920 |

Reiff, W.-E. - Roth, H. - Lucas, K., Phase equilibria in the binary system carbon disulfide-carbon dioxide, Fluid Phase Equilibria 3 (1992) 323-338. doi:10.1016/0378-3812(92)80016-3

**T / K = 285.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.040 | 0.0240 | 0.9366 |
| 10.18 | 0.0476 | 0.9642 |
| 19.98 | 0.0950 | 0.9782 |
| 38.73 | 0.3130 | 0.9834 |
| 39.79 | 0.3804 | 0.9835 |
| 40.02 | 0.4258 | 0.9824 |
| 40.08 | 0.7506 | 0.9841 |
| 40.83 | 0.8343 | 0.9847 |
| 42.43 | 0.9055 | 0.9875 |

Reiff, W.-E. - Roth, H. - Lucas, K., Phase equilibria in the binary system carbon disulfide-carbon dioxide, Fluid Phase Equilibria 3 (1992) 323-338. doi:10.1016/0378-3812(92)80016-3

**T / K = 290.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.120 | 0.0200 | 0.9258 |
| 15.02 | 0.0632 | 0.9701 |
| 25.21 | 0.1181 | 0.9785 |
| 34.68 | 0.1918 | 0.9813 |
| 38.23 | 0.2351 | 0.9814 |
| 41.33 | 0.2921 | 0.9816 |
| 44.08 | 0.4454 | 0.9824 |
| 45.98 | 0.8613 | 0.9839 |
| 46.90 | 0.8891 | 0.9850 |
| 48.24 | 0.9244 | 0.9869 |

Reiff, W.-E. - Roth, H. - Lucas, K., Phase equilibria in the binary system carbon disulfide-carbon dioxide, Fluid Phase Equilibria 3 (1992) 323-338. doi:10.1016/0378-3812(92)80016-3

**T / K = 299.88**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.300 | 0.0165 | 0.8945 |
| 10.00 | 0.0350 | 0.9400 |
| 15.04 | 0.0530 | 0.9567 |
| 20.20 | 0.0750 | 0.9646 |
| 30.00 | 0.1249 | 0.9720 |
| 40.05 | 0.1907 | 0.9753 |
| 45.78 | 0.2524 | 0.9740 |
| 52.86 | 0.4699 | 0.9747 |
| 53.39 | 0.5565 | 0.9754 |
| 54.28 | 0.7397 | 0.9753 |
| 56.21 | 0.8458 | 0.9769 |
| 58.34 | 0.8986 | 0.9789 |

Reiff, W.-E. - Roth, H. - Lucas, K., Phase equilibria in the binary system carbon disulfide-carbon dioxide, Fluid Phase Equilibria 3 (1992) 323-338. doi:10.1016/0378-3812(92)80016-3

**T / K = 310.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.180 | 0.0148 | 0.8465 |
| 10.31 | 0.0321 | 0.9183 |
| 20.20 | 0.0695 | 0.9489 |
| 30.05 | 0.1123 | 0.9611 |
| 40.12 | 0.1684 | 0.9665 |

| | | |
|---|---|---|
| 50.85 | 0.2480 | 0.9672 |
| 60.22 | 0.3839 | 0.9660 |
| 62.70 | 0.4810 | 0.9663 |
| 64.33 | 0.6500 | 0.9662 |
| 67.22 | 0.8267 | 0.9664 |
| 70.33 | 0.8907 | 0.9683 |
| 74.00 | 0.9363 | 0.9711 |

Reiff, W.-E. - Roth, H. - Lucas, K., Phase equilibria in the binary system carbon disulfide-carbon dioxide, Fluid Phase Equilibria 3 (1992) 323-338. doi:10.1016/0378-3812(92)80016-3

**T / K = 330.01**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.00 | 0.0254 | 0.8413 |
| 20.30 | 0.0571 | 0.9117 |
| 30.27 | 0.0898 | 0.9332 |
| 40.77 | 0.1295 | 0.9434 |
| 53.94 | 0.1886 | 0.9473 |
| 64.95 | 0.2518 | 0.9476 |
| 74.95 | 0.3389 | 0.9453 |
| 80.20 | 0.4029 | 0.9422 |
| 85.40 | 0.5171 | 0.9377 |
| 88.00 | 0.6290 | 0.9334 |
| 90.20 | 0.7393 | 0.9273 |
| 92.20 | 0.8101 | 0.9202 |
| 93.00 | 0.8269 | 0.9148 |
| 93.80 | 0.8496 | 0.9042 |

Reiff, W.-E. - Roth, H. - Lucas, K., Phase equilibria in the binary system carbon disulfide-carbon dioxide, Fluid Phase Equilibria 3 (1992) 323-338. doi:10.1016/0378-3812(92)80016-3

**T / K = 360.01**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.18 | 0.0302 | 0.7598 |
| 35.66 | 0.0848 | 0.8737 |
| 54.80 | 0.1441 | 0.8994 |
| 69.70 | 0.1980 | 0.9068 |
| 84.60 | 0.2634 | 0.9060 |
| 100.40 | 0.3539 | 0.8972 |
| 108.60 | 0.4110 | 0.8891 |
| 115.30 | 0.4768 | 0.8748 |
| 120.10 | 0.5396 | 0.8589 |
| 122.40 | 0.5788 | 0.8467 |
| 125.30 | 0.6471 | 0.8157 |
| 125.90 | 0.6674 | 0.8054 |

Reiff, W.-E. - Roth, H. - Lucas, K., Phase equilibria in the binary system carbon disulfide-carbon dioxide, Fluid Phase Equilibria 3 (1992) 323-338. doi:10.1016/0378-3812(92)80016-3

**T / K = 410.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 14.95 | 0.0121 | 0.3262 |
| 25.90 | 0.0371 | 0.5729 |
| 40.74 | 0.0724 | 0.6973 |
| 49.92 | 0.0952 | 0.7396 |
| 61.16 | 0.1230 | 0.7673 |
| 76.40 | 0.1639 | 0.7876 |
| 87.10 | 0.1945 | 0.7954 |
| 94.20 | 0.2171 | 0.7990 |
| 104.20 | 0.2493 | 0.7991 |
| 117.60 | 0.2954 | 0.7931 |
| 125.50 | 0.3297 | 0.7869 |
| 135.80 | 0.3771 | 0.7719 |
| 145.00 | 0.4304 | 0.7549 |
| 149.50 | 0.4579 | 0.7400 |
| 154.90 | 0.5083 | 0.7036 |
| 156.70 | 0.5318 | 0.6904 |
| 158.90 | 0.6008 | 0.6391 |

Reiff, W.-E. - Roth, H. - Lucas, K., Phase equilibria in the binary system carbon disulfide-carbon dioxide, Fluid Phase Equilibria 3 (1992) 323-338. doi:10.1016/0378-3812(92)80016-3

**T / K = 448.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 40.40 | 0.0485 | 0.4477 |
| 55.80 | 0.0851 | 0.5580 |
| 70.30 | 0.1209 | 0.6123 |
| 84.70 | 0.1537 | 0.6431 |
| 99.10 | 0.1909 | 0.6625 |
| 114.90 | 0.2359 | 0.6639 |
| 130.10 | 0.2886 | 0.6513 |
| 144.80 | 0.3495 | 0.6245 |
| 156.30 | 0.4402 | 0.5606 |

Reiff, W.-E. - Roth, H. - Lucas, K., Phase equilibria in the binary system carbon disulfide-carbon dioxide, Fluid Phase Equilibria 3 (1992) 323-338. doi:10.1016/0378-3812(92)80016-3

**T / K = 473.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 48.80 | 0.0495 | 0.3452 |
| 57.60 | 0.0695 | 0.4095 |
| 70.00 | 0.0955 | 0.4748 |
| 79.70 | 0.1194 | 0.5075 |
| 90.90 | 0.1439 | 0.5279 |
| 99.50 | 0.1732 | 0.5425 |

| | | |
|---|---|---|
| 110.50 | 0.2001 | 0.5500 |
| 119.60 | 0.2272 | 0.5499 |
| 129.40 | 0.2629 | 0.5422 |
| 139.50 | 0.3091 | 0.5158 |
| 142.40 | 0.3288 | 0.5063 |
| 145.00 | 0.3490 | 0.4876 |

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**Enthalpy of mixing**

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Wormald, C.J. - Hodgetts, R.W., Measurements of HmE for {xCO2+(1−x)CS2} in the liquid region up to T=300.15 K and p=7.5 MPa, Fluid Phase Equilibria 2 (2003) 303-308. doi:10.1016/S0378-3812(02)00266-2

**T / K = 270.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 779.00 | 0.1570 |
| 822.00 | 0.1690 |
| 874.00 | 0.1880 |
| 917.00 | 0.1960 |
| 967.00 | 0.2110 |
| 1015.0 | 0.2290 |
| 1077.0 | 0.2500 |
| 1127.0 | 0.3200 |
| 1137.0 | 0.3730 |
| 1164.0 | 0.4320 |
| 1160.0 | 0.5340 |
| 1144.0 | 0.5760 |
| 1125.0 | 0.6190 |
| 1094.0 | 0.6850 |
| 1017.0 | 0.7720 |
| 978.00 | 0.8020 |
| 934.00 | 0.8250 |
| 865.00 | 0.8440 |
| 807.00 | 0.8580 |
| 755.00 | 0.8710 |

Wormald, C.J. - Hodgetts, R.W., Measurements of HmE for {xCO2+(1−x)CS2} in the liquid region up to T=300.15 K and p=7.5 MPa, Fluid Phase Equilibria 2 (2003) 303-308. doi:10.1016/S0378-3812(02)00266-2

**T / K = 290.15**

**P / bar = 75.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 724.00 | 0.1710 |
| 764.00 | 0.1820 |
| 806.00 | 0.1980 |
| 849.00 | 0.2140 |
| 896.00 | 0.2320 |
| 958.00 | 0.2540 |
| 1014.0 | 0.2800 |
| 1079.0 | 0.3120 |
| 1140.0 | 0.3620 |
| 1157.0 | 0.3820 |
| 1173.0 | 0.4180 |
| 1183.0 | 0.4340 |
| 1156.0 | 0.5140 |
| 1136.0 | 0.5460 |
| 1107.0 | 0.5880 |
| 1074.0 | 0.6110 |
| 1061.0 | 0.6420 |
| 1002.0 | 0.6830 |
| 976.00 | 0.7080 |
| 911.00 | 0.7520 |
| 843.00 | 0.7710 |
| 776.00 | 0.8020 |
| 722.00 | 0.8250 |
| 666.00 | 0.8430 |
| 629.00 | 0.8580 |

Wormald, C.J. - Hodgetts, R.W., Measurements of HmE for {xCO2+(1−x)CS2} in the liquid region up to T=300.15 K and p=7.5 MPa, Fluid Phase Equilibria 2 (2003) 303-308. doi:10.1016/S0378-3812(02)00266-2

**T / K = 295.15**

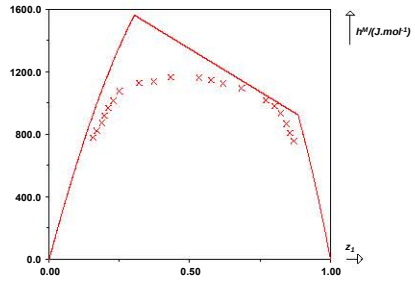
**P / bar = 75.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 666.00 | 0.1710 |
| 710.00 | 0.1850 |
| 754.00 | 0.2010 |
| 808.00 | 0.2210 |
| 862.00 | 0.2450 |
| 927.00 | 0.2740 |
| 994.00 | 0.3120 |
| 1004.0 | 0.3290 |
| 1092.0 | 0.4050 |
| 1105.0 | 0.4760 |
| 1111.0 | 0.5310 |
| 1106.0 | 0.5750 |
| 1034.0 | 0.6190 |
| 982.00 | 0.6710 |
| 860.00 | 0.7300 |
| 664.00 | 0.8020 |
| 604.00 | 0.8250 |
| 554.00 | 0.8430 |

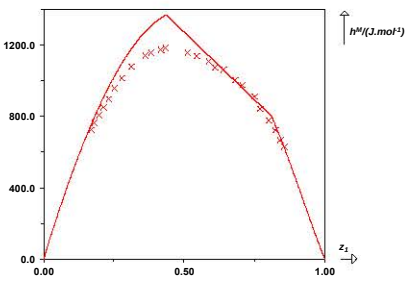
Wormald, C.J. - Hodgetts, R.W., Measurements of HmE for {xCO2+(1−x)CS2} in the liquid region up to T=300.15 K and p=7.5 MPa, Fluid Phase Equilibria 2 (2003) 303-308. doi:10.1016/S0378-3812(02)00266-2

| **T / K =** | **300.15** |
|---|---|
| **P / bar =** | **75.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 631.00 | 0.1770 |
| 668.00 | 0.1930 |
| 715.00 | 0.2110 |
| 766.00 | 0.2320 |
| 802.00 | 0.2540 |
| 840.00 | 0.2800 |
| 904.00 | 0.3120 |
| 939.00 | 0.3530 |
| 963.00 | 0.4050 |
| 965.00 | 0.4760 |
| 951.00 | 0.5220 |
| 915.00 | 0.5760 |
| 829.00 | 0.6300 |
| 757.00 | 0.6710 |
| 702.00 | 0.7030 |
| 633.00 | 0.7300 |
| 544.00 | 0.7710 |
| 466.00 | 0.8020 |
| 402.00 | 0.8250 |

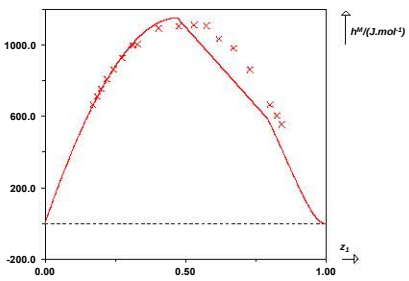
T/K = 270.15 - P/bar = 50.00



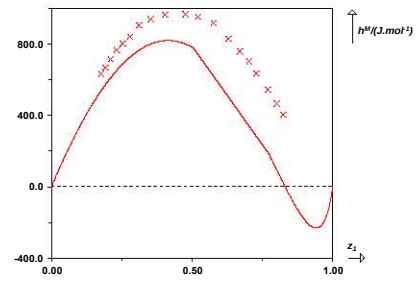

T/K = 290.15 - P/bar = 75.00



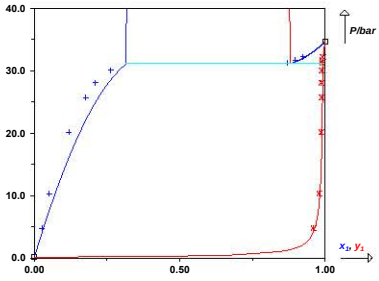

T/K = 295.15 - P/bar = 75.00



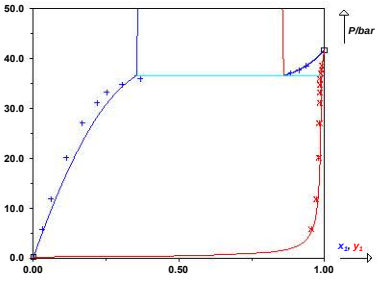

T/K = 300.15 - P/bar = 75.00



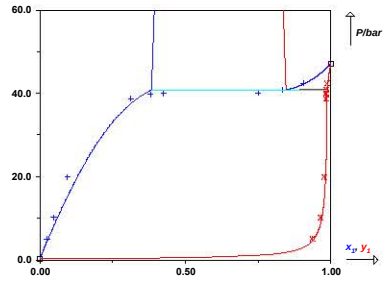

T/K = 273.15



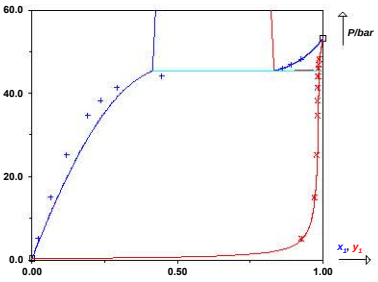

T/K = 280.00



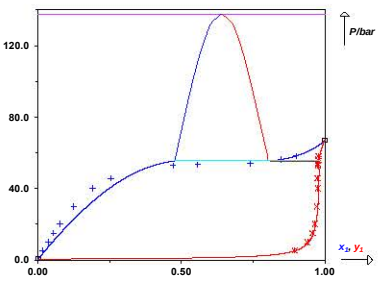

T/K = 285.00



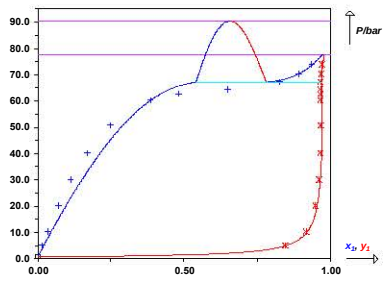

T/K = 290.00



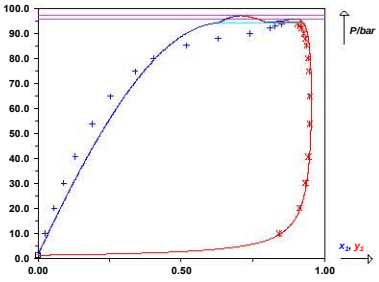

T/K = 299.88



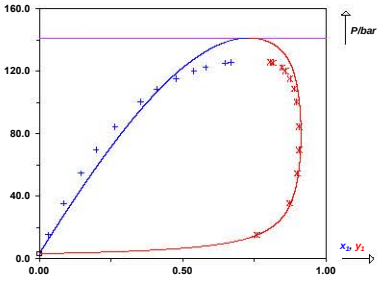

T/K = 310.00



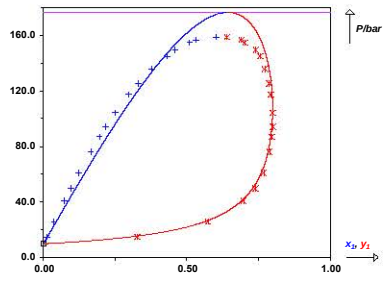

T/K = 330.01



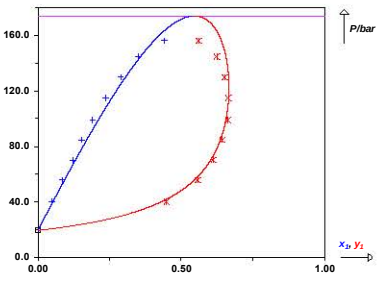

T/K = 360.01



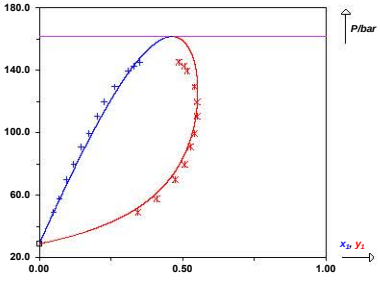

T/K = 410.00




T/K = 448.15




T/K = 473.15



## CARBON DIOXIDE (1) + DIMETHYL CARBONATE (2)

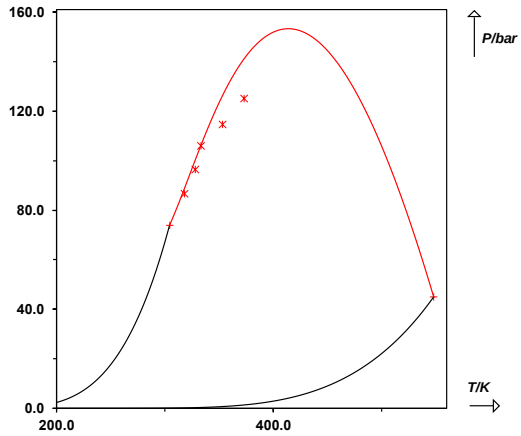
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 616-38-6 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | IEJIGPNLZYLLBP-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 548.00 |
| **$P_c$ / bar** | 73.83 | 45.00 |
| **ω** | 0.224 | 0.385 |

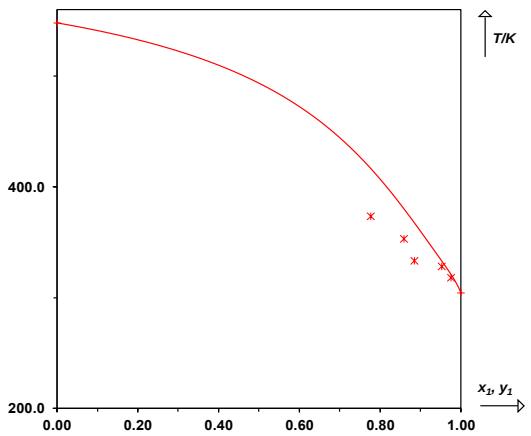
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = -60.3
B/MPa = -501

*Deviations*
MAPE on x = 6.2 %
MAPE on y = 20 %
MAPE on $x_c$ = 21 %
MAPE on $P_c$ = 5.9 %
MAPE on $h^M$ = 8.6 %



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**Isothermal phase equilibrium data**

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Lee, Min Hee - Yim, Joon-Hyuk - Kang, Jeong Won - Lim, Jong Sung, Measurement of VLE data of carbon dioxide+dimethyl carbonate system for the direct synthesis of dimethyl carbonate using supercritical CO2 and methanol, Fluid Phase Equilibria (2012) 77-82. doi:10.1016/j.fluid.2012.01.020

**T / K = 278.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.300 | 0.0790 | 0.9840 |
| 6.000 | 0.2220 | 0.9940 |
| 9.690 | 0.3580 | 0.9960 |
| 29.30 | 0.8470 | 0.9980 |
| 36.48 | 0.9410 | 0.9990 |

Lee, Min Hee - Yim, Joon-Hyuk - Kang, Jeong Won - Lim, Jong Sung, Measurement of VLE data of carbon dioxide+dimethyl carbonate system for the direct synthesis of dimethyl carbonate using supercritical CO2 and methanol, Fluid Phase Equilibria (2012) 77-82. doi:10.1016/j.fluid.2012.01.020

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.800 | 0.0670 | 0.9770 |
| 6.700 | 0.1870 | 0.9900 |
| 29.99 | 0.7720 | 0.9960 |
| 33.78 | 0.8450 | 0.9970 |
| 38.70 | 0.9160 | 0.9980 |

Lee, Min Hee - Yim, Joon-Hyuk - Kang, Jeong Won - Lim, Jong Sung, Measurement of VLE data of carbon dioxide+dimethyl carbonate system for the direct synthesis of dimethyl carbonate using supercritical CO2 and methanol, Fluid Phase Equilibria (2012) 77-82. doi:10.1016/j.fluid.2012.01.020

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.900 | 0.0350 | 0.9590 |
| 9.310 | 0.1900 | 0.9900 |
| 13.96 | 0.3100 | 0.9920 |
| 23.03 | 0.4720 | 0.9940 |
| 32.54 | 0.6470 | 0.9960 |

Lee, Min Hee - Yim, Joon-Hyuk - Kang, Jeong Won - Lim, Jong Sung, Measurement of VLE data of carbon dioxide+dimethyl carbonate system for the direct synthesis of dimethyl carbonate using supercritical CO2 and methanol, Fluid Phase Equilibria (2012) 77-82. doi:10.1016/j.fluid.2012.01.020

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 49.64 | 0.9160 | 0.9980 |

Lee, Min Hee - Yim, Joon-Hyuk - Kang, Jeong Won - Lim, Jong Sung, Measurement of VLE data of carbon dioxide+dimethyl carbonate system for the direct synthesis of dimethyl carbonate using supercritical CO2 and methanol, Fluid Phase Equilibria (2012) 77-82. doi:10.1016/j.fluid.2012.01.020

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.410 | 0.0470 | 0.9610 |
| 9.790 | 0.1780 | 0.9850 |
| 14.34 | 0.2640 | 0.9880 |
| 28.27 | 0.4740 | 0.9920 |
| 40.68 | 0.6670 | 0.9950 |

Lee, Min Hee - Yim, Joon-Hyuk - Kang, Jeong Won - Lim, Jong Sung, Measurement of VLE data of carbon dioxide+dimethyl carbonate system for the direct synthesis of dimethyl carbonate using supercritical CO2 and methanol, Fluid Phase Equilibria (2012) 77-82. doi:10.1016/j.fluid.2012.01.020

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 64.12 | 0.9330 | 0.9970 |

Im, Jihoon - Kim, Myungyoun - Lee, Jaewon - Kim, Hwayong, Vapor–Liquid Equilibria of Binary Carbon Dioxide + Alkyl Carbonate Mixture Systems, Journal of Chemical & Engineering Data 2 (2004) 243-245. doi:10.1021/je034089a

**T / K = 310.27**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.630 | 0.1431 | 0.9525 |
| 18.97 | 0.3019 | 0.9818 |
| 25.56 | 0.3919 | 0.9885 |
| 31.90 | 0.4809 | 0.9879 |
| 37.18 | 0.5473 | 0.9907 |
| 43.80 | 0.6273 | 0.9917 |
| 55.47 | 0.7648 | 0.9930 |
| 67.14 | 0.8867 | 0.9931 |
| 72.46 | 0.9290 | 0.9934 |

Lee, Min Hee - Yim, Joon-Hyuk - Kang, Jeong Won - Lim, Jong Sung, Measurement of VLE data of carbon dioxide+dimethyl carbonate system for the direct synthesis of dimethyl carbonate using supercritical CO2 and methanol, Fluid Phase Equilibria (2012) 77-82. doi:10.1016/j.fluid.2012.01.020

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.930 | 0.0610 | 0.9580 |
| 8.620 | 0.1280 | 0.9750 |

| | | |
|---|---|---|
| 16.55 | 0.2470 | 0.9830 |
| 30.48 | 0.4290 | 0.9890 |
| 38.27 | 0.5350 | 0.9920 |
| 49.64 | 0.6820 | 0.9930 |

Im, Jihoon - Kim, Myungyoun - Lee, Jaewon - Kim, Hwayong, Vapor–Liquid Equilibria of Binary Carbon Dioxide + Alkyl Carbonate Mixture Systems, Journal of Chemical & Engineering Data 2 (2004) 243-245. doi:10.1021/je034089a

**T / K = 320.36**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.270 | 0.1140 | 0.9388 |
| 16.64 | 0.2250 | 0.9699 |
| 25.53 | 0.3356 | 0.9778 |
| 32.19 | 0.4144 | 0.9850 |
| 42.50 | 0.5269 | 0.9881 |
| 57.57 | 0.6820 | 0.9885 |
| 70.84 | 0.8162 | 0.9888 |
| 76.97 | 0.8597 | 0.9879 |
| 81.40 | 0.8954 | 0.9866 |

Lee, Min Hee - Yim, Joon-Hyuk - Kang, Jeong Won - Lim, Jong Sung, Measurement of VLE data of carbon dioxide+dimethyl carbonate system for the direct synthesis of dimethyl carbonate using supercritical CO2 and methanol, Fluid Phase Equilibria (2012) 77-82. doi:10.1016/j.fluid.2012.01.020

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.210 | 0.0570 | 0.9350 |
| 19.79 | 0.2170 | 0.9740 |
| 33.78 | 0.3500 | 0.9800 |
| 53.53 | 0.5480 | 0.9840 |
| 64.67 | 0.6470 | 0.9850 |
| 82.32 | 0.7890 | 0.9860 |
| 91.84 | 0.8550 | 0.9830 |
| 94.46 | 0.8720 | 0.9820 |

Im, Jihoon - Kim, Myungyoun - Lee, Jaewon - Kim, Hwayong, Vapor–Liquid Equilibria of Binary Carbon Dioxide + Alkyl Carbonate Mixture Systems, Journal of Chemical & Engineering Data 2 (2004) 243-245. doi:10.1021/je034089a

**T / K = 340.27**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.19 | 0.1076 | 0.9276 |
| 24.03 | 0.2450 | 0.9645 |
| 36.84 | 0.3616 | 0.9741 |
| 48.66 | 0.4667 | 0.9773 |
| 58.52 | 0.5445 | 0.9786 |
| 70.82 | 0.6412 | 0.9787 |
| 82.69 | 0.7353 | 0.9776 |
| 94.13 | 0.8141 | 0.9727 |
| 99.96 | 0.8569 | 0.9630 |

Chen, L. - Zhu, R.J. - Fang, Y. - Yuan, P.F. - Cao, L.Q. - Tian, Y.L., Vapor-Liquid Equilibrium Data for Carbon Dioxide+Dimethyl Carbonate Binary System, Wuli Huaxue Xuebao 1 (2013) 11-16.

**T / K = 353.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 39.80 | 0.3810 | 0.9831 |
| 51.20 | 0.4656 | 0.9811 |
| 65.20 | 0.5549 | 0.9797 |
| 84.50 | 0.6563 | 0.9748 |
| 105.10 | 0.7577 | 0.9481 |
| 118.70 | 0.8332 | 0.9059 |

Chen, L. - Zhu, R.J. - Fang, Y. - Yuan, P.F. - Cao, L.Q. - Tian, Y.L., Vapor-Liquid Equilibrium Data for Carbon Dioxide+Dimethyl Carbonate Binary System, Wuli Huaxue Xuebao 1 (2013) 11-16.

**T / K = 373.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 44.60 | 0.3890 | 0.9782 |
| 54.80 | 0.4598 | 0.9760 |
| 66.20 | 0.5226 | 0.9762 |
| 76.70 | 0.5763 | 0.9688 |
| 88.40 | 0.6195 | 0.9651 |
| 99.40 | 0.6538 | 0.9600 |
| 111.30 | 0.6929 | 0.9504 |

Chen, L. - Zhu, R.J. - Fang, Y. - Yuan, P.F. - Cao, L.Q. - Tian, Y.L., Vapor-Liquid Equilibrium Data for Carbon Dioxide+Dimethyl Carbonate Binary System, Wuli Huaxue Xuebao 1 (2013) 11-16.

**T / K = 393.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 55.70 | 0.4143 | 0.9559 |
| 65.70 | 0.4699 | 0.9600 |
| 80.70 | 0.5245 | 0.9526 |
| 95.60 | 0.5787 | 0.9491 |
| 110.60 | 0.6287 | 0.9294 |
| 125.70 | 0.6878 | 0.9137 |
| 137.50 | 0.7459 | 0.8935 |

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**Enthalpy of mixing**

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Matsuda, Hiroyuki - Yoshii, Shigetaka - Nagashima, Akinori - Kurihara, Kiyofumi - Ochi, Kenji, Excess Molar

Enthalpies of the Binary Carbon Dioxide + Dimethyl Carbonate System at Temperatures of (298.15 to 308.15) K and Pressures of (5.0 to 7.5) MPa, Journal of Chemical & Engineering Data 4 (2005) 1419-1424. doi:10.1021/je050089u

**T / K = 298.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -865.00 | 0.0793 |
| -1787.0 | 0.1538 |
| -2659.0 | 0.2240 |
| -3480.0 | 0.2902 |
| -4257.0 | 0.3528 |
| -4806.0 | 0.4121 |
| -5560.0 | 0.4683 |
| -6179.0 | 0.5216 |
| -6663.0 | 0.5723 |
| -7173.0 | 0.6206 |
| -7625.0 | 0.6666 |
| -8014.0 | 0.7104 |
| -8345.0 | 0.7523 |
| -8669.0 | 0.7924 |
| -8924.0 | 0.8307 |
| -8756.0 | 0.8382 |
| -7087.0 | 0.8674 |
| -5290.0 | 0.9026 |
| -3285.0 | 0.9364 |
| -1605.0 | 0.9688 |
| 64.00 | 0.9969 |

Matsuda, Hiroyuki - Yoshii, Shigetaka - Nagashima, Akinori - Kurihara, Kiyofumi - Ochi, Kenji, Excess Molar Enthalpies of the Binary Carbon Dioxide + Dimethyl Carbonate System at Temperatures of (298.15 to 308.15) K and Pressures of (5.0 to 7.5) MPa, Journal of Chemical & Engineering Data 4 (2005) 1419-1424. doi:10.1021/je050089u

**T / K = 298.15**

**P / bar = 60.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -1626.0 | 0.1557 |
| -2335.0 | 0.2265 |
| -3334.0 | 0.2932 |
| -3788.0 | 0.3561 |
| -4343.0 | 0.4156 |
| -4974.0 | 0.4718 |
| -5395.0 | 0.5252 |
| -5869.0 | 0.5758 |
| -6342.0 | 0.6239 |
| -6759.0 | 0.6697 |
| -7051.0 | 0.7134 |
| -7255.0 | 0.7550 |
| -7515.0 | 0.7947 |
| -7755.0 | 0.8327 |
| -7833.0 | 0.8691 |
| -7913.0 | 0.9039 |
| -7801.0 | 0.9502 |
| -7458.0 | 0.9693 |
| -3615.0 | 0.9817 |

Matsuda, Hiroyuki - Yoshii, Shigetaka - Nagashima, Akinori - Kurihara, Kiyofumi - Ochi, Kenji, Excess Molar Enthalpies of the Binary Carbon Dioxide + Dimethyl Carbonate System at Temperatures of (298.15 to 308.15) K and Pressures of (5.0 to 7.5) MPa, Journal of Chemical & Engineering Data 4 (2005) 1419-1424. doi:10.1021/je050089u

**T / K = 303.15**

**P / bar = 55.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -896.00 | 0.0798 |
| -1834.0 | 0.1548 |
| -2591.0 | 0.2253 |
| -3339.0 | 0.2918 |
| -4139.0 | 0.3546 |
| -4821.0 | 0.4139 |
| -5437.0 | 0.4702 |
| -5913.0 | 0.5235 |
| -6431.0 | 0.5742 |
| -6870.0 | 0.6223 |
| -7338.0 | 0.6682 |
| -7732.0 | 0.7120 |
| -8042.0 | 0.7537 |
| -8269.0 | 0.7936 |
| -8461.0 | 0.8318 |
| -8422.0 | 0.8392 |
| -7900.0 | 0.8466 |
| -6765.0 | 0.8683 |
| -4920.0 | 0.9033 |
| -3067.0 | 0.9368 |
| -1383.0 | 0.9691 |

Matsuda, Hiroyuki - Yoshii, Shigetaka - Nagashima, Akinori - Kurihara, Kiyofumi - Ochi, Kenji, Excess Molar Enthalpies of the Binary Carbon Dioxide + Dimethyl Carbonate System at Temperatures of (298.15 to 308.15) K and Pressures of (5.0 to 7.5) MPa, Journal of Chemical & Engineering Data 4 (2005) 1419-1424. doi:10.1021/je050089u

**T / K = 308.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -1967.0 | 0.1537 |
| -2761.0 | 0.2239 |
| -3576.0 | 0.2901 |
| -5003.0 | 0.4120 |
| -5674.0 | 0.4682 |
| -6236.0 | 0.5215 |
| -7259.0 | 0.6205 |
| -8064.0 | 0.7103 |
| -8095.0 | 0.7189 |
| -7874.0 | 0.7273 |
| -5842.0 | 0.7923 |
| -3575.0 | 0.8674 |
| -1634.0 | 0.9364 |
| -22.00 | 0.9877 |
| 112.00 | 0.9939 |

Matsuda, Hiroyuki - Yoshii, Shigetaka - Nagashima, Akinori - Kurihara, Kiyofumi - Ochi, Kenji, Excess Molar Enthalpies of the Binary Carbon Dioxide + Dimethyl Carbonate System at Temperatures of (298.15 to 308.15) K and Pressures of (5.0 to 7.5) MPa, Journal of Chemical & Engineering Data 4 (2005) 1419-1424. doi:10.1021/je050089u

**T / K = 308.15**

**P / bar = 60.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -1782.0 | 0.1556 |
| -3307.0 | 0.2931 |
| -4696.0 | 0.4154 |
| -5228.0 | 0.4717 |
| -6267.0 | 0.5757 |
| -6714.0 | 0.6238 |
| -7404.0 | 0.7132 |
| -7713.0 | 0.7549 |
| -7982.0 | 0.7946 |
| -8094.0 | 0.8326 |
| -6291.0 | 0.8690 |
| -2992.0 | 0.9372 |
| -1153.0 | 0.9692 |

Matsuda, Hiroyuki - Yoshii, Shigetaka - Nagashima, Akinori - Kurihara, Kiyofumi - Ochi, Kenji, Excess Molar Enthalpies of the Binary Carbon Dioxide + Dimethyl Carbonate System at Temperatures of (298.15 to 308.15) K and Pressures of (5.0 to 7.5) MPa, Journal of Chemical & Engineering Data 4 (2005) 1419-1424. doi:10.1021/je050089u

**T / K = 308.15**

**P / bar = 70.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -870.00 | 0.0812 |
| -1626.0 | 0.1572 |
| -2304.0 | 0.2285 |
| -3020.0 | 0.2956 |
| -3592.0 | 0.3587 |
| -4190.0 | 0.4184 |
| -4626.0 | 0.4747 |
| -5143.0 | 0.5280 |
| -5515.0 | 0.5786 |
| -5933.0 | 0.6266 |
| -6252.0 | 0.6723 |
| -6527.0 | 0.7157 |
| -6760.0 | 0.7571 |
| -6911.0 | 0.7966 |
| -7053.0 | 0.8343 |
| -7136.0 | 0.8703 |
| -7049.0 | 0.9049 |
| -6953.0 | 0.9249 |
| -5649.0 | 0.9443 |
| -5190.0 | 0.9507 |
| -3208.0 | 0.9697 |

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**Critical point**

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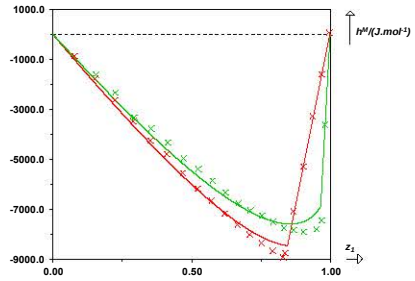
Sun, Yongju - Li, Yanfen - Zhou, Jianguo - Zhu, Rongjiao - Tian, Yiling, Experimental determination and calculation of the critical curves for the binary systems of CO2 containing ketone, alkane, ester and alcohol, respectively, Fluid Phase Equilibria 1 (2011) 72-77. doi:10.1016/j.fluid.2011.05.005

| T / K | P / bar | $x_1$ |
|---|---|---|
| 333.20 | 106.00 | 0.8852 |
| 353.20 | 114.50 | 0.8590 |
| 373.20 | 125.10 | 0.7772 |

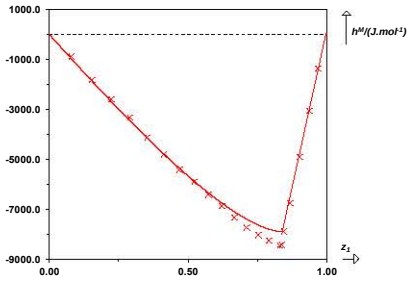
Hou, Yucui - Chen, Xiaoting - Ren, Shuhang - Song, Zhangzuo - Wu, Weize, Phase Behavior, Densities, and Isothermal Compressibility of (Carbon Dioxide + Dimethyl Carbonate), Journal of Chemical & Engineering Data 4 (2010) 1580-1587. doi:10.1021/je900691n

| T / K | P / bar | $x_1$ |
|---|---|---|
| 317.85 | 86.60 | 0.9758 |
| 327.95 | 96.40 | 0.9519 |

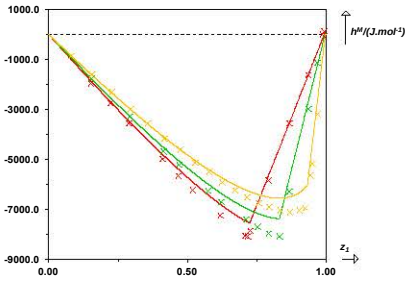
T/K = 298.15 - P/bar = 50.00 60.00



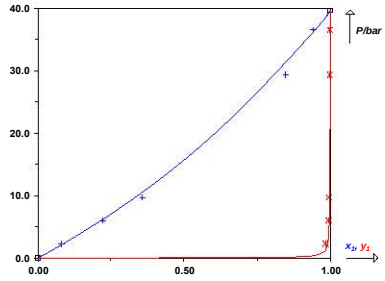

T/K = 303.15 - P/bar = 55.00



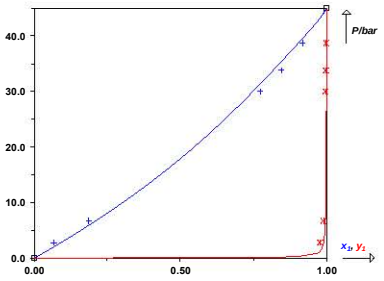

T/K = 308.15 - P/bar = 50.00 60.00 70.00



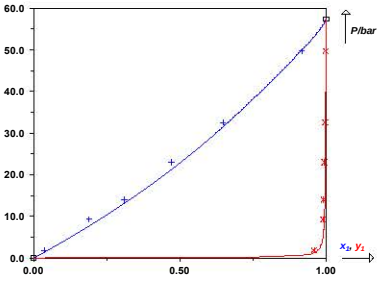

T/K = 278.15



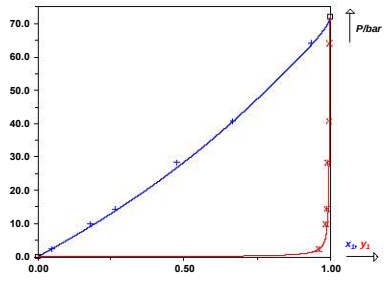

T/K = 283.15



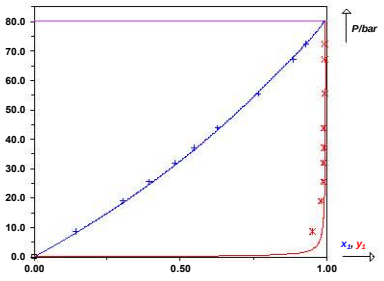

T/K = 293.15



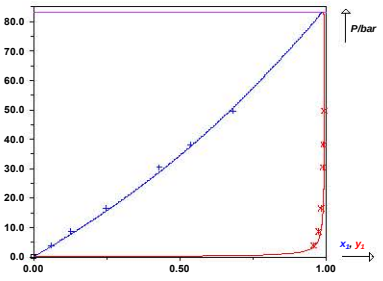

T/K = 303.15



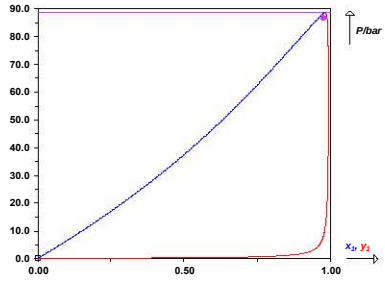

T/K = 310.27



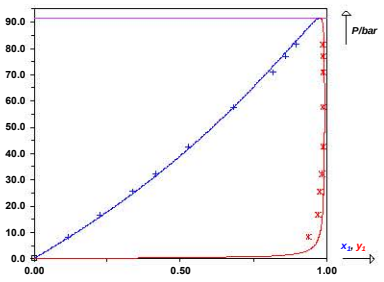

T/K = 313.15



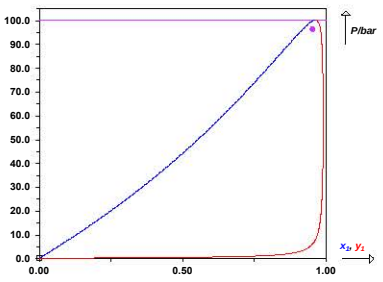

T/K = 317.85



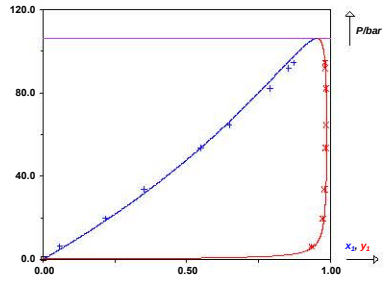

T/K = 320.36



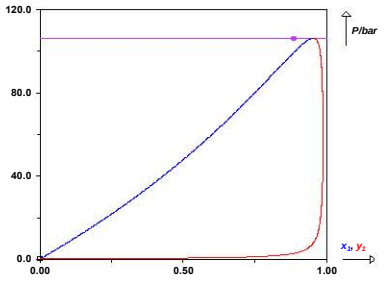

T/K = 327.95



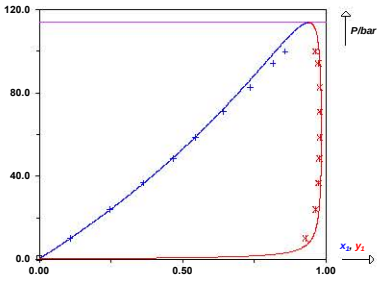

T/K = 333.15

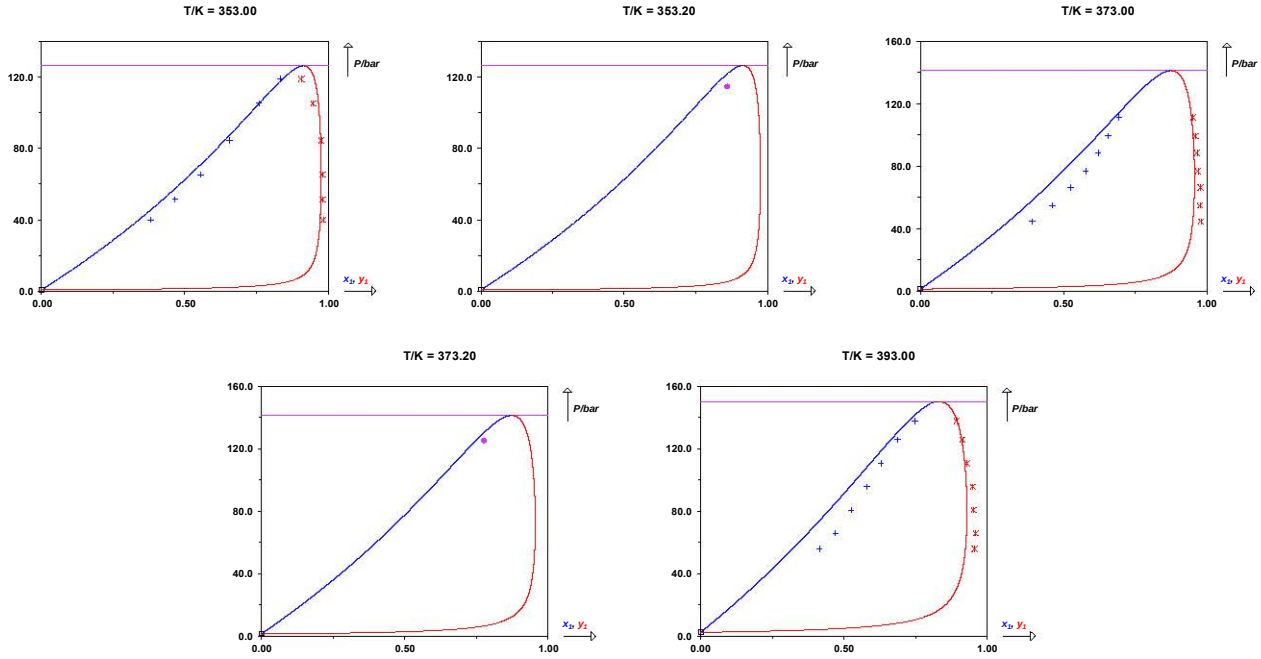



T/K = 333.20




T/K = 340.27




T/K = 353.00
T/K = 353.20
T/K = 373.00
T/K = 373.20
T/K = 393.00
P/bar
x1, y1
0.0
40.0
80.0
120.0
160.0
0.00
0.50
1.00

## CARBON MONOXIDE (1) + CARBON DIOXIDE (2)

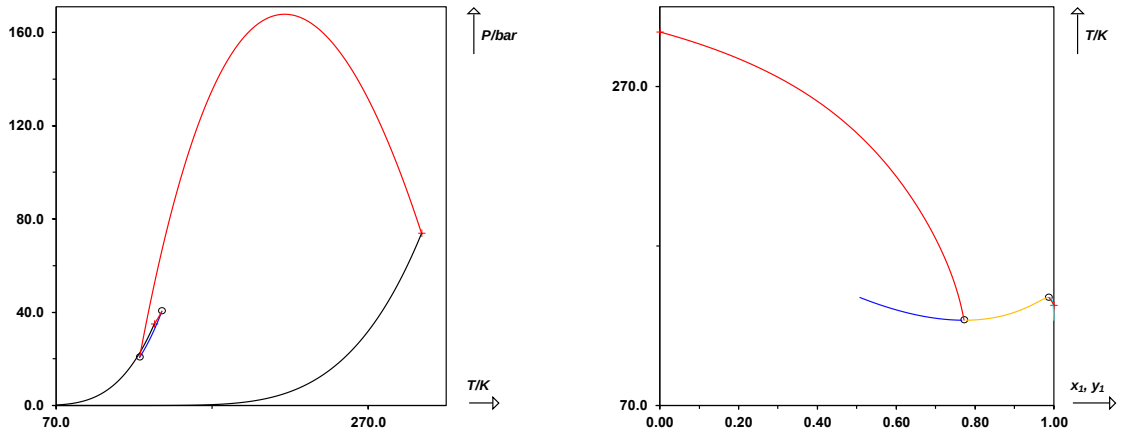
| | | |
|---|---|---|
| **CAS** | 630-08-0 | 124-38-9 |
| **InChiKey** | WSFSSNUMVMOOMR-UHFFFAOYSA-N | CURLTUGMZLYLDI-UHFFFAOYSA-N |
| **$T_c$ / K** | 132.92 | 304.21 |
| **$P_c$ / bar** | 34.99 | 73.83 |
| **ω** | 0.048 | 0.224 |

Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 425
B/MPa = -59

*Deviations*
MAPE on x = 7.4 %
MAPE on y = 3.5 %



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**Isothermal phase equilibrium data**

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Huamin, S., Solubility Of Carbon Monoxide In Methanol And Carbon Dioxide Under High Pressure, Huaxue Gongcheng 6 (1991) 61-69.

**T / K = 223.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.72 | 0.0195 | 0.5059 |
| 29.45 | 0.0516 | 0.6968 |
| 50.05 | 0.0942 | 0.7662 |
| 69.60 | 0.1552 | 0.7908 |

Kaminishi, Gen-Ichi - Arai, Yasuhiko - Saito, Shozaburo - Maeda, Siro, Vapor-Liquid Equilibria For Binary And Ternary Systems Containing Carbon Dioxide, Journal of Chemical Engineering of Japan 2 (1968) 109-116. doi:10.1252/jcej.1.109

**T / K = 223.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 95.45 | 0.2230 | 0.7870 |
| 121.29 | 0.3230 | 0.7550 |

Christiansen, L. J. - Fredenslund, A. - Gardner, N., Gas-Liquid Equilibria of the CO2-CO and CO2-CH4-CO Systems, Advances in Cryogenic Engineering (1995) 309-319.

**T / K = 223.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.268 | 0.0028 | 0.1550 |
| 14.23 | 0.0148 | 0.4910 |
| 22.50 | 0.0318 | 0.6410 |
| 38.34 | 0.0610 | 0.7470 |
| 58.31 | 0.1060 | 0.7900 |
| 81.44 | 0.1610 | 0.8000 |
| 100.72 | 0.2220 | 0.7890 |
| 134.75 | 0.3920 | 0.7000 |
| 141.53 | 0.4630 | 0.6490 |

Christiansen, L. J. - Fredenslund, A. - Gardner, N., Gas-Liquid Equilibria of the CO2-CO and CO2-CH4-CO Systems, Advances in Cryogenic Engineering (1995) 309-319.

**T / K = 243.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 16.46 | 0.0037 | 0.1120 |
| 23.37 | 0.0162 | 0.3380 |
| 34.15 | 0.0360 | 0.5060 |
| 49.36 | 0.0660 | 0.6100 |
| 77.06 | 0.1390 | 0.6660 |
| 99.03 | 0.2050 | 0.6670 |
| 111.77 | 0.2540 | 0.6490 |
| 122.55 | 0.3040 | 0.6190 |
| 130.21 | 0.3640 | 0.5700 |
| 131.42 | 0.3870 | 0.5480 |

Christiansen, L. J. - Fredenslund, A. - Gardner, N., Gas-Liquid Equilibria of the CO2-CO and CO2-CH4-CO Systems, Advances in Cryogenic Engineering (1995) 309-319.

**T / K = 263.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 30.26 | 0.0064 | 0.0930 |
| 37.84 | 0.0189 | 0.2260 |
| 48.87 | 0.0387 | 0.3440 |
| 64.44 | 0.0710 | 0.4320 |
| 81.74 | 0.1160 | 0.4770 |
| 94.98 | 0.1550 | 0.4860 |
| 102.25 | 0.1800 | 0.4800 |
| 109.84 | 0.2140 | 0.4630 |
| 113.55 | 0.2400 | 0.4410 |

Kaminishi, Gen-Ichi - Arai, Yasuhiko - Saito, Shozaburo - Maeda, Siro, Vapor-Liquid Equilibria For Binary And Ternary Systems Containing Carbon Dioxide, Journal of Chemical Engineering of Japan 2 (1968) 109-116. doi:10.1252/jcej.1.109

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 62.01 | 0.0660 | 0.2990 |
| 81.87 | 0.1240 | 0.3710 |
| 99.81 | 0.1910 | 0.3750 |
| 105.78 | 0.2280 | 0.3560 |

Kaminishi, Gen-Ichi - Arai, Yasuhiko - Saito, Shozaburo - Maeda, Siro, Vapor-Liquid Equilibria For Binary And Ternary Systems Containing Carbon Dioxide, Journal of Chemical Engineering of Japan 2 (1968) 109-116. doi:10.1252/jcej.1.109

**T / K = 283.15**

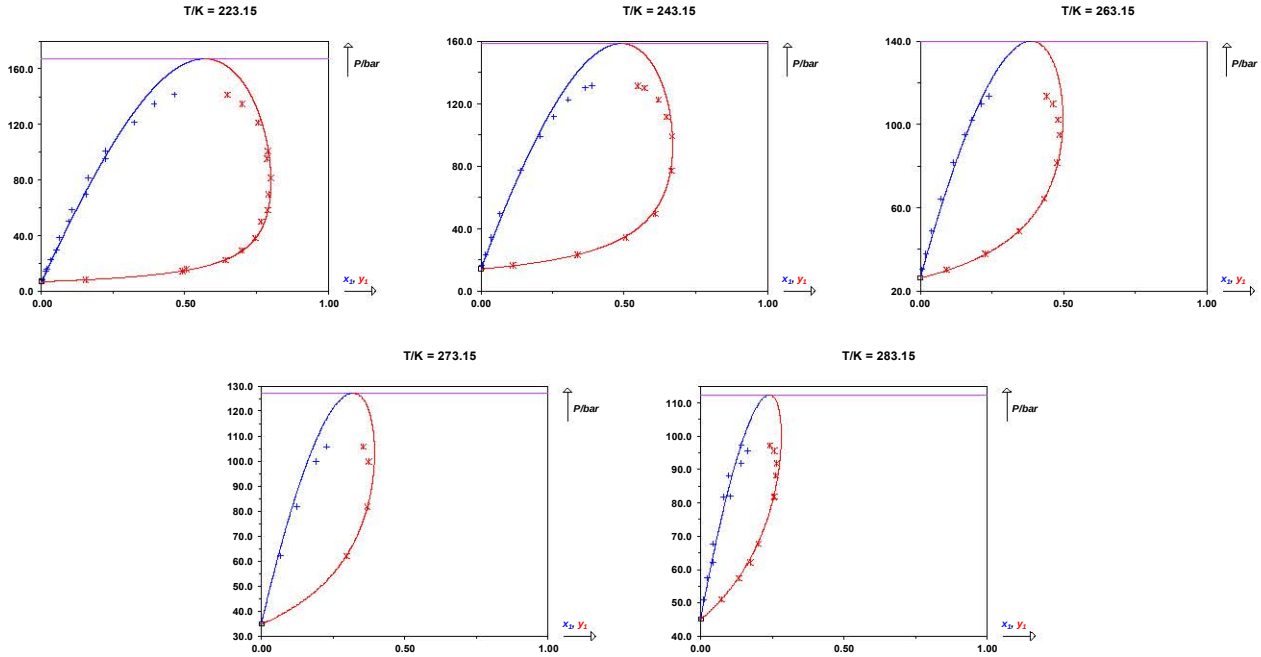
| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 62.01 | 0.0430 | 0.1730 |
| 81.87 | 0.1020 | 0.2570 |
| 91.90 | 0.1420 | 0.2650 |
| 95.65 | 0.1650 | 0.2570 |

Christiansen, L. J. - Fredenslund, A. - Gardner, N., Gas-Liquid Equilibria of the CO2-CO and CO2-CH4-CO Systems, Advances in Cryogenic Engineering (1995) 309-319.

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 50.98 | 0.0106 | 0.0730 |

| | | |
|---|---|---|
| 57.44 | 0.0230 | 0.1330 |
| 67.76 | 0.0436 | 0.2020 |
| 81.75 | 0.0800 | 0.2550 |
| 88.14 | 0.0990 | 0.2630 |
| 97.18 | 0.1410 | 0.2420 |


T/K = 223.15
P/bar
160.0
120.0
80.0
40.0
0.0
0.00
0.50
1.00
x1, y1
T/K = 243.15
P/bar
160.0
120.0
80.0
40.0
0.0
0.00
0.50
1.00
x1, y1
T/K = 263.15
P/bar
140.0
100.0
60.0
20.0
0.00
0.50
1.00
x1, y1
T/K = 273.15
P/bar
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
0.00
0.50
1.00
x1, y1
T/K = 283.15
P/bar
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
0.00
0.50
1.00
x1, y1

## PENTAFLUOROETHANE (1) + 1,1,1,2-TETRAFLUOROETHANE (2)

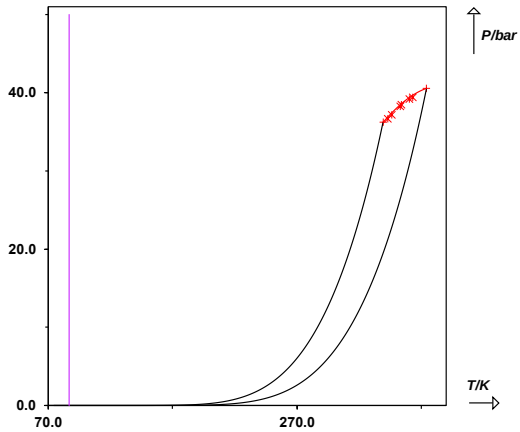
| | | |
|---|---|---|
| **CAS** | 354-33-6 | 811-97-2 |
| **InChiKey** | GTLACDSXYULKMZ-UHFFFAOYSA-N | LVGUZGTVOIAKKC-UHFFFAOYSA-N |
| **$T_c$ / K** | 339.17 | 374.18 |
| **$P_c$ / bar** | 36.20 | 40.56 |
| **ω** | 0.305 | 0.327 |

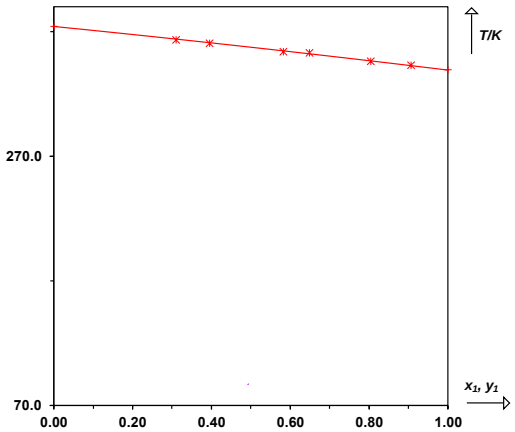
Ideal

**PPR78 results**

*Parameters*
A/MPa = 9.35
B/MPa = 28.4

*Deviations*
MAPE on x = 3.2 %
MAPE on y = 3.5 %
MAPE on $x_c$ = 5.2 %
MAPE on $P_c$ = 0.57 %



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**Isothermal phase equilibrium data**

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Nagel, M. - Bier, K., Vapor-liquid equilibriums of new refrigerant mixtures as alternatives to R 22 and R 502, DKV-Tagungsberichte (1993) 39-59.

**T / K = 203.15**

| P / bar | $y_1$ |
|---|---|
| 0.1415 | 0.5764 |
| 0.1907 | 0.7847 |
| 0.2461 | 0.9126 |

Nagel, M. - Bier, K., Vapor-liquid equilibriums of new refrigerant mixtures as alternatives to R 22 and R 502, DKV-Tagungsberichte (1993) 39-59.

**T / K = 203.15**

| P / bar | $x_1$ |
|---|---|
| 0.1410 | 0.2687 |
| 0.1913 | 0.4924 |
| 0.2458 | 0.7465 |

Nagel, M. - Bier, K., Vapor-liquid equilibriums of new refrigerant mixtures as alternatives to R 22 and R 502, DKV-Tagungsberichte (1993) 39-59.

**T / K = 243.15**

| P / bar | $y_1$ |
|---|---|
| 1.250 | 0.4850 |
| 1.578 | 0.7129 |
| 1.929 | 0.8793 |

Nagel, M. - Bier, K., Vapor-liquid equilibriums of new refrigerant mixtures as alternatives to R 22 and R 502, DKV-Tagungsberichte (1993) 39-59.

**T / K = 243.15**

| P / bar | $x_1$ |
|---|---|
| 1.247 | 0.2679 |
| 1.575 | 0.4897 |
| 1.929 | 0.7447 |

Kim, C.N. - Park, Y.M., Vapor–Liquid Equilibrium of HFC-32/134a And HFC-125/134a Systems, Int. J. Thermophys. 2 (1999) 519-530. doi:10.1023/A:1022605104490

**T / K = 263.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.537 | 0.1853 | 0.3513 |
| 2.946 | 0.3258 | 0.5324 |
| 3.450 | 0.5084 | 0.6921 |
| 3.750 | 0.6265 | 0.7770 |
| 4.317 | 0.8136 | 0.8947 |

Kobayashi, Masanao - Nishiumi, Hideo, Vapor–liquid equilibria for the pure, binary and ternary systems containing HFC32, HFC125 and HFC134a, Fluid Phase Equilibria 1-2 (1998) 191-202. doi:10.1016/S0378-3812(97)00257-4

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.080 | 0.0380 | 0.0770 |
| 3.410 | 0.1260 | 0.2250 |
| 3.900 | 0.2560 | 0.4140 |
| 4.380 | 0.3810 | 0.5570 |
| 4.920 | 0.5190 | 0.6930 |
| 5.420 | 0.6610 | 0.7950 |
| 5.910 | 0.7840 | 0.8790 |
| 6.330 | 0.8960 | 0.9440 |

Kim, C.N. - Park, Y.M., Vapor–Liquid Equilibrium of HFC-32/134a And HFC-125/134a Systems, Int. J. Thermophys. 2 (1999) 519-530. doi:10.1023/A:1022605104490

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.689 | 0.2000 | 0.3622 |
| 4.138 | 0.3258 | 0.5043 |
| 4.833 | 0.5061 | 0.6734 |
| 5.273 | 0.6228 | 0.7663 |
| 6.004 | 0.8120 | 0.8910 |

Kobayashi, Masanao - Nishiumi, Hideo, Vapor–liquid equilibria for the pure, binary and ternary systems containing HFC32, HFC125 and HFC134a, Fluid Phase Equilibria 1-2 (1998) 191-202. doi:10.1016/S0378-3812(97)00257-4

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.420 | 0.0490 | 0.0940 |
| 4.930 | 0.1600 | 0.2710 |
| 5.420 | 0.2640 | 0.4070 |
| 5.910 | 0.3600 | 0.5120 |
| 6.450 | 0.4720 | 0.6310 |
| 7.130 | 0.6090 | 0.7510 |
| 8.020 | 0.7860 | 0.8730 |
| 8.820 | 0.9440 | 0.9700 |

Kim, C.N. - Park, Y.M., Vapor–Liquid Equilibrium of HFC-32/134a And HFC-125/134a Systems, Int. J. Thermophys. 2 (1999) 519-530. doi:10.1023/A:1022605104490

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.139 | 0.1992 | 0.3516 |
| 5.826 | 0.3466 | 0.5064 |

| | | |
|---|---|---|
| 6.597 | 0.4884 | 0.6562 |
| 7.099 | 0.6084 | 0.7482 |
| 8.164 | 0.8102 | 0.8819 |

Kobayashi, Masanao - Nishiumi, Hideo, Vapor–liquid equilibria for the pure, binary and ternary systems containing HFC32, HFC125 and HFC134a, Fluid Phase Equilibria 1-2 (1998) 191-202. doi:10.1016/S0378-3812(97)00257-4

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.060 | 0.0550 | 0.0970 |
| 6.580 | 0.1370 | 0.2300 |
| 7.320 | 0.2550 | 0.3860 |
| 8.160 | 0.3810 | 0.5350 |
| 9.030 | 0.5260 | 0.6620 |
| 9.830 | 0.6570 | 0.7700 |
| 11.58 | 0.9310 | 0.9580 |

Kim, C.N. - Park, Y.M., Vapor–Liquid Equilibrium of HFC-32/134a And HFC-125/134a Systems, Int. J. Thermophys. 2 (1999) 519-530. doi:10.1023/A:1022605104490

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.813 | 0.1794 | 0.3081 |
| 7.793 | 0.3461 | 0.4836 |
| 8.718 | 0.4898 | 0.6324 |
| 9.935 | 0.6646 | 0.7782 |
| 10.84 | 0.8078 | 0.8767 |

Kim, C.N. - Park, Y.M., Vapor–Liquid Equilibrium of HFC-32/134a And HFC-125/134a Systems, Int. J. Thermophys. 2 (1999) 519-530. doi:10.1023/A:1022605104490

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.083 | 0.1786 | 0.2802 |
| 10.22 | 0.3298 | 0.4562 |
| 11.38 | 0.4737 | 0.6215 |
| 12.89 | 0.6597 | 0.7657 |
| 14.09 | 0.8075 | 0.8648 |

Nishiumi, Hideo - Ohno, Takahiro, High pressure vapor-liquid equilibria and critical loci for the HFC125-HFC134a system, Korean Journal of Chemical Engineering 6 (2000) 668-671. doi:10.1007/BF02699115

**T / K = 333.13**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 18.65 | 0.0715 | 0.1705 |
| 19.63 | 0.1685 | 0.3130 |
| 20.42 | 0.2660 | 0.3680 |
| 21.69 | 0.3650 | 0.4755 |
| 23.56 | 0.4910 | 0.5865 |
| 25.71 | 0.6435 | 0.7170 |
| 28.46 | 0.8050 | 0.8505 |
| 30.42 | 0.9380 | 0.9510 |

Nishiumi, Hideo - Ohno, Takahiro, High pressure vapor-liquid equilibria and critical loci for the HFC125-HFC134a system, Korean Journal of Chemical Engineering 6 (2000) 668-671. doi:10.1007/BF02699115

**T / K = 343.13**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 22.48 | 0.0990 | 0.1366 | |
| 24.12 | 0.2023 | 0.2670 | |
| 26.30 | 0.3210 | 0.3940 | |
| 28.02 | 0.4200 | 0.4910 | |
| 29.80 | 0.5153 | 0.5870 | |
| 31.38 | 0.6032 | 0.6643 | |
| 32.74 | 0.6748 | 0.7237 | |
| 34.44 | 0.7688 | 0.7995 | |
| 35.42 | 0.8199 | 0.8410 | |
| 36.69 | 0.9070 | 0.9070 | CRIT |

Nishiumi, Hideo - Ohno, Takahiro, High pressure vapor-liquid equilibria and critical loci for the HFC125-HFC134a system, Korean Journal of Chemical Engineering 6 (2000) 668-671. doi:10.1007/BF02699115

**T / K = 353.13**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 28.23 | 0.1120 | 0.1449 | |
| 28.51 | 0.1240 | 0.1585 | |
| 30.07 | 0.2050 | 0.2548 | |
| 31.60 | 0.2760 | 0.3320 | |
| 33.56 | 0.3700 | 0.4260 | |
| 35.37 | 0.4550 | 0.5050 | |
| 37.09 | 0.5395 | 0.5757 | |
| 38.22 | 0.6490 | 0.6490 | CRIT |

Nishiumi, Hideo - Ohno, Takahiro, High pressure vapor-liquid equilibria and critical loci for the HFC125-HFC134a system, Korean Journal of Chemical Engineering 6 (2000) 668-671. doi:10.1007/BF02699115

**T / K = 363.12**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.94 | 0.1132 | 0.1371 |
| 35.77 | 0.1483 | 0.1766 |
| 37.19 | 0.2022 | 0.2333 |

| | | |
|---|---|---|
| 38.07 | 0.2366 | 0.2677 |
| 39.25 | 0.2892 | 0.3095 |

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**Critical point**

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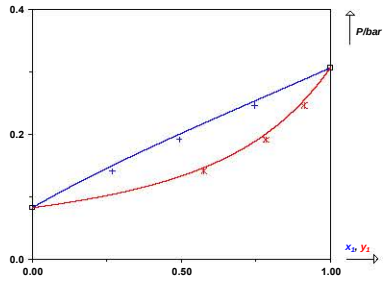
Kato, Ryo - Nishiumi, Hideo, Vapor–liquid equilibria and critical loci of binary and ternary systems composed of CH2F2, C2HF5 and C2H2F4, Fluid Phase Equilibria 1-2 (2006) 140-146. doi:10.1016/j.fluid.2006.07.017

| T / K | P / bar | $x_1$ |
|---|---|---|
| 346.08 | 37.20 | 0.8040 |
| 353.80 | 38.44 | 0.5830 |
| 360.50 | 39.16 | 0.3950 |

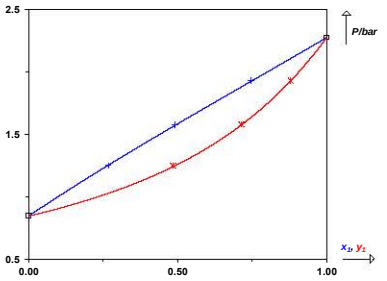
Nishiumi, Hideo - Ohno, Takahiro, High pressure vapor-liquid equilibria and critical loci for the HFC125-HFC134a system, Korean Journal of Chemical Engineering 6 (2000) 668-671. doi:10.1007/BF02699115

| T / K | P / bar | $x_1$ |
|---|---|---|
| 363.16 | 39.42 | 0.3095 |

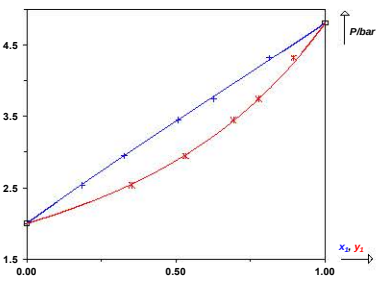
T/K = 203.15



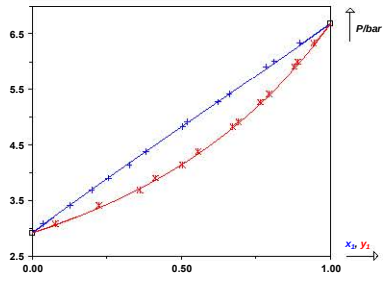

T/K = 243.15



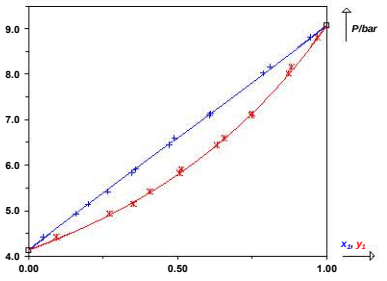

T/K = 263.15



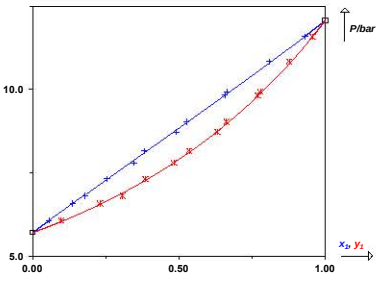

T/K = 273.15



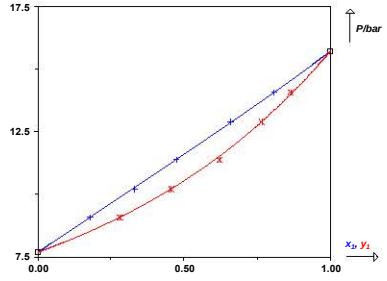

T/K = 283.15



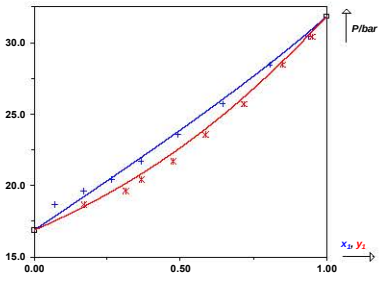

T/K = 293.15



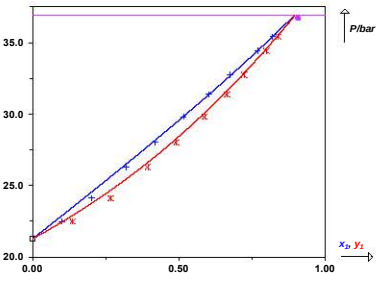

T/K = 303.15



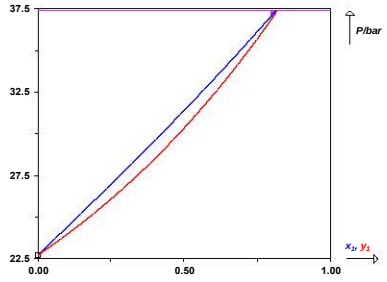

T/K = 333.13



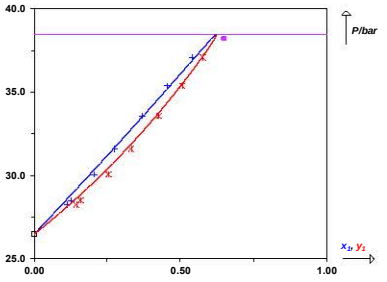

T/K = 343.13



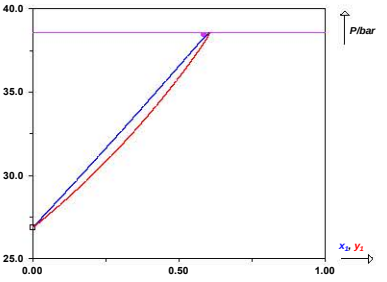

T/K = 346.08



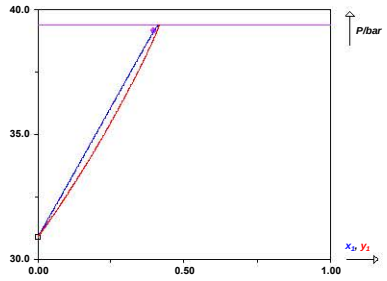

T/K = 353.13



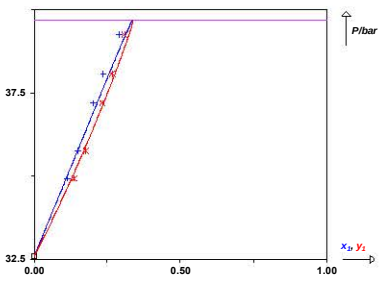

T/K = 353.80



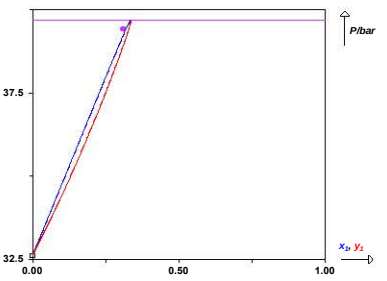

T/K = 360.50




T/K = 363.12




T/K = 363.16



## DIFLUOROMETHANE (1) + PENTAFLUOROETHANE (2)

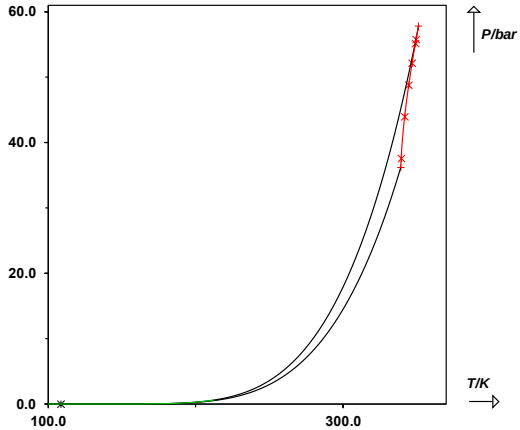
| | | |
|---|---|---|
| **CAS** | 75-10-5 | 354-33-6 |
| **InChiKey** | RWRIWBAIICGTTQ-UHFFFAOYSA-N | GTLACDSXYULKMZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 351.255 | 339.165 |
| **$P_c$ / bar** | 57.84 | 36.199 |
| **ω** | 0.277 | 0.305 |

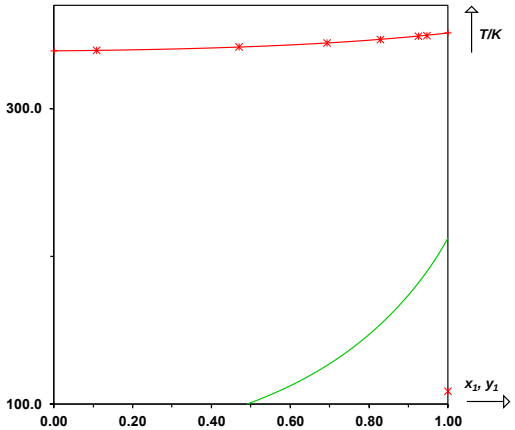
Ideal

**PPR78 results**

*Parameters*
A/MPa = 60.3
B/MPa = -8.45

*Deviations*
MAPE on $x_c$ = 1.8 %
MAPE on $P_c$ = 0.33 %
MAPE on $h^M$ = 22 %



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**Enthalpy of mixing**

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Horstmann, Sven - Wilken, Michael - Fischer, Kai - Gmehling, Jürgen, Isothermal Vapor−Liquid Equilibrium and Excess Enthalpy Data for the Binary Systems Propylene Oxide + 2-Methylpentane and Difluoromethane (R32) + Pentafluoroethane (R125), Journal of Chemical & Engineering Data 6 (2004) 1504-1507. doi:10.1021/je034253u

**T / K = 308.15**

**P / bar = 51.30**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 25.00 | 0.0880 |
| 50.00 | 0.1692 |
| 73.00 | 0.2444 |
| 95.00 | 0.3142 |
| 114.00 | 0.3792 |
| 129.00 | 0.4399 |
| 141.00 | 0.4967 |
| 150.00 | 0.5499 |
| 155.00 | 0.5999 |
| 157.00 | 0.6470 |
| 155.00 | 0.6913 |
| 150.00 | 0.7332 |
| 142.00 | 0.7729 |
| 130.00 | 0.8105 |
| 115.00 | 0.8461 |
| 97.00 | 0.8800 |
| 76.00 | 0.9122 |
| 52.00 | 0.9428 |
| 26.00 | 0.9721 |

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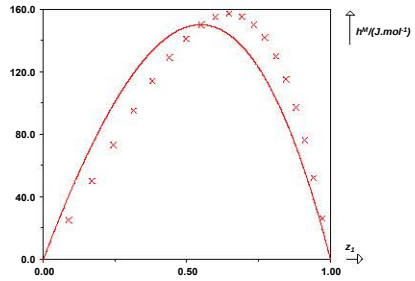
**Critical point**

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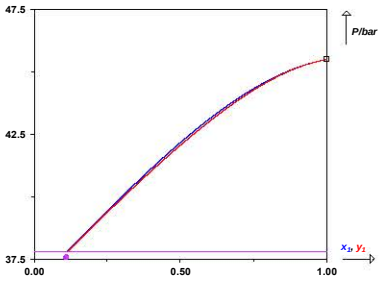
Kato, Ryo - Shirakawa, Katsushi - Nishiumi, Hideo, Critical locus and vapor–liquid equilibria of HFC32–HFC125 system, Fluid Phase Equilibria (2002) 995-1008. doi:10.1016/S0378-3812(01)00788-9

| T / K | P / bar | $x_1$ |
|---|---|---|
| 339.50 | 37.57 | 0.1090 |
| 341.74 | 43.95 | 0.4700 |
| 344.39 | 48.80 | 0.6930 |
| 346.74 | 52.14 | 0.8280 |
| 349.15 | 55.13 | 0.9250 |
| 349.60 | 55.76 | 0.9460 |

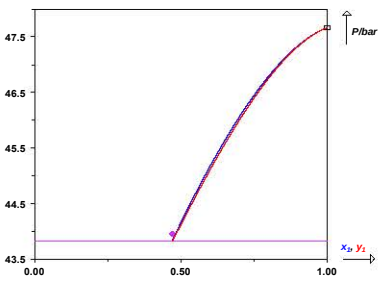
T/K = 308.15 - P/bar = 51.300



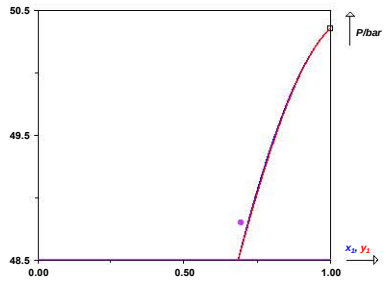

T/K = 339.50



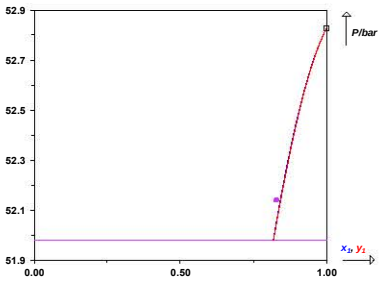

T/K = 341.74



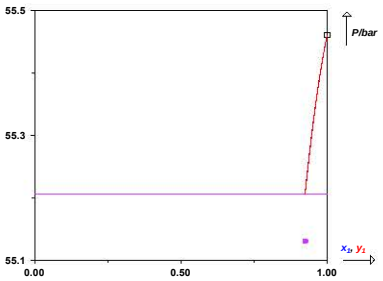

T/K = 344.39



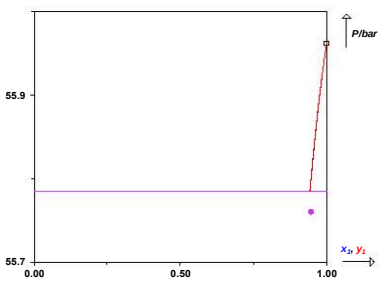

T/K = 346.74




T/K = 349.15




T/K = 349.60



## CHLORODIFLUOROMETHANE (1) + 1,1,1,2-TETRAFLUOROETHANE (2)

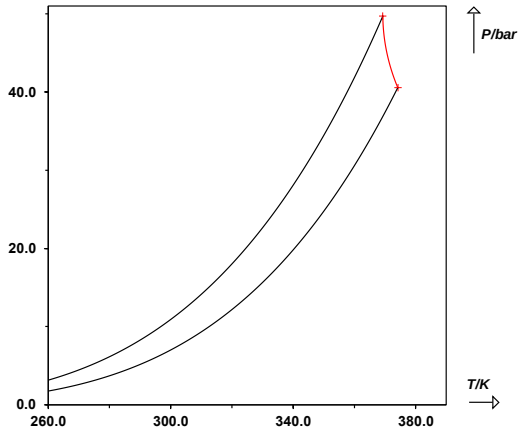
| | | |
|---|---|---|
| **CAS** | 75-45-6 | 811-97-2 |
| **InChiKey** | VOPWNXZWBYDODV-UHFFFAOYSA-N | LVGUZGTVOIAKKC-UHFFFAOYSA-N |
| **$T_c$ / K** | 369.30 | 374.18 |
| **$P_c$ / bar** | 49.71 | 40.56 |
| **ω** | 0.219 | 0.327 |

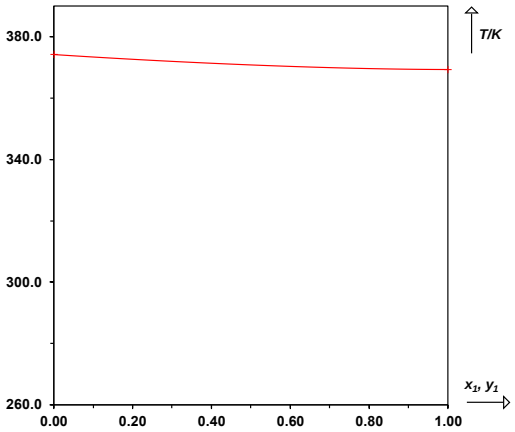
Ideal

**PPR78 results**

*Parameters*
A/MPa = 0.641
B/MPa = -10.1

*Deviations*
MAPE on x = 12 %
MAPE on y = 11 %



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**Isothermal phase equilibrium data**

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Arita, Koji - Tomizawa, Takeshi - Nagakawa, Yuko - Yoshida, Yuji, Vapour—liquid equilibrium of the non-azeotropic refrigerant mixture formed by chlorofluoromethane and 1,1,1,2-tetrafluoroethane, Fluid Phase Equilibria 1-2 (1991) 151-156. doi:10.1016/0378-3812(91)80027-S

**T / K = 298.16**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.011 | 0.2953 | 0.3895 |
| 8.973 | 0.5519 | 0.6436 |
| 9.636 | 0.7460 | 0.8041 |
| 9.872 | 0.8229 | 0.8631 |

Arita, Koji - Tomizawa, Takeshi - Nagakawa, Yuko - Yoshida, Yuji, Vapour—liquid equilibrium of the non-azeotropic refrigerant mixture formed by chlorofluoromethane and 1,1,1,2-tetrafluoroethane, Fluid Phase Equilibria 1-2 (1991) 151-156. doi:10.1016/0378-3812(91)80027-S

**T / K = 323.16**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.33 | 0.2995 | 0.3712 |
| 16.06 | 0.4031 | 0.4832 |
| 17.03 | 0.5657 | 0.6384 |
| 18.07 | 0.7430 | 0.7913 |
| 18.52 | 0.8247 | 0.8630 |

Nishiumi, Hideo - Komatsu, Masahiro - Yokoyama, Taichirou - Kohmatsu, Satoshi, Two- and three-phase equilibria and critical locus for the system of HCFC22-HFC134a, Fluid Phase Equilibria (1993) 109-117. doi:10.1016/0378-3812(93)87013-Q

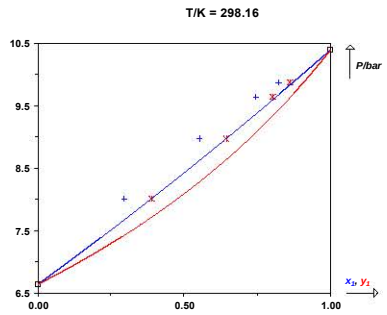
**T / K = 370.15**

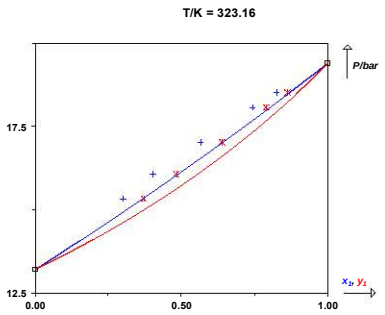
| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 39.61 | 0.1370 | 0.1470 |
| 41.03 | 0.2320 | 0.2440 |
| 42.35 | 0.3350 | 0.3490 |
| 43.63 | 0.4220 | 0.4330 |
| 44.51 | 0.4780 | 0.4840 |
| 44.62 | 0.4970 | 0.5010 |

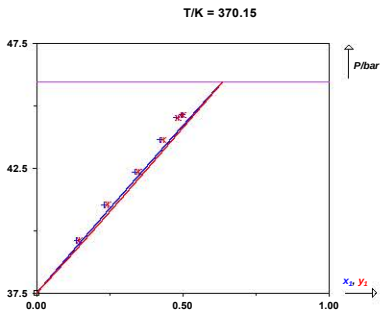
Nishiumi, Hideo - Komatsu, Masahiro - Yokoyama, Taichirou - Kohmatsu, Satoshi, Two- and three-phase equilibria and critical locus for the system of HCFC22-HFC134a, Fluid Phase Equilibria (1993) 109-117. doi:10.1016/0378-3812(93)87013-Q

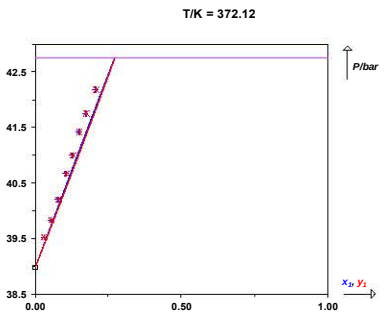
**T / K = 372.12**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 39.52 | 0.0310 | 0.0320 |
| 39.83 | 0.0530 | 0.0550 |
| 40.20 | 0.0760 | 0.0790 |
| 40.67 | 0.1040 | 0.1080 |
| 41.00 | 0.1240 | 0.1300 |
| 41.42 | 0.1480 | 0.1520 |
| 41.75 | 0.1710 | 0.1760 |
| 42.18 | 0.2050 | 0.2090 |


T/K = 298.16
10.5
9.5
8.5
7.5
6.5
P/bar
0.00
0.50
1.00
x1, y1


T/K = 323.16
17.5
12.5
P/bar
0.00
0.50
1.00
x1, y1


T/K = 370.15
47.5
42.5
37.5
P/bar
0.00
0.50
1.00
x1, y1


T/K = 372.12
42.5
41.5
40.5
39.5
38.5
P/bar
0.00
0.50
1.00
x1, y1

## DIFLUOROMETHANE (1) + 1,1,1,2-TETRAFLUOROETHANE (2)

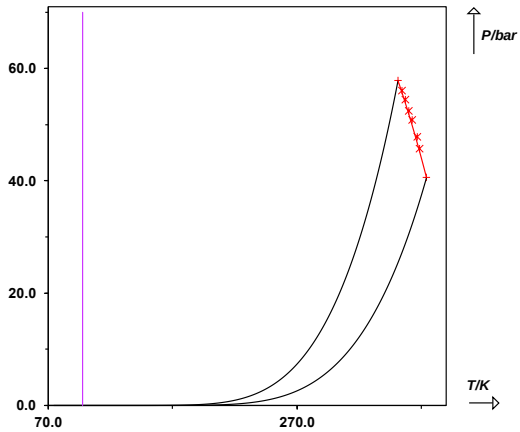
| | | |
|---|---|---|
| **CAS** | 75-10-5 | 811-97-2 |
| **InChiKey** | RWRIWBAIICGTTQ-UHFFFAOYSA-N | LVGUZGTVOIAKKC-UHFFFAOYSA-N |
| **$T_c$ / K** | 351.26 | 374.18 |
| **$P_c$ / bar** | 57.84 | 40.56 |
| **ω** | 0.277 | 0.327 |

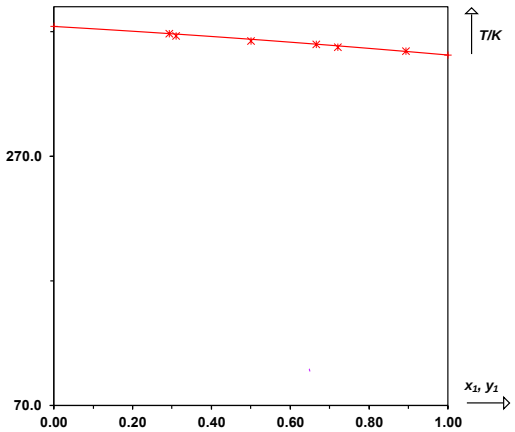
Ideal

**PPR78 results**

*Parameters*
A/MPa = 24.6
B/MPa = 66.5

*Deviations*
MAPE on x = 3.7 %
MAPE on y = 3.4 %
MAPE on $x_c$ = 7.4 %
MAPE on $P_c$ = 1.2 %



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**Isothermal phase equilibrium data**

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Nagel, M. - Bier, K., Vapor-liquid equilibriums of new refrigerant mixtures as alternatives to R 22 and R 502, DKV-Tagungsberichte (1993) 39-59.

**T / K = 203.15**

| P / bar | $y_1$ |
|---|---|
| 0.1492 | 0.5814 |
| 0.2301 | 0.8204 |
| 0.3006 | 0.9342 |

Nagel, M. - Bier, K., Vapor-liquid equilibriums of new refrigerant mixtures as alternatives to R 22 and R 502, DKV-Tagungsberichte (1993) 39-59.

**T / K = 203.15**

| P / bar | $x_1$ |
|---|---|
| 0.1487 | 0.2308 |
| 0.2296 | 0.5124 |
| 0.2989 | 0.7695 |

Nagel, M. - Bier, K., Vapor-liquid equilibriums of new refrigerant mixtures as alternatives to R 22 and R 502, DKV-Tagungsberichte (1993) 39-59.

**T / K = 253.15**

| P / bar | $y_1$ |
|---|---|
| 1.951 | 0.4615 |
| 2.721 | 0.7479 |
| 3.435 | 0.9054 |

Nagel, M. - Bier, K., Vapor-liquid equilibriums of new refrigerant mixtures as alternatives to R 22 and R 502, DKV-Tagungsberichte (1993) 39-59.

**T / K = 253.15**

| P / bar | $x_1$ |
|---|---|
| 1.945 | 0.2315 |
| 2.715 | 0.5117 |
| 3.437 | 0.7735 |

Kim, C.N. - Park, Y.M., Vapor–Liquid Equilibrium of HFC-32/134a And HFC-125/134a Systems, Int. J. Thermophys. 2 (1999) 519-530. doi:10.1023/A:1022605104490

**T / K = 263.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.758 | 0.2021 | 0.4004 |
| 3.490 | 0.4035 | 0.6249 |
| 4.250 | 0.5946 | 0.7798 |
| 5.021 | 0.7876 | 0.9053 |

Chung, Eui-Yeop - Kim, Min Soo, Vapor–Liquid Equilibria for the Difluoromethane (HFC-32) + 1,1,1,2-Tetrafluoroethane (HFC-134a) System, Journal of Chemical & Engineering Data 6 (1997) 1126-1128. doi:10.1021/je970071m

**T / K = 263.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.889 | 0.2245 | 0.4510 |
| 3.450 | 0.3919 | 0.6179 |
| 4.677 | 0.7001 | 0.8538 |

Cui, Xiaolong - Chen, Guangming - Li, Changsheng - Han, Xiaohong, Vapor–liquid equilibrium of difluoromethane +1,1,1,2-tetrafluoroethane systems over a temperature range from 258.15 to 343.15K, Fluid Phase Equilibria 1-2 (2006) 97-103. doi:10.1016/j.fluid.2006.09.017

**T / K = 263.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.934 | 0.2363 | 0.4534 |
| 3.175 | 0.3067 | 0.5335 |
| 3.552 | 0.3869 | 0.6368 |
| 3.964 | 0.4929 | 0.7423 |
| 4.255 | 0.5777 | 0.7978 |
| 4.667 | 0.6912 | 0.8623 |
| 4.927 | 0.7508 | 0.9053 |
| 5.219 | 0.8247 | 0.9313 |
| 5.387 | 0.8741 | 0.9519 |
| 5.526 | 0.9134 | 0.9640 |
| 5.628 | 0.9446 | 0.9749 |

Weber, L. A. - Silva, A. M., Design of a high-pressure ebulliometer, with vapor-liquid equilibrium results for the systems CHF2 Cl + CF3 CH3 and CF3 CH2 F + CH2F2, International Journal of Thermophysics 4 (1996) 873-888. doi:10.1007/BF01439194

**T / K = 280.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.399 | 0.1000 | 0.2240 |
| 5.073 | 0.2000 | 0.3910 |
| 5.745 | 0.3000 | 0.5210 |
| 6.411 | 0.4000 | 0.6250 |
| 7.065 | 0.5000 | 0.7100 |
| 7.704 | 0.6000 | 0.7810 |
| 8.324 | 0.7000 | 0.8420 |
| 8.923 | 0.8000 | 0.8970 |
| 9.503 | 0.9000 | 0.9480 |

Kobayashi, Masanao - Nishiumi, Hideo, Vapor–liquid equilibria for the pure, binary and ternary systems containing HFC32, HFC125 and HFC134a, Fluid Phase Equilibria 1-2 (1998) 191-202. doi:10.1016/S0378-3812(97)00257-4

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.220 | 0.0700 | 0.1270 |
| 6.670 | 0.1300 | 0.2340 |
| 7.470 | 0.2220 | 0.3590 |
| 8.330 | 0.3220 | 0.4790 |
| 9.240 | 0.4310 | 0.5890 |
| 10.76 | 0.5940 | 0.7340 |
| 12.01 | 0.7290 | 0.8330 |
| 13.07 | 0.8330 | 0.9040 |
| 13.30 | 0.8640 | 0.9210 |
| 13.54 | 0.8780 | 0.9310 |

Chung, Eui-Yeop - Kim, Min Soo, Vapor–Liquid Equilibria for the Difluoromethane (HFC-32) + 1,1,1,2-Tetrafluoroethane (HFC-134a) System, Journal of Chemical & Engineering Data 6 (1997) 1126-1128. doi:10.1021/je970071m

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.696 | 0.2376 | 0.4034 |
| 10.62 | 0.5757 | 0.7217 |
| 12.35 | 0.7599 | 0.8568 |

Shimawaki, S. - Fijii, K. - Higashi, Y., Precise Measurements of the Vapor-Liquid Equilibria (VLE) of HFC-32/134a Mixtures Using a New Apparatus, Int. J. Thermophys. 3 (2002) 801-808. doi:10.1023/A:1015407205188

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.848 | 0.1350 | 0.2564 |
| 8.052 | 0.2751 | 0.4587 |
| 8.449 | 0.3181 | 0.5024 |
| 9.270 | 0.4138 | 0.5992 |
| 10.22 | 0.5179 | 0.7031 |
| 11.04 | 0.6095 | 0.7645 |
| 11.42 | 0.6507 | 0.8034 |
| 13.75 | 0.8948 | 0.9473 |
| 13.97 | 0.9211 | 0.9608 |

Weber, L. A. - Silva, A. M., Design of a high-pressure ebulliometer, with vapor-liquid equilibrium results for the systems CHF2 Cl + CF3 CH3 and CF3 CH2 F + CH2F2, International Journal of Thermophysics 4 (1996) 873-888. doi:10.1007/BF01439194

**T / K = 300.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.005 | 0.1000 | 0.1930 |
| 9.022 | 0.2000 | 0.3510 |
| 10.07 | 0.3000 | 0.4820 |
| 11.15 | 0.4000 | 0.5920 |
| 12.26 | 0.5000 | 0.6840 |
| 13.38 | 0.6000 | 0.7630 |
| 14.49 | 0.7000 | 0.8320 |
| 15.60 | 0.8000 | 0.8920 |
| 16.68 | 0.9000 | 0.9460 |

Kato, Ryo - Nishiumi, Hideo, Vapor–liquid equilibria and critical loci of binary and ternary systems composed of CH2F2, C2HF5 and C2H2F4, Fluid Phase Equilibria 1-2 (2006) 140-146. doi:10.1016/j.fluid.2006.07.017

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.76 | 0.0610 | 0.1160 |
| 15.91 | 0.1790 | 0.3230 |
| 17.88 | 0.3140 | 0.4680 |
| 18.84 | 0.3680 | 0.5280 |
| 20.43 | 0.4630 | 0.6130 |
| 21.61 | 0.5240 | 0.6700 |
| 22.38 | 0.5640 | 0.7070 |
| 24.94 | 0.6920 | 0.8030 |

Kobayashi, Masanao - Nishiumi, Hideo, Vapor–liquid equilibria for the pure, binary and ternary systems containing HFC32, HFC125 and HFC134a, Fluid Phase Equilibria 1-2 (1998) 191-202. doi:10.1016/S0378-3812(97)00257-4

**T / K = 363.45**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 38.45 | 0.2020 | 0.2470 |
| 40.00 | 0.2570 | 0.2950 |
| 43.65 | 0.3570 | 0.4200 |
| 46.56 | 0.4330 | 0.4980 |
| 48.10 | 0.4780 | 0.4810 |

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**Critical point**

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Kato, Ryo - Nishiumi, Hideo, Vapor–liquid equilibria and critical loci of binary and ternary systems composed of CH2F2, C2HF5 and C2H2F4, Fluid Phase Equilibria 1-2 (2006) 140-146. doi:10.1016/j.fluid.2006.07.017

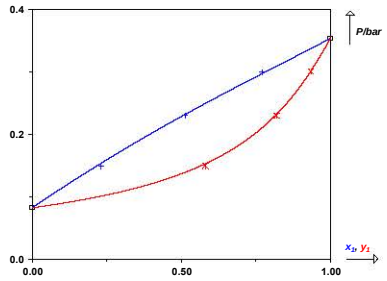
| T / K | P / bar | $x_1$ |
|---|---|---|
| 354.23 | 56.03 | 0.8930 |
| 359.80 | 52.40 | 0.6660 |
| 368.31 | 45.73 | 0.2930 |

Kordikowski, Andreas - Robertson, Duncan G. - Poliakoff, Martyn - DiNoia, Todd D. - McHugh, Mark - Aguiar-Ricardo, Ana, Acoustic Determination of the

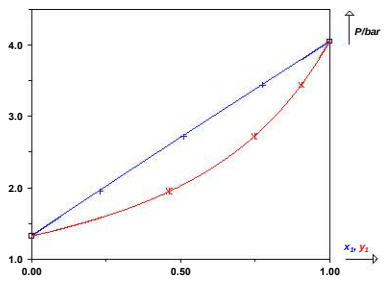
Critical Surfaces in the Ternary Systems CO2 + CH2F2 + CF3CH2F and CO + C2H4 + CH3CHCH2 and in Their Binary Subsystems, The Journal of Physical Chemistry B 30 (1997) 5853-5862. doi:10.1021/jp963061l

| T / K | P / bar | $x_1$ |
|---|---|---|
| 357.30 | 54.50 | 0.7200 |
| 362.50 | 50.80 | 0.5000 |
| 366.70 | 47.80 | 0.3100 |

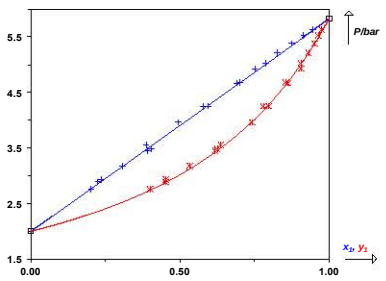
T/K = 203.15



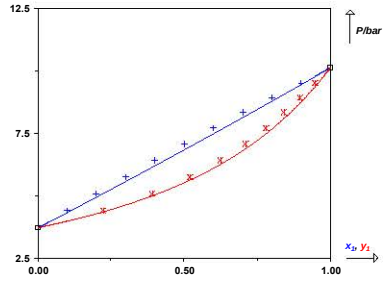

T/K = 253.15



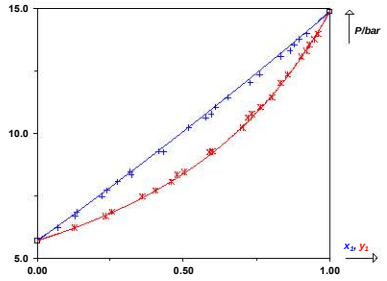

T/K = 263.15



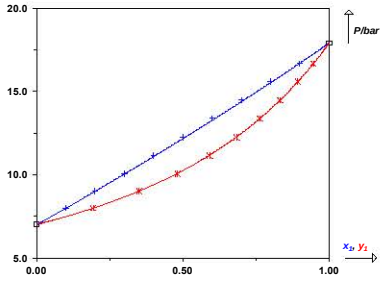

T/K = 280.00



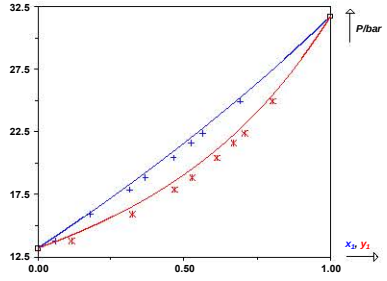

T/K = 293.15



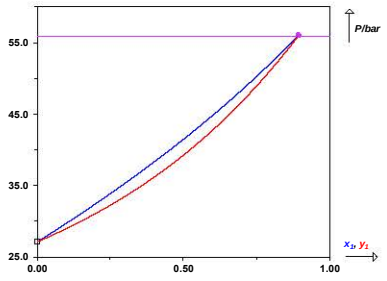

T/K = 300.00



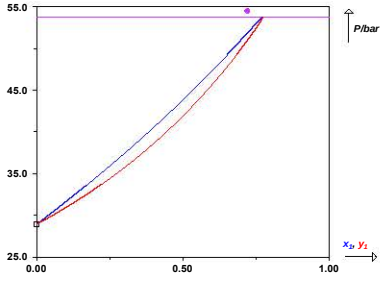

T/K = 323.15



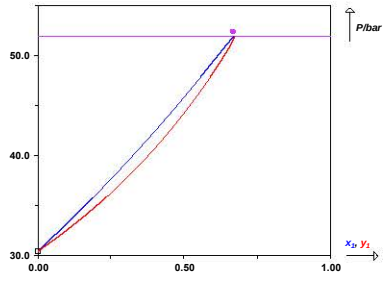

T/K = 354.23



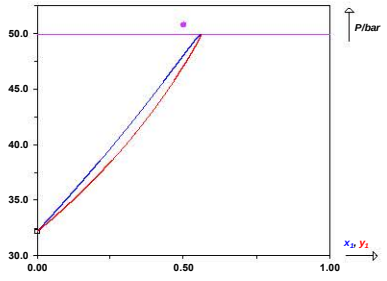

T/K = 357.30



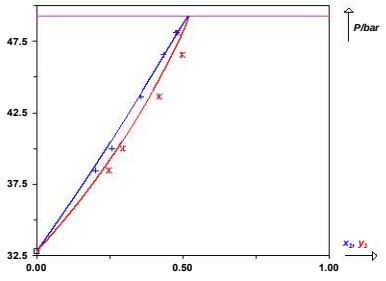

T/K = 359.80



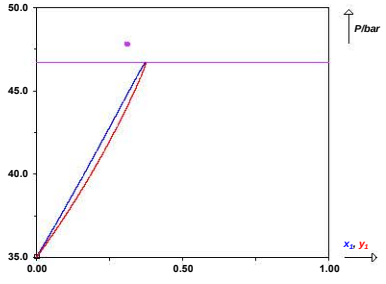

T/K = 362.50



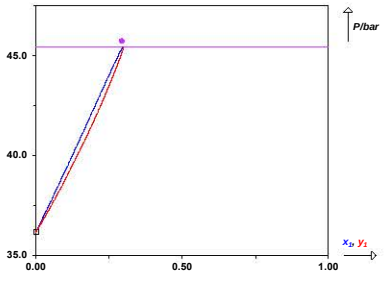

T/K = 363.45




T/K = 366.70




T/K = 368.31



## 1,1,1,2-TETRAFLUOROETHANE (1) + 1,1-DIFLUOROETHANE (2)

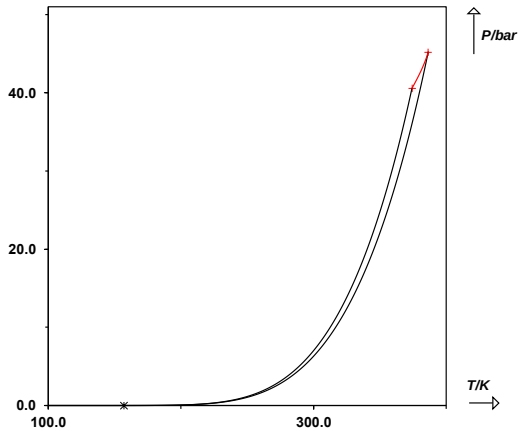
| | | |
|---|---|---|
| **CAS** | 811-97-2 | 75-37-6 |
| **InChiKey** | LVGUZGTVOIAKKC-UHFFFAOYSA-N | NPNPZTNLOVBDOC-UHFFFAOYSA-N |
| **$T_c$ / K** | 374.18 | 386.44 |
| **$P_c$ / bar** | 40.56 | 45.20 |
| **ω** | 0.327 | 0.275 |

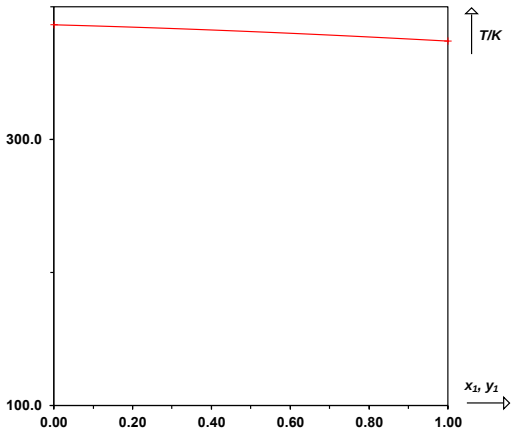
Ideal

**PPR78 results**

*Parameters*
A/MPa = -12.7
B/MPa = 9.89

*Deviations*
MAPE on x = 6.0 %
MAPE on y = 6.3 %



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**Isothermal phase equilibrium data**

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Kleiber, Michael, Vapor-liquid equilibria of binary refrigerant mixtures containing propylene or R134a, Fluid Phase Equilibria (1994) 149-194. doi:10.1016/0378-3812(94)80046-4

**T / K = 255.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.328 | 0.3147 | 0.3298 |
| 1.342 | 0.4489 | 0.4659 |
| 1.354 | 0.5495 | 0.5737 |
| 1.371 | 0.6580 | 0.6736 |
| 1.389 | 0.7594 | 0.7777 |
| 1.414 | 0.8843 | 0.8998 |

Kleiber, Michael, Vapor-liquid equilibria of binary refrigerant mixtures containing propylene or R134a, Fluid Phase Equilibria (1994) 149-194. doi:10.1016/0378-3812(94)80046-4

**T / K = 275.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.883 | 0.3225 | 0.3329 |
| 2.914 | 0.4483 | 0.4664 |
| 2.946 | 0.5502 | 0.5748 |
| 2.983 | 0.6648 | 0.6843 |
| 3.023 | 0.7590 | 0.7782 |
| 3.077 | 0.8874 | 0.8979 |

Kleiber, Michael, Vapor-liquid equilibria of binary refrigerant mixtures containing propylene or R134a, Fluid Phase Equilibria (1994) 149-194. doi:10.1016/0378-3812(94)80046-4

**T / K = 298.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.084 | 0.3195 | 0.3365 |
| 6.162 | 0.4460 | 0.4656 |
| 6.233 | 0.5498 | 0.5686 |
| 6.313 | 0.6626 | 0.6822 |
| 6.394 | 0.7575 | 0.7744 |
| 6.509 | 0.8828 | 0.8940 |
| 6.597 | 0.9777 | 0.9789 |

Shi, Y. - Wang, K. - Liu, H. - Hu, Y., Measurement of vapor-liquid equilibria for 1, 1, 1, 2-tetrafluoroethane-1, 1-difluoroethane binary system, Huadong Ligong Daxue Xuebao 5 (1995) 613-618.

**T / K = 303.09**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.877 | 0.0518 | 0.0554 |
| 6.915 | 0.1132 | 0.1211 |
| 6.963 | 0.1900 | 0.2022 |
| 7.024 | 0.2845 | 0.3007 |
| 7.087 | 0.3817 | 0.4003 |
| 7.155 | 0.4871 | 0.5067 |
| 7.208 | 0.5664 | 0.5862 |
| 7.291 | 0.6798 | 0.6994 |
| 7.339 | 0.7377 | 0.7567 |
| 7.414 | 0.8170 | 0.8339 |
| 7.449 | 0.8495 | 0.8652 |
| 7.554 | 0.9344 | 0.9436 |

Shi, Y. - Wang, K. - Liu, H. - Hu, Y., Measurement of vapor-liquid equilibria for 1, 1, 1, 2-tetrafluoroethane-1, 1-difluoroethane binary system, Huadong Ligong Daxue Xuebao 5 (1995) 613-618.

**T / K = 313.07**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.092 | 0.0518 | 0.0545 |
| 9.132 | 0.1131 | 0.1196 |
| 9.192 | 0.1897 | 0.2011 |
| 9.275 | 0.2841 | 0.3008 |
| 9.369 | 0.3804 | 0.4015 |
| 9.479 | 0.4858 | 0.5092 |
| 9.567 | 0.5653 | 0.5890 |
| 9.699 | 0.6788 | 0.7006 |
| 9.769 | 0.7369 | 0.7566 |
| 9.868 | 0.8164 | 0.8321 |
| 9.909 | 0.8491 | 0.8628 |
| 10.02 | 0.9344 | 0.9412 |

Tillner-Roth, R., An experimental study of the thermodynamic properties of the refrigerant mixture: {1,1,1,2-tetrafluoroethane (R 134a) + 1,1-difluoroethane (R 152a)}, The Journal of Chemical Thermodynamics 12 (1993) 1419-1441. doi:10.1006/jcht.1993.1144

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 12.00 | 0.2416 | 0.2527 |
| 12.31 | 0.4985 | 0.5279 |
| 12.69 | 0.7500 | 0.7665 |

Tillner-Roth, R., An experimental study of the thermodynamic properties of the refrigerant mixture: {1,1,1,2-tetrafluoroethane (R 134a) + 1,1-difluoroethane (R 152a)}, The Journal of Chemical Thermodynamics 12 (1993) 1419-1441. doi:10.1006/jcht.1993.1144

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.32 | 0.2410 | 0.2558 |
| 15.72 | 0.4990 | 0.5155 |
| 16.20 | 0.7495 | 0.7647 |

Tillner-Roth, R., An experimental study of the thermodynamic properties of the refrigerant mixture: {1,1,1,2-tetrafluoroethane (R 134a) + 1,1-difluoroethane (R 152a)}, The Journal of Chemical Thermodynamics 12 (1993) 1419-1441. doi:10.1006/jcht.1993.1144

| **T / K =** | **343.15** | |
|---|---|---|
| P / bar | $x_1$ | $y_1$ |
| 19.28 | 0.2409 | 0.2532 |
| 19.80 | 0.4986 | 0.5152 |
| 20.41 | 0.7495 | 0.7634 |

Tillner-Roth, R., An experimental study of the thermodynamic properties of the refrigerant mixture: {1,1,1,2-tetrafluoroethane (R 134a) + 1,1-difluoroethane (R 152a)}, The Journal of Chemical Thermodynamics 12 (1993) 1419-1441. doi:10.1006/jcht.1993.1144

| **T / K =** | **353.15** | |
|---|---|---|
| P / bar | $x_1$ | $y_1$ |
| 23.97 | 0.2402 | 0.2541 |
| 24.63 | 0.4978 | 0.5165 |
| 25.39 | 0.7492 | 0.7619 |

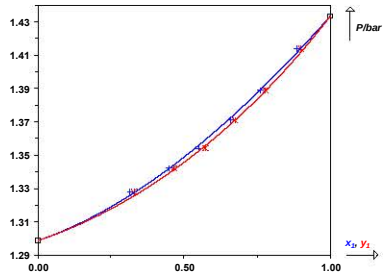
Tillner-Roth, R., An experimental study of the thermodynamic properties of the refrigerant mixture: {1,1,1,2-tetrafluoroethane (R 134a) + 1,1-difluoroethane (R 152a)}, The Journal of Chemical Thermodynamics 12 (1993) 1419-1441. doi:10.1006/jcht.1993.1144

| **T / K =** | **363.15** | |
|---|---|---|
| P / bar | $x_1$ | $y_1$ |
| 29.49 | 0.2400 | 0.2512 |
| 30.33 | 0.4978 | 0.5165 |
| 31.29 | 0.7487 | 0.7608 |

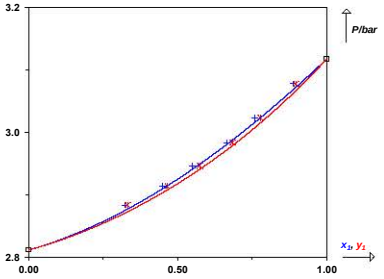
Tillner-Roth, R., An experimental study of the thermodynamic properties of the refrigerant mixture: {1,1,1,2-tetrafluoroethane (R 134a) + 1,1-difluoroethane (R 152a)}, The Journal of Chemical Thermodynamics 12 (1993) 1419-1441. doi:10.1006/jcht.1993.1144

| **T / K =** | **373.15** | |
|---|---|---|
| P / bar | $x_1$ | $y_1$ |
| 35.98 | 0.2402 | 0.2474 |
| 37.05 | 0.4959 | 0.5058 |

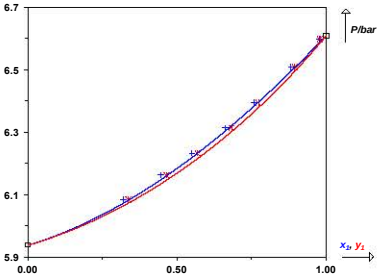
T/K = 255.00



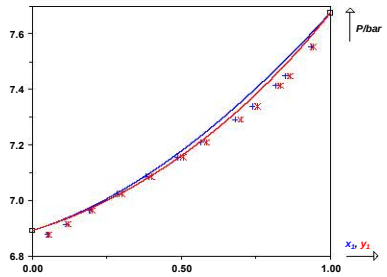

T/K = 275.00



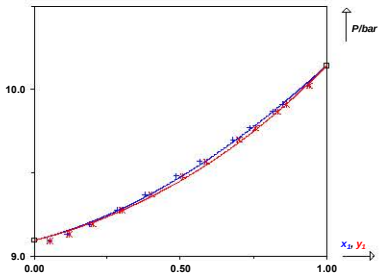

T/K = 298.00



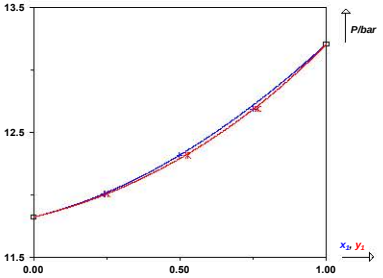

T/K = 303.09



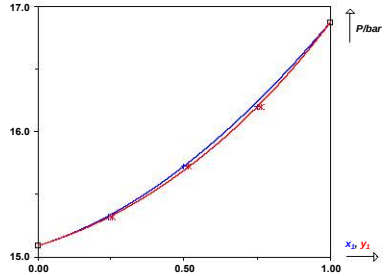

T/K = 313.07



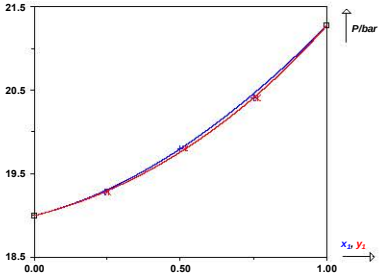

T/K = 323.15



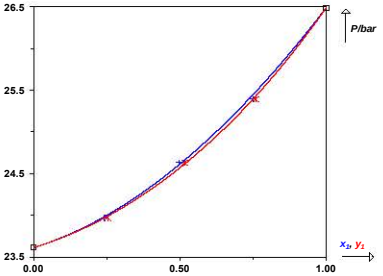

T/K = 333.15



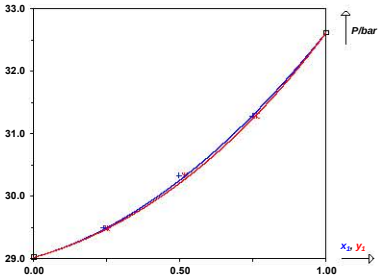

T/K = 343.15



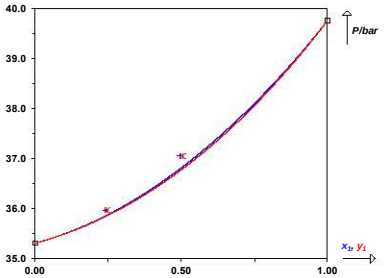

T/K = 353.15




T/K = 363.15




T/K = 373.15



## ETHYL ACETATE (1) + 1,4-DIOXANE (2)

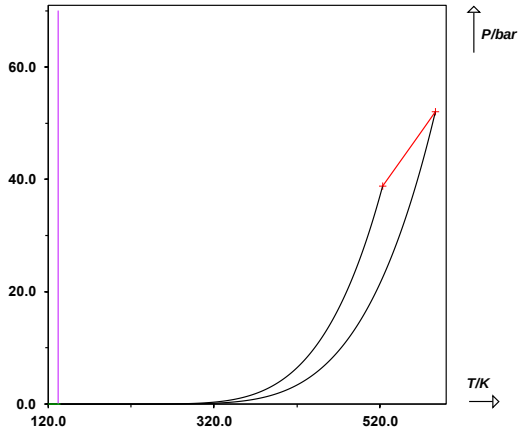
| | | |
|---|---|---|
| **CAS** | 141-78-6 | 123-91-1 |
| **InChiKey** | XEKOWRVHYACXOJ-UHFFFAOYSA-N | RYHBNJHYFVUHQT-UHFFFAOYSA-N |
| **$T_c$ / K** | 523.30 | 587.00 |
| **$P_c$ / bar** | 38.80 | 52.081 |
| **ω** | 0.366 | 0.279 |

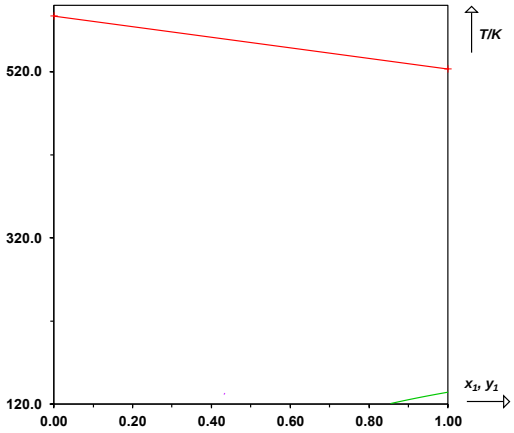
Ideal

**PPR78 results**

*Parameters*
A/MPa = 21.8
B/MPa = 70.2

*Deviations*
MAPE on x = 6.4 %
MAPE on y = 7.9 %
MAPE on $h^M$ = 4.4 %



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**Isothermal phase equilibrium data**

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Steinbrecher, M. - Bittrich, H.-J., Das isotherme Flüssigkeits-Dampf-Gleichgewicht der binären Systeme zwischen den Komponenten Tetrachlormethan, Äthylacetat und Dioxan, Zeitschrift für Physikalische Chemie 1 (1966) doi:10.1515/zpch-1966-23228

**T / K = 293.15**

| P / bar | $y_1$ |
|---|---|
| 0.0385 | 0.0600 |
| 0.0407 | 0.1230 |
| 0.0405 | 0.1370 |
| 0.0428 | 0.2030 |
| 0.0468 | 0.2990 |
| 0.0485 | 0.3470 |
| 0.0547 | 0.4720 |
| 0.0552 | 0.5180 |
| 0.0580 | 0.5380 |
| 0.0641 | 0.6230 |
| 0.0659 | 0.6540 |
| 0.0716 | 0.7130 |
| 0.0792 | 0.8090 |
| 0.0849 | 0.8800 |
| 0.0953 | 0.9740 |

Steinbrecher, M. - Bittrich, H.-J., Das isotherme Flüssigkeits-Dampf-Gleichgewicht der binären Systeme zwischen den Komponenten Tetrachlormethan, Äthylacetat und Dioxan, Zeitschrift für Physikalische Chemie 1 (1966) doi:10.1515/zpch-1966-23228

**T / K = 293.15**

| P / bar | $x_1$ |
|---|---|
| 0.0425 | 0.0600 |
| 0.0479 | 0.1230 |
| 0.0485 | 0.1370 |
| 0.0528 | 0.2030 |
| 0.0593 | 0.2990 |
| 0.0623 | 0.3470 |
| 0.0701 | 0.4720 |
| 0.0723 | 0.5180 |
| 0.0744 | 0.5380 |
| 0.0791 | 0.6230 |
| 0.0801 | 0.6540 |
| 0.0829 | 0.7130 |
| 0.0880 | 0.8090 |
| 0.0915 | 0.8800 |
| 0.0968 | 0.9740 |

Engelmann, K. - Bittrich, H.J., Estimation of isothermal mixing functions from isobaric liquid-vapor equilibriums, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1969) 213-218.

**T / K = 335.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2666 | 0.0039 | 0.0109 |
| 0.3333 | 0.1605 | 0.3271 |
| 0.4000 | 0.3484 | 0.5538 |
| 0.4666 | 0.5466 | 0.7333 |
| 0.6000 | 0.9658 | 0.9837 |

Engelmann, K. - Bittrich, H.J., Estimation of isothermal mixing functions from isobaric liquid-vapor equilibriums, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1969) 213-218.

**T / K = 340.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3333 | 0.0233 | 0.0578 |
| 0.4000 | 0.1566 | 0.3159 |
| 0.4666 | 0.3201 | 0.5227 |
| 0.6000 | 0.6624 | 0.8077 |
| 0.6666 | 0.8226 | 0.9065 |

Engelmann, K. - Bittrich, H.J., Estimation of isothermal mixing functions from isobaric liquid-vapor equilibriums, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1969) 213-218.

**T / K = 345.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4000 | 0.0200 | 0.0514 |
| 0.4666 | 0.1397 | 0.2822 |
| 0.6000 | 0.4117 | 0.6061 |
| 0.6666 | 0.5443 | 0.7214 |
| 0.7999 | 0.8391 | 0.9142 |
| 0.8666 | 0.9890 | 0.9933 |

Engelmann, K. - Bittrich, H.J., Estimation of isothermal mixing functions from isobaric liquid-vapor equilibriums, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1969) 213-218.

**T / K = 350.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4666 | 0.0042 | 0.0108 |
| 0.6000 | 0.2107 | 0.3807 |
| 0.6666 | 0.3212 | 0.5136 |
| 0.7999 | 0.5641 | 0.7357 |
| 0.8666 | 0.6737 | 0.8110 |
| 0.9333 | 0.8096 | 0.8969 |
| 1.013 | 0.9698 | 0.9833 |

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**Isobaric phase equilibrium data**

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Engelmann, K. - Bittrich, H.J., Isobaric liquid-vapor equilibriums of the system diethylamine-ethyl acetate, diethylamine-1,4-dioxane and ethyl acetate-1,4-dioxane at reduced pressures, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 289-291.

**P / bar = 0.2666**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 334.70 | 0.0230 | 0.0670 |
| 333.55 | 0.0520 | 0.1320 |
| 332.45 | 0.0850 | 0.1990 |
| 331.20 | 0.1220 | 0.2650 |
| 329.65 | 0.1750 | 0.3500 |
| 328.20 | 0.2300 | 0.4240 |
| 326.15 | 0.3160 | 0.5220 |
| 324.50 | 0.3970 | 0.6000 |
| 322.70 | 0.4850 | 0.6810 |
| 320.90 | 0.5830 | 0.7600 |
| 319.20 | 0.6890 | 0.8300 |
| 317.60 | 0.7950 | 0.8910 |
| 316.60 | 0.8640 | 0.9310 |
| 315.70 | 0.9280 | 0.9660 |

Engelmann, K. - Bittrich, H.J., Isobaric liquid-vapor equilibriums of the system diethylamine-ethyl acetate, diethylamine-1,4-dioxane and ethyl acetate-1,4-dioxane at reduced pressures, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 289-291.

**P / bar = 0.5333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 353.70 | 0.0180 | 0.0550 |
| 352.25 | 0.0550 | 0.1360 |
| 351.20 | 0.0850 | 0.1930 |
| 349.75 | 0.1290 | 0.2690 |
| 348.45 | 0.1700 | 0.3340 |
| 347.05 | 0.2160 | 0.4000 |
| 345.20 | 0.2840 | 0.4850 |
| 343.25 | 0.3640 | 0.5710 |
| 341.50 | 0.4460 | 0.6470 |
| 340.15 | 0.5100 | 0.7000 |
| 338.20 | 0.6110 | 0.7760 |
| 336.50 | 0.7060 | 0.8400 |
| 335.15 | 0.7920 | 0.8910 |
| 334.00 | 0.8650 | 0.9320 |
| 333.05 | 0.9310 | 0.9660 |

Engelmann, K. - Bittrich, H.J., Isobaric liquid-vapor equilibriums of the system diethylamine-ethyl acetate, diethylamine-1,4-dioxane and ethyl acetate-1,4-dioxane at reduced pressures, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 289-291.

**P / bar = 0.7999**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 366.05 | 0.0200 | 0.0440 |
| 365.45 | 0.0370 | 0.0800 |
| 364.65 | 0.0580 | 0.1260 |
| 363.85 | 0.0820 | 0.1700 |
| 362.15 | 0.1280 | 0.2500 |
| 360.65 | 0.1740 | 0.3210 |
| 359.20 | 0.2230 | 0.3890 |
| 358.00 | 0.2650 | 0.4430 |
| 356.15 | 0.3340 | 0.5200 |
| 354.35 | 0.4050 | 0.5990 |
| 352.65 | 0.4740 | 0.6640 |
| 351.05 | 0.5500 | 0.7260 |
| 349.65 | 0.6240 | 0.7800 |
| 348.20 | 0.7060 | 0.8360 |
| 346.65 | 0.7880 | 0.8820 |
| 345.35 | 0.8680 | 0.9310 |
| 344.35 | 0.9260 | 0.9640 |

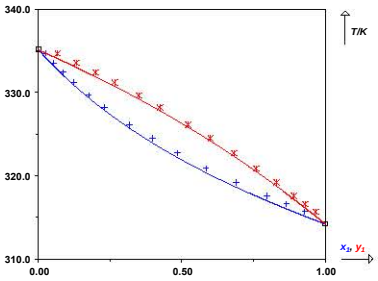
Engelmann, K. - Bittrich, H.J., Isobaric liquid-vapor equilibriums of the systems diethylamine/ethyl acetate, diethylamine/1,4-dioxane, and ethyl acetate /1,4-dioxane at 760 mm, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 148-153.

**P / bar = 1.013**

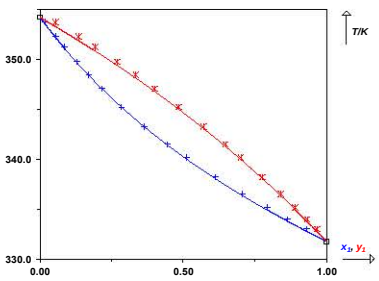
| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 372.90 | 0.0420 | 0.0900 |
| 372.40 | 0.0580 | 0.1200 |
| 371.80 | 0.0690 | 0.1430 |
| 371.45 | 0.0790 | 0.1620 |
| 370.75 | 0.1020 | 0.1980 |
| 370.10 | 0.1170 | 0.2260 |
| 369.45 | 0.1340 | 0.2570 |
| 368.65 | 0.1560 | 0.2910 |
| 367.95 | 0.1810 | 0.3220 |
| 367.00 | 0.2110 | 0.3630 |
| 366.05 | 0.2390 | 0.4150 |
| 364.90 | 0.2810 | 0.4510 |
| 363.95 | 0.3150 | 0.4980 |
| 362.95 | 0.3500 | 0.5290 |
| 361.95 | 0.3900 | 0.5720 |
| 360.95 | 0.4320 | 0.6150 |
| 359.95 | 0.4760 | 0.6550 |
| 358.95 | 0.5160 | 0.6930 |

| | | |
|---|---|---|
| 358.00 | 0.5670 | 0.7290 |
| 356.85 | 0.6240 | 0.7740 |
| 355.85 | 0.6780 | 0.8110 |
| 354.75 | 0.7280 | 0.8470 |
| 353.35 | 0.8120 | 0.8970 |
| 352.05 | 0.8900 | 0.9420 |

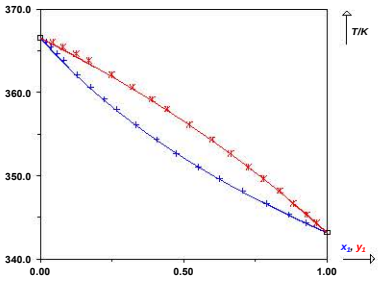
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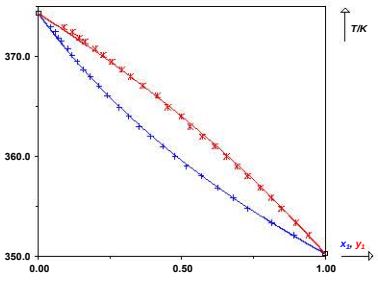

P/bar = 0.53329



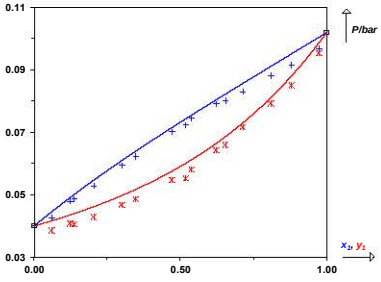

P/bar = 0.79993



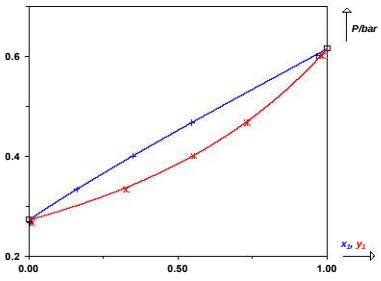

P/bar = 1.01330



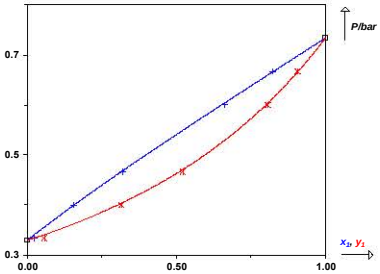

T/K = 293.15



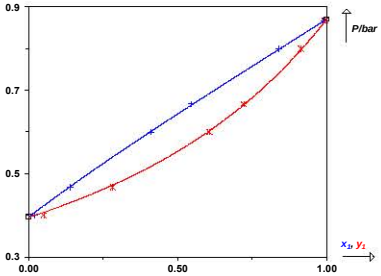

T/K = 335.65



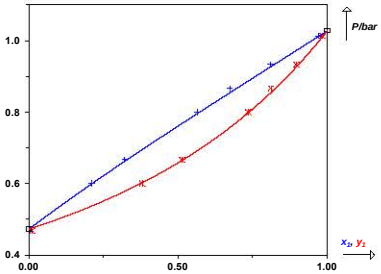

T/K = 340.65




T/K = 345.65




T/K = 350.65



## DIMETHYL CARBONATE (1) + DIETHYL CARBONATE (2)

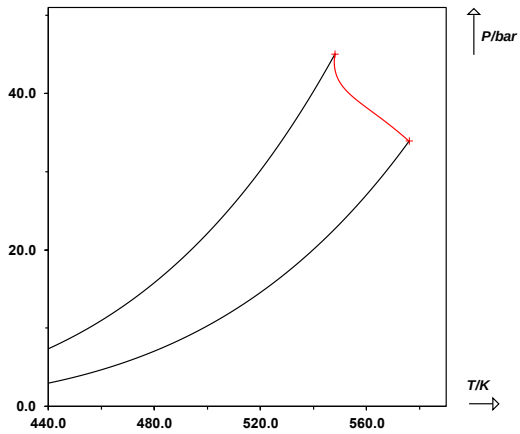
| | | |
|---|---|---|
| **CAS** | 616-38-6 | 105-58-8 |
| **InChiKey** | IEJIGPNLZYLLBP-UHFFFAOYSA-N | OIFBSDVPJOWBCH-UHFFFAOYSA-N |
| **$T_c$ / K** | 548.00 | 576.00 |
| **$P_c$ / bar** | 45.00 | 33.90 |
| **ω** | 0.385 | 0.486 |

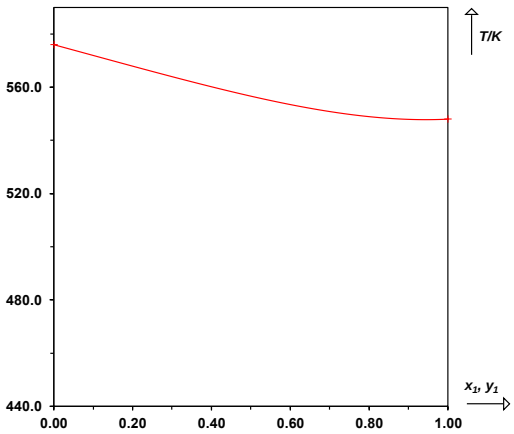
Ideal

**PPR78 results**

*Parameters*
A/MPa = 64
B/MPa = 21.1

*Deviations*
MAPE on x = 14 %
MAPE on y = 18 %
MAPE on $h^M$ = 7.8 %



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**Isothermal phase equilibrium data**

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Comelli, Fabio - Francesconi, Romolo - Ottani, Stefano, Isothermal Vapor−Liquid Equilibria of Dimethyl Carbonate + Diethyl Carbonate in the Range (313.15 to 353.15) K, Journal of Chemical & Engineering Data 3 (1996) 534-536. doi:10.1021/je950287t

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0390 | 0.0250 | 0.1210 |
| 0.0480 | 0.0900 | 0.3360 |
| 0.0515 | 0.1160 | 0.3980 |
| 0.0575 | 0.1570 | 0.4850 |
| 0.0640 | 0.2160 | 0.5760 |
| 0.0715 | 0.2770 | 0.6510 |
| 0.0805 | 0.3490 | 0.7110 |
| 0.0890 | 0.4280 | 0.7700 |
| 0.0995 | 0.5040 | 0.8240 |
| 0.1075 | 0.5830 | 0.8620 |
| 0.1170 | 0.6580 | 0.8950 |
| 0.1235 | 0.7270 | 0.9200 |
| 0.1335 | 0.8030 | 0.9440 |
| 0.1470 | 0.9350 | 0.9830 |

Comelli, Fabio - Francesconi, Romolo - Ottani, Stefano, Isothermal Vapor−Liquid Equilibria of Dimethyl Carbonate + Diethyl Carbonate in the Range (313.15 to 353.15) K, Journal of Chemical & Engineering Data 3 (1996) 534-536. doi:10.1021/je950287t

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0650 | 0.0270 | 0.1150 |
| 0.0810 | 0.1040 | 0.3460 |
| 0.0885 | 0.1510 | 0.4450 |
| 0.0975 | 0.2010 | 0.5320 |
| 0.1130 | 0.2800 | 0.6430 |
| 0.1210 | 0.3250 | 0.6800 |
| 0.1290 | 0.3710 | 0.7190 |
| 0.1450 | 0.4620 | 0.7850 |
| 0.1600 | 0.5430 | 0.8320 |
| 0.1690 | 0.5940 | 0.8600 |
| 0.1820 | 0.6600 | 0.8910 |
| 0.1940 | 0.7330 | 0.9160 |
| 0.2060 | 0.8090 | 0.9440 |
| 0.2190 | 0.8880 | 0.9680 |
| 0.2305 | 0.9730 | 0.9920 |

Comelli, Fabio - Francesconi, Romolo - Ottani, Stefano, Isothermal Vapor−Liquid Equilibria of Dimethyl Carbonate + Diethyl Carbonate in the Range (313.15 to 353.15) K, Journal of Chemical & Engineering Data 3 (1996) 534-536. doi:10.1021/je950287t

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1100 | 0.0630 | 0.2060 |
| 0.1180 | 0.0930 | 0.2860 |
| 0.1443 | 0.1830 | 0.4750 |
| 0.1650 | 0.2550 | 0.5810 |
| 0.1895 | 0.3440 | 0.6840 |
| 0.2005 | 0.3860 | 0.7220 |
| 0.2175 | 0.4490 | 0.7670 |
| 0.2360 | 0.5150 | 0.8120 |
| 0.2515 | 0.5710 | 0.8440 |
| 0.2705 | 0.6460 | 0.8800 |
| 0.2880 | 0.7110 | 0.9080 |
| 0.3040 | 0.7840 | 0.9300 |
| 0.3140 | 0.8260 | 0.9460 |
| 0.3360 | 0.9270 | 0.9760 |

Comelli, Fabio - Francesconi, Romolo - Ottani, Stefano, Isothermal Vapor−Liquid Equilibria of Dimethyl Carbonate + Diethyl Carbonate in the Range (313.15 to 353.15) K, Journal of Chemical & Engineering Data 3 (1996) 534-536. doi:10.1021/je950287t

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1560 | 0.0300 | 0.1000 |
| 0.1740 | 0.0670 | 0.2150 |
| 0.1880 | 0.1000 | 0.3010 |
| 0.2140 | 0.1620 | 0.4250 |
| 0.2390 | 0.2300 | 0.5430 |
| 0.2600 | 0.2800 | 0.6050 |
| 0.2760 | 0.3270 | 0.6470 |
| 0.3070 | 0.4040 | 0.7210 |
| 0.3775 | 0.5740 | 0.8320 |
| 0.4005 | 0.6300 | 0.8600 |
| 0.4180 | 0.6720 | 0.8840 |
| 0.4420 | 0.7420 | 0.9100 |
| 0.4730 | 0.8280 | 0.9440 |
| 0.4825 | 0.8620 | 0.9560 |
| 0.4960 | 0.9080 | 0.9720 |
| 0.5035 | 0.9350 | 0.9800 |

Comelli, Fabio - Francesconi, Romolo - Ottani, Stefano, Isothermal Vapor−Liquid Equilibria of Dimethyl Carbonate + Diethyl Carbonate in the Range (313.15 to 353.15) K, Journal of Chemical & Engineering Data 3 (1996) 534-536. doi:10.1021/je950287t

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|

| | | |
|---|---|---|
| 0.2400 | 0.0430 | 0.1500 |
| 0.2855 | 0.1190 | 0.3380 |
| 0.3120 | 0.1700 | 0.4250 |
| 0.3520 | 0.2410 | 0.5380 |
| 0.3705 | 0.2750 | 0.5800 |
| 0.3945 | 0.3240 | 0.6220 |
| 0.4525 | 0.4200 | 0.7190 |
| 0.4800 | 0.4750 | 0.7570 |
| 0.5185 | 0.5430 | 0.8000 |
| 0.5765 | 0.6670 | 0.8660 |
| 0.6100 | 0.7270 | 0.8970 |
| 0.6380 | 0.7830 | 0.9250 |
| 0.6730 | 0.8500 | 0.9500 |
| 0.7000 | 0.9040 | 0.9680 |

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**Isobaric phase equilibrium data**

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Zhao, X. - Yang, Y. - Guo, R., Measurement and correlation for vapor-liquid equilibrium of binary system for dimethyl carbonate-diethyl carbonate, Huaxue Gongcheng 8 (2008) 44-46.

**P / bar = 1.0000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 397.20 | 0.0477 | 0.0981 |
| 396.00 | 0.0776 | 0.1530 |
| 394.40 | 0.1168 | 0.2324 |
| 391.60 | 0.1887 | 0.3594 |
| 374.60 | 0.6356 | 0.8531 |
| 373.40 | 0.6664 | 0.8737 |
| 372.30 | 0.6984 | 0.8863 |
| 370.50 | 0.7568 | 0.9175 |
| 369.90 | 0.7761 | 0.9237 |
| 368.70 | 0.8128 | 0.9432 |
| 367.50 | 0.8546 | 0.9624 |
| 366.40 | 0.8897 | 0.9724 |
| 365.10 | 0.9365 | 0.9870 |
| 364.00 | 0.9776 | 0.9977 |

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**Enthalpy of mixing**

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Francesconi, Romolo - Comelli, Fabio, Excess Molar Enthalpies, Densities, and Excess Molar Volumes of Binary Mixtures Containing Esters of Carbonic Acid at 298.15 and 313.15 K, Journal of Chemical & Engineering Data 4 (1995) 811-814. doi:10.1021/je00020a016

**T / K = 298.15**

**P / bar = 1.010**

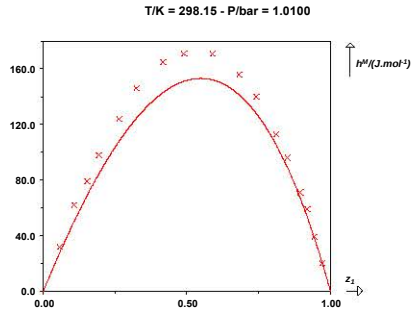
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 32.00 | 0.0565 |
| 62.00 | 0.1070 |
| 79.00 | 0.1523 |
| 98.00 | 0.1934 |
| 124.00 | 0.2645 |
| 146.00 | 0.3241 |
| 165.00 | 0.4184 |
| 171.00 | 0.4896 |
| 171.00 | 0.5899 |
| 156.00 | 0.6834 |
| 140.00 | 0.7421 |
| 113.00 | 0.8119 |
| 96.00 | 0.8520 |
| 71.00 | 0.8962 |
| 59.00 | 0.9201 |
| 39.00 | 0.9453 |
| 20.00 | 0.9719 |

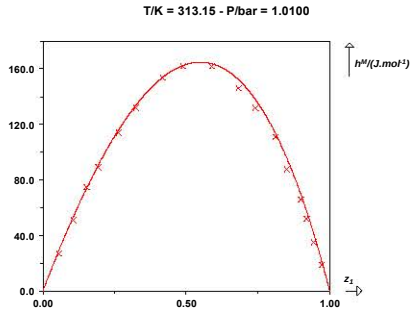
Francesconi, Romolo - Comelli, Fabio, Excess Molar Enthalpies, Densities, and Excess Molar Volumes of Binary Mixtures Containing Esters of Carbonic Acid at 298.15 and 313.15 K, Journal of Chemical & Engineering Data 4 (1995) 811-814. doi:10.1021/je00020a016

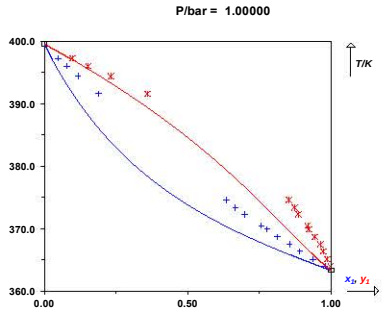
**T / K = 313.15**

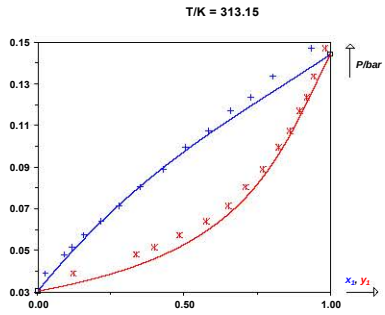
**P / bar = 1.010**

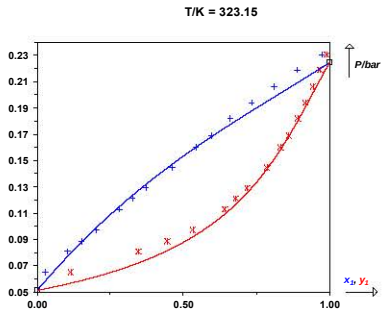
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 27.00 | 0.0565 |
| 51.00 | 0.1069 |
| 75.00 | 0.1522 |
| 89.00 | 0.1932 |
| 114.00 | 0.2643 |
| 132.00 | 0.3238 |
| 154.00 | 0.4181 |
| 162.00 | 0.4892 |
| 162.00 | 0.5896 |
| 146.00 | 0.6831 |
| 132.00 | 0.7418 |
| 111.00 | 0.8117 |
| 88.00 | 0.8518 |
| 66.00 | 0.8995 |
| 52.00 | 0.9200 |
| 35.00 | 0.9452 |
| 19.00 | 0.9718 |

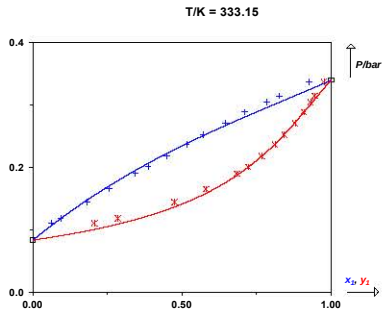

T/K = 298.15 - P/bar = 1.0100
$h^M$/(J.mol$^{-1}$)
$z_1$

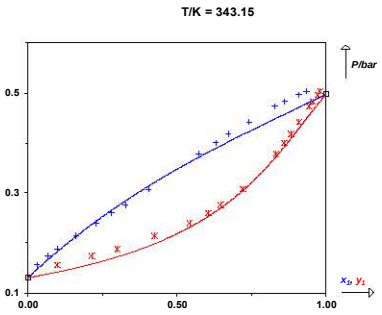

T/K = 313.15 - P/bar = 1.0100
$h^M$/(J.mol$^{-1}$)
$z_1$

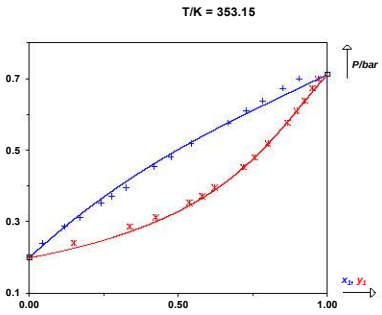

P/bar = 1.00000
T/K
$x_1$, $y_1$


T/K = 313.15
P/bar
$x_1$, $y_1$


T/K = 323.15
P/bar
$x_1$, $y_1$


T/K = 333.15
P/bar
$x_1$, $y_1$


T/K = 343.15
P/bar
$x_1$, $y_1$


T/K = 353.15
P/bar
$x_1$, $y_1$

## 1,2-EPOXYBUTANE (1) + DIMETHYL CARBONATE (2)

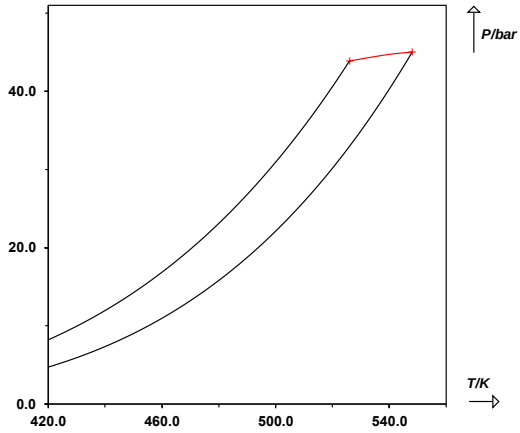
| | | |
|---|---|---|
| **CAS** | 106-88-7 | 616-38-6 |
| **InChiKey** | RBACIKXCRWGCBB-UHFFFAOYSA-N | IEJIGPNLZYLLBP-UHFFFAOYSA-N |
| **$T_c$ / K** | 526.00 | 548.00 |
| **$P_c$ / bar** | 43.90 | 45.00 |
| **ω** | 0.235 | 0.385 |

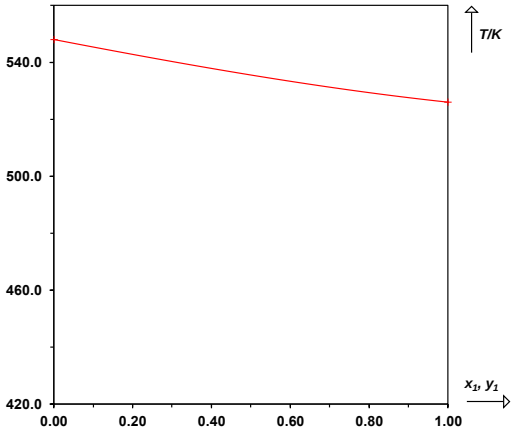
Ideal

**PPR78 results**

*Parameters*
A/MPa = 39.2
B/MPa = 52.2

*Deviations*
MAPE on x = 15 %
MAPE on y = 11 %
MAPE on $h^M$ = 21 %



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**Isothermal phase equilibrium data**

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Francesconi, Romolo - Comelli, Fabio, Vapor−Liquid Equilibria, Excess Molar Enthalpies, and Excess Molar Volumes of Dimethyl Carbonate + 1,2-Epoxybutane at 288.15, 298.15, or 313.15 K, Journal of Chemical & Engineering Data 4 (1996) 736-740. doi:10.1021/je950298m

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0815 | 0.0350 | 0.1410 |
| 0.0915 | 0.0770 | 0.2550 |
| 0.0970 | 0.1120 | 0.3300 |
| 0.1070 | 0.1590 | 0.4210 |
| 0.1190 | 0.2250 | 0.5160 |
| 0.1345 | 0.3070 | 0.6020 |
| 0.1485 | 0.3920 | 0.6820 |
| 0.1600 | 0.4710 | 0.7370 |
| 0.1755 | 0.5680 | 0.7960 |
| 0.1820 | 0.6160 | 0.8210 |
| 0.1900 | 0.6770 | 0.8540 |
| 0.1990 | 0.7420 | 0.8780 |
| 0.2090 | 0.8060 | 0.9100 |
| 0.2160 | 0.8470 | 0.9320 |
| 0.2205 | 0.8820 | 0.9450 |
| 0.2240 | 0.9120 | 0.9580 |
| 0.2300 | 0.9550 | 0.9810 |

Francesconi, Romolo - Comelli, Fabio, Vapor−Liquid Equilibria, Excess Molar Enthalpies, and Excess Molar Volumes of Dimethyl Carbonate + 1,2-Epoxybutane at 288.15, 298.15, or 313.15 K, Journal of Chemical & Engineering Data 4 (1996) 736-740. doi:10.1021/je950298m

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1660 | 0.0280 | 0.1110 |
| 0.1790 | 0.0620 | 0.1980 |
| 0.2020 | 0.1260 | 0.3350 |
| 0.2170 | 0.1730 | 0.4100 |
| 0.2260 | 0.1960 | 0.4460 |
| 0.2510 | 0.2760 | 0.5460 |
| 0.2695 | 0.3370 | 0.6110 |
| 0.2835 | 0.3870 | 0.6490 |
| 0.2970 | 0.4340 | 0.6870 |
| 0.3120 | 0.4870 | 0.7250 |
| 0.3275 | 0.5430 | 0.7630 |
| 0.3530 | 0.6370 | 0.8190 |
| 0.3720 | 0.7120 | 0.8600 |
| 0.3885 | 0.7770 | 0.8920 |
| 0.4025 | 0.8300 | 0.9180 |
| 0.4135 | 0.8820 | 0.9410 |
| 0.4260 | 0.9350 | 0.9700 |

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**Enthalpy of mixing**

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Miyanaga, Shoji - Tamura, Katsutoshi - Murakami, Sachio, Excess enthalpies and excess isobaric heat capacities of (2,2,2-trifluoroethan-1-ol + benzene), (benzene + dimethylsulfoxide), and (2,2,2,-trifluoroethan-1-ol + dimethylsulfoxide), at the temperature 298.15 K, The Journal of Chemical Thermodynamics 3 (1992) 291-296. doi:10.1016/S0021-9614(05)80069-2

**T / K = 288.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 16.20 | 0.0388 |
| 40.80 | 0.0748 |
| 69.50 | 0.1081 |
| 99.80 | 0.1390 |
| 154.90 | 0.1951 |
| 192.70 | 0.2443 |
| 247.70 | 0.3265 |
| 277.60 | 0.3926 |
| 295.00 | 0.4889 |
| 283.90 | 0.5863 |
| 260.90 | 0.6567 |
| 212.50 | 0.7416 |
| 175.20 | 0.7928 |
| 122.90 | 0.8516 |
| 92.60 | 0.8844 |
| 58.30 | 0.9209 |
| 28.50 | 0.9588 |

Miyanaga, Shoji - Tamura, Katsutoshi - Murakami, Sachio, Excess enthalpies and excess isobaric heat capacities of (2,2,2-trifluoroethan-1-ol + benzene), (benzene + dimethylsulfoxide), and (2,2,2,-trifluoroethan-1-ol + dimethylsulfoxide), at the temperature 298.15 K, The Journal of Chemical Thermodynamics 3 (1992) 291-296. doi:10.1016/S0021-9614(05)80069-2

**T / K = 298.15**

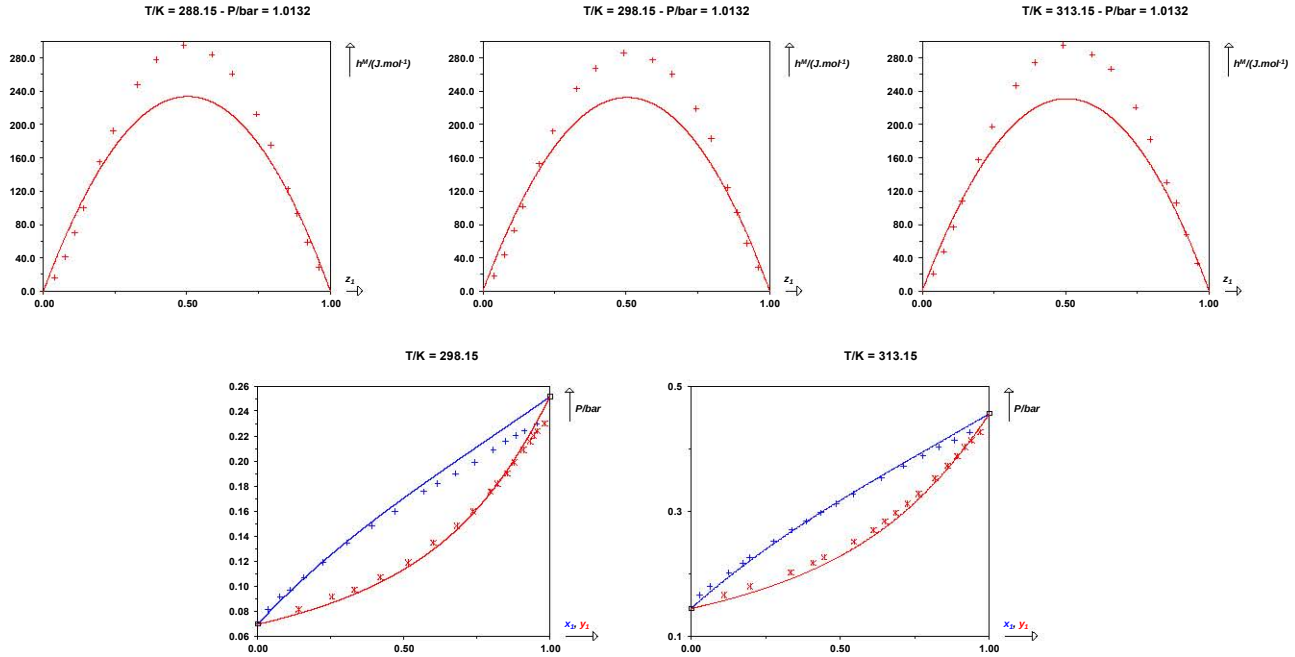
**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 18.20 | 0.0388 |
| 43.80 | 0.0747 |
| 73.00 | 0.1080 |

| | |
|---|---|
| 101.70 | 0.1390 |
| 152.80 | 0.1950 |
| 192.10 | 0.2441 |
| 242.80 | 0.3263 |
| 266.90 | 0.3923 |
| 285.70 | 0.4921 |
| 277.20 | 0.5924 |
| 260.20 | 0.6596 |
| 219.20 | 0.7440 |
| 182.90 | 0.7949 |
| 124.50 | 0.8532 |
| 94.60 | 0.8857 |
| 57.70 | 0.9208 |
| 28.20 | 0.9588 |

Miyanaga, Shoji - Tamura, Katsutoshi - Murakami, Sachio, Excess enthalpies and excess isobaric heat capacities of (2,2,2-trifluoroethan-1-ol + benzene), (benzene + dimethylsulfoxide), and (2,2,2,-trifluoroethan-1-ol + dimethylsulfoxide), at the temperature 298.15 K, The Journal of Chemical Thermodynamics 3 (1992) 291-296. doi:10.1016/S0021-9614(05)80069-2

| **T / K =** | **313.15** |
|---|---|
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| 20.90 | 0.0387 |
| 47.40 | 0.0746 |
| 76.70 | 0.1079 |
| 108.20 | 0.1388 |
| 157.50 | 0.1947 |
| 197.30 | 0.2438 |
| 246.20 | 0.3260 |
| 274.40 | 0.3920 |
| 294.80 | 0.4917 |
| 283.90 | 0.5920 |
| 266.70 | 0.6592 |
| 220.70 | 0.7437 |
| 181.80 | 0.7946 |
| 130.40 | 0.8530 |
| 106.20 | 0.8856 |
| 68.10 | 0.9207 |
| 33.50 | 0.9587 |


T/K = 288.15 - P/bar = 1.0132
T/K = 298.15 - P/bar = 1.0132
T/K = 313.15 - P/bar = 1.0132
T/K = 298.15
T/K = 313.15
P/bar

## DIMETHYL ETHER (1) + SULFUR DIOXIDE (2)

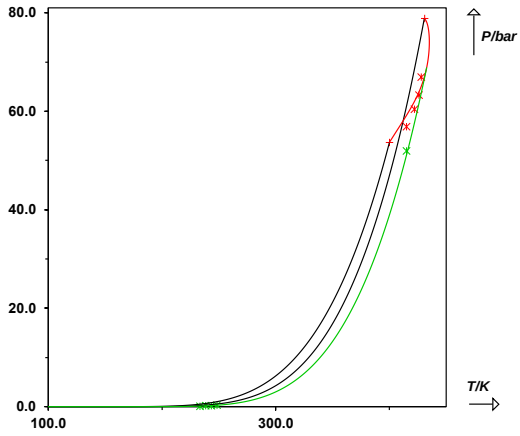
| | | |
|---|---|---|
| **CAS** | 115-10-6 | 05/09/7446 |
| **InChiKey** | LCGLNKUTAGEVQW-UHFFFAOYSA-N | RAHZWNYVWXNFOC-UHFFFAOYSA-N |
| **$T_c$ / K** | 400.10 | 430.75 |
| **$P_c$ / bar** | 53.70 | 78.84 |
| **ω** | 0.200 | 0.245 |

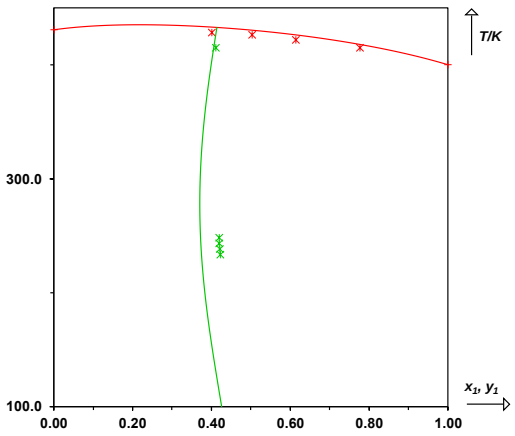
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = -669
B/MPa = -1870

*Deviations*
MAPE on x = 11 %
MAPE on y = 13 %
MAPE on $x_c$ = 43 %
MAPE on $P_c$ = 5.5 %
MAPE on $x_{az}$ = 9.3 %
MAPE on $P_{az}$ = 0.21 %



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**Isothermal phase equilibrium data**

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Pupezin, J. - Ribnikar, S. - Knezevic, Z. - Dokic, V., Liquid-vapor equilibrium and thermodynamic properties of the system sulfur dioxide + dimethyl ether, Bull. Boris Kidric Inst. Nucl. Sci. 4 (1966) 297-309.

**T / K = 233.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2017 | 0.0670 | 0.0100 | |
| 0.1786 | 0.1520 | 0.0320 | |
| 0.1351 | 0.2980 | 0.1480 | |
| 0.1200 | 0.3600 | 0.2350 | |
| 0.1141 | 0.4050 | 0.3600 | |
| 0.1133 | 0.4220 | 0.4220 | AZEO |
| 0.1237 | 0.5000 | 0.6720 | |
| 0.1755 | 0.5960 | 0.8720 | |
| 0.2538 | 0.6850 | 0.9530 | |
| 0.3555 | 0.7880 | 0.9880 | |

Pupezin, J. - Ribnikar, S. - Knezevic, Z. - Dokic, V., Liquid-vapor equilibrium and thermodynamic properties of the system sulfur dioxide + dimethyl ether, Bull. Boris Kidric Inst. Nucl. Sci. 4 (1966) 297-309.

**T / K = 238.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2693 | 0.0680 | 0.0120 | |
| 0.2407 | 0.1530 | 0.0360 | |
| 0.1838 | 0.2990 | 0.1580 | |
| 0.1647 | 0.3600 | 0.2440 | |
| 0.1582 | 0.4050 | 0.3620 | |
| 0.1572 | 0.4210 | 0.4210 | AZEO |
| 0.1700 | 0.5010 | 0.6600 | |
| 0.2322 | 0.5950 | 0.8620 | |
| 0.3264 | 0.6850 | 0.9430 | |
| 0.4546 | 0.7860 | 0.9840 | |

Pupezin, J. - Ribnikar, S. - Knezevic, Z. - Dokic, V., Liquid-vapor equilibrium and thermodynamic properties of the system sulfur dioxide + dimethyl ether, Bull. Boris Kidric Inst. Nucl. Sci. 4 (1966) 297-309.

**T / K = 243.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.3545 | 0.0700 | 0.0140 | |
| 0.3183 | 0.1540 | 0.0390 | |
| 0.2461 | 0.3000 | 0.1630 | |
| 0.2224 | 0.3610 | 0.2500 | |
| 0.2152 | 0.4050 | 0.3660 | |
| 0.2141 | 0.4200 | 0.4200 | AZEO |
| 0.2293 | 0.4990 | 0.6470 | |
| 0.3027 | 0.5890 | 0.8450 | |
| 0.4151 | 0.6790 | 0.9340 | |
| 0.5729 | 0.7820 | 0.9790 | |

Pupezin, J. - Ribnikar, S. - Knezevic, Z. - Dokic, V., Liquid-vapor equilibrium and thermodynamic properties of the system sulfur dioxide + dimethyl ether, Bull. Boris Kidric Inst. Nucl. Sci. 4 (1966) 297-309.

**T / K = 248.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.4605 | 0.0720 | 0.0170 | |
| 0.4143 | 0.1560 | 0.0420 | |
| 0.3246 | 0.3010 | 0.1730 | |
| 0.2960 | 0.3610 | 0.2600 | |
| 0.2877 | 0.4060 | 0.3700 | |
| 0.2865 | 0.4190 | 0.4190 | AZEO |
| 0.3044 | 0.4960 | 0.6340 | |
| 0.3897 | 0.5850 | 0.8300 | |
| 0.5227 | 0.6760 | 0.9250 | |
| 0.7127 | 0.7790 | 0.9740 | |

Noles, Joe R. - Zollweg, John A., Isothermal vapor-liquid equilibrium for dimethyl ether + sulfur dioxide, Fluid Phase Equilibria 3 (1991) 275-289. doi:10.1016/0378-3812(91)85061-X

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.980 | 0.1732 | 0.0702 |
| 1.820 | 0.2391 | 0.1215 |
| 1.630 | 0.3224 | 0.2249 |
| 1.540 | 0.3905 | 0.3533 |
| 1.530 | 0.4420 | 0.4620 |
| 1.660 | 0.5304 | 0.6511 |
| 2.030 | 0.6391 | 0.8315 |
| 2.470 | 0.7355 | 0.9230 |
| 3.370 | 0.9180 | 0.9855 |

Noles, Joe R. - Zollweg, John A., Isothermal vapor-liquid equilibrium for dimethyl ether + sulfur dioxide, Fluid Phase Equilibria 3 (1991) 275-289. doi:10.1016/0378-3812(91)85061-X

**T / K = 323.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.980 | 0.0980 | 0.0468 |
| 7.690 | 0.1482 | 0.0791 |
| 7.000 | 0.2635 | 0.1819 |
| 6.590 | 0.3547 | 0.3079 |
| 6.480 | 0.4463 | 0.4577 |

| | | |
|---|---|---|
| 6.670 | 0.5169 | 0.5802 |
| 7.040 | 0.5853 | 0.6877 |
| 8.350 | 0.7304 | 0.8615 |

Noles, Joe R. - Zollweg, John A., Isothermal vapor-liquid equilibrium for dimethyl ether + sulfur dioxide, Fluid Phase Equilibria 3 (1991) 275-289. doi:10.1016/0378-3812(91)85061-X

**T / K = 363.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.00 | 0.1977 | 0.1360 |
| 19.31 | 0.2598 | 0.1968 |
| 18.62 | 0.3436 | 0.2989 |
| 18.27 | 0.4137 | 0.3986 |
| 18.20 | 0.4678 | 0.4751 |
| 21.44 | 0.7370 | 0.8135 |
| 22.80 | 0.8023 | 0.8721 |

Noles, Joe R. - Zollweg, John A., Isothermal vapor-liquid equilibrium for dimethyl ether + sulfur dioxide, Fluid Phase Equilibria 3 (1991) 275-289. doi:10.1016/0378-3812(91)85061-X

**T / K = 405.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 48.60 | 0.0769 | 0.0598 |
| 45.48 | 0.2093 | 0.1776 |
| 43.79 | 0.2962 | 0.2826 |
| 42.86 | 0.3995 | 0.4036 |
| 43.00 | 0.5084 | 0.5295 |
| 44.94 | 0.6576 | 0.6885 |
| 46.09 | 0.7051 | 0.7425 |
| 48.58 | 0.7909 | 0.8226 |
| 50.25 | 0.8414 | 0.8626 |
| 52.79 | 0.9019 | 0.9117 |
| 53.61 | 0.9228 | 0.9302 |

Noles, Joe R. - Zollweg, John A., Isothermal vapor-liquid equilibrium for dimethyl ether + sulfur dioxide, Fluid Phase Equilibria 3 (1991) 275-289. doi:10.1016/0378-3812(91)85061-X

**T / K = 415.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 57.64 | 0.1021 | 0.0847 | |
| 55.35 | 0.1865 | 0.1668 | |
| 53.08 | 0.2987 | 0.2825 | |
| 51.94 | 0.4104 | 0.4092 | |
| 51.94 | 0.4110 | 0.4110 | AZEO |
| 52.65 | 0.5736 | 0.5910 | |
| 54.01 | 0.6494 | 0.6732 | |
| 55.77 | 0.7209 | 0.7405 | |
| 55.91 | 0.7300 | 0.7449 | |
| 56.48 | 0.7604 | 0.7713 | |

Noles, Joe R. - Zollweg, John A., Isothermal vapor-liquid equilibrium for dimethyl ether + sulfur dioxide, Fluid Phase Equilibria 3 (1991) 275-289. doi:10.1016/0378-3812(91)85061-X

**T / K = 425.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 68.03 | 0.1041 | 0.0932 |
| 65.72 | 0.1811 | 0.1639 |
| 64.25 | 0.2362 | 0.2240 |
| 62.90 | 0.3017 | 0.2929 |
| 62.24 | 0.3501 | 0.3457 |
| 61.79 | 0.4070 | 0.4045 |
| 61.71 | 0.4641 | 0.4686 |
| 61.86 | 0.5044 | 0.5086 |

Noles, Joe R. - Zollweg, John A., Isothermal vapor-liquid equilibrium for dimethyl ether + sulfur dioxide, Fluid Phase Equilibria 3 (1991) 275-289. doi:10.1016/0378-3812(91)85061-X

**T / K = 428.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 71.52 | 0.1059 | 0.0962 |
| 69.28 | 0.1791 | 0.1687 |
| 66.82 | 0.2773 | 0.2709 |
| 65.46 | 0.3373 | 0.3333 |
| 65.11 | 0.3670 | 0.3648 |

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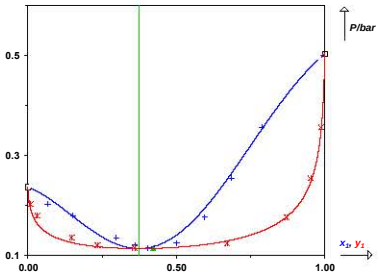
**Critical point**

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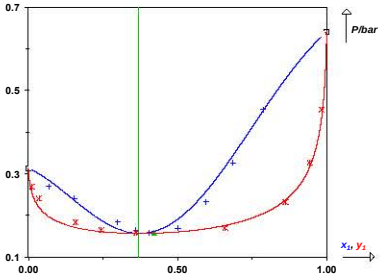
Glowka, S. - Zawisza, A.C., Liquid-vapor equilibriums and thermodynamic functions of methyl ethyl ether-sulfur dioxide system up to 300.deg. and 77.81 atm, Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques 9 (1970) 555-560.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 415.03 | 56.80 | 0.7768 |
| 422.05 | 60.40 | 0.6139 |
| 426.06 | 63.22 | 0.5036 |
| 428.20 | 66.91 | 0.4014 |

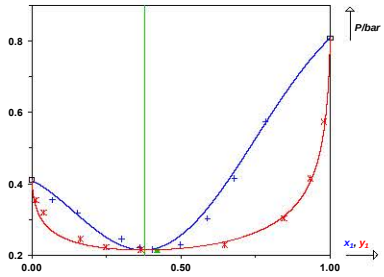
T/K = 233.15



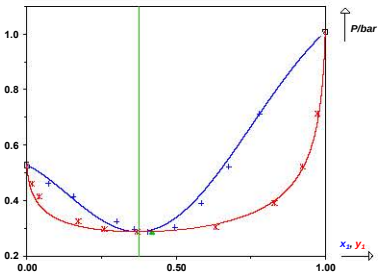

T/K = 238.15



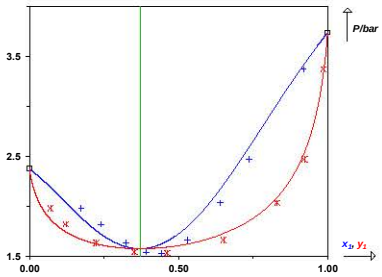

T/K = 243.15



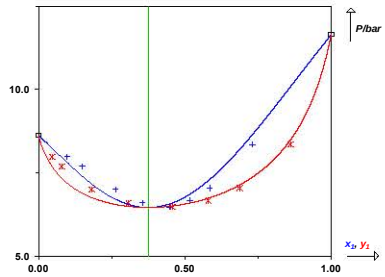

T/K = 248.15



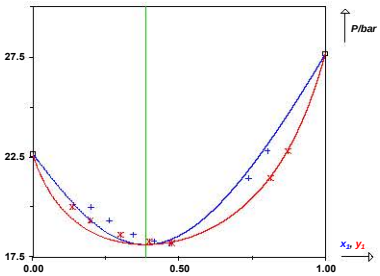

T/K = 283.15



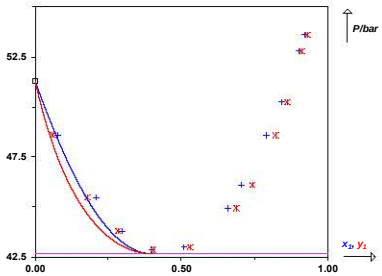

T/K = 323.59



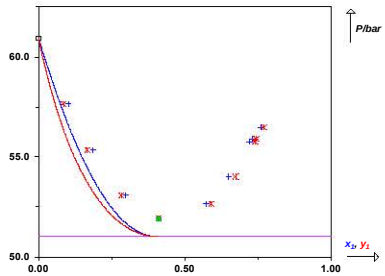

T/K = 363.15



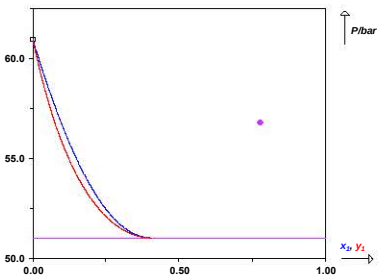

T/K = 405.00



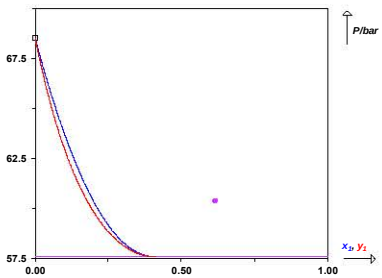

T/K = 415.00



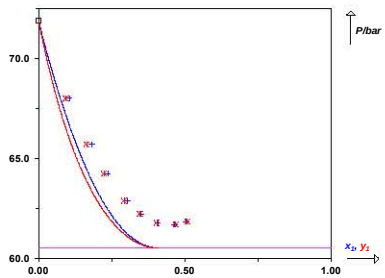

T/K = 415.03



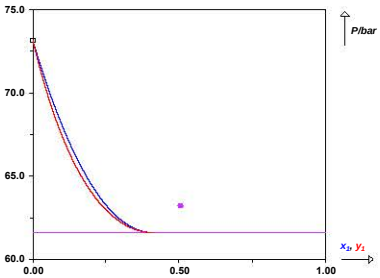

T/K = 422.05



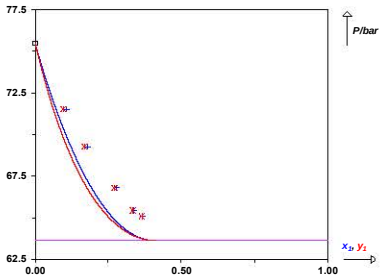

T/K = 425.00



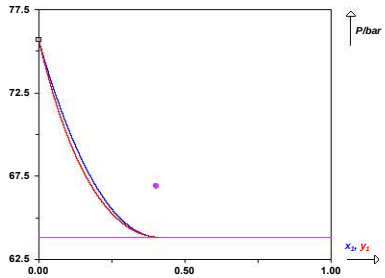

T/K = 426.06




T/K = 428.00




T/K = 428.20



## TRIFLUOROMETHANE (1) + CHLORODIFLUOROMETHANE (2)

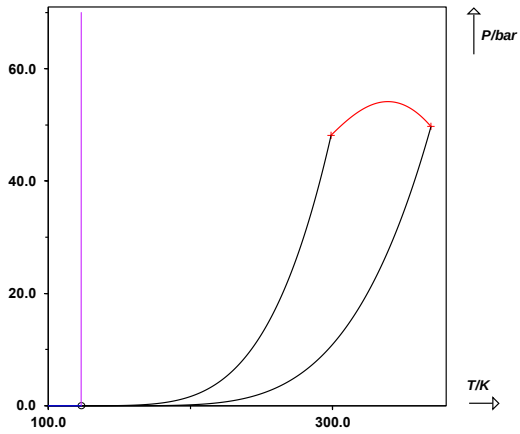
| | | |
|---|---|---|
| **CAS** | 75-46-7 | 75-45-6 |
| **InChiKey** | XPDWGBQVDMORPB-UHFFFAOYSA-N | VOPWNXZWBYDODV-UHFFFAOYSA-N |
| **$T_c$ / K** | 299.01 | 369.30 |
| **$P_c$ / bar** | 48.16 | 49.71 |
| **ω** | 0.264 | 0.219 |

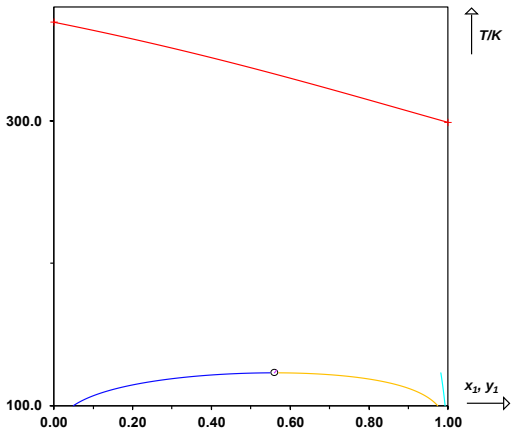
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 51.6
B/MPa = 139

*Deviations*
MAPE on x = 1.6 %
MAPE on y = 1.6 %



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**Isothermal phase equilibrium data**

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Feng Yaosheng - Li, C. - Shou, Z., Vapor-Liquid Equilibrium for Trifluoromethane and Chlorodifluoromethane, Huaxue Gongcheng 3 (1984) 41-47.

**T / K = 248.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.594 | 0.0475 | 0.2520 |
| 3.506 | 0.1250 | 0.4810 |
| 4.712 | 0.2310 | 0.6510 |
| 5.553 | 0.3250 | 0.7340 |
| 6.363 | 0.4080 | 0.7920 |
| 7.143 | 0.4890 | 0.8330 |
| 7.620 | 0.5390 | 0.8540 |
| 8.795 | 0.6610 | 0.8960 |
| 10.11 | 0.8150 | 0.9450 |
| 10.66 | 0.8700 | 0.9610 |

Feng Yaosheng - Li, C. - Shou, Z., Vapor-Liquid Equilibrium for Trifluoromethane and Chlorodifluoromethane, Huaxue Gongcheng 3 (1984) 41-47.

**T / K = 258.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.942 | 0.0630 | 0.2800 |
| 4.468 | 0.0990 | 0.3840 |
| 6.880 | 0.2650 | 0.6560 |
| 8.299 | 0.3680 | 0.7460 |
| 9.322 | 0.4580 | 0.7980 |
| 10.63 | 0.5470 | 0.8430 |
| 11.86 | 0.6590 | 0.8900 |
| 13.13 | 0.7590 | 0.9240 |
| 14.85 | 0.8770 | 0.9610 |
| 15.35 | 0.9130 | 0.9720 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.25 | 0.0903 | 0.2463 |
| 20.20 | 0.2279 | 0.4668 |
| 25.10 | 0.3668 | 0.6042 |
| 29.90 | 0.4962 | 0.7002 |
| 35.15 | 0.6394 | 0.7811 |
| 40.00 | 0.7547 | 0.8445 |
| 45.00 | 0.8608 | 0.9036 |
| 48.05 | 0.9215 | 0.9361 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 24.30 | 0.0984 | 0.2217 |
| 30.20 | 0.2181 | 0.3955 |
| 35.60 | 0.3273 | 0.5050 |
| 39.95 | 0.4122 | 0.5768 |
| 45.75 | 0.5240 | 0.6442 |
| 49.90 | 0.6039 | 0.6822 |
| 51.70 | 0.6414 | 0.6933 |
| 52.55 | 0.6601 | 0.6911 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

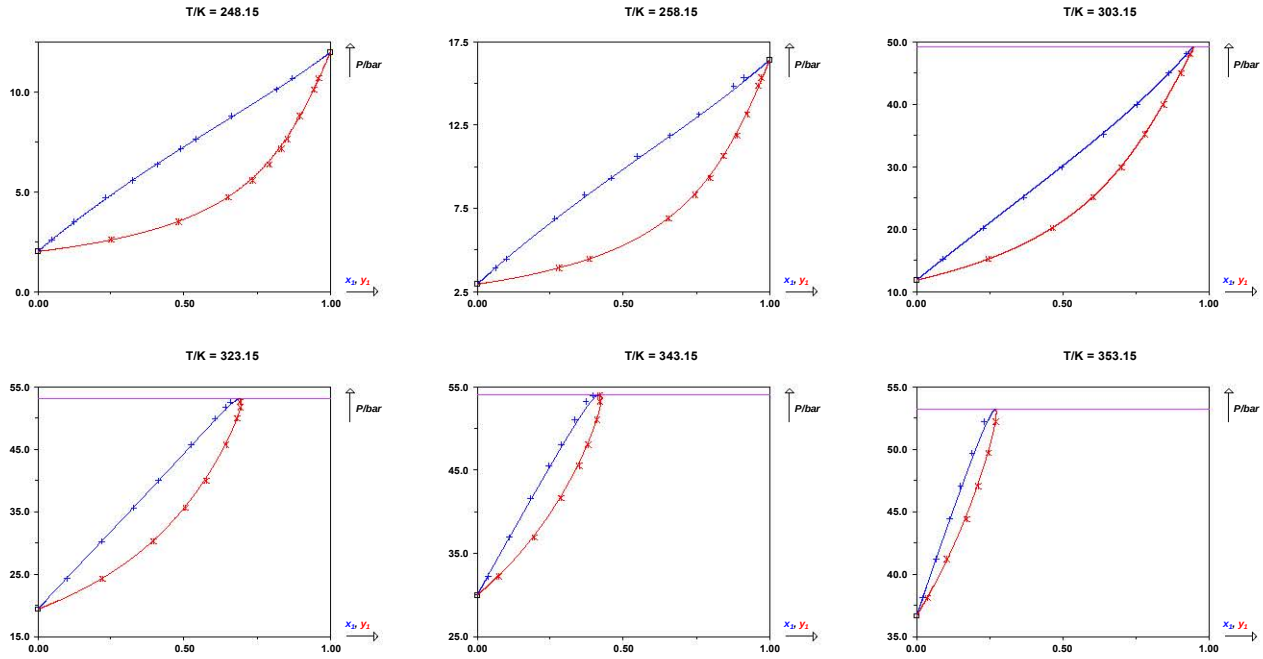
**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 32.25 | 0.0368 | 0.0752 |
| 36.90 | 0.1089 | 0.1961 |
| 41.60 | 0.1819 | 0.2873 |
| 45.50 | 0.2448 | 0.3488 |
| 48.05 | 0.2864 | 0.3803 |
| 51.05 | 0.3337 | 0.4098 |
| 53.20 | 0.3720 | 0.4196 |
| 53.95 | 0.3960 | 0.4191 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 38.10 | 0.0218 | 0.0388 |
| 41.20 | 0.0660 | 0.1036 |
| 44.40 | 0.1125 | 0.1715 |
| 47.05 | 0.1496 | 0.2106 |
| 49.70 | 0.1898 | 0.2453 |
| 52.20 | 0.2309 | 0.2711 |


T/K = 248.15
P/bar
10.0
5.0
0.0
0.00
0.50
1.00
x1, y1
T/K = 258.15
P/bar
17.5
12.5
7.5
2.5
0.00
0.50
1.00
x1, y1
T/K = 303.15
P/bar
50.0
40.0
30.0
20.0
10.0
0.00
0.50
1.00
x1, y1
T/K = 323.15
P/bar
55.0
45.0
35.0
25.0
15.0
0.00
0.50
1.00
x1, y1
T/K = 343.15
P/bar
55.0
45.0
35.0
25.0
0.00
0.50
1.00
x1, y1
T/K = 353.15
P/bar
55.0
50.0
45.0
40.0
35.0
0.00
0.50
1.00
x1, y1

## DIETHYL ETHER (1) + ACETONE (2)

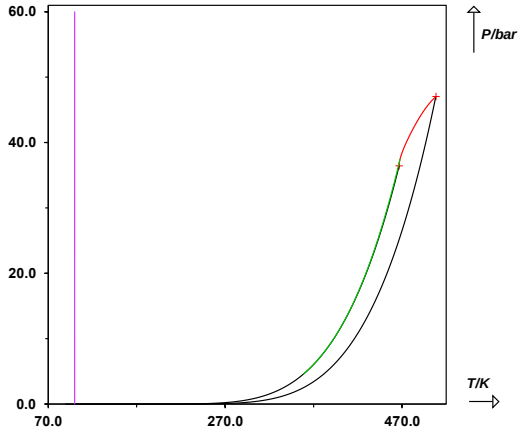
| | | |
|---|---|---|
| **CAS** | 60-29-7 | 67-64-1 |
| **InChiKey** | RTZKZFJDLAIYFH-UHFFFAOYSA-N | CSCPPACGZOOCGX-UHFFFAOYSA-N |
| **$T_c$ / K** | 466.70 | 508.20 |
| **$P_c$ / bar** | 36.40 | 47.01 |
| **ω** | 0.281 | 0.307 |

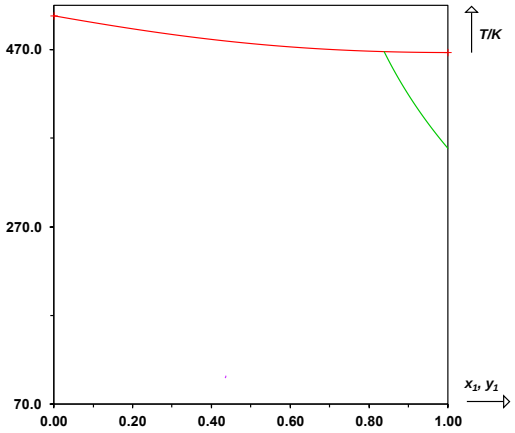
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 138
B/MPa = 103

*Deviations*
MAPE on x = 6.2 %
MAPE on y = 2.9 %
MAPE on $h^M$ = 12 %



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**Isothermal phase equilibrium data**

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Gerrits, G.C., On Px-Curves of Mixtures of Acetone and Ethyl Ether and of Carbon Tetrachloride and Acetone at 0 °C, Proc. K. Ned. Akad. Wet. Nat. Sci. (1905) 162-173.

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1070 | 0.0240 | 0.1730 |
| 0.1307 | 0.0830 | 0.3420 |
| 0.1427 | 0.1240 | 0.4210 |
| 0.1693 | 0.2320 | 0.5530 |
| 0.1792 | 0.2950 | 0.5900 |
| 0.2196 | 0.5610 | 0.7480 |
| 0.2402 | 0.7960 | 0.8460 |

Sameshima, Jitsusaburo, On The System Acetone—Ethyl Ether., Journal of the American Chemical Society 10 (1918) 1482-1503. doi:10.1021/ja02243a002

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2479 | 0.0041 | 0.0098 |
| 0.2624 | 0.0210 | 0.0784 |
| 0.2950 | 0.0642 | 0.2090 |
| 0.2970 | 0.0683 | 0.2168 |
| 0.3301 | 0.1117 | 0.3219 |
| 0.3621 | 0.1584 | 0.4089 |
| 0.4453 | 0.3338 | 0.5951 |
| 0.4682 | 0.3879 | 0.6389 |
| 0.5160 | 0.5430 | 0.7283 |
| 0.5609 | 0.7510 | 0.8332 |
| 0.5812 | 0.8729 | 0.9042 |
| 0.5890 | 0.9480 | 0.9557 |

Sameshima, Jitsusaburo, On The System Acetone—Ethyl Ether., Journal of the American Chemical Society 10 (1918) 1482-1503. doi:10.1021/ja02243a002

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3965 | 0.0201 | 0.0698 |
| 0.4346 | 0.0472 | 0.1696 |
| 0.4504 | 0.0663 | 0.2101 |
| 0.5461 | 0.1619 | 0.4066 |
| 0.6396 | 0.2953 | 0.5545 |
| 0.6702 | 0.3493 | 0.5997 |
| 0.7437 | 0.5042 | 0.6996 |
| 0.7959 | 0.6546 | 0.7782 |
| 0.8225 | 0.7491 | 0.8270 |
| 0.8493 | 0.8673 | 0.8960 |
| 0.8603 | 0.9613 | 0.9663 |

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**Enthalpy of mixing**

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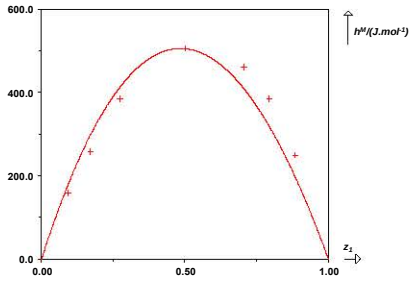
Hirobe, H., Thermochemical studies, J. Fac. Sci. Univ. Tokyo Sect. 1 4 (1926) 155-222.

**T / K = 298.15**

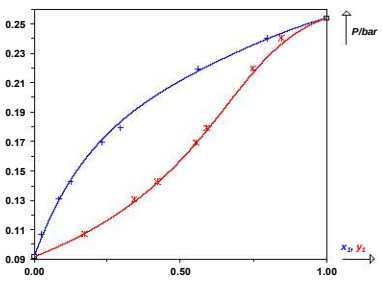
**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 158.68 | 0.0923 |
| 257.91 | 0.1705 |
| 385.19 | 0.2731 |
| 505.35 | 0.5002 |
| 461.38 | 0.7057 |
| 384.77 | 0.7932 |
| 249.53 | 0.8845 |

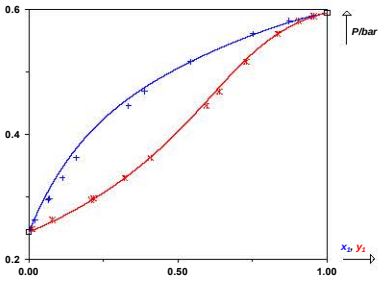
T/K = 298.15 - P/bar = 1.0132



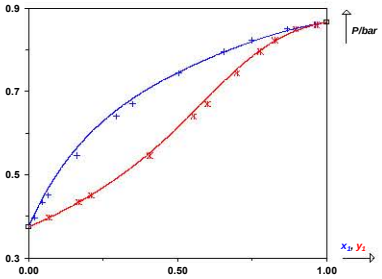

T/K = 273.15




T/K = 293.15




T/K = 303.15



## CARBON DISULFIDE (1) + ACETONE (2)

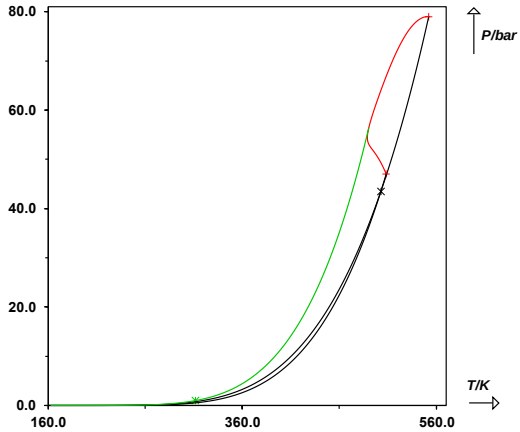
| | | |
|---|---|---|
| **CAS** | 75-15-0 | 67-64-1 |
| **InChiKey** | QGJOPFRUJISHPQ-UHFFFAOYSA-N | CSCPPACGZOOCGX-UHFFFAOYSA-N |
| **$T_c$ / K** | 552.00 | 508.20 |
| **$P_c$ / bar** | 79.00 | 47.01 |
| **ω** | 0.111 | 0.307 |

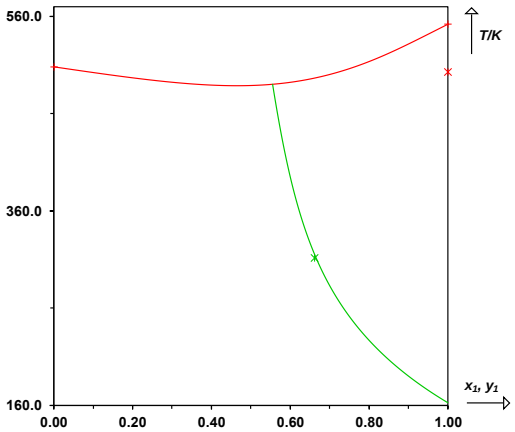
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 405
B/MPa = -41.6

*Deviations*
MAPE on x = 6.6 %
MAPE on y = 1.7 %
MAPE on $x_{az}$ = 0.87 %
MAPE on $P_{az}$ = 0.0016 %



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**Isothermal phase equilibrium data**

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Litvinov, N.D., Isothermal equilibrium of vapor and liquid in systems of three fully miscible liquids, Zh. Fiz. Khim. 10 (1952) 1405-1412.

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4206 | 0.1000 | 0.3520 |
| 0.5032 | 0.2000 | 0.5050 |
| 0.5533 | 0.3000 | 0.5830 |
| 0.5792 | 0.4000 | 0.6250 |
| 0.5905 | 0.5000 | 0.6480 |
| 0.5942 | 0.6000 | 0.6620 |
| 0.5946 | 0.7000 | 0.6740 |
| 0.5901 | 0.8000 | 0.6980 |
| 0.5649 | 0.9000 | 0.7650 |

Zawidzki, Jan von, Über die Dampfdrücke binärer Flüssigkeitsgemische, Zeitschrift für Physikalische Chemie 1 (1900) doi:10.1515/zpch-1900-3514

**T / K = 308.32**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5889 | 0.0624 | 0.2506 |
| 0.5966 | 0.0670 | 0.2674 |
| 0.6024 | 0.0711 | 0.2724 |
| 0.6735 | 0.1212 | 0.3794 |
| 0.6863 | 0.1330 | 0.4012 |
| 0.7383 | 0.1857 | 0.4666 |
| 0.7499 | 0.1991 | 0.4834 |
| 0.7563 | 0.2085 | 0.5005 |
| 0.7979 | 0.2761 | 0.5403 |
| 0.8038 | 0.2869 | 0.5452 |
| 0.8295 | 0.3502 | 0.5759 |
| 0.8311 | 0.3551 | 0.5795 |
| 0.8454 | 0.4058 | 0.5986 |
| 0.8467 | 0.4141 | 0.6015 |
| 0.8541 | 0.4474 | 0.6094 |
| 0.8557 | 0.4530 | 0.6141 |
| 0.8613 | 0.4933 | 0.6242 |
| 0.8615 | 0.4974 | 0.6254 |
| 0.8693 | 0.5702 | 0.6433 |
| 0.8699 | 0.5730 | 0.6441 |
| 0.8718 | 0.6124 | 0.6529 |
| 0.8733 | 0.6713 | 0.6682 |
| 0.8601 | 0.8280 | 0.7207 |
| 0.8187 | 0.9191 | 0.7989 |
| 0.8137 | 0.9245 | 0.8029 |
| 0.8017 | 0.9350 | 0.8181 |
| 0.7939 | 0.9407 | 0.8261 |
| 0.7761 | 0.9549 | 0.8523 |
| 0.7655 | 0.9620 | 0.8723 |
| 0.7519 | 0.9692 | 0.8902 |

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**Isobaric phase equilibrium data**

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Loiseleur, Henri - Merlin, Jean-Claude - Paris, René A., Diagrammes d'ébullition-rosée (sous 740 mm) des systèmes acétone-sulfure de carbone, acétone-tétrachloréthylène et cycopentanone-sulfure de carbone, Journal de Chimie Physique (1964) 1231-1233. doi:10.1051/jcp/1964611231

**P / bar = 0.9866**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 324.75 | 0.0340 | 0.1570 |
| 321.25 | 0.0740 | 0.2760 |
| 318.45 | 0.1170 | 0.3780 |
| 316.15 | 0.1700 | 0.4460 |
| 313.75 | 0.2630 | 0.5340 |
| 312.35 | 0.3770 | 0.5880 |
| 311.65 | 0.5070 | 0.6270 |
| 311.50 | 0.5930 | 0.6470 |
| 311.65 | 0.8100 | 0.7010 |
| 312.85 | 0.9140 | 0.7630 |
| 314.65 | 0.9630 | 0.8440 |

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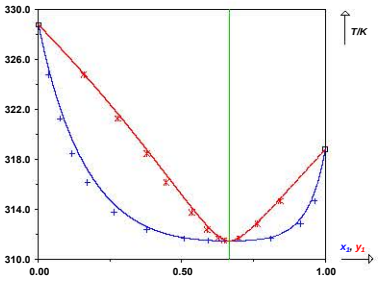
**Azeotropic point**

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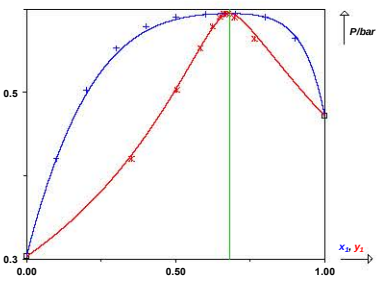
Loiseleur, Henri - Merlin, Jean-Claude - Paris, René A., Diagrammes d'ébullition-rosée (sous 740 mm) des systèmes acétone-sulfure de carbone, acétone-tétrachloréthylène et cycopentanone-sulfure de carbone, Journal de Chimie Physique (1964) 1231-1233. doi:10.1051/jcp/1964611231

| T / K | P / bar | $x_1$ |
|---|---|---|
| 311.45 | 0.9866 | 0.6620 |

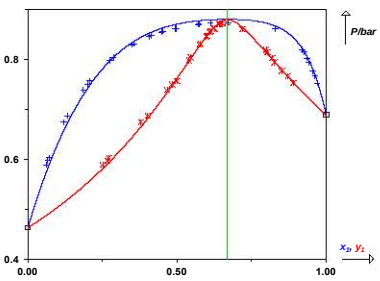
P/bar = 0.98659



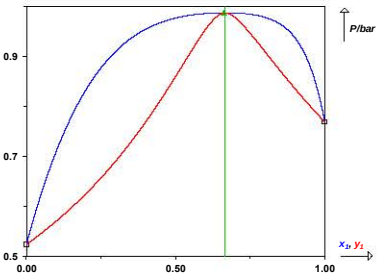

T/K = 298.15




T/K = 308.32




T/K = 311.45



## TRIETHYLAMINE (1) + 1,4-DIOXANE (2)

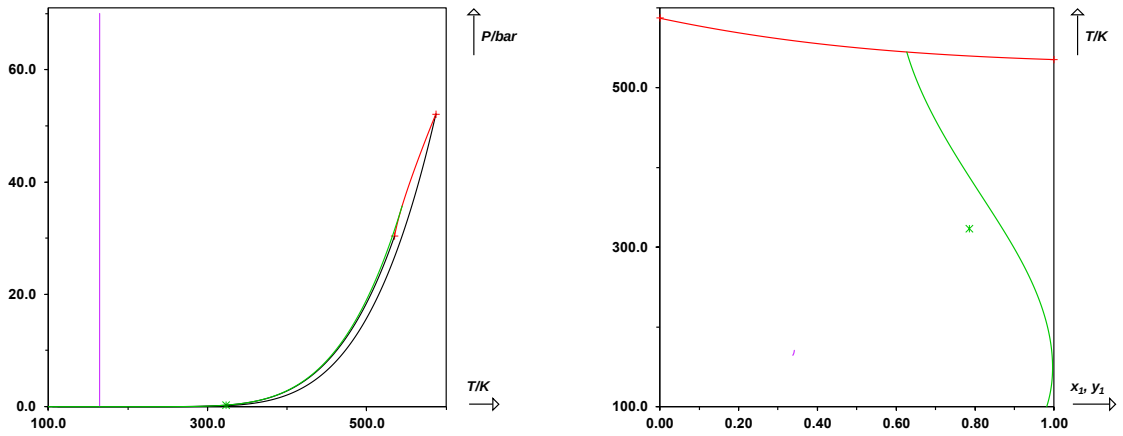
| | | |
|---|---|---|
| **CAS** | 121-44-8 | 123-91-1 |
| **InChiKey** | ZMANZCXQSJIPKH-UHFFFAOYSA-N | RYHBNJHYFVUHQT-UHFFFAOYSA-N |
| **$T_c$ / K** | 535.15 | 587.00 |
| **$P_c$ / bar** | 30.40 | 52.08 |
| **ω** | 0.316 | 0.279 |

Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 138
B/MPa = 155

*Deviations*
MAPE on x = 14 %
MAPE on y = 15 %
MAPE on $x_{az}$ = 25 %
MAPE on $P_{az}$ = 0.66 %
MAPE on $h^M$ = 56 %
MAPE on $c_p^M$ = 100 %



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**Isothermal phase equilibrium data**

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Bittrich, H. J. - Rodrigues, L. F. T. G., Dampf-Flüssigkeit-Gleichgewichte der Mischungen von Triethylamin mit Tetrahydrofuran und 1,4-Dioxan, Zeitschrift für Physikalische Chemie 1 (1988) doi:10.1515/zpch-1988-26997

**T / K = 323.20**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2252 | 0.1880 | 0.4350 | |
| 0.2464 | 0.3240 | 0.5420 | |
| 0.2576 | 0.4430 | 0.5960 | |
| 0.2716 | 0.6760 | 0.7160 | |
| 0.2734 | 0.7700 | 0.7800 | |
| 0.2733 | 0.7820 | 0.7840 | |
| 0.2733 | 0.7850 | 0.7850 | AZEO |
| 0.2727 | 0.8220 | 0.8280 | |
| 0.2709 | 0.9080 | 0.8940 | |

Bittrich, H. J. - Rodrigues, L. F. T. G., Dampf-Flüssigkeit-Gleichgewichte der Mischungen von Triethylamin mit Tetrahydrofuran und 1,4-Dioxan, Zeitschrift für Physikalische Chemie 1 (1988) doi:10.1515/zpch-1988-26997

**T / K = 343.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3660 | 0.0120 | 0.0700 |
| 0.3882 | 0.0350 | 0.1550 |
| 0.4109 | 0.0700 | 0.2380 |
| 0.4368 | 0.1080 | 0.2840 |
| 0.4821 | 0.2160 | 0.4180 |
| 0.4954 | 0.2480 | 0.4500 |
| 0.5229 | 0.3450 | 0.5200 |
| 0.5360 | 0.4060 | 0.5360 |
| 0.5485 | 0.4740 | 0.5920 |
| 0.5524 | 0.5100 | 0.6220 |
| 0.5541 | 0.5320 | 0.6140 |
| 0.5563 | 0.5460 | 0.6380 |
| 0.5640 | 0.6400 | 0.6740 |
| 0.5668 | 0.7000 | 0.7060 |
| 0.5672 | 0.7720 | 0.7770 |
| 0.5614 | 0.8760 | 0.8860 |
| 0.5510 | 0.9740 | 0.9600 |

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**Enthalpy of mixing**

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Kimura, T. - Khan, M. A. - Kamiyama, T., Enthalpic changes on mixing two couples of S- and R-enantiomers which contained amino groups at 298.15 K, Journal of Thermal Analysis and Calorimetry 3 (2006) 575-580. doi:10.1007/s10973-006-7657-4

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 185.17 | 0.0960 |
| 199.36 | 0.1170 |
| 471.25 | 0.3080 |
| 550.02 | 0.4170 |
| 529.38 | 0.5310 |
| 495.30 | 0.5990 |
| 495.31 | 0.6050 |
| 391.74 | 0.6910 |
| 269.58 | 0.8050 |
| 106.39 | 0.9320 |

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**Heat capacity of mixing**

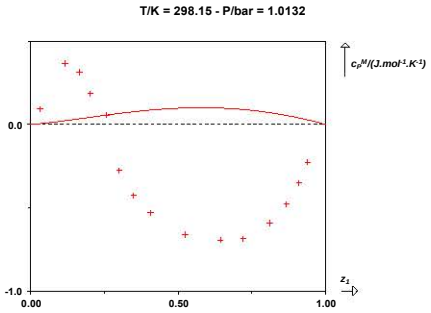
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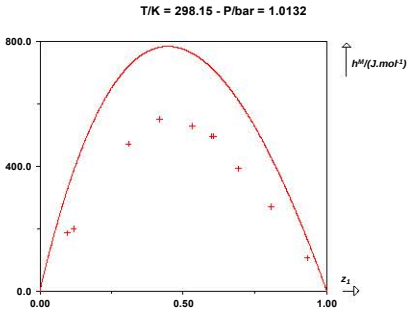
Grolier, J. -P. E. - Roux-Desgranges, G. - Berkane, M. - Wilhelm, Emmerich, Heat capacities and densities of mixtures of very polar substances. 3. Mixtures containing either trichloromethane or 1,4-dioxane or diisopropylether, Journal of Solution Chemistry 2 (1994) 153-166. doi:10.1007/BF00973543

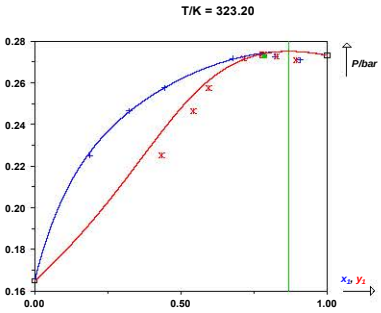
**T / K = 298.15**

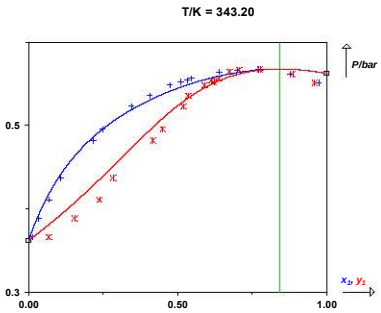
**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.0920 | 0.0319 |
| 0.3640 | 0.1166 |
| 0.3140 | 0.1654 |
| 0.1850 | 0.2032 |
| 0.0560 | 0.2567 |
| -0.2780 | 0.3007 |
| -0.4270 | 0.3497 |
| -0.5290 | 0.4072 |
| -0.6630 | 0.5233 |
| -0.6930 | 0.6436 |
| -0.6860 | 0.7207 |
| -0.5930 | 0.8110 |
| -0.4790 | 0.8687 |
| -0.3510 | 0.9103 |
| -0.2280 | 0.9390 |


T/K = 298.15 - P/bar = 1.0132
$c_P^M$/(J.mol$^{-1}$.K$^{-1}$)
0.0
-1.0
0.00
0.50
1.00
$z_1$


T/K = 298.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
800.0
400.0
0.0
0.00
0.50
1.00
$z_1$


T/K = 323.20
P/bar
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.00
0.50
1.00
$x_1$, $y_1$


T/K = 343.20
P/bar
0.5
0.3
0.00
0.50
1.00
$x_1$, $y_1$

## TETRAHYDROFURAN (1) + N,N-DIMETHYLFORMAMIDE (2)

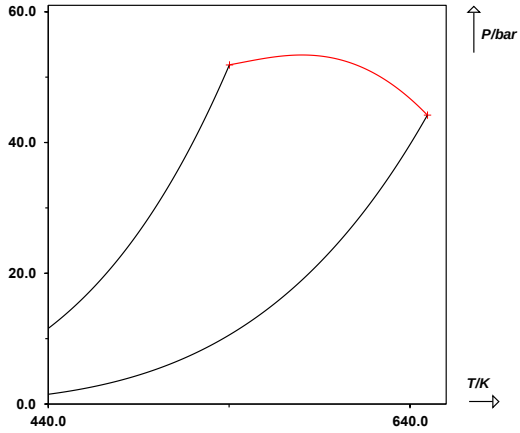
| | | |
|---|---|---|
| **CAS** | 109-99-9 | 68-12-2 |
| **InChiKey** | WYURNTSHIVDZCO-UHFFFAOYSA-N | ZMXDDKWLCZADIW-UHFFFAOYSA-N |
| **$T_c$ / K** | 540.15 | 649.60 |
| **$P_c$ / bar** | 51.90 | 44.20 |
| **ω** | 0.225 | 0.318 |

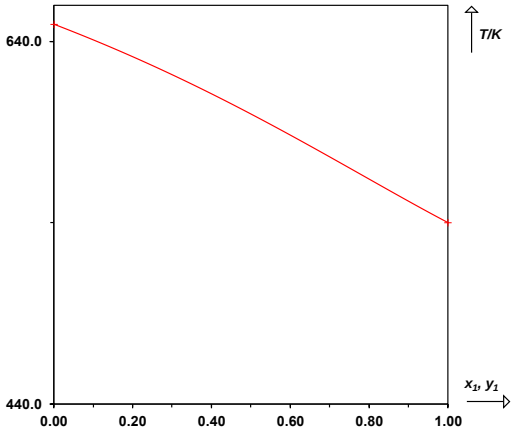
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 88.2
B/MPa = 77.4

*Deviations*
MAPE on x = 5.6 %
MAPE on y = 6.4 %
MAPE on $h^M$ = 5.4 %



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**Isothermal phase equilibrium data**

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Geier, K. - Bittrich, H.-J., Zur Thermodynamik der Flüssig-Dampf-Gleichgewichte der binären Systeme n-Hexan/Benzol, Cyclohexan/Benzol und Tetrahydrofuran mit n-hexan, cyclohexan, benzol und dimethylformamid, Zeitschrift für Physikalische Chemie 1 (1979) doi:10.1515/zpch-1979-26094

**T / K =** **313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1121 | 0.1560 | 0.9020 |
| 0.1725 | 0.2970 | 0.9440 |
| 0.2272 | 0.4440 | 0.9630 |
| 0.2678 | 0.5630 | 0.9740 |
| 0.2970 | 0.6550 | 0.9800 |
| 0.3177 | 0.7260 | 0.9850 |
| 0.3341 | 0.7800 | 0.9870 |
| 0.3468 | 0.8250 | 0.9890 |
| 0.3597 | 0.8610 | 0.9920 |
| 0.3702 | 0.8950 | 0.9930 |
| 0.3769 | 0.9170 | 0.9940 |
| 0.3844 | 0.9400 | 0.9960 |
| 0.3898 | 0.9550 | 0.9970 |
| 0.3960 | 0.9740 | 0.9980 |

Geier, K. - Bittrich, H.-J., Zur Thermodynamik der Flüssig-Dampf-Gleichgewichte der binären Systeme n-Hexan/Benzol, Cyclohexan/Benzol und Tetrahydrofuran mit n-hexan, cyclohexan, benzol und dimethylformamid, Zeitschrift für Physikalische Chemie 1 (1979) doi:10.1515/zpch-1979-26094

**T / K =** **333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1032 | 0.0450 | 0.6820 |
| 0.1217 | 0.0580 | 0.7330 |
| 0.1552 | 0.0870 | 0.7990 |
| 0.1704 | 0.1000 | 0.8200 |
| 0.2139 | 0.1400 | 0.8630 |
| 0.2564 | 0.1800 | 0.8890 |
| 0.3040 | 0.2300 | 0.9100 |
| 0.3522 | 0.2840 | 0.9280 |
| 0.4220 | 0.3750 | 0.9450 |
| 0.4673 | 0.4380 | 0.9530 |
| 0.5442 | 0.5500 | 0.9660 |
| 0.7226 | 0.8250 | 0.9880 |
| 0.7681 | 0.8950 | 0.9930 |

---

**Enthalpy of mixing**

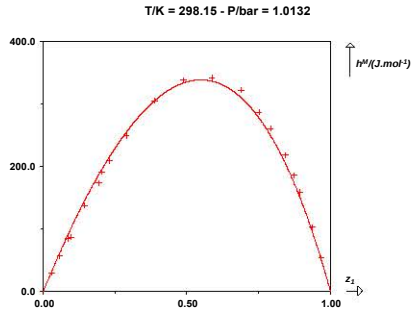
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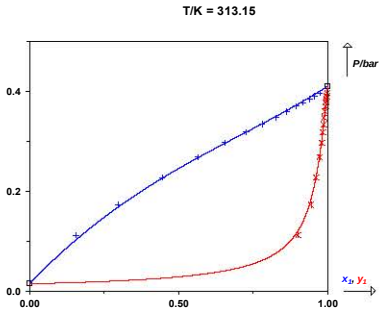
Conti, G. - Gianni, P. - Matteoli, E., Excess enthalpies and excess heat capacities of (N,N-dimethylformamide + tetrahydrofuran + cyclohexane) at the temperature 298.15 K, The Journal of Chemical Thermodynamics 12 (1994) 1249-1257. doi:10.1006/jcht.1994.1142

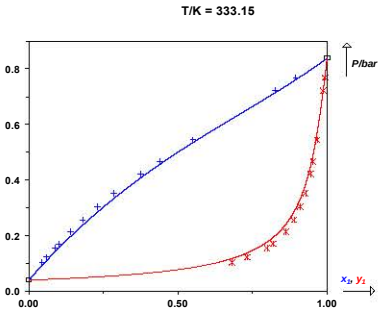
**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 29.30 | 0.0285 |
| 56.40 | 0.0572 |
| 84.10 | 0.0859 |
| 86.30 | 0.0953 |
| 137.10 | 0.1435 |
| 173.00 | 0.1916 |
| 190.70 | 0.2014 |
| 208.20 | 0.2305 |
| 248.50 | 0.2889 |
| 304.80 | 0.3873 |
| 337.60 | 0.4867 |
| 341.60 | 0.5871 |
| 321.40 | 0.6887 |
| 286.30 | 0.7502 |
| 260.20 | 0.7913 |
| 217.80 | 0.8431 |
| 184.70 | 0.8743 |
| 158.30 | 0.8951 |
| 102.40 | 0.9369 |
| 53.10 | 0.9684 |


T/K = 298.15 - P/bar = 1.0132
400.0
200.0
0.0
0.00
0.50
1.00
$h^M$/(J.mol$^{-1}$)
$z_1$


T/K = 313.15
0.4
0.2
0.0
0.00
0.50
1.00
P/bar
$x_1$, $y_1$


T/K = 333.15
0.8
0.6
0.4
0.2
0.0
0.00
0.50
1.00
P/bar
$x_1$, $y_1$

## n-BUTYL ACETATE (1) + N,N-DIMETHYLFORMAMIDE (2)

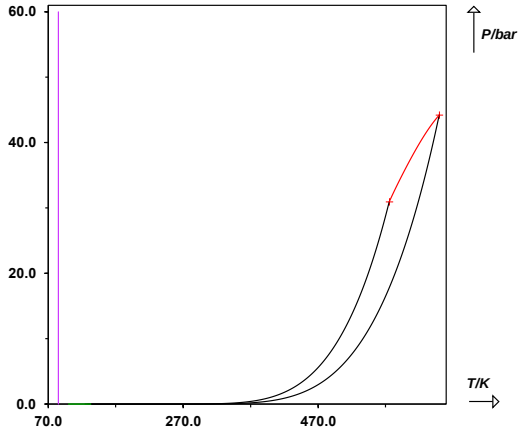
| | | |
|---|---|---|
| **CAS** | 123-86-4 | 68-12-2 |
| **InChiKey** | DKPFZGUDAPQIHT-UHFFFAOYSA-N | ZMXDDKWLCZADIW-UHFFFAOYSA-N |
| **$T_c$ / K** | 575.40 | 649.60 |
| **$P_c$ / bar** | 30.90 | 44.20 |
| **ω** | 0.439 | 0.318 |

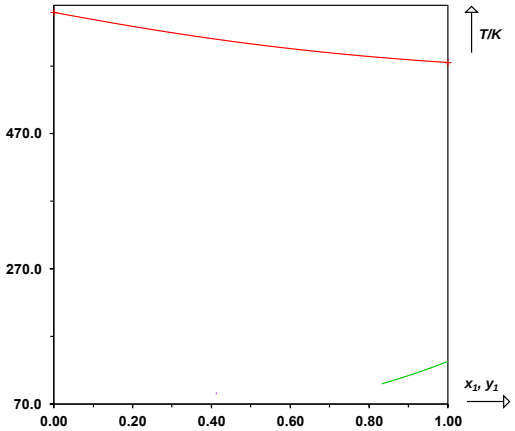
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 84.2
B/MPa = 64.7

*Deviations*
MAPE on x = 11 %
MAPE on y = 14 %
MAPE on $h^M$ = 6.1 %



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**Isothermal phase equilibrium data**

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Shealy, Glenn S. - Sandler, Stanley I., Vapor-liquid equilibrium for four mixtures containing N,N-dimethylformamide, Journal of Chemical & Engineering Data 4 (1985) 455-459. doi:10.1021/je00042a026

**T / K = 363.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1347 | 0.0103 | 0.0473 |
| 0.1435 | 0.0291 | 0.1206 |
| 0.1588 | 0.0629 | 0.2309 |
| 0.1765 | 0.1105 | 0.3410 |
| 0.1962 | 0.1733 | 0.4414 |
| 0.2093 | 0.2222 | 0.5074 |
| 0.2148 | 0.2540 | 0.5339 |
| 0.2305 | 0.3143 | 0.5956 |
| 0.2446 | 0.3906 | 0.6497 |
| 0.2584 | 0.4720 | 0.6991 |
| 0.2713 | 0.5601 | 0.7481 |
| 0.2824 | 0.6536 | 0.7947 |
| 0.2933 | 0.7491 | 0.8399 |
| 0.3016 | 0.8287 | 0.8790 |
| 0.3069 | 0.8899 | 0.9217 |
| 0.3110 | 0.9409 | 0.9556 |
| 0.3130 | 0.9771 | 0.9811 |

Shealy, Glenn S. - Sandler, Stanley I., Vapor-liquid equilibrium for four mixtures containing N,N-dimethylformamide, Journal of Chemical & Engineering Data 4 (1985) 455-459. doi:10.1021/je00042a026

**T / K = 388.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3355 | 0.0118 | 0.0440 |
| 0.3534 | 0.0299 | 0.1138 |
| 0.3855 | 0.0641 | 0.2187 |
| 0.4220 | 0.1095 | 0.3196 |
| 0.4581 | 0.1610 | 0.4120 |
| 0.5031 | 0.2363 | 0.5054 |
| 0.5414 | 0.3119 | 0.5754 |
| 0.5775 | 0.3957 | 0.6391 |
| 0.6070 | 0.4760 | 0.6833 |
| 0.6335 | 0.5578 | 0.7325 |
| 0.6617 | 0.6572 | 0.7832 |
| 0.6855 | 0.7504 | 0.8360 |
| 0.7035 | 0.8327 | 0.8826 |
| 0.7184 | 0.9020 | 0.9260 |
| 0.7266 | 0.9531 | 0.9622 |
| 0.7307 | 0.9852 | 0.9871 |

---

**Enthalpy of mixing**

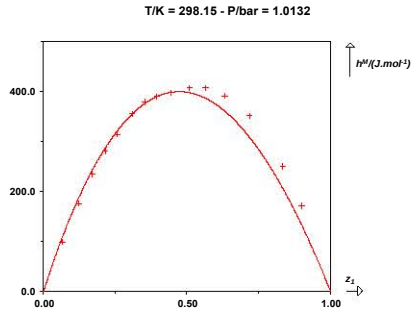
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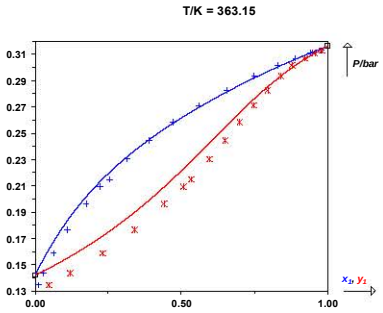
Venkatesu, P. - Ramadevi, R. S. - Prabhakara Rao, M. V. - Prasad, D. H. L., Excess Molar Enthalpies of N,N-Dimethylformamide with Chloroethanes and Acetates at 298.15 K, Journal of Chemical & Engineering Data 4 (2000) 515-517. doi:10.1021/je990286r

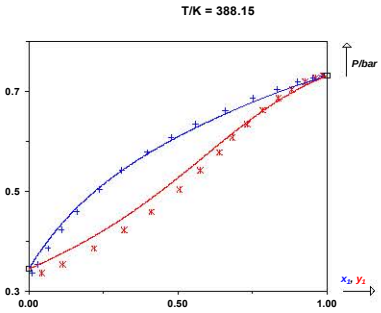
**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 170.00 | 0.8998 |
| 250.00 | 0.8344 |
| 351.00 | 0.7179 |
| 391.00 | 0.6326 |
| 407.00 | 0.5656 |
| 407.00 | 0.5092 |
| 397.00 | 0.4454 |
| 389.00 | 0.3956 |
| 379.00 | 0.3536 |
| 355.00 | 0.3089 |
| 314.00 | 0.2558 |
| 279.00 | 0.2151 |
| 234.00 | 0.1702 |
| 175.00 | 0.1208 |
| 98.00 | 0.0650 |


T/K = 298.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
400.0
200.0
0.0
0.00
0.50
1.00
$z_1$


T/K = 363.15
P/bar
0.31
0.29
0.27
0.25
0.23
0.21
0.19
0.17
0.15
0.13
0.00
0.50
1.00
$x_1$, $y_1$


T/K = 388.15
P/bar
0.7
0.5
0.3
0.00
0.50
1.00
$x_1$, $y_1$

## THIOPHENE (1) + SULFOLANE (2)

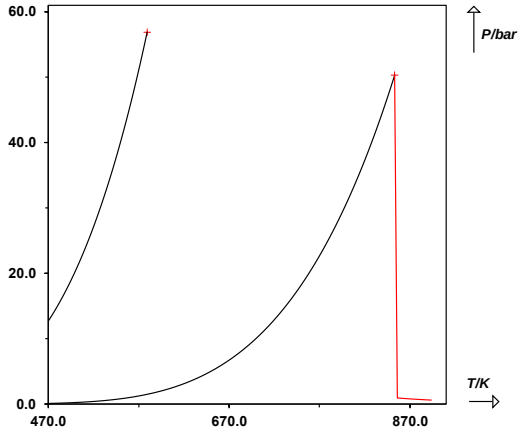
| | | |
|---|---|---|
| **CAS** | 110-02-1 | 126-33-0 |
| **InChiKey** | YTPLMLYBLZKORZ-UHFFFAOYSA-N | HXJUTPCZVOIRIF-UHFFFAOYSA-N |
| **$T_c$ / K** | 579.35 | 853.00 |
| **$P_c$ / bar** | 56.90 | 50.30 |
| **ω** | 0.197 | 0.382 |

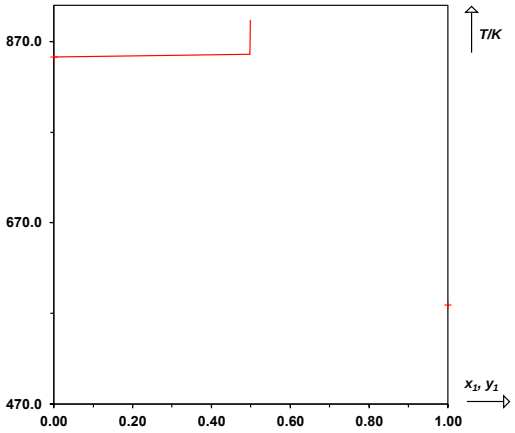
Non ideal with entropic causes

**PPR78 results**

*Parameters*
A/MPa = 2.16
B/MPa = -23.7

*Deviations*
MAPE on x = 1.7 %
MAPE on y = 17 %
MAPE on $h^M$ = 17 %



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**Isothermal phase equilibrium data**

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Ahlers, S., Systematische Messung thermodynamischer Daten für das System Thiophen - Sulfolan zur Erweiterung der Gruppenbeitragsmethode Modified UNIFAC (Dortmund) (2009)

**T / K = 353.15**

| P / bar | $y_1$ |
|---|---|
| 0.0087 | 0.9240 |
| 0.0157 | 0.9610 |
| 0.0302 | 0.9800 |
| 0.0548 | 0.9890 |
| 0.0800 | 0.9930 |
| 0.1074 | 0.9950 |
| 0.1402 | 0.9960 |
| 0.1824 | 0.9970 |

Ahlers, S., Systematische Messung thermodynamischer Daten für das System Thiophen - Sulfolan zur Erweiterung der Gruppenbeitragsmethode Modified UNIFAC (Dortmund) (2009)

**T / K = 413.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0712 | 0.0090 | 0.7700 |
| 0.1300 | 0.0180 | 0.8740 |
| 0.1941 | 0.0280 | 0.9160 |
| 0.3944 | 0.0580 | 0.9580 |
| 0.5995 | 0.0920 | 0.9730 |
| 0.8256 | 0.1290 | 0.9800 |
| 1.043 | 0.1660 | 0.9840 |
| 1.296 | 0.2120 | 0.9870 |
| 1.604 | 0.2700 | 0.9890 |
| 1.924 | 0.3340 | 0.9910 |
| 2.246 | 0.4030 | 0.9920 |
| 3.386 | 0.7180 | 0.9960 |

---

**Enthalpy of mixing**

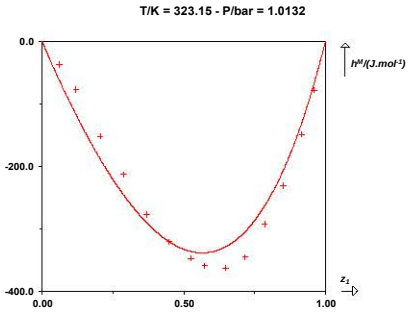
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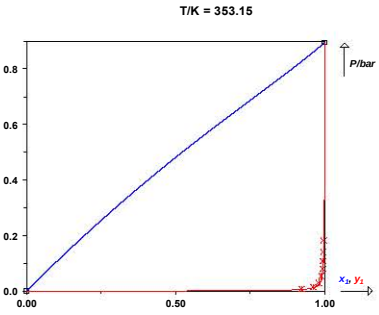
Ahlers, S., Systematische Messung thermodynamischer Daten für das System Thiophen - Sulfolan zur Erweiterung der Gruppenbeitragsmethode Modified UNIFAC (Dortmund) (2009)

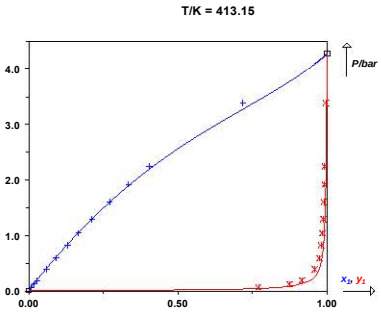
**T / K = 323.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -37.38 | 0.0603 |
| -77.26 | 0.1192 |
| -151.89 | 0.2054 |
| -213.24 | 0.2888 |
| -277.19 | 0.3697 |
| -320.59 | 0.4482 |
| -347.35 | 0.5244 |
| -359.45 | 0.5739 |
| -362.97 | 0.6464 |
| -345.56 | 0.7168 |
| -292.75 | 0.7852 |
| -231.14 | 0.8517 |
| -148.88 | 0.9164 |
| -78.40 | 0.9586 |


T/K = 323.15 - P/bar = 1.0132
0.0
-200.0
-400.0
0.00
0.50
1.00
hᴱ/(J.mol⁻¹)
z₁


T/K = 353.15
0.8
0.6
0.4
0.2
0.0
0.00
0.50
1.00
P/bar
x₁, y₁


T/K = 413.15
4.0
3.0
2.0
1.0
0.0
0.00
0.50
1.00
P/bar
x₁, y₁

# Annexe B-2

# Banque de données des systèmes binaires
# Systèmes associés

# SA-NA systems (AC = 5)

## n-BUTANE (1) + WATER (2)

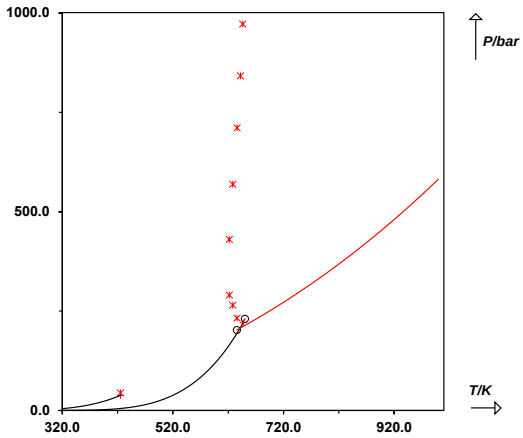
| | | |
|---|---|---|
| **CAS** | 106-97-8 | 7732-18-5 |
| **InChiKey** | IJDNQMDRQITEOD-UHFFFAOYSA-N | XLYOFNOQVPJJNP-UHFFFAOYSA-N |
| **$T_c$ / K** | 425.12 | 647.096 |
| **$P_c$ / bar** | 37.96 | 220.64 |
| **ω** | 0.200 | 0.345 |

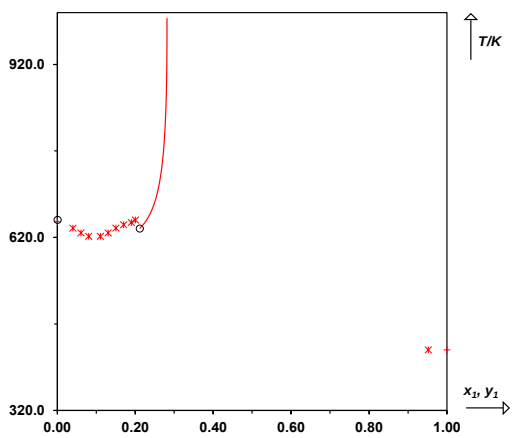
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 9880
B/MPa = 10100

*Deviations*
MAPE on x = 52 %
MAPE on y = 51 %
MAPE on $x_c$ = 87 %
MAPE on $P_c$ = 55 %
MAPE on $h^M$ = 20 %



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**Isothermal phase equilibrium data**

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Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. n-Butane-Water System in the Two-Phase Region., Industrial & Engineering Chemistry 3 (1952) 609-615. doi:10.1021/ie50507a049

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.379 | 0.0000 | 0.9535 |
| 2.758 | 0.0000 | 0.9772 |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. n-Butane-Water System in the Two-Phase Region., Industrial & Engineering Chemistry 3 (1952) 609-615. doi:10.1021/ie50507a049

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.379 | 0 | 0.7650 |
| 2.758 | 0 | 0.8850 |
| 4.137 | 0 | 0.9243 |
| 5.516 | 0.0001 | 0.9443 |
| 6.895 | 0.0001 | 0.9562 |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. n-Butane-Water System in the Two-Phase Region., Industrial & Engineering Chemistry 3 (1952) 609-615. doi:10.1021/ie50507a049

**T / K = 377.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.379 | 0 | 0.1420 |
| 2.758 | 0 | 0.5730 |
| 4.137 | 0 | 0.7280 |
| 5.516 | 0 | 0.7910 |
| 6.895 | 0.0001 | 0.8340 |
| 13.79 | 0.0001 | 0.9244 |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. n-Butane-Water System in the Two-Phase Region., Industrial & Engineering Chemistry 3 (1952) 609-615. doi:10.1021/ie50507a049

**T / K = 410.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.137 | 0 | 0.1800 |
| 5.516 | 0 | 0.3860 |
| 6.895 | 0 | 0.5090 |
| 13.79 | 0.0001 | 0.7610 |
| 20.68 | 0.0001 | 0.8520 |
| 27.58 | 0.0002 | 0.9009 |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. n-Butane-Water System in the Two-Phase Region., Industrial & Engineering Chemistry 3 (1952) 609-615. doi:10.1021/ie50507a049

**T / K = 444.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.79 | 0.0001 | 0.4060 |
| 20.68 | 0.0002 | 0.6090 |
| 27.58 | 0.0002 | 0.7250 |
| 34.47 | 0.0003 | 0.8020 |
| 41.37 | 0.0003 | 0.8580 |
| 55.16 | 0.0004 | 0.9184 |
| 68.95 | 0.0004 | 0.9382 |
| 86.18 | 0.0004 | 0.9455 |
| 103.42 | 0.0004 | 0.9503 |
| 120.66 | 0.0004 | 0.9539 |
| 137.90 | 0.0004 | 0.9567 |
| 172.37 | 0.0004 | 0.9603 |
| 206.84 | 0.0004 | 0.9631 |
| 275.79 | 0.0005 | 0.9667 |
| 344.74 | 0.0005 | 0.9601 |
| 413.69 | 0.0005 | 0.9713 |
| 482.63 | 0.0005 | 0.9734 |
| 551.58 | 0.0005 | 0.9752 |
| 620.53 | 0.0005 | 0.9767 |
| 689.48 | 0.0005 | 0.9779 |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. n-Butane-Water System in the Two-Phase Region., Industrial & Engineering Chemistry 3 (1952) 609-615. doi:10.1021/ie50507a049

**T / K = 477.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.68 | 0.0001 | 0.1690 |
| 27.58 | 0.0002 | 0.3650 |
| 34.47 | 0.0003 | 0.4880 |
| 41.37 | 0.0004 | 0.5770 |
| 55.16 | 0.0005 | 0.6970 |
| 68.95 | 0.0006 | 0.7750 |
| 86.18 | 0.0006 | 0.8320 |
| 103.42 | 0.0007 | 0.8600 |
| 120.66 | 0.0007 | 0.8770 |
| 137.90 | 0.0007 | 0.8900 |
| 172.37 | 0.0008 | 0.9052 |
| 206.84 | 0.0008 | 0.9150 |
| 275.79 | 0.0009 | 0.9264 |

| | | |
|---|---|---|
| 344.74 | 0.0009 | 0.9335 |
| 413.69 | 0.0009 | 0.9390 |
| 482.63 | 0.0009 | 0.9421 |
| 551.58 | 0.0010 | 0.9453 |
| 620.53 | 0.0010 | 0.9481 |
| 689.48 | 0.0010 | 0.9503 |

Reamer, H. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. n-Butane-Water System in the Two-Phase Region., Industrial & Engineering Chemistry 3 (1952) 609-615. doi:10.1021/ie50507a049

**T / K = 510.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.47 | 0.0001 | 0.0560 |
| 41.37 | 0.0003 | 0.1890 |
| 55.16 | 0.0006 | 0.3770 |
| 68.95 | 0.0008 | 0.5070 |
| 86.18 | 0.0010 | 0.6180 |
| 103.42 | 0.0011 | 0.6890 |
| 120.66 | 0.0011 | 0.7320 |
| 137.90 | 0.0012 | 0.7620 |
| 172.37 | 0.0013 | 0.7980 |
| 206.84 | 0.0013 | 0.8210 |
| 275.79 | 0.0014 | 0.8500 |
| 344.74 | 0.0015 | 0.8650 |
| 413.69 | 0.0016 | 0.8740 |
| 482.63 | 0.0016 | 0.8800 |
| 551.58 | 0.0016 | 0.8850 |
| 620.53 | 0.0017 | 0.8890 |
| 689.48 | 0.0017 | 0.8920 |

Danneil, A. - Tödheide, K. - Franck, E. U., Verdampfungsgleichgewichte und kritische Kurven in den Systemen Äthan/Wasser und n-Butan/Wasser bei hohen Drücken, Chemie Ingenieur Technik - CIT 13 (1967) 816-822. doi:10.1002/cite.330391309

**T / K = 628.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 255.00 | 0.0250 | 0.1240 |
| 295.00 | 0.0480 | 0.1050 |
| 590.00 | 0.0430 | 0.2870 |

Danneil, A. - Tödheide, K. - Franck, E. U., Verdampfungsgleichgewichte und kritische Kurven in den Systemen Äthan/Wasser und n-Butan/Wasser bei hohen Drücken, Chemie Ingenieur Technik - CIT 13 (1967) 816-822. doi:10.1002/cite.330391309

**T / K = 637.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 690.00 | 0.0770 | 0.2560 |
| 830.00 | 0.0410 | 0.3180 |

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**Enthalpy of mixing**

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Lancaster, N.M - Wormald, C.J, Excess molar enthalpies for {xH2O + (1 − x)C3H6}(g), {xH2O + (1 − x)C3H8}(g), and {xH2O + (1 − x)C4H10}(g), The Journal of Chemical Thermodynamics 6 (1986) 545-550. doi:10.1016/0021-9614(86)90137-0

**T / K = 393.20**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 54.30 | 0.3180 |
| 56.40 | 0.3610 |
| 57.40 | 0.3990 |
| 60.20 | 0.4310 |
| 61.00 | 0.4580 |
| 61.60 | 0.4950 |
| 61.50 | 0.5410 |
| 60.20 | 0.5660 |
| 58.50 | 0.6350 |
| 51.60 | 0.7020 |

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**Critical point**

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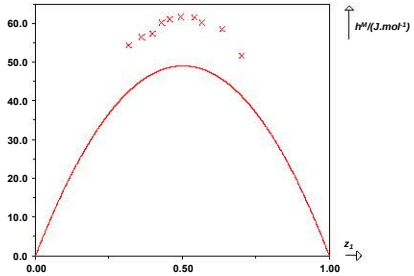
Tian, Yiling - Zhao, Xuefeng - Chen, Li - Zhu, Hugang - Fu, Huafeng, High pressure phase equilibria and critical phenomena of water + iso-butane and water + n-butane systems to 695 K and 306 MPa, The Journal of Supercritical Fluids 2 (2004) 145-153. doi:10.1016/j.supflu.2003.09.002

| T / K | P / bar | $x_1$ |
|---|---|---|
| 650.00 | 1060.0 | 0.2000 |
| 646.00 | 972.00 | 0.1900 |
| 642.00 | 842.00 | 0.1700 |
| 636.00 | 711.00 | 0.1500 |
| 628.00 | 569.00 | 0.1300 |
| 622.00 | 430.00 | 0.1100 |
| 622.00 | 290.00 | 0.0800 |
| 628.00 | 265.00 | 0.0600 |
| 636.00 | 232.00 | 0.0400 |

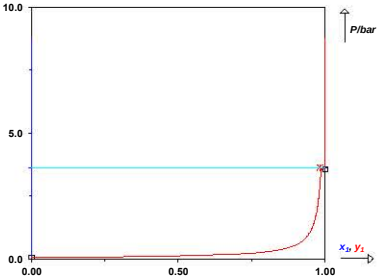
Reamer, H. H. - Olds, R. H. - Sage, B. H. - Lacey, W. N., Phase Equilibria in Hydrocarbon Systems. n-Butane–Water System in Three-Phase Region, Industrial & Engineering Chemistry 4 (1944) 381-383. doi:10.1021/ie50412a024

| T / K | P / bar | $x_1$ |
|---|---|---|
| 425.15 | 43.95 | 0.9517 |

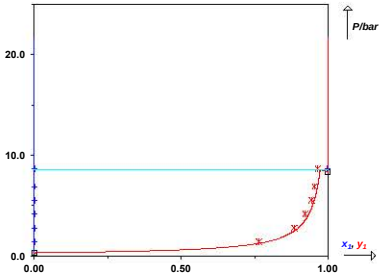
T/K = 393.20 - P/bar = 1.0100



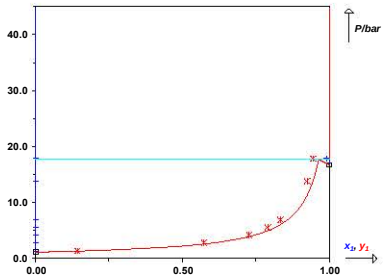

T/K = 310.93



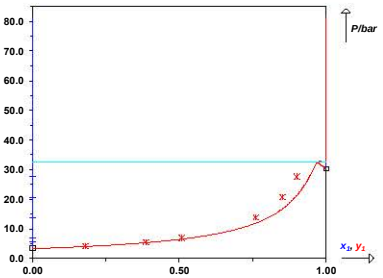

T/K = 344.26



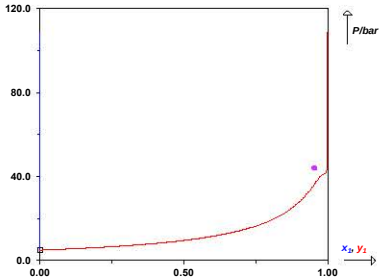

T/K = 377.59



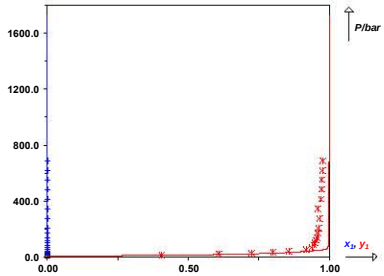

T/K = 410.93



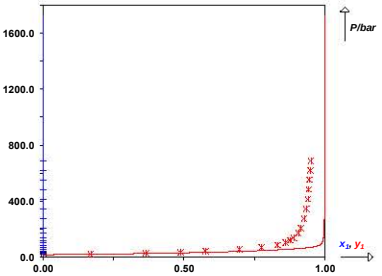

T/K = 425.15



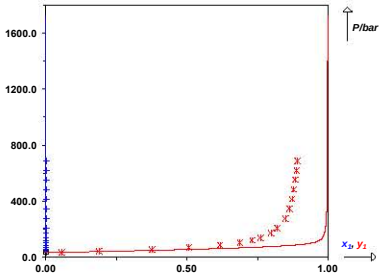

T/K = 444.26



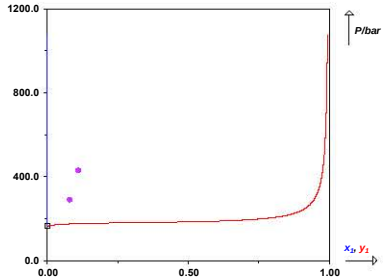

T/K = 477.59



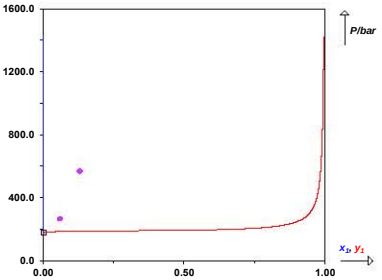

T/K = 510.93



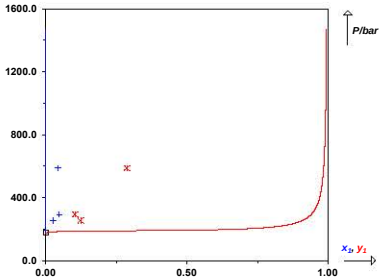

T/K = 622.00

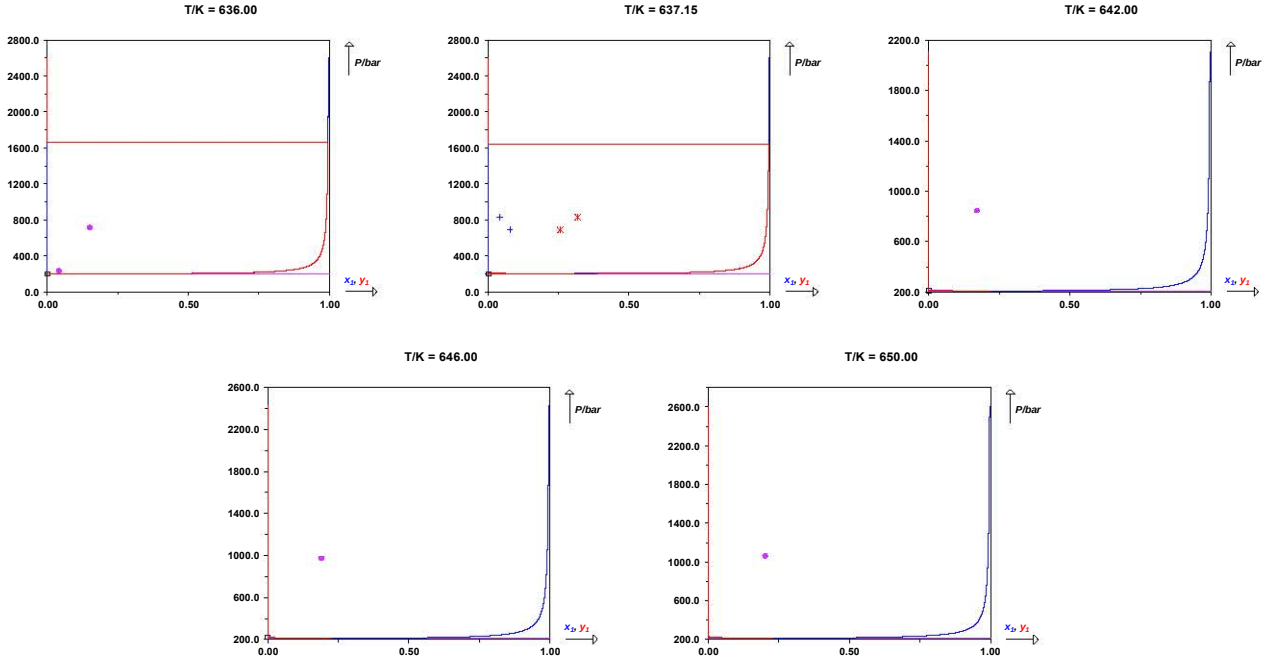



T/K = 628.00




T/K = 628.15




T/K = 636.00
T/K = 637.15
T/K = 642.00
T/K = 646.00
T/K = 650.00
P/bar
x1, y1

## WATER (1) + BENZENE (2)

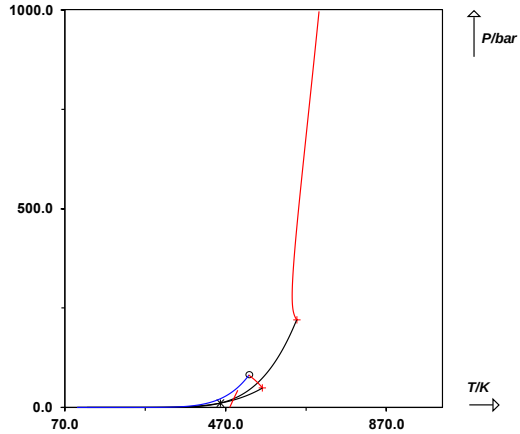
| | | |
|---|---|---|
| **CAS** | 7732-18-5 | 71-43-2 |
| **InChiKey** | XLYOFNOQVPJJNP-UHFFFAOYSA-N | UHOVQNZJYSORNB-UHFFFAOYSA-N |
| **$T_c$ / K** | 647.10 | 562.05 |
| **$P_c$ / bar** | 220.64 | 48.95 |
| **ω** | 0.345 | 0.210 |

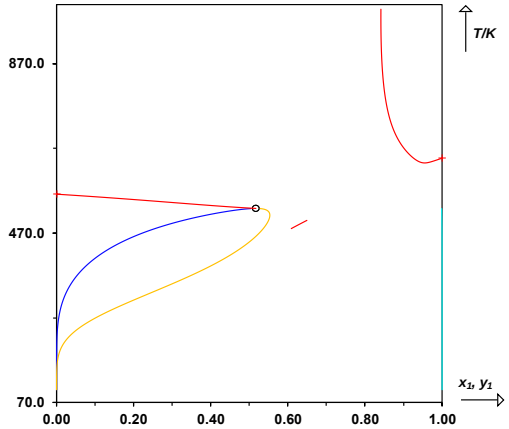
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 3460
B/MPa = 4300

*Deviations*
MAPE on x = 50 %
MAPE on y = 33 %
MAPE on $h^M$ = 23 %



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**Isobaric phase equilibrium data**

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Thompson, W. H. - Snyder, J. R., Mutual Solubilities of Benzene and Water. Equilibria in the Two Phase Liquid - Liquid Region., Journal of Chemical & Engineering Data 4 (1964) 516-520. doi:10.1021/je60023a013

**P / bar = 68.95**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 310.93 | 0.9996 | 0.0042 |
| 310.98 | 0.9995 | 0.0047 |
| 311.09 | 0.9996 | 0.0049 |
| 311.48 | 0.9995 | 0.0042 |
| 344.26 | 0.9993 | 0.0121 |
| 344.43 | 0.9993 | 0.0124 |
| 410.93 | 0.9981 | 0.0558 |
| 444.26 | 0.9964 | 0.1000 |
| 477.59 | 0.9918 | 0.1780 |

Thompson, W. H. - Snyder, J. R., Mutual Solubilities of Benzene and Water. Equilibria in the Two Phase Liquid - Liquid Region., Journal of Chemical & Engineering Data 4 (1964) 516-520. doi:10.1021/je60023a013

**P / bar = 344.74**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 344.26 | 0.9991 | 0.0106 |
| 377.98 | 0.9993 | 0.0124 |
| 443.87 | 0.9957 | 0.0959 |
| 444.26 | 0.9957 | 0.0905 |
| 477.59 | 0.9902 | 0.1620 |
| 477.98 | 0.9902 | 0.1530 |
| 511.32 | 0.9735 | 0.4320 |
| 510.93 | 0.9745 | 0.4500 |
| 510.76 | 0.9752 | 0.4600 |

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**Enthalpy of mixing**

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Wormald, C. J. - Lancaster, N. M. - Sowden, C. J., Benzene–water association Excess molar enthalpy and second virial cross-coefficients for (benzene–water)(g) and (cyclohexane–water)(g), Journal of the Chemical Society, Faraday Transactions 10 (1997) 1921-1926. doi:10.1039/a608259i

**T / K = 403.20**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 62.00 | 0.6180 |
| 65.20 | 0.5570 |
| 65.40 | 0.4940 |
| 64.50 | 0.4530 |
| 63.60 | 0.3990 |

Wormald, C. J. - Lancaster, N. M. - Sowden, C. J., Benzene–water association Excess molar enthalpy and second virial cross-coefficients for (benzene–water)(g) and (cyclohexane–water)(g), Journal of the Chemical Society, Faraday Transactions 10 (1997) 1921-1926. doi:10.1039/a608259i

**T / K = 413.20**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 57.00 | 0.6350 |
| 58.30 | 0.5910 |
| 59.70 | 0.5040 |
| 60.80 | 0.4480 |
| 57.10 | 0.4200 |

Wormald, C.J. - Slater, J., Excess enthalpies for (water + benzene) in the liquid and supercritical regions at T= 503 K to T= 592 K and p= 16.4 MPa, The Journal of Chemical Thermodynamics 6 (1996) 627-636. doi:10.1006/jcht.1996.0059

**T / K = 503.00**

**P / bar = 164.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 395.00 | 0.9720 |
| 692.00 | 0.9380 |
| 1020.0 | 0.8930 |
| 1434.0 | 0.8340 |
| 1681.0 | 0.7970 |
| 1967.0 | 0.7500 |
| 2294.0 | 0.6960 |
| 2473.0 | 0.6630 |
| 2707.0 | 0.6270 |
| 2971.0 | 0.5850 |
| 3250.0 | 0.5370 |
| 3575.0 | 0.4840 |
| 3959.0 | 0.4180 |
| 4294.0 | 0.3610 |
| 4520.0 | 0.3260 |
| 4724.0 | 0.2900 |
| 4858.0 | 0.2710 |
| 4709.0 | 0.2520 |
| 4194.0 | 0.2100 |

Wormald, C.J. - Slater, J., Excess enthalpies for (water + benzene) in the liquid and supercritical regions at T= 503 K to T= 592 K and p= 16.4 MPa, The Journal of Chemical Thermodynamics 6 (1996) 627-636. doi:10.1006/jcht.1996.0059

**T / K = 521.00**

**P / bar = 164.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 355.00 | 0.9870 |
| 587.00 | 0.9720 |
| 1012.0 | 0.9380 |
| 1465.0 | 0.8940 |
| 2047.0 | 0.8340 |
| 2358.0 | 0.7970 |
| 2772.0 | 0.7520 |
| 3260.0 | 0.6980 |
| 3438.0 | 0.6650 |
| 3843.0 | 0.6200 |
| 4199.0 | 0.5870 |
| 4566.0 | 0.5390 |
| 5064.0 | 0.4830 |
| 5602.0 | 0.4200 |
| 6160.0 | 0.3600 |
| 6156.0 | 0.3440 |
| 5981.0 | 0.3280 |
| 5006.0 | 0.2540 |

Wormald, C.J. - Slater, J., Excess enthalpies for (water + benzene) in the liquid and supercritical regions at T= 503 K to T= 592 K and p= 16.4 MPa, The Journal of Chemical Thermodynamics 6 (1996) 627-636. doi:10.1006/jcht.1996.0059

**T / K = 544.00**

**P / bar = 164.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 927.00 | 0.9730 |
| 606.00 | 0.9690 |
| 1566.0 | 0.9400 |
| 2271.0 | 0.8950 |
| 3049.0 | 0.8370 |
| 3584.0 | 0.7990 |
| 4207.0 | 0.7550 |
| 4929.0 | 0.7000 |
| 5475.0 | 0.6670 |
| 5832.0 | 0.6310 |
| 6445.0 | 0.5890 |
| 7037.0 | 0.5420 |
| 7656.0 | 0.5070 |
| 7785.0 | 0.4840 |
| 7636.0 | 0.4610 |
| 7426.0 | 0.4200 |
| 6453.0 | 0.3280 |
| 5410.0 | 0.2530 |

Wormald, C.J. - Slater, J., Excess enthalpies for (water + benzene) in the liquid and supercritical regions at T= 503 K to T= 592 K and p= 16.4 MPa, The Journal of Chemical Thermodynamics 6 (1996) 627-636. doi:10.1006/jcht.1996.0059

**T / K = 560.00**

**P / bar = 164.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 2349.0 | 0.9390 |
| 3302.0 | 0.8950 |
| 4482.0 | 0.8370 |
| 5297.0 | 0.7990 |
| 6243.0 | 0.7550 |
| 7233.0 | 0.7010 |
| 8556.0 | 0.6280 |
| 8803.0 | 0.5890 |
| 8727.0 | 0.5370 |
| 8067.0 | 0.4180 |
| 6899.0 | 0.3300 |
| 5694.0 | 0.2520 |

Wormald, C.J. - Slater, J., Excess enthalpies for (water + benzene) in the liquid and supercritical regions at T= 503 K to T= 592 K and p= 16.4 MPa, The Journal of Chemical Thermodynamics 6 (1996) 627-636. doi:10.1006/jcht.1996.0059

**T / K = 576.00**

**P / bar = 164.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 2407.0 | 0.9490 |
| 4244.0 | 0.9000 |
| 5627.0 | 0.8520 |
| 5947.0 | 0.8390 |
| 7167.0 | 0.8010 |
| 8073.0 | 0.7580 |
| 9199.0 | 0.7040 |
| 9779.0 | 0.6680 |
| 10132.0 | 0.6370 |
| 10060.0 | 0.6360 |
| 10175.0 | 0.6000 |
| 9971.0 | 0.5390 |
| 9599.0 | 0.4860 |
| 8869.0 | 0.4290 |
| 8958.0 | 0.4270 |
| 7676.0 | 0.3470 |
| 6009.0 | 0.2570 |

Wormald, C.J. - Slater, J., Excess enthalpies for (water + benzene) in the liquid and supercritical regions at T= 503 K to T= 592 K and p= 16.4 MPa, The Journal of

Chemical Thermodynamics 6 (1996) 627-636. doi:10.1006/jcht.1996.0059

**T / K = 581.00**

**P / bar = 164.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 1413.0 | 0.9730 |
| 2932.0 | 0.9390 |
| 4626.0 | 0.8960 |
| 6594.0 | 0.8370 |
| 7771.0 | 0.8000 |
| 9192.0 | 0.7540 |
| 10315.0 | 0.7000 |
| 10458.0 | 0.6990 |
| 10998.0 | 0.6310 |
| 11162.0 | 0.5900 |
| 10846.0 | 0.5420 |
| 10097.0 | 0.4870 |
| 9229.0 | 0.4230 |
| 7637.0 | 0.3300 |
| 6165.0 | 0.2560 |

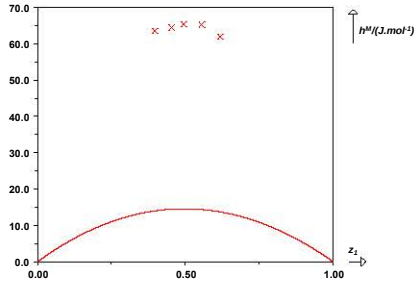
Wormald, C.J. - Slater, J., Excess enthalpies for (water + benzene) in the liquid and supercritical regions at T= 503 K to T= 592 K and p= 16.4 MPa, The Journal of Chemical Thermodynamics 6 (1996) 627-636. doi:10.1006/jcht.1996.0059

**T / K = 592.00**

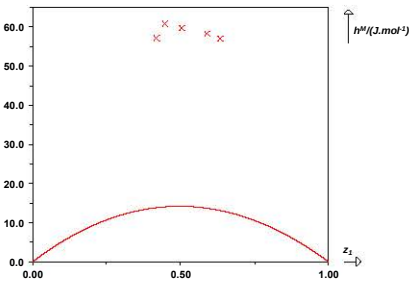
**P / bar = 164.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 1674.0 | 0.9730 |
| 3400.0 | 0.9390 |
| 3728.0 | 0.9310 |
| 4314.0 | 0.9190 |
| 5651.0 | 0.8950 |
| 6546.0 | 0.8800 |
| 6923.0 | 0.8680 |
| 7791.0 | 0.8590 |
| 8039.0 | 0.8500 |
| 8315.0 | 0.8430 |
| 8764.0 | 0.8370 |
| 9506.0 | 0.8300 |
| 9732.0 | 0.8230 |
| 10136.0 | 0.8150 |
| 10754.0 | 0.8080 |
| 11313.0 | 0.7960 |
| 12791.0 | 0.7550 |
| 13589.0 | 0.7230 |
| 13680.0 | 0.6990 |
| 13180.0 | 0.6300 |
| 12758.0 | 0.5890 |
| 11697.0 | 0.5210 |
| 9890.0 | 0.4220 |
| 8007.0 | 0.3290 |
| 6478.0 | 0.2550 |

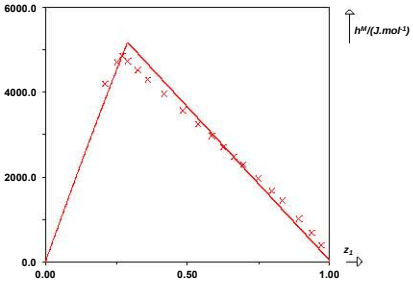
T/K = 403.20 - P/bar = 1.0100



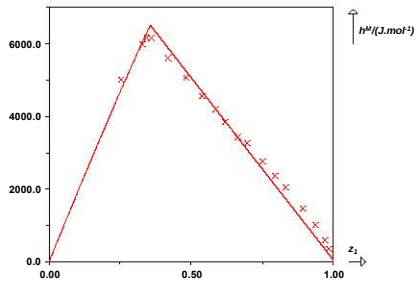

T/K = 413.20 - P/bar = 1.0100



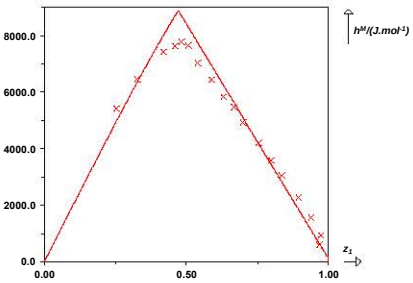

T/K = 503.00 - P/bar = 164.00



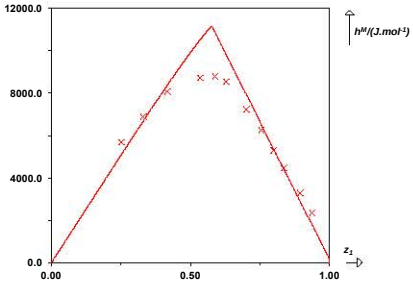

T/K = 521.00 - P/bar = 164.00



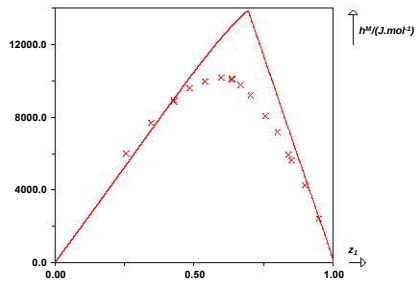

T/K = 544.00 - P/bar = 164.00



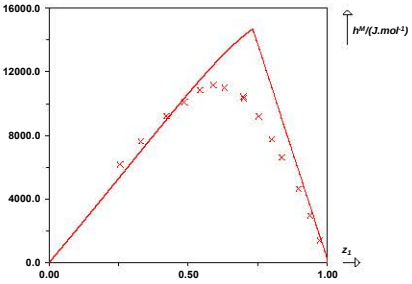

T/K = 560.00 - P/bar = 164.00



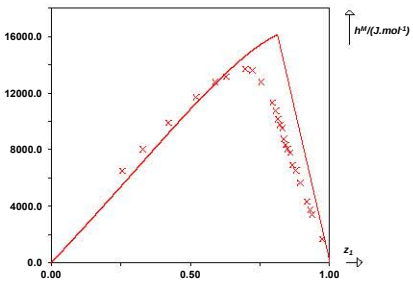

T/K = 576.00 - P/bar = 164.00



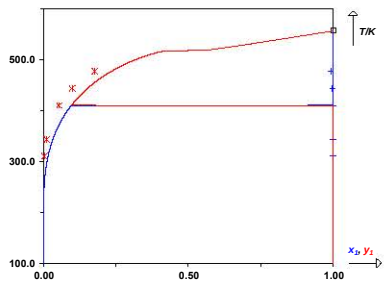

T/K = 581.00 - P/bar = 164.00



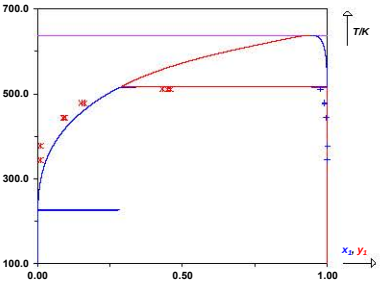

T/K = 592.00 - P/bar = 164.00



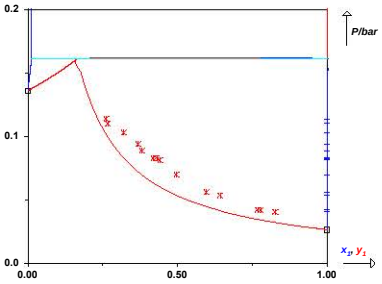

P/bar = 68.94800




P/bar = 344.74000




T/K = 298.15



## ETHANE (1) + 1-PROPANOL (2)

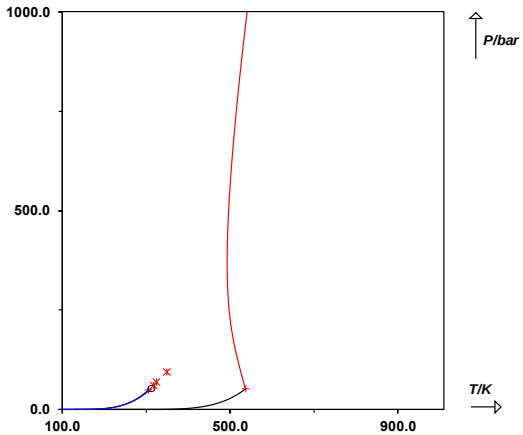
| | | |
|---|---|---|
| **CAS** | 74-84-0 | 71-23-8 |
| **InChiKey** | OTMSDBZUPAUEDD-UHFFFAOYSA-N | BDERNNFJNOPAEC-UHFFFAOYSA-N |
| **$T_c$ / K** | 305.32 | 536.80 |
| **$P_c$ / bar** | 48.72 | 51.69 |
| **ω** | 0.099 | 0.621 |

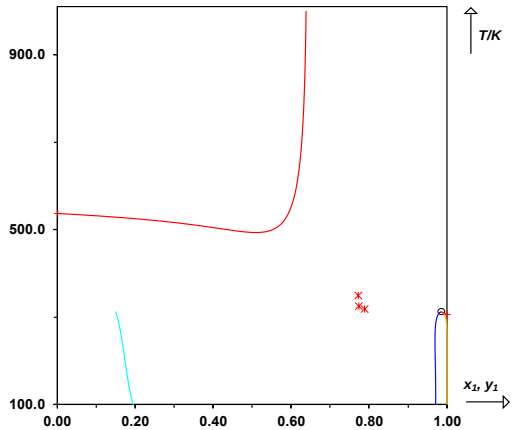
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 529
B/MPa = -51.6

*Deviations*
MAPE on x = 170 %
MAPE on y = 17 %
MAPE on $h^M$ = 97 %



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**Isothermal phase equilibrium data**

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Jiménez-Gallegos, Rodrigo - Galicia-Luna, Luis A. - Bouchot, Christian - Camacho-Camacho, Luis E. - Elizalde-Solis, Octavio, Experimental Determination and Correlation of Phase Equilibria for the Ethane + 1-Propanol and Propane + 1-Propanol Systems, Journal of Chemical & Engineering Data 5 (2006) 1629-1633. doi:10.1021/je060112r

**T / K = 317.59**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 28.17 | 0.2210 | 0.9930 | |
| 48.36 | 0.4350 | 0.9930 | |
| 53.36 | 0.5250 | 0.9920 | |
| 55.95 | 0.5870 | 0.9770 | |
| 57.27 | 0.6500 | 0.9680 | |
| 57.73 | 0.6570 | 0.9600 | |
| 58.68 | 0.6880 | 0.9230 | |
| 59.57 | 0.7080 | 0.8720 | |
| 59.78 | 0.7890 | 0.7890 | CRIT |

Jiménez-Gallegos, Rodrigo - Galicia-Luna, Luis A. - Bouchot, Christian - Camacho-Camacho, Luis E. - Elizalde-Solis, Octavio, Experimental Determination and Correlation of Phase Equilibria for the Ethane + 1-Propanol and Propane + 1-Propanol Systems, Journal of Chemical & Engineering Data 5 (2006) 1629-1633. doi:10.1021/je060112r

**T / K = 324.51**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 32.43 | 0.2320 | 0.9910 | |
| 52.41 | 0.4200 | 0.9910 | |
| 58.80 | 0.5070 | 0.9880 | |
| 61.11 | 0.5510 | 0.9850 | |
| 63.62 | 0.5900 | 0.9650 | |
| 65.46 | 0.6440 | 0.9440 | |
| 66.76 | 0.6750 | 0.9250 | |
| 67.82 | 0.7040 | 0.8800 | |
| 68.24 | 0.7340 | 0.8450 | |
| 69.32 | 0.7740 | 0.7740 | CRIT |

Suzuki, Kazuhiko - Sue, Haruhusa - Itou, Masahiro - Smith, Richard L. - Inomata, Hiroshi - Arai, Kunio - Saito, Shozaburo, Isothermal vapor-liquid equilibrium data for binary systems at high pressures: carbon dioxide-methanol, carbon dioxide-ethanol, carbon dioxide-1-propanol, methane-ethanol, methane-1-propanol, ethane-ethanol, and ethane-1-propanol systems, Journal of Chemical & Engineering Data 1 (1990) 63-66. doi:10.1021/je00059a020

**T / K = 333.40**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.56 | 0.0800 | 0.9840 |
| 28.11 | 0.1740 | 0.9900 |
| 59.67 | 0.4210 | 0.9890 |
| 67.42 | 0.5030 | 0.9710 |

Jiménez-Gallegos, Rodrigo - Galicia-Luna, Luis A. - Bouchot, Christian - Camacho-Camacho, Luis E. - Elizalde-Solis, Octavio, Experimental Determination and Correlation of Phase Equilibria for the Ethane + 1-Propanol and Propane + 1-Propanol Systems, Journal of Chemical & Engineering Data 5 (2006) 1629-1633. doi:10.1021/je060112r

**T / K = 348.68**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 8.410 | 0.0410 | 0.9460 | |
| 18.17 | 0.0920 | 0.9680 | |
| 28.09 | 0.1420 | 0.9770 | |
| 36.03 | 0.1880 | 0.9790 | |
| 43.44 | 0.2290 | 0.9800 | |
| 50.57 | 0.2680 | 0.9790 | |
| 57.11 | 0.3070 | 0.9780 | |
| 63.24 | 0.3450 | 0.9760 | |
| 70.76 | 0.3970 | 0.9710 | |
| 76.82 | 0.4550 | 0.9650 | |
| 85.29 | 0.5480 | 0.9480 | |
| 89.29 | 0.6000 | 0.9190 | |
| 91.70 | 0.6570 | 0.8870 | |
| 93.96 | 0.7060 | 0.8660 | |
| 94.88 | 0.7720 | 0.7720 | CRIT |

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**Enthalpy of mixing**

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McFall, T.A. - Post, M.E. - Christensen, J.J. - Izatt, R.M., The excess enthalpies of eight (ethane + alcohol) mixtures at 298.15 K, The Journal of Chemical Thermodynamics 5 (1981) 441-446. doi:10.1016/0021-9614(81)90051-3

**T / K = 298.15**

**P / bar = 69.00**

$h^M$ / $z_1$

$J.mol^{-1}$

| | |
|---|---|
| -15.39 | 0.0182 |
| -57.04 | 0.0730 |
| -96.91 | 0.1285 |
| -137.32 | 0.1846 |
| -171.08 | 0.2414 |
| -204.25 | 0.2989 |
| -228.87 | 0.3570 |
| -240.33 | 0.4158 |
| -249.67 | 0.4753 |
| -246.26 | 0.5053 |
| -248.97 | 0.5355 |
| -241.51 | 0.5659 |
| -235.20 | 0.5964 |
| -224.27 | 0.6272 |
| -212.87 | 0.6581 |
| -194.66 | 0.6892 |
| -175.50 | 0.7205 |
| -152.57 | 0.7520 |
| -132.93 | 0.7837 |
| -100.67 | 0.8156 |
| -74.47 | 0.8477 |
| -37.36 | 0.8799 |
| -3.940 | 0.9124 |
| 28.13 | 0.9342 |
| 43.98 | 0.9451 |
| 58.48 | 0.9560 |
| 73.39 | 0.9670 |
| 84.97 | 0.9780 |
| 86.11 | 0.9890 |

Ott, J.B. - Lemon, L.R. - Sipowska, J.T. - Brown, P.R., Excess enthalpies and excess volumes for (ethane + propan-1-ol) at the temperatures (298.15, 323.15, and 348.15) K and at the pressures (5, 10, 12.5, and 15) MPa, The Journal of Chemical Thermodynamics 9 (1995) 1033-1045. doi:10.1006/jcht.1995.0108

**T / K = 298.15**

**P / bar = 125.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -12.00 | 0.0167 |
| -18.60 | 0.0500 |
| -32.30 | 0.0834 |
| -44.60 | 0.1334 |
| -56.90 | 0.1667 |
| -62.40 | 0.2168 |
| -69.10 | 0.2501 |
| -72.40 | 0.2834 |
| -74.50 | 0.3334 |
| -76.20 | 0.3668 |
| -71.50 | 0.4168 |
| -67.10 | 0.4501 |
| -56.80 | 0.4835 |
| -45.00 | 0.5335 |
| -31.70 | 0.5668 |
| -11.60 | 0.6168 |
| 5.200 | 0.6501 |
| 22.40 | 0.6834 |
| 49.90 | 0.7334 |
| 65.60 | 0.7668 |
| 92.60 | 0.8167 |
| 105.90 | 0.8501 |
| 119.60 | 0.8834 |
| 130.10 | 0.9334 |
| 127.80 | 0.9667 |

Ott, J.B. - Lemon, L.R. - Sipowska, J.T. - Brown, P.R., Excess enthalpies and excess volumes for (ethane + propan-1-ol) at the temperatures (298.15, 323.15, and 348.15) K and at the pressures (5, 10, 12.5, and 15) MPa, The Journal of Chemical Thermodynamics 9 (1995) 1033-1045. doi:10.1006/jcht.1995.0108

**T / K = 323.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -170.37 | 0.0297 |
| -340.01 | 0.0597 |
| -519.93 | 0.0899 |
| -772.10 | 0.1356 |
| -960.54 | 0.1664 |
| -1271.2 | 0.2130 |
| -1432.7 | 0.2443 |
| -1692.6 | 0.2918 |
| -1956.2 | 0.3398 |
| -2172.6 | 0.3721 |
| -2211.4 | 0.4047 |
| -2091.6 | 0.4541 |
| -1908.0 | 0.4873 |
| -1710.1 | 0.5376 |
| -1583.2 | 0.5715 |
| -1431.7 | 0.6056 |
| -1212.0 | 0.6574 |
| -1087.9 | 0.6922 |
| -935.85 | 0.7273 |
| -793.69 | 0.7627 |

| | |
|---|---|
| -565.67 | 0.8164 |
| -410.60 | 0.8525 |
| -261.31 | 0.8889 |
| -104.29 | 0.9256 |
| 53.68 | 0.9627 |
| 127.57 | 0.9819 |
| 153.53 | 0.9863 |
| 165.49 | 0.9890 |

Ott, J.B. - Lemon, L.R. - Sipowska, J.T. - Brown, P.R., Excess enthalpies and excess volumes for (ethane + propan-1-ol) at the temperatures (298.15, 323.15, and 348.15) K and at the pressures (5, 10, 12.5, and 15) MPa, The Journal of Chemical Thermodynamics 9 (1995) 1033-1045. doi:10.1006/jcht.1995.0108

**T / K = 348.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -161.98 | 0.0297 |
| -309.57 | 0.0597 |
| -453.42 | 0.0899 |
| -698.92 | 0.1356 |
| -885.53 | 0.1664 |
| -1092.6 | 0.2130 |
| -1226.3 | 0.2443 |
| -1390.5 | 0.2918 |
| -1371.8 | 0.2918 |
| -1270.1 | 0.3398 |
| -1167.9 | 0.3721 |
| -1022.8 | 0.4047 |
| -918.96 | 0.4541 |
| -831.57 | 0.4873 |
| -688.40 | 0.5376 |
| -599.92 | 0.5715 |
| -500.69 | 0.6056 |
| -353.27 | 0.6574 |
| -256.95 | 0.6922 |
| -151.07 | 0.7273 |
| -60.82 | 0.7627 |
| 91.25 | 0.8164 |
| 211.33 | 0.8525 |
| 290.49 | 0.8889 |
| 339.82 | 0.9072 |
| 402.64 | 0.9256 |
| 509.79 | 0.9627 |
| 552.02 | 0.9813 |
| 568.07 | 0.9860 |
| 409.83 | 0.9888 |
| 320.68 | 0.9906 |
| 293.28 | 0.9920 |

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**Three-phase line**

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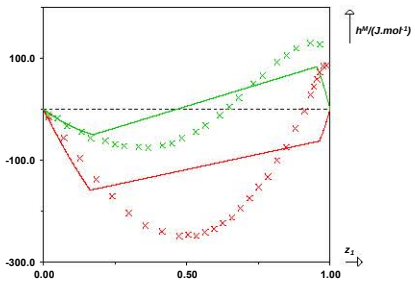
D. Kodama - H. Tanaka - M. Kato - High Pressure Phase Equilibrium for Ethane + 1-Propanol at 314.15 K, Journal of Chemical & Engineering Data. 46 (2001) 1280–1282. doi:10.1021/je010077i.

| T / K | P / bar | $x_{1a}$ | $x_{1b}$ | $y_1$ |
|---|---|---|---|---|
| 314.15 | 54.89 | 0.7990 | 0.9030 | 0.9650 |

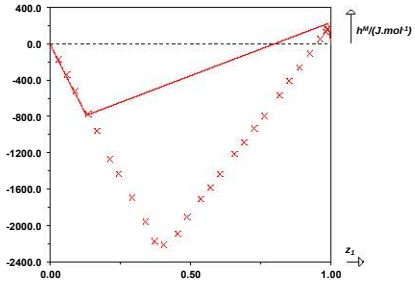
D.H. Lam, A. Jangkamolkulchai, K.D. Luks, Liquid-liquid-vapor phase equilibrium behavior of certain binary ethane + n-alkanol mixtures, Fluid Phase Equilibria. 59 (1990) 263–277. doi:10.1016/0378-3812(90)80003-T.

| T / K | P / bar | $x_{1a}$ | $x_{1b}$ | $y_1$ |
|---|---|---|---|---|
| 313.75 | 54.57 | 0.8046 | 0.8741 | 0.9918 |
| 313.95 | 54.79 | 0.7893 | 0.8892 | 0.9877 |
| 314.15 | 55.01 | 0.7798 | 0.8996 | 0.9850 |
| 314.35 | 55.24 | 0.7716 | 0.9081 | 0.9889 |
| 314.55 | 55.46 | 0.7656 | 0.9161 | 0.9855 |
| 314.75 | 55.67 | 0.7605 | 0.9227 | 0.9841 |
| 315.01 | 55.97 | 0.7533 | 0.9331 | 0.9837 |
| 315.15 | 56.11 | 0.7505 | 0.9375 | 0.9812 |
| 315.35 | 56.34 | 0.7467 | 0.9457 | 0.9762 |

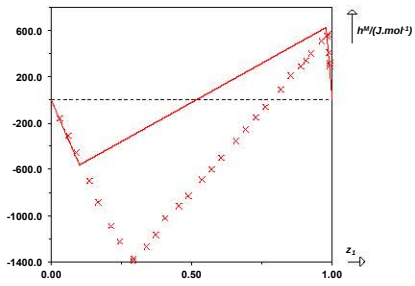
T/K = 298.15 - P/bar = 69.00 125.00



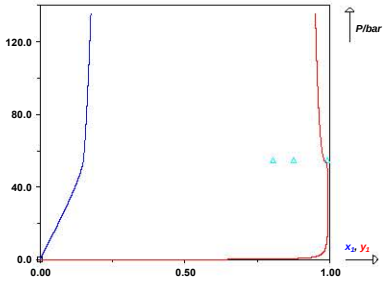

T/K = 323.15 - P/bar = 50.00



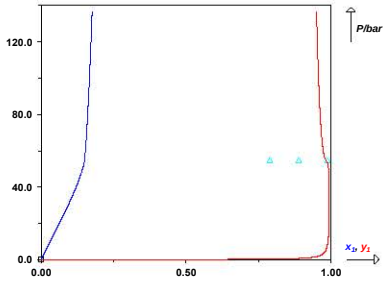

T/K = 348.15 - P/bar = 50.00



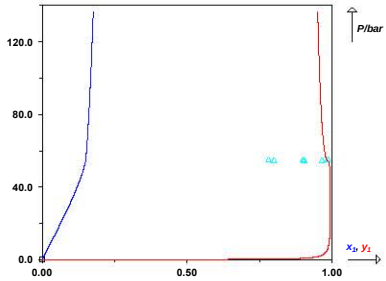

T/K = 313.75



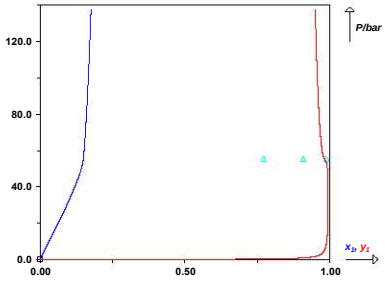

T/K = 313.95



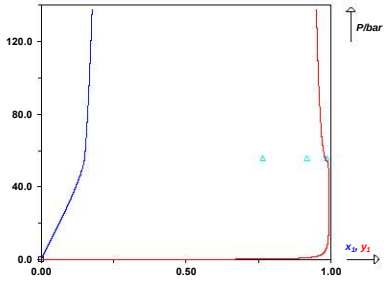

T/K = 314.15



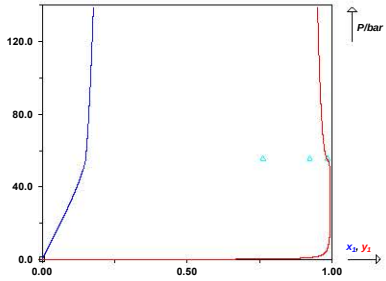

T/K = 314.35



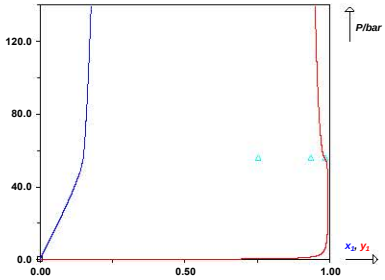

T/K = 314.55



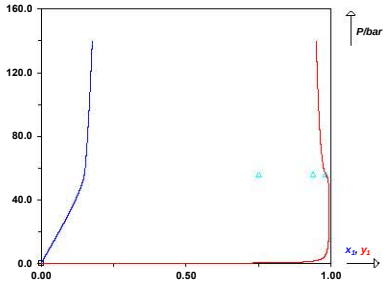

T/K = 314.75



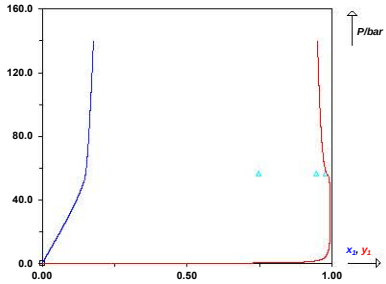

T/K = 315.01



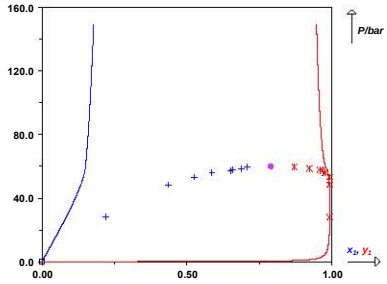

T/K = 315.15



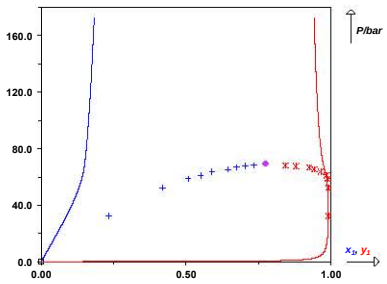

T/K = 315.35



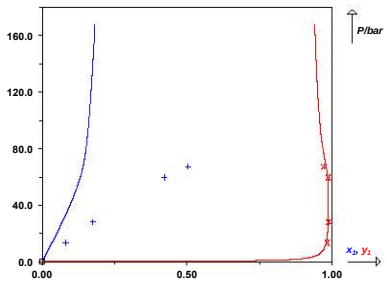
T/K = 317.59



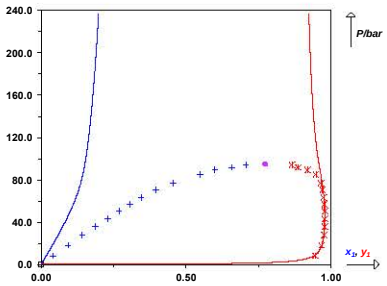

T/K = 324.51




T/K = 333.40




T/K = 348.68



## NITROGEN (1) + AMMONIA (2)

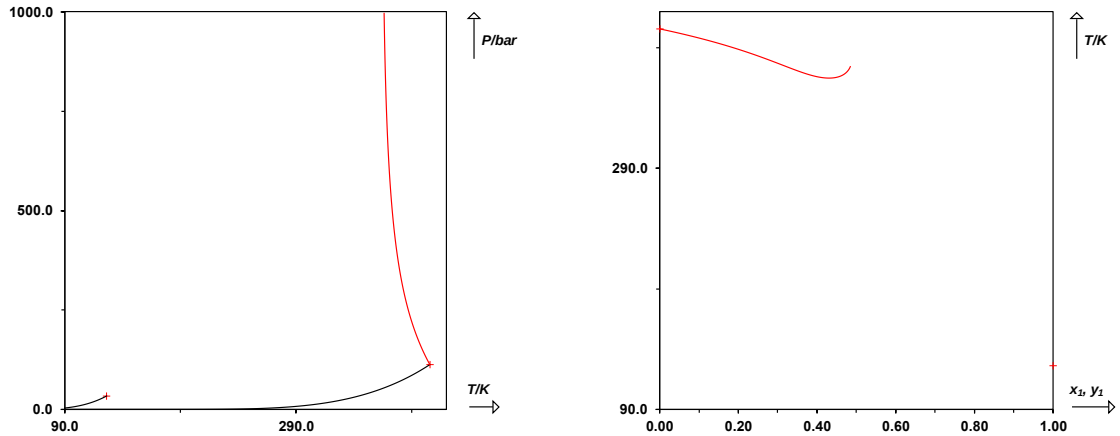
| | | |
|---|---|---|
| **CAS** | 7727-37-9 | 7664-41-7 |
| **InChiKey** | MDFFNEOEWAXZRQ-UHFFFAOYSA-N | QGZKDVFQNNGYKY-UHFFFAOYSA-N |
| **$T_c$ / K** | 126.20 | 405.65 |
| **$P_c$ / bar** | 34.00 | 112.80 |
| **ω** | 0.038 | 0.253 |

Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 2020
B/MPa = 5930

*Deviations*
MAPE on x = 17 %
MAPE on y = 6.5 %
MAPE on $h^M$ = 20 %



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**Isothermal phase equilibrium data**

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Reamer, H. H. - Sage, B. H., Phase Behavior in the Nitrogen-Ammonia System., Journal of Chemical & Engineering Data 4 (1959) 303-305. doi:10.1021/je60004a005

**T / K = 277.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.48 | 0.0021 | 0.8364 |
| 68.95 | 0.0043 | 0.9064 |
| 103.42 | 0.0064 | 0.9270 |
| 137.90 | 0.0083 | 0.9361 |
| 172.37 | 0.0101 | 0.9395 |
| 206.85 | 0.0117 | 0.9400 |
| 241.31 | 0.0131 | 0.9405 |
| 275.79 | 0.0142 | 0.9408 |
| 310.27 | 0.0152 | 0.9410 |
| 344.74 | 0.0161 | 0.9415 |
| 379.21 | 0.0168 | 0.9420 |
| 413.69 | 0.0175 | 0.9430 |

Reamer, H. H. - Sage, B. H., Phase Behavior in the Nitrogen-Ammonia System., Journal of Chemical & Engineering Data 4 (1959) 303-305. doi:10.1021/je60004a005

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.48 | 0.0027 | 0.5200 |
| 68.95 | 0.0071 | 0.7180 |
| 103.42 | 0.0113 | 0.7905 |
| 137.90 | 0.0152 | 0.8275 |
| 172.37 | 0.0188 | 0.8461 |
| 206.85 | 0.0221 | 0.8550 |
| 241.31 | 0.0251 | 0.8605 |
| 275.79 | 0.0278 | 0.8635 |
| 310.27 | 0.0303 | 0.8655 |
| 344.74 | 0.0327 | 0.8675 |
| 379.21 | 0.0349 | 0.8690 |
| 413.69 | 0.0369 | 0.8700 |

Lindroos, A.E. - Dodge, B.F., Phase-equilibria at high pressures; the system nitrogen-ammonia at pressures above 1000 atmospheres, Chem. Eng. Progr. Symp. Ser. 3 (1952) 10-17.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 978.29 | 0.0720 | 0.8490 |
| 1160.2 | 0.0710 | 0.8580 |
| 1365.9 | 0.0740 | 0.8670 |
| 1844.1 | 0.0820 | 0.9080 |
| 2270.2 | 0.0770 | 0.9190 |
| 2854.3 | 0.0600 | 0.9150 |
| 3286.0 | 0.0620 | 0.9120 |
| 3810.3 | 0.0730 | 0.9380 |

Reamer, H. H. - Sage, B. H., Phase Behavior in the Nitrogen-Ammonia System., Journal of Chemical & Engineering Data 4 (1959) 303-305. doi:10.1021/je60004a005

**T / K = 344.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 34.48 | 0.0001 | 0.0103 |
| 68.95 | 0.0084 | 0.4090 |
| 103.42 | 0.0162 | 0.5408 |
| 137.90 | 0.0239 | 0.6055 |
| 172.37 | 0.0315 | 0.6452 |
| 206.85 | 0.0389 | 0.6695 |
| 241.31 | 0.0463 | 0.6820 |
| 275.79 | 0.0530 | 0.6885 |
| 310.27 | 0.0595 | 0.6920 |
| 344.74 | 0.0658 | 0.6940 |
| 379.21 | 0.0718 | 0.6950 |
| 413.69 | 0.0777 | 0.6955 |

Reamer, H. H. - Sage, B. H., Phase Behavior in the Nitrogen-Ammonia System., Journal of Chemical & Engineering Data 4 (1959) 303-305. doi:10.1021/je60004a005

**T / K = 377.59**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 68.95 | 0.0005 | 0.0105 |
| 103.42 | 0.0163 | 0.1975 |
| 137.90 | 0.0324 | 0.2850 |
| 172.37 | 0.0502 | 0.3333 |
| 206.85 | 0.0700 | 0.3540 |
| 241.31 | 0.0944 | 0.3640 |
| 275.79 | 0.1262 | 0.3628 |
| 310.27 | 0.1555 | 0.3200 |

Reamer, H. H. - Sage, B. H., Phase Behavior in the Nitrogen-Ammonia System., Journal of Chemical & Engineering Data 4 (1959) 303-305. doi:10.1021/je60004a005

**T / K = 394.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 103.42 | 0.0089 | 0.0510 |
| 137.90 | 0.0379 | 0.1290 |
| 172.37 | 0.0696 | 0.1315 |

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**Enthalpy of mixing**

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Naumowicz-Węglińska, E - Wóycicki, W, Excess enthalpies of gaseous mixtures containing ammonia 2. (Ammonia + nitrogen) and (ammonia + methane), The Journal of Chemical Thermodynamics 11 (1986) 1047-1052. doi:10.1016/0021-9614(86)90019-4

**T / K = 313.15**

**P / bar = 8.110**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 81.90 | 0.1220 |
| 110.40 | 0.1960 |
| 130.40 | 0.2850 |
| 135.90 | 0.3340 |
| 149.50 | 0.4230 |
| 142.70 | 0.5030 |
| 129.50 | 0.5830 |
| 124.90 | 0.6340 |
| 93.60 | 0.7090 |
| 87.40 | 0.7600 |

Naumowicz-Węglińska, E - Wóycicki, W, Excess enthalpies of gaseous mixtures containing ammonia 2. (Ammonia + nitrogen) and (ammonia + methane), The Journal of Chemical Thermodynamics 11 (1986) 1047-1052. doi:10.1016/0021-9614(86)90019-4

**T / K = 313.50**

**P / bar = 11.15**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 137.50 | 0.1450 |
| 152.80 | 0.1850 |
| 167.00 | 0.2090 |
| 213.20 | 0.3710 |
| 213.30 | 0.4350 |
| 198.20 | 0.5610 |
| 194.70 | 0.6170 |
| 160.40 | 0.6920 |

Naumowicz-Węglińska, E - Wóycicki, W, Excess enthalpies of gaseous mixtures containing ammonia 2. (Ammonia + nitrogen) and (ammonia + methane), The Journal of Chemical Thermodynamics 11 (1986) 1047-1052. doi:10.1016/0021-9614(86)90019-4

**T / K = 333.15**

**P / bar = 8.110**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 26.70 | 0.0470 |
| 81.60 | 0.1890 |
| 94.70 | 0.2740 |
| 105.20 | 0.3920 |
| 102.70 | 0.5380 |
| 79.80 | 0.6890 |

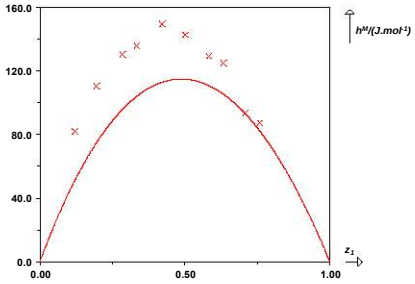
Naumowicz-Węglińska, E - Wóycicki, W, Excess enthalpies of gaseous mixtures containing ammonia 2. (Ammonia + nitrogen) and (ammonia + methane), The Journal of Chemical Thermodynamics 11 (1986) 1047-1052. doi:10.1016/0021-9614(86)90019-4

**T / K = 333.15**

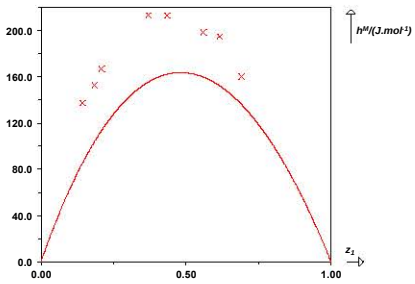
**P / bar = 14.19**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 87.70 | 0.0890 |
| 144.00 | 0.1590 |
| 199.10 | 0.3220 |
| 204.60 | 0.4250 |
| 169.00 | 0.6180 |
| 125.80 | 0.7350 |

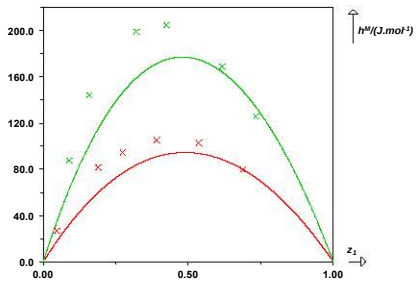
T/K = 313.15 - P/bar = 8.1100



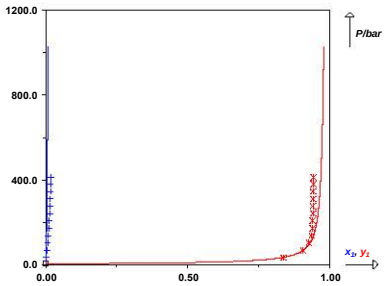

T/K = 313.50 - P/bar = 11.1500



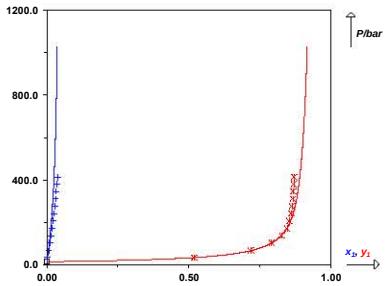

T/K = 333.15 - P/bar = 8.1100 14.1900



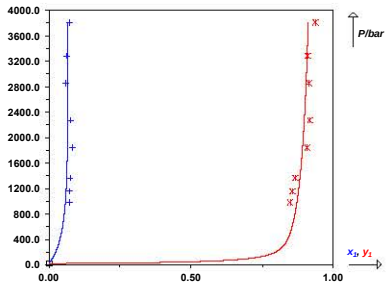

T/K = 277.59



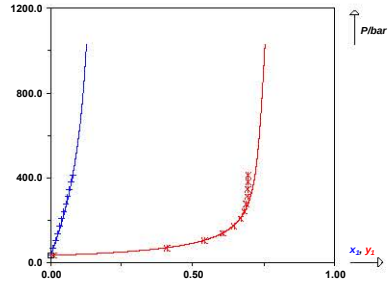

T/K = 310.93



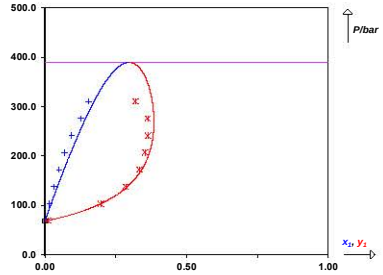

T/K = 323.15



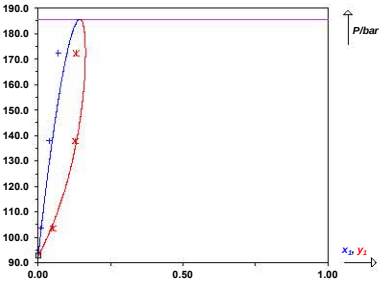

T/K = 344.26




T/K = 377.59




T/K = 394.26



## ETHANE (1) + WATER (2)

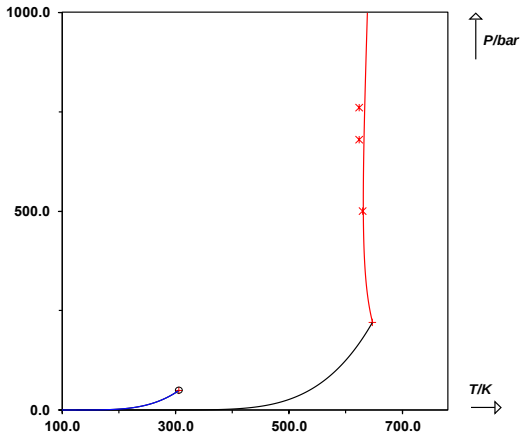
| | | |
|---|---|---|
| **CAS** | 74-84-0 | 7732-18-5 |
| **InChiKey** | OTMSDBZUPAUEDD-UHFFFAOYSA-N | XLYOFNOQVPJJNP-UHFFFAOYSA-N |
| **$T_c$ / K** | 305.32 | 647.096 |
| **$P_c$ / bar** | 48.72 | 220.64 |
| **ω** | 0.099 | 0.345 |

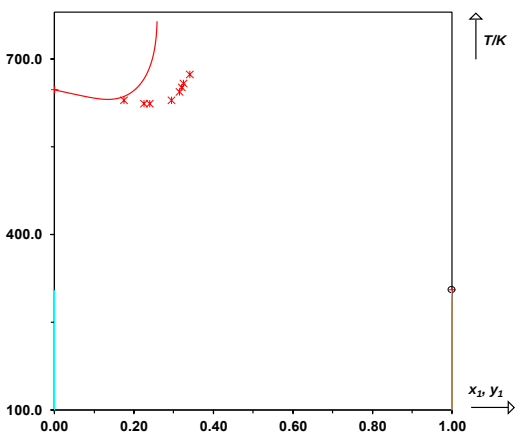
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 5630
B/MPa = 10800

*Deviations*
MAPE on x = 12 %
MAPE on y = 33 %
MAPE on $x_c$ = 25 %
MAPE on $P_c$ = 13 %



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**Isothermal phase equilibrium data**

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Danneil, A. - Tödheide, K. - Franck, E. U., Verdampfungsgleichgewichte und kritische Kurven in den Systemen Äthan/Wasser und n-Butan/Wasser bei hohen Drücken, Chemie Ingenieur Technik - CIT 13 (1967) 816-822. doi:10.1002/cite.330391309

**T / K = 523.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 200.00 | 0.0070 | 0.6900 |
| 500.00 | 0.0100 | 0.7810 |
| 1000.0 | 0.0125 | 0.8500 |
| 1500.0 | 0.0150 | 0.8850 |

Danneil, A. - Tödheide, K. - Franck, E. U., Verdampfungsgleichgewichte und kritische Kurven in den Systemen Äthan/Wasser und n-Butan/Wasser bei hohen Drücken, Chemie Ingenieur Technik - CIT 13 (1967) 816-822. doi:10.1002/cite.330391309

**T / K = 573.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 200.00 | 0.0100 | 0.4540 |
| 500.00 | 0.0200 | 0.5870 |
| 1000.0 | 0.0240 | 0.7340 |
| 1500.0 | 0.0280 | 0.8280 |

Danneil, A. - Tödheide, K. - Franck, E. U., Verdampfungsgleichgewichte und kritische Kurven in den Systemen Äthan/Wasser und n-Butan/Wasser bei hohen Drücken, Chemie Ingenieur Technik - CIT 13 (1967) 816-822. doi:10.1002/cite.330391309

**T / K = 623.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 200.00 | 0.0090 | 0.1500 | |
| 300.00 | 0.0350 | 0.2300 | |
| 400.00 | 0.0650 | 0.2750 | |
| 500.00 | 0.0990 | 0.3020 | |
| 600.00 | 0.1430 | 0.3050 | |
| 800.00 | 0.1250 | 0.3200 | |
| 900.00 | 0.0970 | 0.4230 | |
| 1000.0 | 0.0850 | 0.4890 | |
| 1500.0 | 0.0750 | 0.6780 | |
| 2000.0 | 0.0730 | 0.7380 | |
| 2500.0 | 0.0720 | 0.7560 | |
| 680.00 | 0.2250 | 0.2250 | CRIT |

Danneil, A. - Tödheide, K. - Franck, E. U., Verdampfungsgleichgewichte und kritische Kurven in den Systemen Äthan/Wasser und n-Butan/Wasser bei hohen Drücken, Chemie Ingenieur Technik - CIT 13 (1967) 816-822. doi:10.1002/cite.330391309

**T / K = 629.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 200.00 | 0.0090 | 0.1350 | |
| 300.00 | 0.0370 | 0.2100 | |
| 400.00 | 0.0800 | 0.2270 | |
| 1300.0 | 0.1170 | 0.5420 | |
| 1400.0 | 0.1060 | 0.5920 | |
| 1500.0 | 0.1040 | 0.6250 | |
| 2000.0 | 0.0970 | 0.7040 | |
| 2500.0 | 0.0900 | 0.7300 | |
| 500.00 | 0.1750 | 0.1750 | CRIT |

Danneil, A. - Tödheide, K. - Franck, E. U., Verdampfungsgleichgewichte und kritische Kurven in den Systemen Äthan/Wasser und n-Butan/Wasser bei hohen Drücken, Chemie Ingenieur Technik - CIT 13 (1967) 816-822. doi:10.1002/cite.330391309

**T / K = 643.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3500.0 | 0.0900 | 0.7220 | |
| 3000.0 | 0.0930 | 0.7120 | |
| 2500.0 | 0.0960 | 0.6840 | |
| 2000.0 | 0.1140 | 0.6190 | |
| 1900.0 | 0.1230 | 0.5890 | |
| 1800.0 | 0.1350 | 0.5370 | |
| 1700.0 | 0.2110 | 0.3670 | |
| 1680.0 | 0.3150 | 0.3150 | CRIT |

Danneil, A. - Tödheide, K. - Franck, E. U., Verdampfungsgleichgewichte und kritische Kurven in den Systemen Äthan/Wasser und n-Butan/Wasser bei hohen Drücken, Chemie Ingenieur Technik - CIT 13 (1967) 816-822. doi:10.1002/cite.330391309

**T / K = 651.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3500.0 | 0.0960 | 0.6920 | |
| 3000.0 | 0.0990 | 0.6900 | |
| 2500.0 | 0.1020 | 0.6530 | |
| 2200.0 | 0.1180 | 0.5740 | |
| 2100.0 | 0.1370 | 0.5160 | |
| 2000.0 | 0.2140 | 0.3610 | |
| 1990.0 | 0.3200 | 0.3200 | CRIT |

Danneil, A. - Tödheide, K. - Franck, E. U., Verdampfungsgleichgewichte und kritische Kurven in den Systemen Äthan/Wasser und n-Butan/Wasser bei hohen Drücken, Chemie Ingenieur Technik - CIT 13 (1967) 816-822. doi:10.1002/cite.330391309

**T / K = 658.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3500.0 | 0.1200 | 0.6550 |

| | | | |
|---|---|---|---|
| 3000.0 | 0.1330 | 0.6540 | |
| 2500.0 | 0.1520 | 0.6030 | |
| 2400.0 | 0.1580 | 0.5750 | |
| 2300.0 | 0.1670 | 0.5320 | |
| 2200.0 | 0.2020 | 0.4110 | |
| 2190.0 | 0.3250 | 0.3250 | CRIT |

Danneil, A. - Tödheide, K. - Franck, E. U., Verdampfungsgleichgewichte und kritische Kurven in den Systemen Äthan/Wasser und n-Butan/Wasser bei hohen Drücken, Chemie Ingenieur Technik - CIT 13 (1967) 816-822. doi:10.1002/cite.330391309

**T / K = 673.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3700.0 | 0.1320 | 0.6010 | |
| 3500.0 | 0.1350 | 0.5950 | |
| 3400.0 | 0.1380 | 0.5910 | |
| 3300.0 | 0.1450 | 0.5610 | |
| 3215.0 | 0.3400 | 0.3400 | CRIT |

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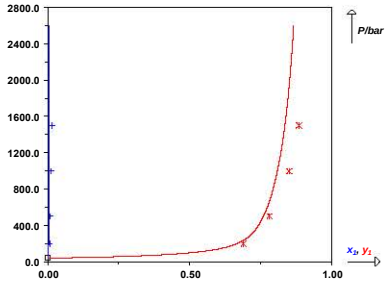
**Critical point**

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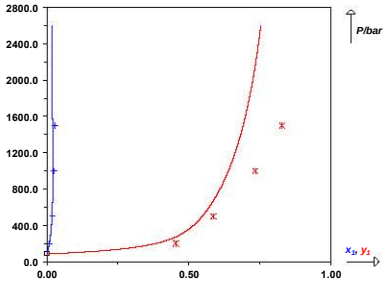
Danneil, A. - Tödheide, K. - Franck, E. U., Verdampfungsgleichgewichte und kritische Kurven in den Systemen Äthan/Wasser und n-Butan/Wasser bei hohen Drücken, Chemie Ingenieur Technik - CIT 13 (1967) 816-822. doi:10.1002/cite.330391309

| T / K | P / bar | $x_1$ |
|---|---|---|
| 623.15 | 760.00 | 0.2400 |
| 629.15 | 1205.0 | 0.2950 |

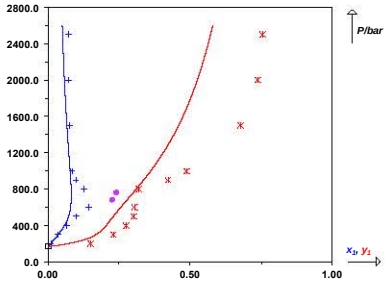
T/K = 523.15



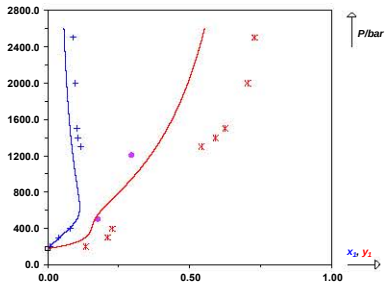

T/K = 573.15



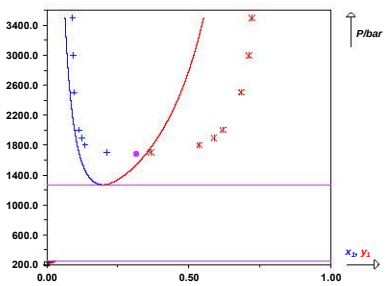

T/K = 623.15



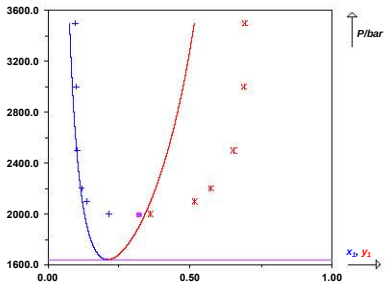

T/K = 629.15



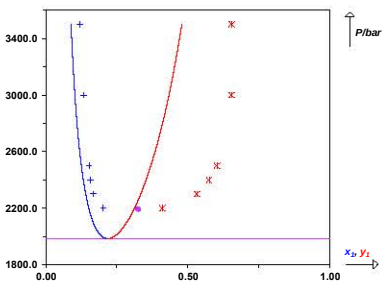

T/K = 643.15



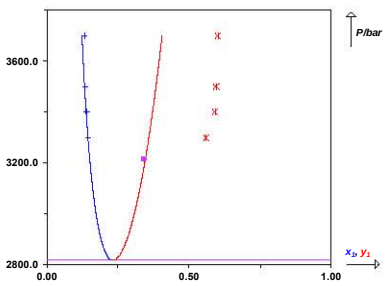

T/K = 651.15




T/K = 658.15




T/K = 673.15



## NITROGEN (1) + WATER (2)

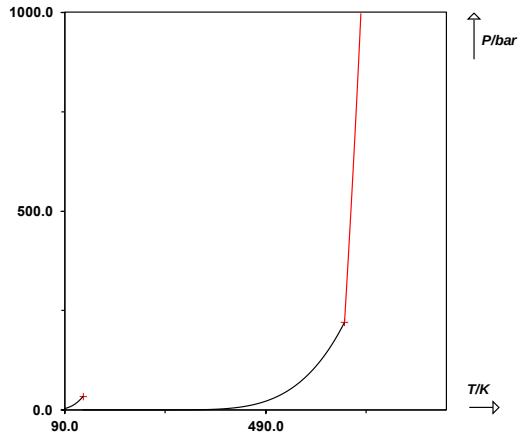
| | | |
|---|---|---|
| **CAS** | 7727-37-9 | 7732-18-5 |
| **InChiKey** | MDFFNEOEWAXZRQ-UHFFFAOYSA-N | XLYOFNOQVPJJNP-UHFFFAOYSA-N |
| **$T_c$ / K** | 126.20 | 647.10 |
| **$P_c$ / bar** | 34.00 | 220.64 |
| **ω** | 0.038 | 0.345 |

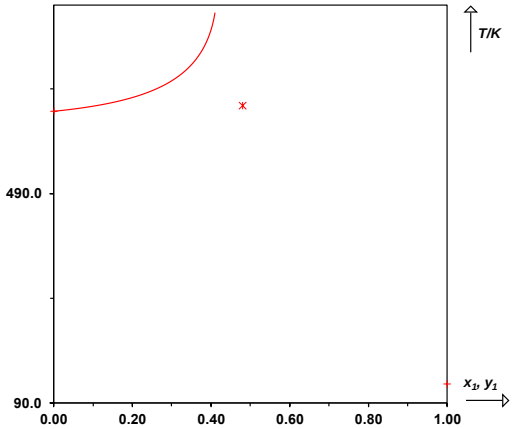
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 6360
B/MPa = 10000

*Deviations*
MAPE on x = 17 %
MAPE on y = 8.8 %
MAPE on $x_c$ = 74 %
MAPE on $P_c$ = 79 %
MAPE on $h^M$ = 39 %



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**Isothermal phase equilibrium data**

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Folas, Georgios K. - Froyna, Einar W. - Lovland, Jorgen - Kontogeorgis, Georgios M. - Solbraa, Even, Data and prediction of water content of high pressure nitrogen, methane and natural gas, Fluid Phase Equilibria 1-2 (2007) 162-174. doi:10.1016/j.fluid.2006.12.018

**T / K = 273.15**

| P / bar | $x_1$ |
|---|---|
| 25.00 | 0.9997 |
| 50.00 | 0.9999 |
| 100.00 | 0.9999 |

Goodman, John B. - Krase, Norman W., Solubility of Nitrogen in Water at High Pressures and Temperatures, Industrial & Engineering Chemistry 4 (1931) 401-404. doi:10.1021/ie50256a015

**T / K = 273.15**

| P / bar | $x_1$ |
|---|---|
| 101.33 | 0.0012 |
| 126.66 | 0.0014 |
| 202.65 | 0.0026 |
| 303.98 | 0.0029 |

Rigby, Maurice - Prausnitz, John M., Solubility of water in compressed nitrogen, argon, and methane, The Journal of Physical Chemistry 1 (1968) 330-334. doi:10.1021/j100847a064

**T / K = 298.15**

| P / bar | $x_1$ |
|---|---|
| 22.49 | 0.9985 |
| 30.90 | 0.9989 |
| 38.70 | 0.9991 |

Maslennikova, V.Ya. - Vdovina, N.A. - Tsiklis, D.S., Solubility of water in compressed nitrogen, Russ. J. Phys. Chem. 9 (1971) 1354-1354.

**T / K = 298.15**

| P / bar | $y_1$ |
|---|---|
| 50.66 | 0.9993 |
| 75.99 | 0.9995 |
| 101.33 | 0.9996 |

Wiebe, R. - Gaddy, V. L. - Heinss, Conrad, Solubility of Nitrogen in Water at 25°C from 25 to 1000 Atmospheres, Industrial & Engineering Chemistry 8 (1932) 927-927. doi:10.1021/ie50272a023

**T / K = 298.15**

| P / bar | $x_1$ |
|---|---|
| 25.33 | 0.0003 |
| 50.66 | 0.0003 |
| 101.33 | 0.0010 |
| 202.65 | 0.0018 |
| 303.98 | 0.0025 |
| 506.62 | 0.0036 |
| 810.60 | 0.0049 |
| 1013.2 | 0.0057 |

Goodman, John B. - Krase, Norman W., Solubility of Nitrogen in Water at High Pressures and Temperatures, Industrial & Engineering Chemistry 4 (1931) 401-404. doi:10.1021/ie50256a015

**T / K = 298.15**

| P / bar | $x_1$ |
|---|---|
| 101.33 | 0.0009 |
| 126.66 | 0.0012 |
| 202.65 | 0.0022 |
| 303.98 | 0.0026 |

Gillespie, P.C. - Wilson, G.M., Vapor-liquid equilibrium data on water-substitute gas components: N2-H2O, H2-H2O, CO-H2O, H2-CO-H2O, and H2S-H2O, GPA Research Report (1980) 1-34.

**T / K = 310.93**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.447 | 0 | 0.9798 |
| 13.79 | 0.0001 | 0.9950 |
| 31.03 | 0.0003 | 0.9976 |
| 65.50 | 0.0006 | 0.9988 |
| 103.42 | 0.0009 | 0.9991 |
| 137.90 | 0.0012 | 0.9993 |

Rigby, Maurice - Prausnitz, John M., Solubility of water in compressed nitrogen, argon, and methane, The Journal of Physical Chemistry 1 (1968) 330-334. doi:10.1021/j100847a064

**T / K = 323.15**

| P / bar | $y_1$ |
|---|---|
| 21.09 | 0.9937 |
| 37.42 | 0.9963 |
| 59.82 | 0.9976 |
| 77.00 | 0.9980 |

Wiebe, R. - Gaddy, V. L. - Heins, Conrad, The Solubility of Nitrogen in Water at 50, 75 and 100° from 25 to 1000 Atmospheres, Journal of the American Chemical Society 3 (1933) 947-953. doi:10.1021/ja01330a011

**T / K = 323.15**

| P / bar | $x_1$ |
|---|---|
| 25.33 | 0.0002 |
| 50.66 | 0.0004 |
| 101.33 | 0.0008 |

| | |
|---|---|
| 202.65 | 0.0015 |
| 303.98 | 0.0020 |
| 506.62 | 0.0030 |
| 810.60 | 0.0042 |
| 1013.2 | 0.0049 |

Maslennikova, V.Ya. - Vdovina, N.A. - Tsiklis, D.S., Solubility of water in compressed nitrogen, Russ. J. Phys. Chem. 9 (1971) 1354-1354.

**T / K = 323.15**

| P / bar | $y_1$ |
|---|---|
| 50.66 | 0.9972 |
| 75.99 | 0.9980 |
| 101.33 | 0.9984 |
| 126.66 | 0.9986 |
| 151.99 | 0.9987 |
| 177.32 | 0.9988 |
| 202.65 | 0.9989 |
| 253.31 | 0.9990 |
| 303.98 | 0.9991 |
| 354.64 | 0.9992 |
| 405.30 | 0.9993 |
| 455.96 | 0.9993 |
| 506.62 | 0.9994 |

Goodman, John B. - Krase, Norman W., Solubility of Nitrogen in Water at High Pressures and Temperatures, Industrial & Engineering Chemistry 4 (1931) 401-404. doi:10.1021/ie50256a015

**T / K = 323.15**

| P / bar | $x_1$ |
|---|---|
| 101.33 | 0.0008 |
| 126.66 | 0.0010 |
| 202.65 | 0.0020 |
| 303.98 | 0.0024 |

Rigby, Maurice - Prausnitz, John M., Solubility of water in compressed nitrogen, argon, and methane, The Journal of Physical Chemistry 1 (1968) 330-334. doi:10.1021/j100847a064

**T / K = 348.15**

| P / bar | $y_1$ |
|---|---|
| 42.21 | 0.9899 |
| 61.15 | 0.9928 |
| 89.72 | 0.9948 |

Wiebe, R. - Gaddy, V. L. - Heins, Conrad, The Solubility of Nitrogen in Water at 50, 75 and 100° from 25 to 1000 Atmospheres, Journal of the American Chemical Society 3 (1933) 947-953. doi:10.1021/ja01330a011

**T / K = 348.15**

| P / bar | $x_1$ |
|---|---|
| 25.33 | 0.0002 |
| 50.66 | 0.0004 |
| 101.33 | 0.0008 |
| 202.65 | 0.0014 |
| 303.98 | 0.0019 |
| 506.62 | 0.0029 |
| 810.60 | 0.0041 |
| 1013.2 | 0.0048 |

Maslennikova, V.Ya. - Vdovina, N.A. - Tsiklis, D.S., Solubility of water in compressed nitrogen, Russ. J. Phys. Chem. 9 (1971) 1354-1354.

**T / K = 348.15**

| P / bar | $y_1$ |
|---|---|
| 50.66 | 0.9917 |
| 75.99 | 0.9940 |
| 101.33 | 0.9950 |
| 126.66 | 0.9954 |
| 151.99 | 0.9954 |
| 177.32 | 0.9955 |
| 202.65 | 0.9955 |
| 253.31 | 0.9957 |
| 303.98 | 0.9959 |
| 354.64 | 0.9960 |
| 405.30 | 0.9962 |
| 455.96 | 0.9964 |
| 506.62 | 0.9966 |

Gillespie, P.C. - Wilson, G.M., Vapor-liquid equilibrium data on water-substitute gas components: N2-H2O, H2-H2O, CO-H2O, H2-CO-H2O, and H2S-H2O, GPA Research Report (1980) 1-34.

**T / K = 366.48**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.447 | 0 | 0.7670 |
| 13.79 | 0.0001 | 0.9395 |
| 31.03 | 0.0002 | 0.9723 |
| 65.50 | 0.0005 | 0.9863 |
| 137.90 | 0.0010 | 0.9925 |

Rigby, Maurice - Prausnitz, John M., Solubility of water in compressed nitrogen, argon, and methane, The Journal of Physical Chemistry 1 (1968) 330-334. doi:10.1021/j100847a064

**T / K = 373.15**

| P / bar | $y_1$ |
|---|---|
| 57.17 | 0.9801 |
| 79.48 | 0.9850 |
| 101.52 | 0.9878 |

Wiebe, R. - Gaddy, V. L. - Heins, Conrad, The Solubility of Nitrogen in Water at 50, 75 and 100° from 25 to 1000 Atmospheres, Journal of the American Chemical Society 3 (1933) 947-953. doi:10.1021/ja01330a011

**T / K = 373.15**

| P / bar | $x_1$ |
|---|---|
| 25.33 | 0.0002 |
| 50.66 | 0.0004 |
| 101.33 | 0.0008 |
| 202.65 | 0.0015 |
| 303.98 | 0.0020 |
| 506.62 | 0.0030 |
| 810.60 | 0.0043 |
| 1013.2 | 0.0050 |

Maslennikova, V.Ya. - Vdovina, N.A. - Tsiklis, D.S., Solubility of water in compressed nitrogen, Russ. J. Phys. Chem. 9 (1971) 1354-1354.

**T / K = 373.15**

| P / bar | $y_1$ |
|---|---|
| 50.66 | 0.9785 |
| 75.99 | 0.9850 |
| 101.33 | 0.9883 |
| 126.66 | 0.9900 |
| 151.99 | 0.9913 |
| 177.32 | 0.9923 |
| 202.65 | 0.9931 |
| 253.31 | 0.9943 |
| 303.98 | 0.9947 |
| 354.64 | 0.9952 |
| 405.30 | 0.9956 |
| 455.96 | 0.9956 |
| 506.62 | 0.9958 |

Goodman, John B. - Krase, Norman W., Solubility of Nitrogen in Water at High Pressures and Temperatures, Industrial & Engineering Chemistry 4 (1931) 401-404. doi:10.1021/ie50256a015

**T / K = 373.15**

| P / bar | $x_1$ |
|---|---|
| 101.33 | 0.0008 |
| 126.66 | 0.0009 |
| 202.65 | 0.0018 |
| 303.98 | 0.0023 |

Maslennikova, V.Ya., Solubility of nitrogen in water, Tr. Gos. Nauchno Issled. Proektn. Inst. Azotn. Promst. Prod. Org. Sin. (1971) 82-87.

**T / K = 473.15**

| P / bar | $x_1$ |
|---|---|
| 105.38 | 0.0019 |
| 214.81 | 0.0038 |
| 253.31 | 0.0046 |

Maslennikova, V.Ya. - Vdovina, N.A. - Tsiklis, D.S., Solubility of water in compressed nitrogen, Russ. J. Phys. Chem. 9 (1971) 1354-1354.

**T / K = 473.15**

| P / bar | $y_1$ |
|---|---|
| 50.66 | 0.7790 |
| 75.99 | 0.8300 |
| 101.33 | 0.8570 |
| 126.66 | 0.8690 |
| 151.99 | 0.8780 |
| 177.32 | 0.8870 |
| 202.65 | 0.8950 |
| 253.31 | 0.9080 |
| 303.98 | 0.9180 |
| 354.64 | 0.9250 |
| 405.30 | 0.9320 |
| 455.96 | 0.9370 |
| 506.62 | 0.9410 |

Maslennikova, V.Ya., Solubility of nitrogen in water, Tr. Gos. Nauchno Issled. Proektn. Inst. Azotn. Promst. Prod. Org. Sin. (1971) 82-87.

**T / K = 543.15**

| P / bar | $x_1$ |
|---|---|
| 166.17 | 0.0035 |
| 192.52 | 0.0040 |
| 214.81 | 0.0048 |

Maslennikova, V.Ya. - Vdovina, N.A. - Tsiklis, D.S., Solubility of water in compressed nitrogen, Russ. J. Phys. Chem. 9 (1971) 1354-1354.

**T / K = 543.15**

| P / bar | $y_1$ |
|---|---|
| 75.99 | 0.2300 |
| 101.33 | 0.5000 |
| 126.66 | 0.5980 |
| 151.99 | 0.6510 |
| 177.32 | 0.6880 |
| 202.65 | 0.7180 |
| 253.31 | 0.7570 |
| 303.98 | 0.7870 |
| 354.64 | 0.8040 |
| 405.30 | 0.8150 |
| 455.96 | 0.8210 |
| 506.62 | 0.8250 |

Maslennikova, V.Ya., Solubility of nitrogen in water, Tr. Gos. Nauchno Issled. Proektn. Inst. Azotn. Promst. Prod. Org. Sin. (1971) 82-87.

**T / K = 573.15**

| P / bar | $x_1$ |
|---|---|
| 158.07 | 0.0040 |
| 197.58 | 0.0055 |
| 212.78 | 0.0061 |
| 293.84 | 0.0098 |
| 314.11 | 0.0108 |
| 374.90 | 0.0136 |
| 466.10 | 0.0179 |

Maslennikova, V.Ya. - Vdovina, N.A. - Tsiklis, D.S., Solubility of water in compressed nitrogen, Russ. J. Phys. Chem. 9 (1971) 1354-1354.

**T / K = 573.15**

| P / bar | $y_1$ |
|---|---|
| 101.33 | 0.1000 |
| 126.66 | 0.2980 |
| 151.99 | 0.4270 |
| 177.32 | 0.5100 |
| 202.65 | 0.5680 |
| 253.31 | 0.6320 |
| 303.98 | 0.6690 |
| 354.64 | 0.6950 |
| 405.30 | 0.7140 |
| 455.96 | 0.7290 |
| 506.62 | 0.7390 |

Maslennikova, V.Ya., Solubility of nitrogen in water, Tr. Gos. Nauchno Issled. Proektn. Inst. Azotn. Promst. Prod. Org. Sin. (1971) 82-87.

**T / K = 603.15**

| P / bar | $x_1$ |
|---|---|
| 280.67 | 0.0137 |
| 283.71 | 0.0138 |
| 352.61 | 0.0191 |
| 380.98 | 0.0209 |
| 455.96 | 0.0256 |
| 488.39 | 0.0277 |
| 498.52 | 0.0281 |

Maslennikova, V.Ya. - Vdovina, N.A. - Tsiklis, D.S., Solubility of water in compressed nitrogen, Russ. J. Phys. Chem. 9 (1971) 1354-1354.

**T / K = 603.15**

| P / bar | $y_1$ |
|---|---|
| 151.99 | 0.1140 |
| 177.32 | 0.2320 |
| 202.65 | 0.3200 |
| 253.31 | 0.4180 |
| 303.98 | 0.4860 |
| 354.64 | 0.5330 |
| 405.30 | 0.5650 |
| 455.96 | 0.5870 |
| 506.62 | 0.6000 |

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**Enthalpy of mixing**

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Richards, P. - Wormald, C.J. - Yerlett, T.K., The excess enthalpy of (water + nitrogen) vapour and (water + n-heptane) vapour, The Journal of Chemical Thermodynamics 7 (1981) 623-628. doi:10.1016/0021-9614(81)90032-X

**T / K = 400.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 34.40 | 0.3230 |
| 35.60 | 0.3640 |
| 36.50 | 0.4060 |
| 38.00 | 0.4600 |
| 37.80 | 0.5140 |
| 36.60 | 0.5840 |
| 33.80 | 0.6480 |
| 32.50 | 0.6860 |

Richards, P. - Wormald, C.J. - Yerlett, T.K., The excess enthalpy of (water + nitrogen) vapour and (water + n-heptane) vapour, The Journal of Chemical Thermodynamics 7 (1981) 623-628. doi:10.1016/0021-9614(81)90032-X

**T / K = 410.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 25.20 | 0.2550 |
| 28.50 | 0.3060 |
| 32.00 | 0.3530 |
| 33.10 | 0.3680 |
| 33.80 | 0.4260 |
| 36.30 | 0.4500 |
| 36.00 | 0.4840 |
| 35.20 | 0.5070 |
| 33.60 | 0.5760 |

Wormald, C.J - Colling, C.N, Excess enthalpies for (water + nitrogen)(g) up to 698.2 K and 12.6 MPa, The Journal of Chemical Thermodynamics 8 (1983) 725-737. doi:10.1016/0021-9614(83)90139-8

**T / K = 548.20**

**P / bar = 42.40**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 548.90 | 0.3020 |
| 640.40 | 0.4010 |
| 676.30 | 0.4990 |
| 646.70 | 0.6000 |
| 545.10 | 0.6980 |

Wormald, C.J - Colling, C.N, Excess enthalpies for (water + nitrogen)(g) up to 698.2 K and 12.6 MPa, The Journal of Chemical Thermodynamics 8 (1983) 725-737. doi:10.1016/0021-9614(83)90139-8

**T / K = 648.20**

**P / bar = 100.30**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 820.80 | 0.2950 |
| 944.00 | 0.3990 |
| 968.50 | 0.5010 |
| 909.60 | 0.6050 |
| 787.50 | 0.7000 |

Wormald, C.J - Colling, C.N, Excess enthalpies for (water + nitrogen)(g) up to 698.2 K and 12.6 MPa, The Journal of Chemical Thermodynamics 8 (1983) 725-737. doi:10.1016/0021-9614(83)90139-8

**T / K = 648.20**

**P / bar = 125.80**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 1157.0 | 0.2950 |
| 1304.0 | 0.3970 |
| 1315.0 | 0.5000 |
| 1273.0 | 0.6000 |
| 1083.0 | 0.7000 |

Wormald, C.J - Colling, C.N, Excess enthalpies for (water + nitrogen)(g) up to 698.2 K and 12.6 MPa, The Journal of Chemical Thermodynamics 8 (1983) 725-737. doi:10.1016/0021-9614(83)90139-8

**T / K = 698.20**

**P / bar = 104.40**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 697.10 | 0.4000 |
| 722.00 | 0.5020 |
| 692.50 | 0.6010 |
| 595.80 | 0.7000 |
| 452.50 | 0.7980 |

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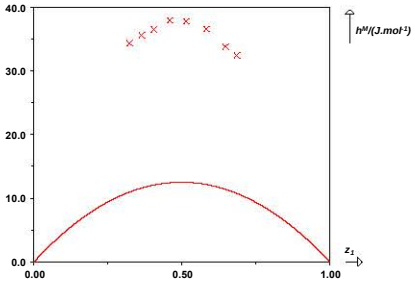
**Critical point**

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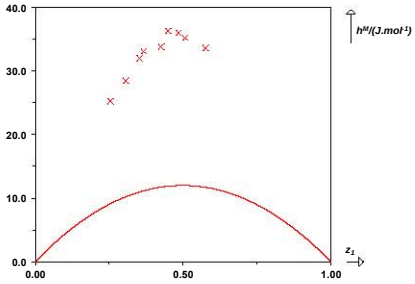
Prokhorova, V.M. - Tsiklis, D.S., Vapor− vapor equilibrium in the system nitrogen− water, Zh. Fiz. Khim. 8 (1970) 2069-2070.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 658.15 | 2229.2 | 0.4800 |

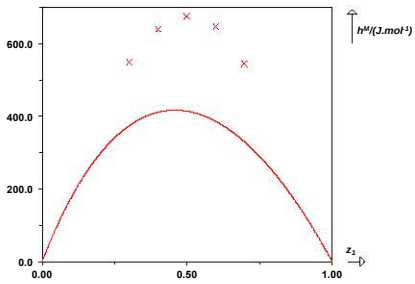
T/K = 400.15 - P/bar = 1.0100



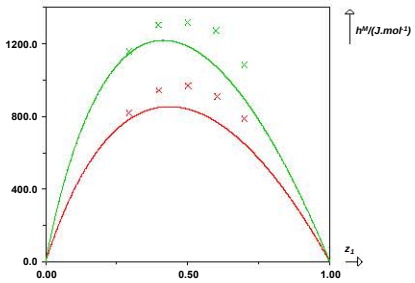

T/K = 410.15 - P/bar = 1.0100



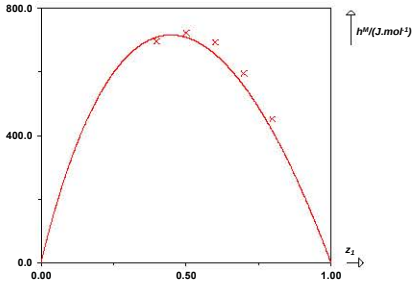

T/K = 548.20 - P/bar = 42.400



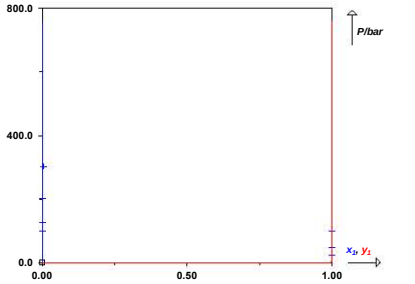

T/K = 648.20 - P/bar = 100.300 125.800



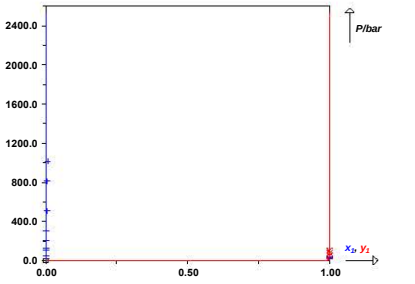

T/K = 698.20 - P/bar = 104.400



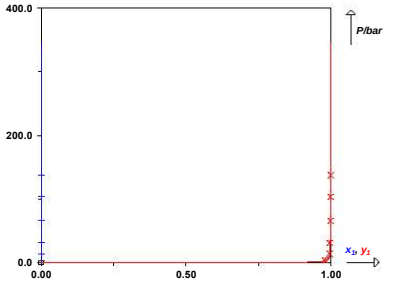

T/K = 273.15



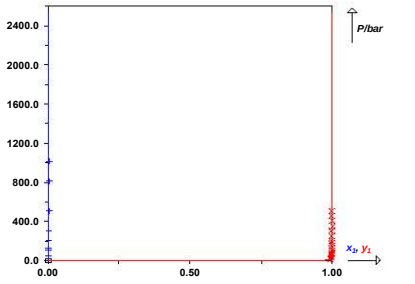

T/K = 298.15



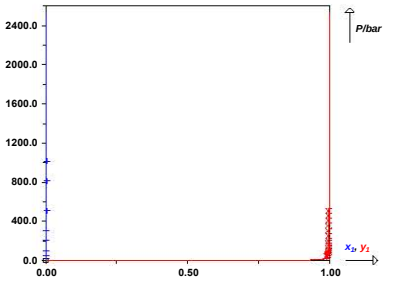

T/K = 310.93



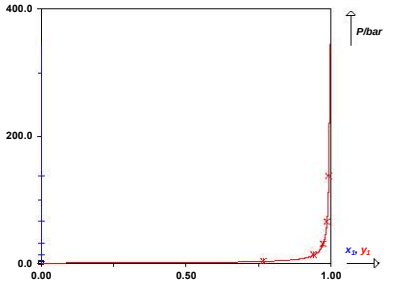

T/K = 323.15



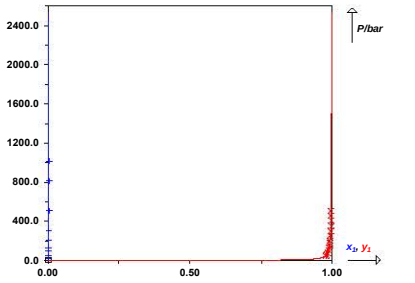

T/K = 348.15

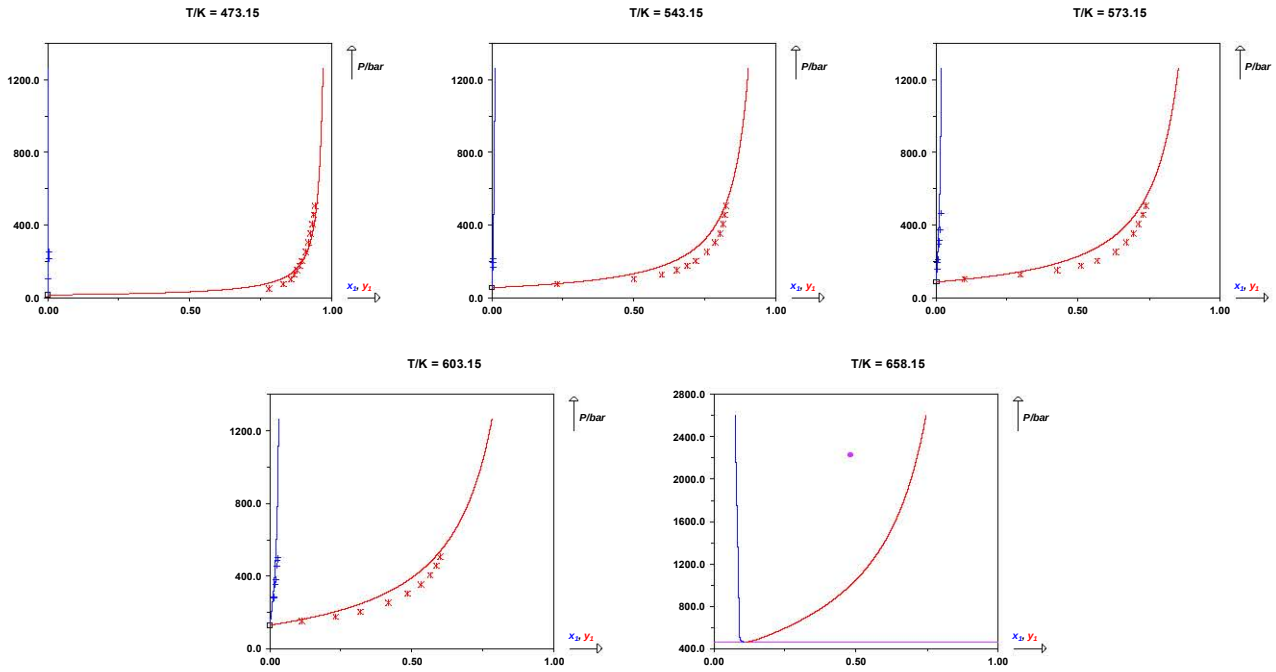



T/K = 366.48




T/K = 373.15




T/K = 473.15
P/bar
1200.0
800.0
400.0
0.0
0.00
0.50
1.00
x1, y1
T/K = 543.15
P/bar
1200.0
800.0
400.0
0.0
0.00
0.50
1.00
x1, y1
T/K = 573.15
P/bar
1200.0
800.0
400.0
0.0
0.00
0.50
1.00
x1, y1
T/K = 603.15
P/bar
1200.0
800.0
400.0
0.0
0.00
0.50
1.00
x1, y1
T/K = 658.15
P/bar
2800.0
2400.0
2000.0
1600.0
1200.0
800.0
400.0
0.00
0.50
1.00
x1, y1

## 1,2,3,4-TETRAHYDRONAPHTHALENE (1) + QUINOLINE (2)

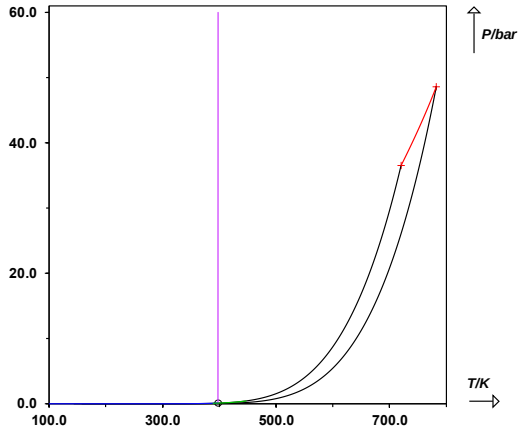
| | | |
|---|---|---|
| **CAS** | 119-64-2 | 91-22-5 |
| **InChiKey** | CXWXQJXEFPUFDZ-UHFFFAOYSA-N | SMWDFEZZVXVKRB-UHFFFAOYSA-N |
| **$T_c$ / K** | 720.00 | 782.15 |
| **$P_c$ / bar** | 36.50 | 48.60 |
| **ω** | 0.335 | 0.346 |

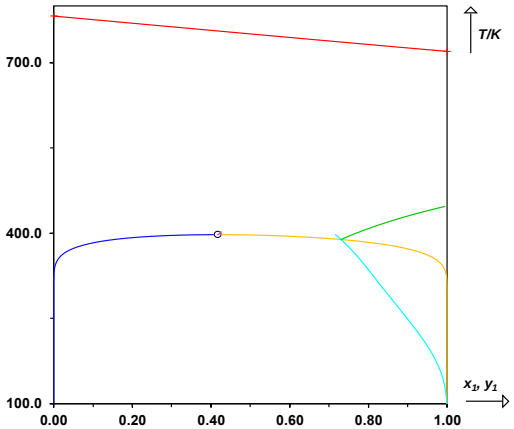
Ideal

**PPR78 results**

*Parameters*
A/MPa = 1310
B/MPa = 8010

*Deviations*
MAPE on x = 6.2 %
MAPE on y = 5.4 %



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**Isothermal phase equilibrium data**

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Niesen, Vicki G. - Yesavage, Victor F., Vapor-liquid equilibria for m-cresol/tetralin and tetralin/quinoline at temperatures between 523 and 598 K, Journal of Chemical & Engineering Data 3 (1988) 253-258. doi:10.1021/je00053a009

**T / K = 523.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.407 | 0.0410 | 0.0870 |
| 1.510 | 0.1020 | 0.1880 |
| 1.613 | 0.1800 | 0.3040 |
| 2.235 | 0.6910 | 0.7850 |
| 2.356 | 0.8260 | 0.8790 |
| 2.388 | 0.8880 | 0.9240 |

Niesen, Vicki G. - Yesavage, Victor F., Vapor-liquid equilibria for m-cresol/tetralin and tetralin/quinoline at temperatures between 523 and 598 K, Journal of Chemical & Engineering Data 3 (1988) 253-258. doi:10.1021/je00053a009

**T / K = 548.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.296 | 0.0360 | 0.0740 |
| 2.434 | 0.0990 | 0.1770 |
| 2.647 | 0.1870 | 0.3040 |
| 2.860 | 0.3050 | 0.4420 |
| 3.138 | 0.4470 | 0.5800 |
| 3.372 | 0.5830 | 0.6920 |
| 3.534 | 0.6890 | 0.7790 |
| 3.697 | 0.8170 | 0.8720 |
| 3.798 | 0.9050 | 0.9320 |

Niesen, Vicki G. - Yesavage, Victor F., Vapor-liquid equilibria for m-cresol/tetralin and tetralin/quinoline at temperatures between 523 and 598 K, Journal of Chemical & Engineering Data 3 (1988) 253-258. doi:10.1021/je00053a009

**T / K = 573.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.554 | 0.0320 | 0.0560 |
| 3.731 | 0.0790 | 0.1370 |
| 3.939 | 0.1460 | 0.2360 |
| 4.167 | 0.2200 | 0.3310 |
| 4.479 | 0.3320 | 0.4540 |
| 4.747 | 0.4370 | 0.5460 |
| 5.017 | 0.5510 | 0.6620 |
| 5.226 | 0.6540 | 0.7410 |
| 5.444 | 0.7600 | 0.8210 |
| 5.715 | 0.9130 | 0.9360 |

Niesen, Vicki G. - Yesavage, Victor F., Vapor-liquid equilibria for m-cresol/tetralin and tetralin/quinoline at temperatures between 523 and 598 K, Journal of Chemical & Engineering Data 3 (1988) 253-258. doi:10.1021/je00053a009

**T / K = 598.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.534 | 0.0750 | 0.1230 |
| 5.842 | 0.1430 | 0.2240 |
| 6.163 | 0.2220 | 0.3190 |
| 6.568 | 0.3280 | 0.4420 |
| 6.918 | 0.4300 | 0.5390 |
| 7.235 | 0.5370 | 0.6330 |
| 7.626 | 0.6560 | 0.7330 |
| 7.898 | 0.7590 | 0.8150 |
| 8.266 | 0.9160 | 0.9360 |

Mahmood, Shaukat - Zhao, Qingwen - Kabadi, Vinayak N., High-Temperature VLE for the Tetralin−Quinoline System, Journal of Chemical & Engineering Data 4 (2001) 994-999. doi:10.1021/je000069m

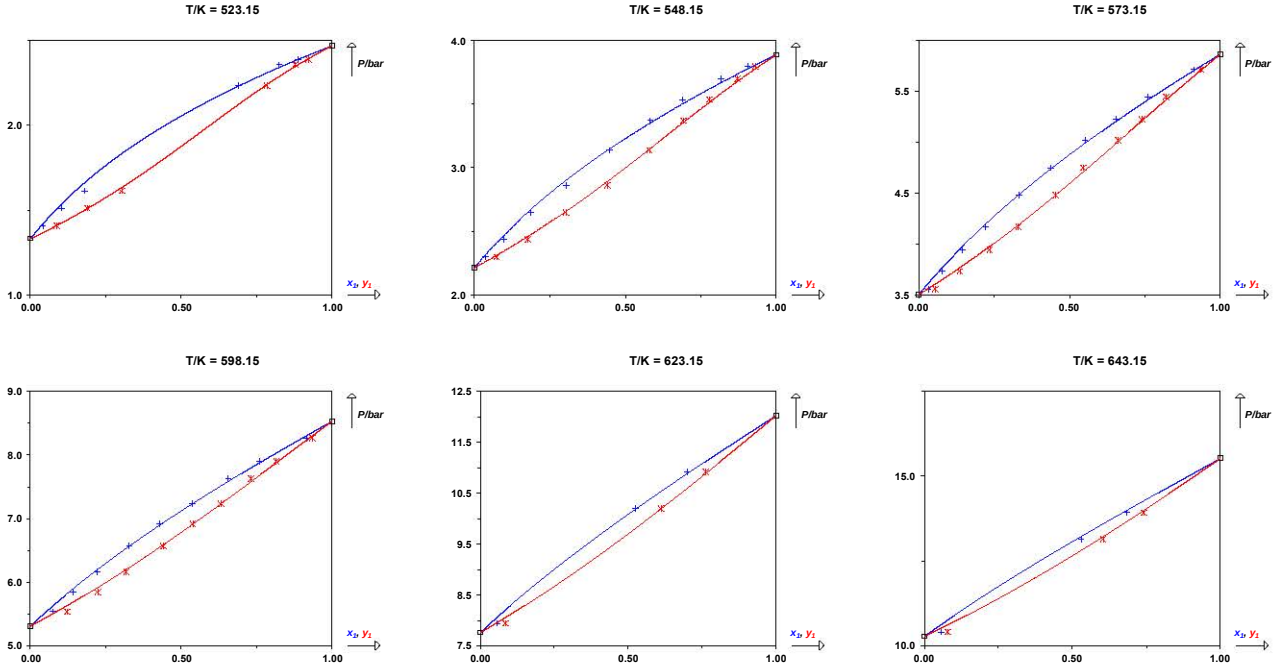
**T / K = 623.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.940 | 0.0570 | 0.0860 |
| 10.20 | 0.5250 | 0.6110 |
| 10.92 | 0.7000 | 0.7630 |

Mahmood, Shaukat - Zhao, Qingwen - Kabadi, Vinayak N., High-Temperature VLE for the Tetralin−Quinoline System, Journal of Chemical & Engineering Data 4 (2001) 994-999. doi:10.1021/je000069m

**T / K = 643.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.40 | 0.0570 | 0.0800 |
| 13.15 | 0.5300 | 0.6050 |
| 13.92 | 0.6850 | 0.7430 |


T/K = 523.15
P/bar
2.0
1.0
0.00
0.50
1.00
x1, y1
T/K = 548.15
P/bar
4.0
3.0
2.0
0.00
0.50
1.00
x1, y1
T/K = 573.15
P/bar
5.5
4.5
3.5
0.00
0.50
1.00
x1, y1
T/K = 598.15
P/bar
9.0
8.0
7.0
6.0
5.0
0.00
0.50
1.00
x1, y1
T/K = 623.15
P/bar
12.5
11.5
10.5
9.5
8.5
7.5
0.00
0.50
1.00
x1, y1
T/K = 643.15
P/bar
15.0
10.0
0.00
0.50
1.00
x1, y1

## DIETHYLAMINE (1) + BENZENE (2)

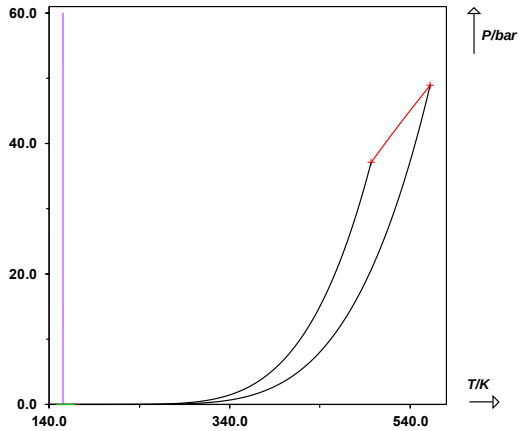
| | | |
|---|---|---|
| **CAS** | 109-89-7 | 71-43-2 |
| **InChiKey** | HPNMFZURTQLUMO-UHFFFAOYSA-N | UHOVQNZJYSORNB-UHFFFAOYSA-N |
| **$T_c$ / K** | 496.60 | 562.05 |
| **$P_c$ / bar** | 37.10 | 48.95 |
| **ω** | 0.304 | 0.210 |

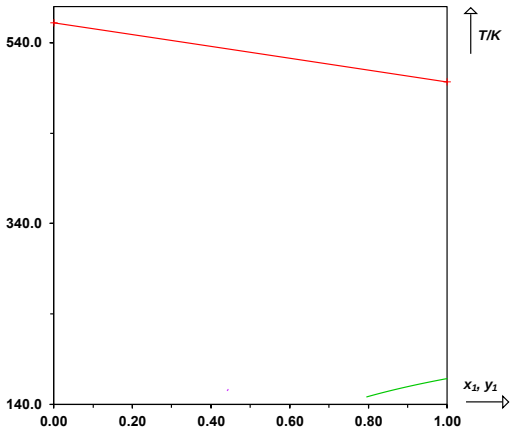
Ideal

**PPR78 results**

*Parameters*
A/MPa = 22.4
B/MPa = 89.6

*Deviations*
MAPE on x = 3.9 %
MAPE on y = 2.8 %
MAPE on $h^M$ = 9.8 %



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**Isothermal phase equilibrium data**

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Bayles, John W. - Letcher, Trevor M., Thermodynamics of some binary liquid mixtures containing aliphatic amines, Journal of Chemical & Engineering Data 3 (1971) 266-271. doi:10.1021/je60050a026

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2080 | 0.0310 | 0.0760 |
| 0.2277 | 0.0930 | 0.2070 |
| 0.2333 | 0.1110 | 0.2410 |
| 0.2660 | 0.2160 | 0.4080 |
| 0.3000 | 0.3310 | 0.5490 |
| 0.3133 | 0.3770 | 0.5970 |
| 0.3334 | 0.4480 | 0.6620 |
| 0.3602 | 0.5440 | 0.7400 |
| 0.3816 | 0.6240 | 0.7950 |
| 0.4042 | 0.7060 | 0.8460 |
| 0.4234 | 0.7810 | 0.8870 |
| 0.4397 | 0.8480 | 0.9210 |
| 0.4534 | 0.9000 | 0.9480 |

Bayles, John W. - Letcher, Trevor M., Thermodynamics of some binary liquid mixtures containing aliphatic amines, Journal of Chemical & Engineering Data 3 (1971) 266-271. doi:10.1021/je60050a026

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4668 | 0.0470 | 0.1060 |
| 0.4930 | 0.0880 | 0.1880 |
| 0.5241 | 0.1380 | 0.2750 |
| 0.5336 | 0.1550 | 0.3020 |
| 0.5601 | 0.1980 | 0.3665 |
| 0.6520 | 0.3540 | 0.5590 |
| 0.6662 | 0.3800 | 0.5850 |
| 0.7133 | 0.4620 | 0.6620 |
| 0.7387 | 0.5070 | 0.6990 |
| 0.7737 | 0.5700 | 0.7480 |
| 0.8533 | 0.7140 | 0.8430 |
| 0.9205 | 0.8410 | 0.9150 |
| 0.9389 | 0.8750 | 0.9340 |

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**Isobaric phase equilibrium data**

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Siedler, R. - Grote, L. - Kauert, E. - Werner, U. - Bittrich, H. J., Zur Thermodynamik der binären Systeme von Benzol mit Diäthylamin und Triäthylamin, Zeitschrift für Physikalische Chemie 1 (1969) doi:10.1515/zpch-1969-24127

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 351.55 | 0.0420 | 0.0830 |
| 350.55 | 0.0820 | 0.1500 |
| 348.65 | 0.1250 | 0.2290 |
| 346.95 | 0.1750 | 0.3060 |
| 335.65 | 0.5870 | 0.7500 |
| 334.95 | 0.6230 | 0.7800 |
| 332.75 | 0.7340 | 0.8600 |
| 331.85 | 0.7850 | 0.8920 |
| 330.75 | 0.8490 | 0.9230 |
| 329.95 | 0.9000 | 0.9540 |

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**Enthalpy of mixing**

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Siedler, R. - Grote, L. - Kauert, E. - Werner, U. - Bittrich, H. J., Zur Thermodynamik der binären Systeme von Benzol mit Diäthylamin und Triäthylamin, Zeitschrift für Physikalische Chemie 1 (1969) doi:10.1515/zpch-1969-24127

**T / K = 293.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 335.00 | 0.2290 |
| 385.00 | 0.3400 |
| 429.00 | 0.4500 |
| 433.00 | 0.5050 |
| 426.00 | 0.5410 |
| 424.00 | 0.5450 |
| 344.00 | 0.7150 |
| 297.00 | 0.7640 |
| 280.00 | 0.7670 |

Bayles, John W. - Letcher, Trevor M., Thermodynamics of some binary liquid mixtures containing aliphatic amines, Journal of Chemical & Engineering Data 3 (1971) 266-271. doi:10.1021/je60050a026

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 236.00 | 0.2070 |
| 335.00 | 0.3660 |
| 333.00 | 0.4690 |
| 294.00 | 0.6220 |
| 232.00 | 0.7640 |
| 180.00 | 0.7990 |

Kiyohara, Osamu - Anand, S.C - Benson, G.C, The thermodynamic properties of acetone + cyclopentanol

mixtures at 298.15 K, The Journal of Chemical Thermodynamics 4 (1974) 355-360. doi:10.1016/0021-9614(74)90164-5

**T / K =** **303.15**

**P / bar =** **1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 60.00 | 0.0499 |
| 166.00 | 0.1388 |
| 193.00 | 0.1704 |
| 248.00 | 0.2520 |
| 260.00 | 0.2826 |
| 304.00 | 0.3890 |
| 307.00 | 0.4757 |
| 308.00 | 0.5494 |
| 255.00 | 0.6660 |
| 199.00 | 0.7720 |
| 143.00 | 0.8549 |

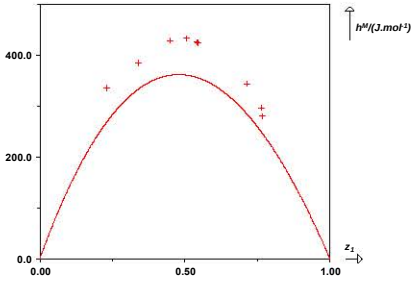
Bayles, John W. - Letcher, Trevor M., Thermodynamics of some binary liquid mixtures containing aliphatic amines, Journal of Chemical & Engineering Data 3 (1971) 266-271. doi:10.1021/je60050a026

**T / K =** **318.15**

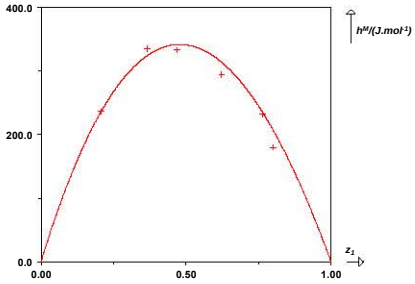
**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 240.00 | 0.2330 |
| 277.00 | 0.3010 |
| 315.00 | 0.3960 |
| 320.00 | 0.4620 |
| 319.00 | 0.4920 |
| 305.00 | 0.5560 |
| 224.00 | 0.7310 |

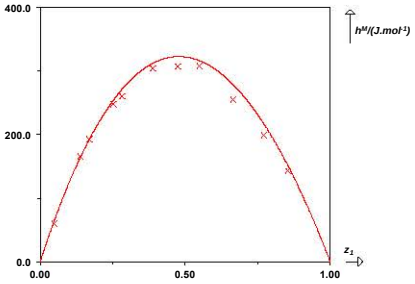
T/K = 293.15 - P/bar = 1.0132



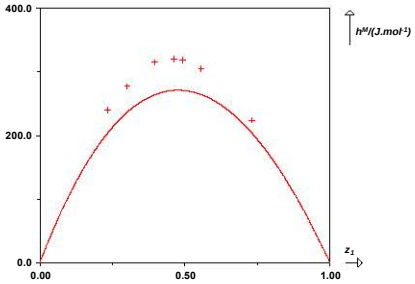

T/K = 298.15 - P/bar = 1.0132



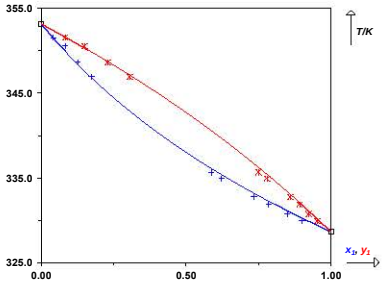

T/K = 303.15 - P/bar = 1.0100



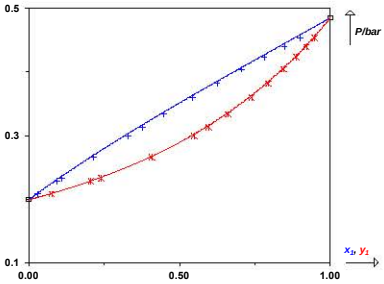

T/K = 318.15 - P/bar = 1.0132



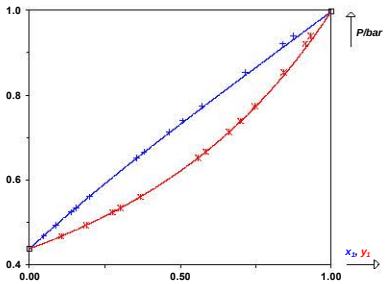

P/bar = 1.01330




T/K = 308.15




T/K = 328.15



## DIETHYLAMINE (1) + MONOCHLOROBENZENE (2)

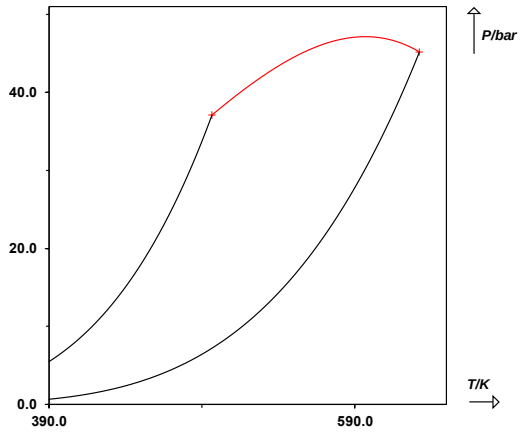
| | | |
|---|---|---|
| **CAS** | 109-89-7 | 108-90-7 |
| **InChiKey** | HPNMFZURTQLUMO-UHFFFAOYSA-N | MVPPADPHJFYWMZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 496.60 | 632.35 |
| **$P_c$ / bar** | 37.10 | 45.191 |
| **ω** | 0.304 | 0.25 |

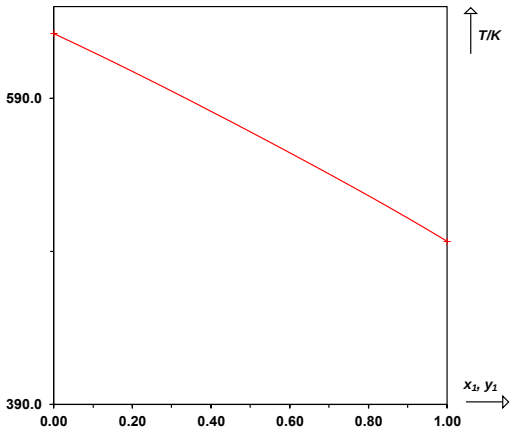
Ideal

**PPR78 results**

*Parameters*
A/MPa = 6.79
B/MPa = -17

*Deviations*
MAPE on x = 1.8 %
MAPE on y = 2.7 %
MAPE on $h^M$ = 3.4 %



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**Isothermal phase equilibrium data**

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Dehmelt, Ch. - Finke, M. - Bittrich, H. J., Untersuchungen zur zwischenmolekularen Wechselwirkung in Systemen von Diäthylamin mit aromatischen Komponenten, Zeitschrift für Physikalische Chemie 1 (1974) doi:10.1515/zpch-1974-25533

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0813 | 0.1250 | 0.6950 |
| 0.1636 | 0.2975 | 0.8835 |
| 0.2329 | 0.4540 | 0.9400 |
| 0.3363 | 0.6875 | 0.9785 |
| 0.4047 | 0.8300 | 0.9925 |

Bayles, John W. - Letcher, Trevor M., Thermodynamics of some binary liquid mixtures containing aliphatic amines, Journal of Chemical & Engineering Data 3 (1971) 266-271. doi:10.1021/je60050a026

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1763 | 0.2390 | 0.8450 |
| 0.2055 | 0.2920 | 0.8760 |
| 0.2308 | 0.3370 | 0.8960 |
| 0.2513 | 0.3740 | 0.9090 |
| 0.2673 | 0.4030 | 0.9180 |
| 0.2861 | 0.4360 | 0.9280 |
| 0.3338 | 0.5230 | 0.9470 |
| 0.3694 | 0.5900 | 0.9580 |
| 0.3864 | 0.6210 | 0.9625 |
| 0.4073 | 0.6610 | 0.9675 |
| 0.4601 | 0.7600 | 0.9790 |
| 0.4974 | 0.8320 | 0.9860 |
| 0.5212 | 0.8780 | 0.9900 |

Bayles, John W. - Letcher, Trevor M., Thermodynamics of some binary liquid mixtures containing aliphatic amines, Journal of Chemical & Engineering Data 3 (1971) 266-271. doi:10.1021/je60050a026

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1415 | 0.0445 | 0.3980 |
| 0.1525 | 0.0530 | 0.4450 |
| 0.2003 | 0.0950 | 0.5950 |
| 0.2701 | 0.1550 | 0.7180 |
| 0.2814 | 0.1650 | 0.7320 |
| 0.3334 | 0.2110 | 0.7850 |
| 0.3857 | 0.2570 | 0.8240 |
| 0.4368 | 0.3020 | 0.8535 |
| 0.4880 | 0.3480 | 0.8765 |
| 0.5248 | 0.3820 | 0.8910 |
| 0.5336 | 0.3900 | 0.8940 |
| 0.5621 | 0.4150 | 0.9030 |
| 0.6053 | 0.4550 | 0.9155 |
| 0.6484 | 0.4920 | 0.9255 |
| 0.6835 | 0.5260 | 0.9335 |
| 0.7337 | 0.5770 | 0.9445 |
| 0.7870 | 0.6220 | 0.9530 |
| 0.8327 | 0.6650 | 0.9600 |
| 0.8958 | 0.7250 | 0.9690 |
| 0.9330 | 0.7600 | 0.9730 |
| 1.000 | 0.8210 | 0.9810 |

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**Enthalpy of mixing**

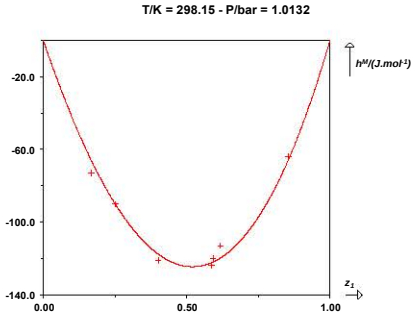
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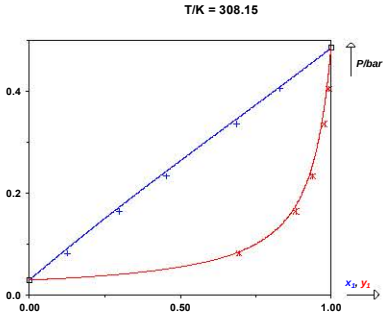
Bayles, John W. - Letcher, Trevor M., Thermodynamics of some binary liquid mixtures containing aliphatic amines, Journal of Chemical & Engineering Data 3 (1971) 266-271. doi:10.1021/je60050a026

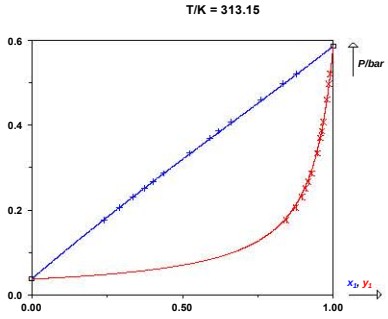
**T / K = 298.15**

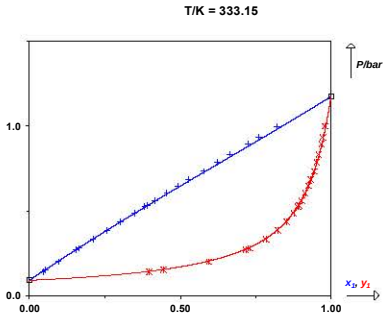
**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -73.00 | 0.1670 |
| -90.00 | 0.2510 |
| -121.00 | 0.4010 |
| -124.00 | 0.5860 |
| -120.00 | 0.5920 |
| -113.00 | 0.6180 |
| -64.00 | 0.8560 |


T/K = 298.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
-20.0
-60.0
-100.0
-140.0
0.00
0.50
1.00
$z_1$


T/K = 308.15
P/bar
0.4
0.2
0.0
0.00
0.50
1.00
$x_1$, $y_1$


T/K = 313.15
P/bar
0.6
0.4
0.2
0.0
0.00
0.50
1.00
$x_1$, $y_1$


T/K = 333.15
P/bar
1.0
0.0
0.00
0.50
1.00
$x_1$, $y_1$

## ETHANE (1) + METHANOL (2)

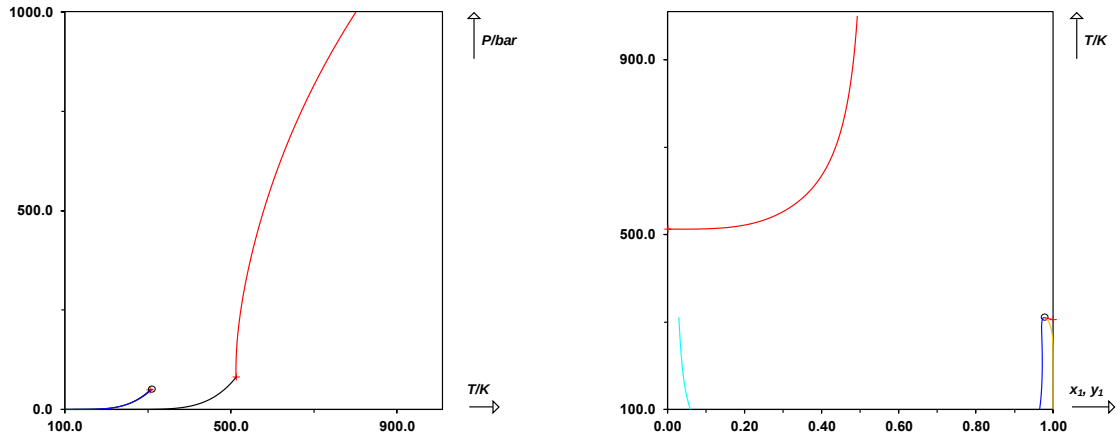
| | | |
|---|---|---|
| **CAS** | 74-84-0 | 67-56-1 |
| **InChiKey** | OTMSDBZUPAUEDD-UHFFFAOYSA-N | OKKJLVBELUTLKV-UHFFFAOYSA-N |
| **$T_c$ / K** | 305.32 | 512.50 |
| **$P_c$ / bar** | 48.72 | 80.84 |
| **ω** | 0.099 | 0.566 |

Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 989
B/MPa = -224

*Deviations*
MAPE on x = 130 %
MAPE on y = 21 %
MAPE on $h^M$ = 110 %



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**Isothermal phase equilibrium data**

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Ruffine, L., Équilibres de phases à basse température de systèmes complexes CO2 - hydrocarbures légers - méthanol - eau : mesures et modélisation (2005)

**T / K = 241.40**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.700 | 0.0346 | 0.9917 |
| 3.160 | 0.0582 | 0.9998 |
| 6.260 | 0.1348 | 0.9999 |
| 9.320 | 0.3267 | 0.9996 |

Ohgaki, Kazunari - Sano, Fumihiko - Katayama, Takashi, Isothermal vapor-liquid equilibrium data for binary systems containing ethane at high pressures, Journal of Chemical & Engineering Data 1 (1976) 55-58. doi:10.1021/je60068a016

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.94 | 0.0403 | 0.9822 |
| 21.02 | 0.0880 | 0.9887 |
| 31.43 | 0.1755 | 0.9914 |
| 38.56 | 0.2728 | 0.9921 |
| 41.25 | 0.3511 | 0.9922 |

Ishihara, Katsuo - Tanaka, Hiroyuki - Kato, Masahiro, Phase equilibrium properties of ethane+methanol system at 298.15 K, Fluid Phase Equilibria 1-2 (1998) 131-136. doi:10.1016/S0378-3812(97)00251-3

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.630 | 0.0530 | 0.9590 |
| 20.58 | 0.1130 | 0.9780 |
| 30.61 | 0.1990 | 0.9860 |
| 34.10 | 0.2410 | 0.9910 |
| 41.33 | 0.9720 | 0.9970 |
| 41.55 | 0.9880 | 0.9980 |

Ma, Yi Hua. - Kohn, James P., Multiphase and Volumetric Equilibria of the Ethane-Methanol System at Temperatures between -40° and 100°C., Journal of Chemical & Engineering Data 1 (1964) 3-5. doi:10.1021/je60020a002

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.26 | 0.0619 | 0.9070 |
| 30.39 | 0.0990 | 0.9430 |
| 40.52 | 0.1454 | 0.9600 |
| 50.65 | 0.2045 | 0.9700 |
| 60.78 | 0.2753 | 0.9780 |

Ma, Yi Hua. - Kohn, James P., Multiphase and Volumetric Equilibria of the Ethane-Methanol System at Temperatures between -40° and 100°C., Journal of Chemical & Engineering Data 1 (1964) 3-5. doi:10.1021/je60020a002

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.26 | 0.0433 | 0.8550 |
| 30.39 | 0.0718 | 0.8970 |
| 40.52 | 0.1015 | 0.9260 |
| 50.65 | 0.1332 | 0.9440 |
| 60.78 | 0.1738 | 0.9490 |

Ma, Yi Hua. - Kohn, James P., Multiphase and Volumetric Equilibria of the Ethane-Methanol System at Temperatures between -40° and 100°C., Journal of Chemical & Engineering Data 1 (1964) 3-5. doi:10.1021/je60020a002

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.26 | 0.0284 | 0.6870 |
| 30.39 | 0.0510 | 0.7560 |
| 40.52 | 0.0719 | 0.8080 |
| 50.65 | 0.0967 | 0.8420 |
| 60.78 | 0.1290 | 0.8640 |

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**Enthalpy of mixing**

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Sipowska, J.T - Graham, R.C - Neely, B.J - Ott, J.B - Izatt, R.M, Excess enthalpies for (ethane + methanol) at 298.15 and 348.15 K and 7.5 and 15 MPa, and at 323.15 K at 7.5, 10, and 15 MPa, The Journal of Chemical Thermodynamics 10 (1989) 1085-1093. doi:10.1016/0021-9614(89)90095-5

**T / K = 298.15**

**P / bar = 75.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 8.760 | 0.0265 |
| 16.52 | 0.0542 |
| 21.58 | 0.0835 |
| 26.72 | 0.1143 |
| 29.23 | 0.1468 |

| | |
|---|---|
| 28.46 | 0.1812 |
| 26.68 | 0.2175 |
| 23.45 | 0.2560 |
| 19.30 | 0.2970 |
| 13.70 | 0.3405 |
| 8.500 | 0.3869 |
| 6.570 | 0.4195 |
| 9.210 | 0.4607 |
| 14.63 | 0.4895 |
| 20.32 | 0.5155 |
| 27.55 | 0.5464 |
| 32.96 | 0.5744 |
| 44.59 | 0.6076 |
| 48.33 | 0.6378 |
| 59.17 | 0.6737 |
| 65.62 | 0.7064 |
| 79.14 | 0.7452 |
| 85.40 | 0.7807 |
| 96.78 | 0.8229 |
| 101.32 | 0.8503 |
| 117.61 | 0.8784 |
| 129.39 | 0.9075 |
| 138.46 | 0.9374 |
| 138.37 | 0.9682 |
| 137.16 | 0.9731 |
| 134.70 | 0.9745 |

McFall, T.A. - Post, M.E. - Christensen, J.J. - Izatt, R.M., The excess enthalpies of eight (ethane + alcohol) mixtures at 298.15 K, The Journal of Chemical Thermodynamics 5 (1981) 441-446. doi:10.1016/0021-9614(81)90051-3

**T / K = 298.15**

**P / bar = 69.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 4.170 | 0.0099 |
| 12.29 | 0.0410 |
| 18.76 | 0.0740 |
| 22.14 | 0.1093 |
| 23.40 | 0.1471 |
| 19.89 | 0.1877 |
| 16.14 | 0.2313 |
| 7.030 | 0.2784 |
| 1.010 | 0.3293 |
| -4.650 | 0.3846 |
| -6.970 | 0.4141 |
| -5.180 | 0.4448 |
| -1.850 | 0.4770 |
| 4.870 | 0.5106 |
| 14.21 | 0.5459 |
| 25.44 | 0.5829 |
| 35.90 | 0.6218 |
| 43.43 | 0.6626 |
| 56.08 | 0.7057 |
| 67.33 | 0.7510 |
| 71.22 | 0.7667 |
| 80.19 | 0.7989 |
| 88.70 | 0.8324 |
| 93.98 | 0.8496 |
| 111.35 | 0.8850 |
| 117.56 | 0.9032 |
| 127.45 | 0.9218 |
| 134.39 | 0.9408 |
| 136.17 | 0.9601 |
| 131.89 | 0.9798 |

Sipowska, J.T - Graham, R.C - Neely, B.J - Ott, J.B - Izatt, R.M, Excess enthalpies for (ethane + methanol) at 298.15 and 348.15 K and 7.5 and 15 MPa, and at 323.15 K at 7.5, 10, and 15 MPa, The Journal of Chemical Thermodynamics 10 (1989) 1085-1093. doi:10.1016/0021-9614(89)90095-5

**T / K = 323.15**

**P / bar = 100.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 6.400 | 0.0560 |
| 8.100 | 0.0861 |
| 6.900 | 0.1177 |
| 5.000 | 0.1511 |
| 0.7000 | 0.1862 |
| -4.900 | 0.2233 |
| -13.30 | 0.2625 |
| -18.10 | 0.3040 |
| -19.50 | 0.3480 |
| -20.20 | 0.3948 |
| -17.00 | 0.4447 |
| 8.700 | 0.4978 |
| 41.40 | 0.5547 |
| 72.90 | 0.6156 |
| 112.10 | 0.6810 |
| 155.50 | 0.7515 |
| 196.90 | 0.8277 |
| 231.80 | 0.8654 |
| 275.40 | 0.9103 |
| 292.70 | 0.9393 |

| | |
|---|---|
| 292.60 | 0.9512 |
| 263.20 | 0.9768 |

Sipowska, J.T - Graham, R.C - Neely, B.J - Ott, J.B - Izatt, R.M, Excess enthalpies for (ethane + methanol) at 298.15 and 348.15 K and 7.5 and 15 MPa, and at 323.15 K at 7.5, 10, and 15 MPa, The Journal of Chemical Thermodynamics 10 (1989) 1085-1093. doi:10.1016/0021-9614(89)90095-5

**T / K = 348.15**

**P / bar = 75.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -20.00 | 0.0087 |
| -44.70 | 0.0175 |
| -69.00 | 0.0265 |
| -152.80 | 0.0542 |
| -235.40 | 0.0835 |
| -325.10 | 0.1143 |
| -422.80 | 0.1468 |
| -530.70 | 0.1812 |
| -635.30 | 0.2175 |
| -650.40 | 0.2301 |
| -597.10 | 0.2560 |
| -508.80 | 0.2969 |
| -417.20 | 0.3404 |
| -316.20 | 0.3869 |
| -209.10 | 0.4364 |
| -96.30 | 0.4895 |
| 155.40 | 0.6076 |
| 301.70 | 0.6737 |
| 443.40 | 0.7452 |
| 514.50 | 0.7807 |
| 620.10 | 0.8229 |
| 688.90 | 0.8614 |
| 791.60 | 0.9075 |
| 858.20 | 0.9374 |
| 866.50 | 0.9435 |
| 885.50 | 0.9496 |
| 901.10 | 0.9558 |
| 831.10 | 0.9620 |
| 753.10 | 0.9682 |

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**Three-phase line**

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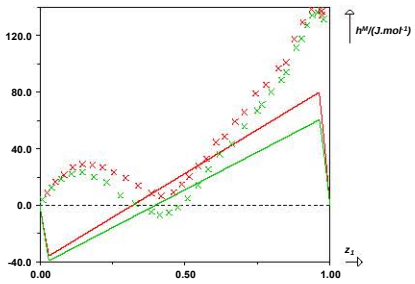
Y.H. Ma - J.P. Kohn, Multiphase and Volumetric Equilibria of the Ethane-Methanol System at Temperatures between -40° and 100°C., Journal of Chemical & Engineering Data. 9 (1964) 3–5. doi:10.1021/je60020a002.

| T / K | P / bar | $x_{1a}$ | $x_{1b}$ | $y_1$ |
|---|---|---|---|---|
| 233.15 | 7.28 | 0.3600 | 0.9570 | 0.9920 |
| 242.45 | 10.13 | 0.3760 | 0.9360 | 0.9910 |
| 267.50 | 20.27 | 0.4100 | 0.9340 | 0.9900 |
| 283.95 | 30.40 | 0.3570 | 0.9360 | 0.9890 |
| 296.93 | 40.53 | 0.3540 | 0.9410 | 0.9880 |
| 308.40 | 50.66 | 0.3480 | 0.9620 | 0.9860 |
| 309.57 | 51.76 | 0.3510 | 0.9790 | 0.9790 |

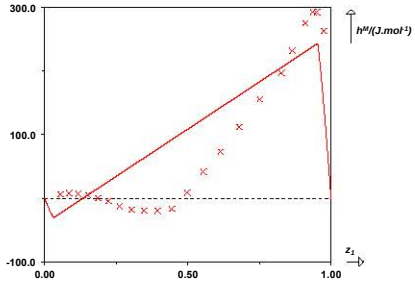
L. Ruffine - A. Barreau - I. Brunella - P. Mougin - J. Jose, New Apparatus for Low-Temperature Investigations: Measurements of the Multiphase Equilibrium of Mixtures Containing Methane, Ethane, Propane, Butane, Methanol, and Carbon Dioxide, Industrial & Engineering Chemistry Research. 44 (2005) 8387–8392. doi:10.1021/ie0506365.

| T / K | P / bar | $x_{1a}$ | $x_{1b}$ | $y_1$ |
|---|---|---|---|---|
| 241.00 | 9.40 | 0.4202 | 0.8876 | 0.9888 |
| 258.95 | 15.95 | 0.4245 | 0.8843 | 0.9999 |
| 273.15 | 23.26 | 0.4269 | 0.8829 | 0.9998 |
| 283.43 | 29.27 | 0.4165 | 0.9339 | 0.9998 |

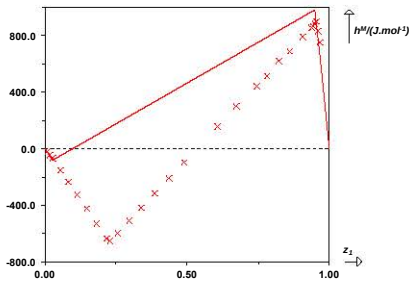
T/K = 298.15 - P/bar = 75.00 69.00



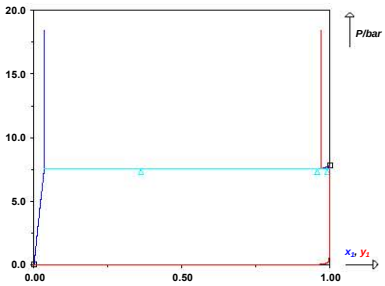

T/K = 323.15 - P/bar = 100.00



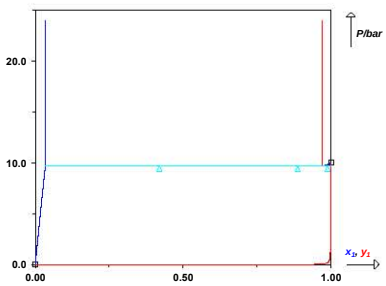

T/K = 348.15 - P/bar = 75.00



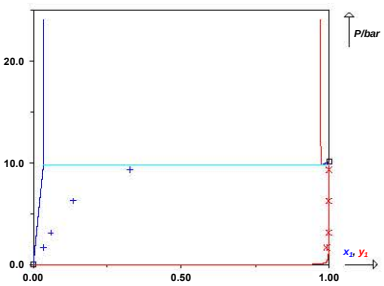

T/K = 233.15



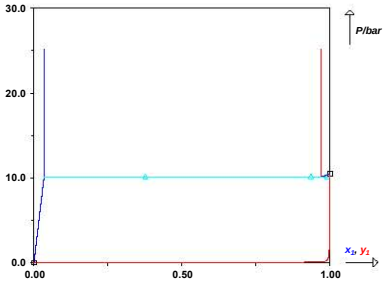

T/K = 241.00



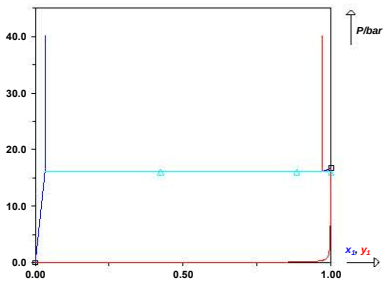

T/K = 241.40



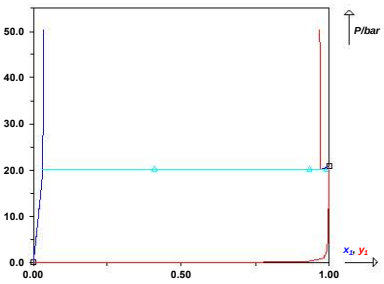

T/K = 242.45



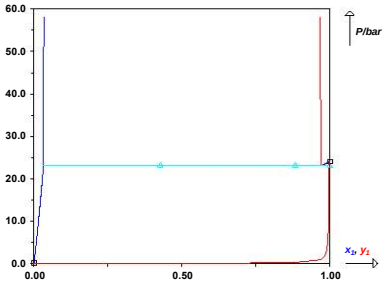

T/K = 258.95



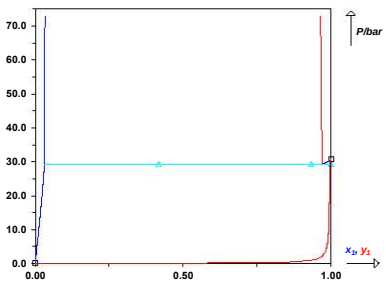

T/K = 267.50



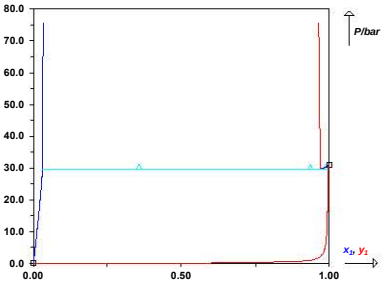

T/K = 273.15



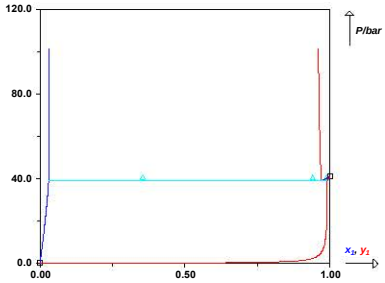

T/K = 283.43



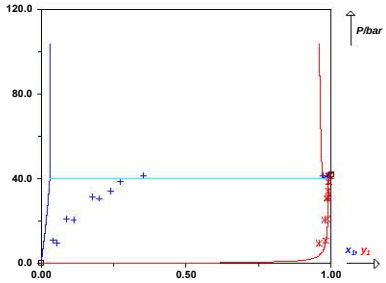

T/K = 283.95



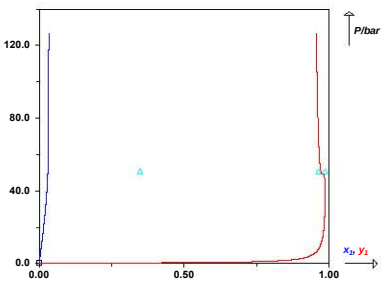

T/K = 296.93

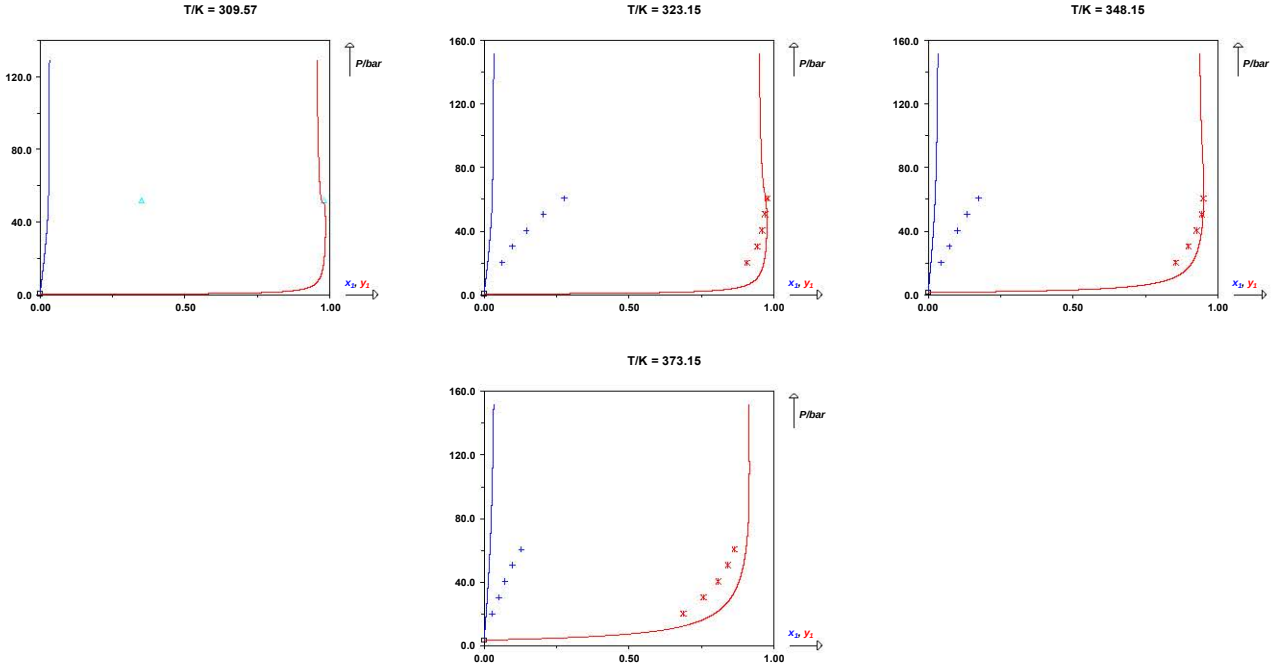



T/K = 298.15




T/K = 308.40




T/K = 309.57
P/bar
120.0
80.0
40.0
0.0
0.00
0.50
1.00
x1, y1
T/K = 323.15
P/bar
160.0
120.0
80.0
40.0
0.0
0.00
0.50
1.00
x1, y1
T/K = 348.15
P/bar
160.0
120.0
80.0
40.0
0.0
0.00
0.50
1.00
x1, y1
T/K = 373.15
P/bar
160.0
120.0
80.0
40.0
0.0
0.00
0.50
1.00
x1, y1

## PROPANE (1) + METHANOL (2)

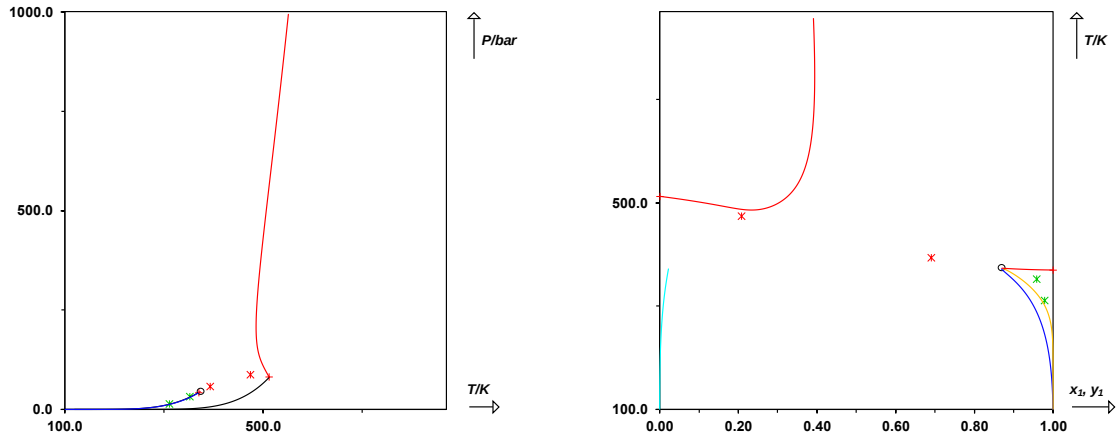
| | | |
|---|---|---|
| **CAS** | 74-98-6 | 67-56-1 |
| **InChiKey** | ATUOYWHBWRKTHZ-UHFFFAOYSA-N | OKKJLVBELUTLKV-UHFFFAOYSA-N |
| **$T_c$ / K** | 369.83 | 512.50 |
| **$P_c$ / bar** | 42.48 | 80.84 |
| **ω** | 0.152 | 0.566 |

Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 1060
B/MPa = 728

*Deviations*
MAPE on x = 87 %
MAPE on y = 11 %
MAPE on $h^M$ = 35 %



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**Isothermal phase equilibrium data**

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Lev, Ah-Dong - Robinson, Donald B. - Chung, Samuels Y.-K. - Chen, C.-J., The equilibrium phase properties of the propane-methanol and n-Butane-methanol binary systems, The Canadian Journal of Chemical Engineering 2 (1992) 330-334. doi:10.1002/cjce.5450700217

**T / K = 310.70**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 2.120 | 0.0160 | 0.8220 | |
| 5.050 | 0.0460 | 0.9220 | |
| 9.230 | 0.1240 | 0.9600 | |
| 11.37 | 0.2160 | 0.9640 | |
| 11.73 | 0.2390 | 0.9680 | |
| 12.36 | 0.3480 | 0.9600 | |
| 12.84 | 0.5320 | 0.9610 | |
| 13.04 | 0.7540 | 0.9580 | |
| 13.29 | 0.8970 | 0.9700 | |
| 13.43 | 0.9440 | 0.9740 | |
| 13.50 | 0.9790 | 0.9790 | AZEO |
| 13.41 | 0.9840 | 0.9800 | |

Galivel-Solastiouk, Francine - Laugier, Serge - Richon, Dominique, Vapor-liquid equilibrium data for the propane-methanol and propane-methanol-carbon dioxide system, Fluid Phase Equilibria 1 (1986) 73-85. doi:10.1016/0378-3812(86)85069-5

**T / K = 313.10**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.500 | 0.0252 | 0.8780 |
| 5.100 | 0.0386 | 0.9000 |
| 6.200 | 0.0520 | 0.9270 |
| 7.120 | 0.0750 | 0.9370 |
| 8.400 | 0.0840 | 0.9470 |
| 10.60 | 0.1460 | 0.9560 |
| 11.51 | 0.1950 | 0.9650 |
| 12.50 | 0.2630 | 0.9660 |
| 13.10 | 0.3870 | 0.9690 |
| 13.23 | 0.4110 | 0.9720 |
| 13.30 | 0.4490 | 0.9680 |
| 13.60 | 0.7520 | 0.9650 |

Joung, Seung Nam - Shin, Hun Yong - Kim, Han Seok - Yoo, Ki-Pung, High-Pressure Vapor−Liquid Equilibrium Data and Modeling of Propane + Methanol and Propane + Ethanol Systems, Journal of Chemical & Engineering Data 3 (2004) 426-429. doi:10.1021/je0340506

**T / K = 327.95**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.500 | 0.0192 | 0.7501 |
| 6.600 | 0.0493 | 0.8721 |
| 9.400 | 0.0791 | 0.9085 |
| 11.70 | 0.1102 | 0.9165 |
| 14.60 | 0.1697 | 0.9402 |
| 17.50 | 0.2946 | 0.9518 |
| 18.30 | 0.4059 | 0.9540 |
| 18.80 | 0.5083 | 0.9549 |
| 19.00 | 0.7414 | 0.9566 |

Joung, Seung Nam - Shin, Hun Yong - Kim, Han Seok - Yoo, Ki-Pung, High-Pressure Vapor−Liquid Equilibrium Data and Modeling of Propane + Methanol and Propane + Ethanol Systems, Journal of Chemical & Engineering Data 3 (2004) 426-429. doi:10.1021/je0340506

**T / K = 343.21**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.000 | 0.0143 | 0.6380 |
| 7.400 | 0.0374 | 0.7864 |
| 11.30 | 0.0684 | 0.8610 |
| 14.60 | 0.1006 | 0.8933 |
| 17.90 | 0.1468 | 0.9112 |
| 21.30 | 0.2068 | 0.9253 |
| 22.30 | 0.2455 | 0.9333 |
| 23.60 | 0.3187 | 0.9363 |
| 24.80 | 0.4068 | 0.9387 |
| 25.40 | 0.6108 | 0.9367 |
| 25.80 | 0.7627 | 0.9455 |

Lev, Ah-Dong - Robinson, Donald B. - Chung, Samuels Y.-K. - Chen, C.-J., The equilibrium phase properties of the propane-methanol and n-Butane-methanol binary systems, The Canadian Journal of Chemical Engineering 2 (1992) 330-334. doi:10.1002/cjce.5450700217

**T / K = 352.20**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.600 | 0.0200 | 0.6600 | |
| 11.37 | 0.0510 | 0.8170 | |
| 17.27 | 0.0970 | 0.8680 | |
| 23.89 | 0.1850 | 0.9050 | |
| 27.89 | 0.2920 | 0.9180 | |
| 30.66 | 0.5430 | 0.9210 | |
| 31.31 | 0.7250 | 0.9270 | |
| 31.73 | 0.9570 | 0.9550 | |
| 31.80 | 0.9580 | 0.9580 | AZEO |
| 31.56 | 0.9750 | 0.9660 | |

Galivel-Solastiouk, Francine - Laugier, Serge - Richon, Dominique, Vapor-liquid equilibrium data for the propane-methanol and propane-methanol-carbon dioxide system, Fluid Phase Equilibria 1 (1986) 73-85. doi:10.1016/0378-3812(86)85069-5

**T / K = 373.10**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.800 | 0.0210 | 0.5370 |
| 18.60 | 0.0670 | 0.7540 |
| 22.60 | 0.0920 | 0.7960 |
| 30.40 | 0.1560 | 0.8470 |
| 34.90 | 0.2130 | 0.8630 |
| 39.00 | 0.3060 | 0.8900 |
| 40.20 | 0.3570 | 0.8760 |
| 42.80 | 0.6480 | 0.8420 |

Lev, Ah-Dong - Robinson, Donald B. - Chung, Samuels Y.-K. - Chen, C.-J., The equilibrium phase properties of the propane-methanol and n-Butane-methanol binary systems, The Canadian Journal of Chemical Engineering 2 (1992) 330-334. doi:10.1002/cjce.5450700217

**T / K = 393.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 14.46 | 0.0270 | 0.5020 | |
| 22.04 | 0.0540 | 0.6340 | |
| 31.01 | 0.0950 | 0.7180 | |
| 41.83 | 0.1710 | 0.7700 | |
| 48.65 | 0.2420 | 0.7930 | |
| 54.13 | 0.3710 | 0.7920 | |
| 56.92 | 0.5440 | 0.7710 | |
| 57.32 | 0.5890 | 0.7640 | |
| 58.10 | 0.6900 | 0.6900 | CRIT |

Lev, Ah-Dong - Robinson, Donald B. - Chung, Samuels Y.-K. - Chen, C.-J., The equilibrium phase properties of the propane-methanol and n-Butane-methanol binary systems, The Canadian Journal of Chemical Engineering 2 (1992) 330-334. doi:10.1002/cjce.5450700217

**T / K = 474.30**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 53.01 | 0.0280 | 0.1460 | |
| 60.65 | 0.0500 | 0.1990 | |
| 65.96 | 0.0660 | 0.2310 | |
| 75.20 | 0.1000 | 0.2650 | |
| 81.03 | 0.1320 | 0.2740 | |
| 85.42 | 0.1550 | 0.2610 | |
| 86.63 | 0.1730 | 0.2400 | |
| 87.30 | 0.2080 | 0.2080 | CRIT |

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**Enthalpy of mixing**

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Sipowska, J.T. - Ott, J.B. - Woolley, A.T. - Marchant, B.G. - Gruszkiewicz, M.S., Excess enthalpies for (propane + methanol) at the pressure 5 MPa and the temperatures (253.15, 258.15, 263.15, and 273.15) K. The effect of water as an impurity on the (liquid + liquid) equilibria in (propane + methanol), The Journal of Chemical Thermodynamics 8 (1993) 999-1004. doi:10.1006/jcht.1993.1095

**T / K = 253.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 62.10 | 0.0323 |
| 153.70 | 0.0948 |
| 198.00 | 0.1346 |
| 234.00 | 0.1778 |
| 274.10 | 0.2500 |
| 296.40 | 0.3328 |
| 299.70 | 0.4118 |
| 295.40 | 0.4463 |
| 291.20 | 0.4828 |
| 281.00 | 0.5213 |
| 272.30 | 0.5621 |
| 259.20 | 0.6053 |
| 245.90 | 0.6512 |
| 235.60 | 0.6752 |
| 218.60 | 0.7256 |
| 198.10 | 0.7794 |
| 182.50 | 0.8077 |
| 148.80 | 0.8673 |
| 103.70 | 0.9312 |
| 70.60 | 0.9650 |

Sipowska, J.T. - Ott, J.B. - Woolley, A.T. - Marchant, B.G. - Gruszkiewicz, M.S., Excess enthalpies for (propane + methanol) at the pressure 5 MPa and the temperatures (253.15, 258.15, 263.15, and 273.15) K. The effect of water as an impurity on the (liquid + liquid) equilibria in (propane + methanol), The Journal of Chemical Thermodynamics 8 (1993) 999-1004. doi:10.1006/jcht.1993.1095

**T / K = 283.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 57.80 | 0.0323 |
| 151.60 | 0.0948 |
| 193.80 | 0.1346 |
| 233.10 | 0.1778 |
| 278.90 | 0.2500 |

| | |
|---|---|
| 310.00 | 0.3328 |
| 325.50 | 0.4118 |
| 329.30 | 0.4828 |
| 326.50 | 0.5621 |
| 312.90 | 0.6512 |
| 287.40 | 0.7256 |
| 264.00 | 0.8077 |
| 213.10 | 0.8987 |
| 143.70 | 0.9650 |

Sipowska, J.T. - Ott, J.B. - Neely, B.J. - Izatt, R.M., Excess enthalpies for (propane + methanol) at the temperatures (298.15, 323.15, 348.15, and 373.15) K and pressures (5, 10, and 15) MPa, and at 363.15K and (5 and 15) MPa, The Journal of Chemical Thermodynamics 6 (1991) 551-559. doi:10.1016/S0021-9614(05)80098-9

| **T / K =** | **298.15** |
|---|---|
| **P / bar =** | **150.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 48.90 | 0.0245 |
| 97.10 | 0.0504 |
| 144.00 | 0.0777 |
| 186.10 | 0.1066 |
| 227.70 | 0.1373 |
| 263.30 | 0.1699 |
| 304.60 | 0.2166 |
| 332.80 | 0.2543 |
| 355.00 | 0.2947 |
| 376.80 | 0.3379 |
| 386.70 | 0.3685 |
| 399.90 | 0.4173 |
| 407.60 | 0.4520 |
| 410.80 | 0.4885 |
| 413.40 | 0.5270 |
| 416.50 | 0.5677 |
| 409.00 | 0.6107 |
| 404.10 | 0.6564 |
| 400.10 | 0.6802 |
| 389.20 | 0.7302 |
| 380.80 | 0.7563 |
| 355.00 | 0.8112 |
| 341.20 | 0.8401 |
| 325.90 | 0.8699 |
| 291.20 | 0.9007 |
| 263.30 | 0.9326 |
| 211.50 | 0.9657 |
| 197.40 | 0.9742 |

Sipowska, J.T. - Ott, J.B. - Neely, B.J. - Izatt, R.M., Excess enthalpies for (propane + methanol) at the temperatures (298.15, 323.15, 348.15, and 373.15) K and pressures (5, 10, and 15) MPa, and at 363.15K and (5 and 15) MPa, The Journal of Chemical Thermodynamics 6 (1991) 551-559. doi:10.1016/S0021-9614(05)80098-9

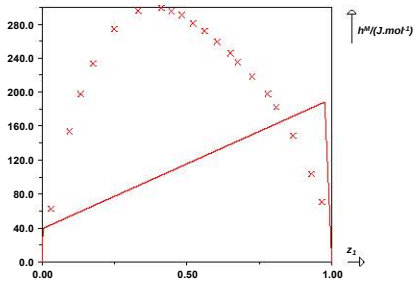
| **T / K =** | **348.15** |
|---|---|
| **P / bar =** | **50.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 56.10 | 0.0239 |
| 106.90 | 0.0492 |
| 162.90 | 0.0759 |
| 217.10 | 0.1042 |
| 273.10 | 0.1343 |
| 342.00 | 0.1774 |
| 390.80 | 0.2123 |
| 444.60 | 0.2495 |
| 497.00 | 0.2894 |
| 550.30 | 0.3322 |
| 610.60 | 0.3784 |
| 644.80 | 0.4111 |
| 679.40 | 0.4457 |
| 721.70 | 0.4821 |
| 759.10 | 0.5206 |
| 795.40 | 0.5614 |
| 833.80 | 0.6046 |
| 869.70 | 0.6506 |
| 899.70 | 0.6994 |
| 924.20 | 0.7356 |
| 936.60 | 0.7790 |
| 943.60 | 0.8073 |
| 933.70 | 0.8366 |
| 915.70 | 0.8670 |
| 873.40 | 0.8984 |
| 820.10 | 0.9178 |
| 781.80 | 0.9310 |
| 677.90 | 0.9512 |
| 573.40 | 0.9649 |

Sipowska, J.T. - Ott, J.B. - Neely, B.J. - Izatt, R.M., Excess enthalpies for (propane + methanol) at the temperatures (298.15, 323.15, 348.15, and 373.15) K and pressures (5, 10, and 15) MPa, and at 363.15K and (5 and 15) MPa, The Journal of Chemical Thermodynamics 6 (1991) 551-559. doi:10.1016/S0021-9614(05)80098-9

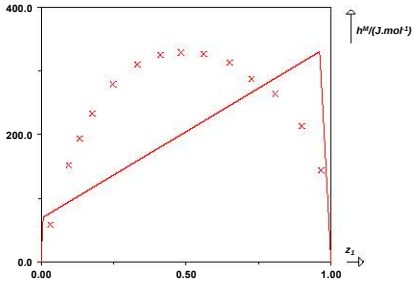
| **T / K =** | **363.15** |
|---|---|
| **P / bar =** | **150.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 56.20 | 0.0162 |

| | |
|---|---|
| 198.80 | 0.0594 |
| 297.70 | 0.0970 |
| 405.40 | 0.1376 |
| 489.80 | 0.1702 |
| 596.60 | 0.2170 |
| 676.00 | 0.2548 |
| 754.70 | 0.2952 |
| 838.20 | 0.3384 |
| 884.80 | 0.3691 |
| 967.20 | 0.4179 |
| 1023.2 | 0.4525 |
| 1066.6 | 0.4891 |
| 1112.3 | 0.5276 |
| 1159.7 | 0.5682 |
| 1196.1 | 0.6113 |
| 1226.4 | 0.6569 |
| 1238.6 | 0.6807 |
| 1252.6 | 0.7306 |
| 1249.5 | 0.7567 |
| 1245.3 | 0.7837 |
| 1221.3 | 0.8116 |
| 1191.5 | 0.8404 |
| 1139.7 | 0.8701 |
| 1064.2 | 0.9009 |
| 928.30 | 0.9328 |
| 791.70 | 0.9525 |
| 651.10 | 0.9658 |

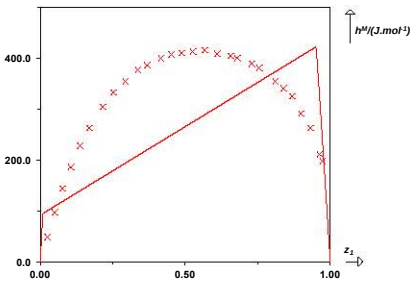
T/K = 253.15 - P/bar = 50.00



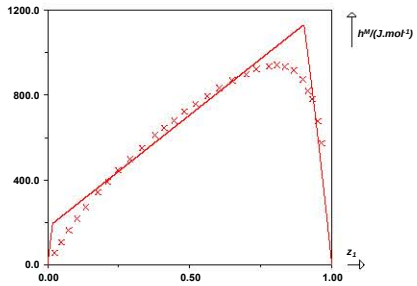

T/K = 283.15 - P/bar = 50.00



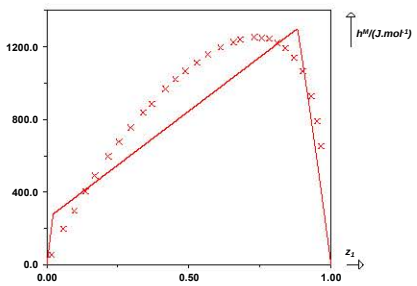

T/K = 298.15 - P/bar = 150.00



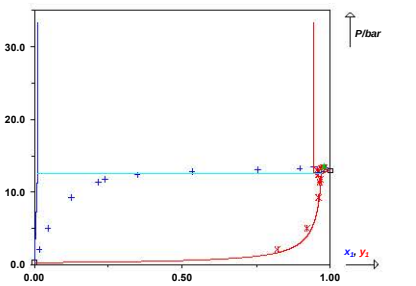

T/K = 348.15 - P/bar = 50.00



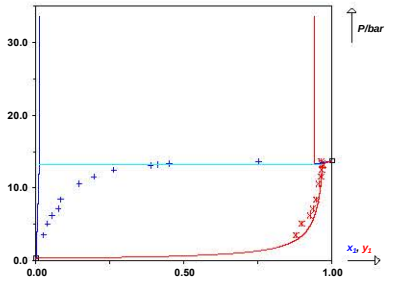

T/K = 363.15 - P/bar = 150.00



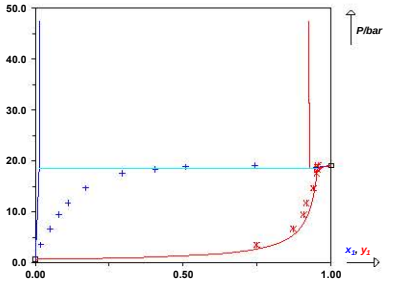

T/K = 310.70



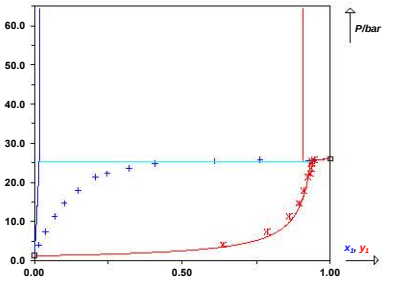

T/K = 313.10



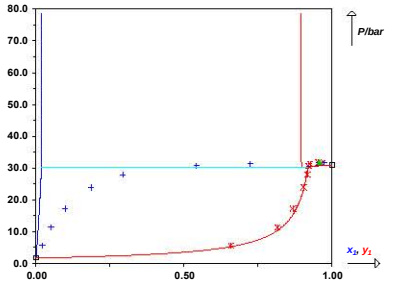

T/K = 327.95



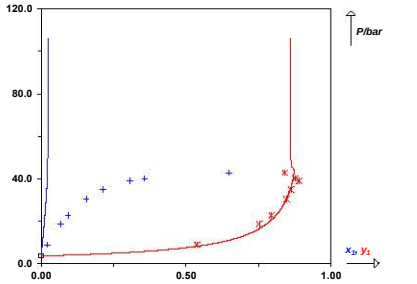

T/K = 343.21



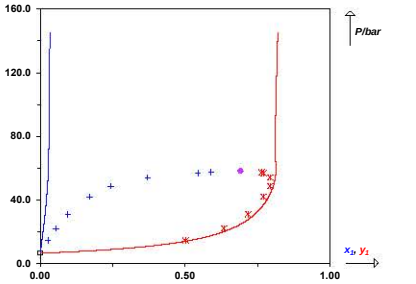

T/K = 352.20



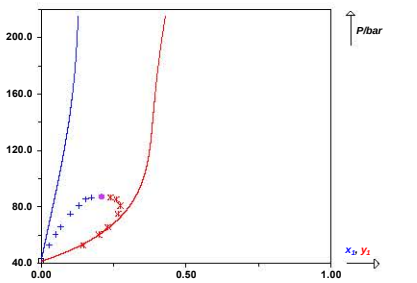

T/K = 373.10




T/K = 393.00




T/K = 474.30



## 1-PROPANOL (1) + BENZENE (2)

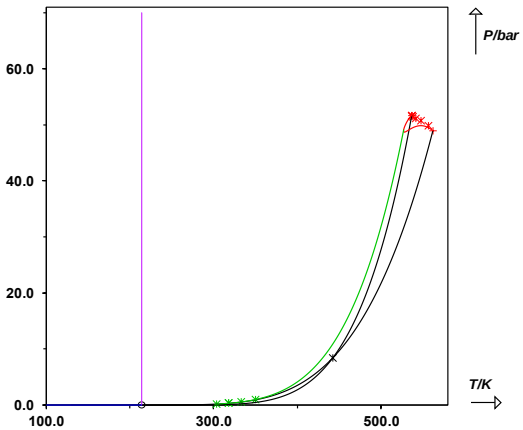
| | | |
|---|---|---|
| **CAS** | 71-23-8 | 71-43-2 |
| **InChiKey** | BDERNNFJNOPAEC-UHFFFAOYSA-N | UHOVQNZJYSORNB-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.80 | 562.05 |
| **$P_c$ / bar** | 51.69 | 48.95 |
| **ω** | 0.621 | 0.210 |

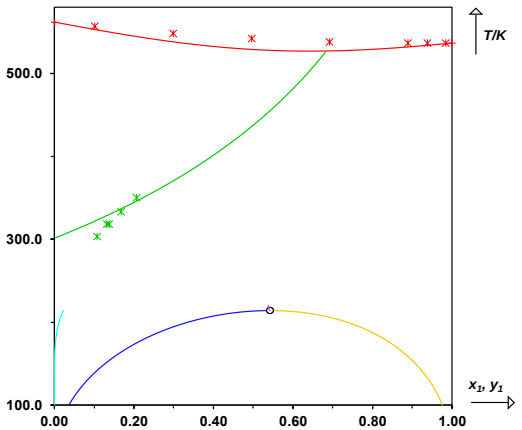
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 268
B/MPa = 202

*Deviations*
MAPE on x = 19 %
MAPE on y = 14 %
MAPE on $x_c$ = 50 %
MAPE on $P_c$ = 2.3 %
MAPE on $x_{az}$ = 15 %
MAPE on $P_{az}$ = 4.7 %
MAPE on $h^M$ = 30 %
MAPE on $c_P^M$ = 87 %



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**Isothermal phase equilibrium data**

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Udovenko, V.V. - Mazanko, T.F., Liquid-vapor equilibrium in propyl alcohol-water and propyl alcohol-benzene systems, Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol. 11 (1972) 1654-1658.

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1028 | 0.8664 | 0.3545 | |
| 0.1143 | 0.8088 | 0.2910 | |
| 0.1327 | 0.7161 | 0.2336 | |
| 0.1459 | 0.6232 | 0.1984 | |
| 0.1597 | 0.4538 | 0.1734 | |
| 0.1652 | 0.3246 | 0.1481 | |
| 0.1680 | 0.1866 | 0.1201 | |
| 0.1685 | 0.1070 | 0.1070 | AZEO |
| 0.1683 | 0.0804 | 0.0991 | |
| 0.1667 | 0.0425 | 0.0703 | |
| 0.1651 | 0.0194 | 0.0476 | |

Brown, I - Smith, F, Liquid-Vapour Equilibria. IX. The Systems n-Propanol + Benzene and n-Butanol + Benzene at 45°C, Australian Journal of Chemistry 3 (1959) doi:10.1071/CH9590407

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1628 | 0.9140 | 0.5252 | |
| 0.2267 | 0.7982 | 0.3437 | |
| 0.2595 | 0.7033 | 0.2790 | |
| 0.2814 | 0.6053 | 0.2402 | |
| 0.2939 | 0.5252 | 0.2185 | |
| 0.2988 | 0.4807 | 0.2080 | |
| 0.3060 | 0.4061 | 0.1935 | |
| 0.3132 | 0.2973 | 0.1728 | |
| 0.3167 | 0.2144 | 0.1560 | |
| 0.3186 | 0.1320 | 0.1320 | AZEO |
| 0.3178 | 0.0977 | 0.1194 | |
| 0.3137 | 0.0470 | 0.0843 | |

Udovenko, V.V. - Mazanko, T.F., Liquid-vapor equilibrium in propyl alcohol-water and propyl alcohol-benzene systems, Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol. 11 (1972) 1654-1658.

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1193 | 0.9752 | 0.7976 | |
| 0.1545 | 0.9293 | 0.5769 | |
| 0.2055 | 0.8429 | 0.3881 | |
| 0.2447 | 0.7520 | 0.2910 | |
| 0.2808 | 0.6137 | 0.2336 | |
| 0.3024 | 0.4642 | 0.2114 | |
| 0.3126 | 0.3555 | 0.1878 | |
| 0.3160 | 0.2648 | 0.1746 | |
| 0.3184 | 0.1866 | 0.1518 | |
| 0.3189 | 0.1457 | 0.1384 | |
| 0.3189 | 0.1370 | 0.1370 | AZEO |
| 0.3184 | 0.1015 | 0.1213 | |
| 0.3133 | 0.0476 | 0.0841 | |
| 0.3077 | 0.0258 | 0.0488 | |

Strubl, K. - Svoboda, V. - Holub, R. - Pick, J., Liquid-vapour equilibrium in the benzene-n-propanol system, Collection of Czechoslovak Chemical Communications 6 (1975) 1647-1656. doi:10.1135/cccc19751647

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1712 | 0.9895 | 0.9120 |
| 0.1956 | 0.9694 | 0.7831 |
| 0.2023 | 0.9635 | 0.7525 |
| 0.2185 | 0.9486 | 0.6866 |
| 0.2321 | 0.9352 | 0.6372 |
| 0.2560 | 0.9109 | 0.5652 |
| 0.2720 | 0.8929 | 0.5240 |
| 0.2885 | 0.8676 | 0.4796 |
| 0.3293 | 0.8140 | 0.4024 |
| 0.3369 | 0.8050 | 0.3873 |
| 0.3576 | 0.7665 | 0.3587 |
| 0.3973 | 0.6659 | 0.2952 |
| 0.4242 | 0.5620 | 0.2596 |
| 0.4456 | 0.4499 | 0.2260 |
| 0.4633 | 0.3465 | 0.1990 |
| 0.4641 | 0.2557 | 0.1850 |
| 0.4697 | 0.1747 | 0.1690 |
| 0.4672 | 0.0896 | 0.1272 |
| 0.4636 | 0.0320 | 0.0710 |
| 0.4561 | 0.0079 | 0.0240 |

Kurihara, Kiyofumi - Uchiyama, Masanori - Kojima, Kazuo, Isothermal Vapor−Liquid Equilibria for Benzene + Cyclohexane + 1-Propanol and for Three Constituent Binary Systems, Journal of Chemical & Engineering Data 1 (1997) 149-154. doi:10.1021/je9602475

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2861 | 0.9430 | 0.6790 |
| 0.3616 | 0.8690 | 0.5070 |
| 0.3759 | 0.8560 | 0.4770 |
| 0.4303 | 0.7810 | 0.3910 |
| 0.4443 | 0.7580 | 0.3730 |

| | | | |
|---|---|---|---|
| 0.4592 | 0.7300 | 0.3520 | |
| 0.4723 | 0.6940 | 0.3340 | |
| 0.5056 | 0.6180 | 0.2940 | |
| 0.5091 | 0.6080 | 0.2870 | |
| 0.5241 | 0.5520 | 0.2700 | |
| 0.5275 | 0.5430 | 0.2660 | |
| 0.5353 | 0.4900 | 0.2540 | |
| 0.5471 | 0.4330 | 0.2390 | |
| 0.5496 | 0.4160 | 0.2340 | |
| 0.5519 | 0.3970 | 0.2300 | |
| 0.5546 | 0.3770 | 0.2250 | |
| 0.5583 | 0.3440 | 0.2180 | |
| 0.5622 | 0.3030 | 0.2070 | |
| 0.5655 | 0.2350 | 0.1910 | |
| 0.5661 | 0.2170 | 0.1860 | |
| 0.5668 | 0.1970 | 0.1800 | |
| 0.5670 | 0.1680 | 0.1680 | AZEO |
| 0.5667 | 0.1420 | 0.1570 | |
| 0.5662 | 0.1260 | 0.1510 | |
| 0.5652 | 0.1110 | 0.1430 | |
| 0.5637 | 0.0960 | 0.1340 | |
| 0.5628 | 0.0910 | 0.1300 | |
| 0.5624 | 0.0870 | 0.1270 | |
| 0.5613 | 0.0810 | 0.1220 | |
| 0.5596 | 0.0720 | 0.1150 | |
| 0.5591 | 0.0680 | 0.1110 | |
| 0.5584 | 0.0660 | 0.1100 | |
| 0.5543 | 0.0500 | 0.0940 | |

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**Isobaric phase equilibrium data**

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Strubl, K. - Svoboda, V. - Holub, R. - Pick, J., Liquid-vapour equilibrium in the benzene-n-propanol system, Collection of Czechoslovak Chemical Communications 6 (1975) 1647-1656. doi:10.1135/cccc19751647

**P / bar = 0.4533**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 348.06 | 0.9807 | 0.8908 |
| 345.20 | 0.9529 | 0.7683 |
| 343.34 | 0.9330 | 0.6951 |
| 341.45 | 0.9077 | 0.6194 |
| 338.08 | 0.8569 | 0.5036 |
| 334.55 | 0.7908 | 0.4024 |
| 332.28 | 0.7258 | 0.3363 |
| 331.07 | 0.6659 | 0.3054 |
| 329.86 | 0.5817 | 0.2607 |
| 328.69 | 0.4988 | 0.2305 |
| 328.37 | 0.4614 | 0.2192 |
| 327.82 | 0.3928 | 0.2014 |
| 327.36 | 0.3163 | 0.1906 |
| 327.16 | 0.2646 | 0.1703 |
| 327.12 | 0.0880 | 0.1229 |
| 327.44 | 0.0513 | 0.0984 |
| 328.05 | 0.0210 | 0.0542 |
| 328.65 | 0.0039 | 0.0160 |

Strubl, K. - Svoboda, V. - Holub, R. - Pick, J., Liquid-vapour equilibrium in the benzene-n-propanol system, Collection of Czechoslovak Chemical Communications 6 (1975) 1647-1656. doi:10.1135/cccc19751647

**P / bar = 0.6949**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 358.33 | 0.9799 | 0.9000 |
| 355.48 | 0.9474 | 0.7777 |
| 353.56 | 0.9261 | 0.7068 |
| 352.03 | 0.9000 | 0.6463 |
| 348.91 | 0.8474 | 0.5353 |
| 345.66 | 0.7826 | 0.4367 |
| 343.67 | 0.7134 | 0.3790 |
| 342.38 | 0.6633 | 0.3477 |
| 340.95 | 0.5724 | 0.2992 |
| 340.14 | 0.4943 | 0.2726 |
| 339.83 | 0.4522 | 0.2595 |
| 339.38 | 0.3918 | 0.2416 |
| 338.95 | 0.3110 | 0.2207 |
| 338.80 | 0.2401 | 0.1990 |
| 338.73 | 0.1707 | 0.1739 |
| 338.75 | 0.1410 | 0.1568 |
| 338.97 | 0.0807 | 0.1289 |
| 339.53 | 0.0522 | 0.0930 |
| 340.18 | 0.0200 | 0.0524 |
| 340.93 | 0.0058 | 0.0160 |

Hiaki, Toshihiko - Tochigi, Katsumi - Kojima, Kazuo, Measurement of vapor-liquid equilibria and determination of azeotropic point, Fluid Phase Equilibria 1 (1986) 83-102. doi:10.1016/0378-3812(86)85006-3

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 361.87 | 0.8960 | 0.6600 |
| 357.02 | 0.7840 | 0.4860 |
| 355.46 | 0.7330 | 0.4370 |
| 353.00 | 0.6300 | 0.3680 |
| 351.69 | 0.5210 | 0.3110 |
| 350.78 | 0.4330 | 0.2750 |
| 350.76 | 0.4190 | 0.2690 |
| 350.66 | 0.3960 | 0.2650 |

| | | |
|---|---|---|
| 350.47 | 0.3580 | 0.2520 |
| 350.36 | 0.3370 | 0.2440 |
| 350.30 | 0.3170 | 0.2360 |
| 350.20 | 0.2960 | 0.2300 |
| 350.11 | 0.2470 | 0.2170 |
| 350.07 | 0.2320 | 0.2140 |
| 350.07 | 0.2130 | 0.2090 |
| 350.06 | 0.2030 | 0.2050 |
| 350.07 | 0.2000 | 0.2040 |
| 350.09 | 0.1940 | 0.2020 |
| 350.14 | 0.1350 | 0.1800 |
| 350.47 | 0.1010 | 0.1570 |
| 351.74 | 0.0310 | 0.0700 |

Shouyu Wang - Chenpu Zao, VLE data for benzene-n-propanol-lithium chloride system, Huaxue Gongcheng 2 (1991) 72-76.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 366.15 | 0.9580 | 0.8140 |
| 362.05 | 0.9030 | 0.6770 |
| 358.95 | 0.8500 | 0.5610 |
| 357.05 | 0.8020 | 0.4940 |
| 353.95 | 0.7020 | 0.3940 |
| 352.35 | 0.5840 | 0.3300 |
| 351.15 | 0.4820 | 0.2930 |
| 350.45 | 0.3620 | 0.2590 |
| 350.25 | 0.2830 | 0.2340 |
| 350.05 | 0.1900 | 0.2000 |
| 350.25 | 0.1400 | 0.1740 |
| 350.45 | 0.0830 | 0.1300 |
| 351.35 | 0.0500 | 0.0990 |

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**Enthalpy of mixing**

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Cen, P. - Zhu, Z., The Measurement of Mixing Heat and the Prediction of Vapor-Liquid Equilibrium Data for Hydrocarbon - Alcohol Systems, Huagong Xuebao 1 (1984) 51-65.

**T / K = 288.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 72.50 | 0.9639 |
| 152.00 | 0.9217 |
| 254.00 | 0.8643 |
| 370.00 | 0.8059 |
| 488.40 | 0.7464 |
| 585.00 | 0.6851 |
| 683.60 | 0.6229 |
| 756.40 | 0.5592 |
| 802.80 | 0.4669 |
| 833.50 | 0.4277 |
| 858.80 | 0.3599 |
| 839.30 | 0.2903 |
| 799.60 | 0.2194 |
| 584.10 | 0.0910 |
| 331.90 | 0.0344 |

Chao, J.P. - Dai, M., Studies on thermodynamic properties of binary systems containing alcohols. VII. Temperature dependence of excess enthalpies for n-propanol + benzene an, Thermochimica Acta (1988) 285-291. doi:10.1016/0040-6031(88)80032-7

**T / K = 293.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 145.10 | 0.9312 |
| 241.60 | 0.8891 |
| 332.50 | 0.8463 |
| 417.20 | 0.8028 |
| 502.50 | 0.7587 |
| 589.90 | 0.7138 |
| 669.40 | 0.6682 |
| 743.60 | 0.6218 |
| 808.90 | 0.5747 |
| 869.90 | 0.5268 |
| 906.80 | 0.4945 |
| 934.50 | 0.4617 |
| 958.40 | 0.4286 |
| 971.50 | 0.3951 |
| 977.70 | 0.3612 |
| 976.30 | 0.3270 |
| 966.40 | 0.2923 |
| 947.20 | 0.2573 |
| 914.90 | 0.2218 |
| 868.60 | 0.1859 |
| 808.80 | 0.1496 |
| 722.80 | 0.1129 |
| 602.50 | 0.0757 |

Chao, J.P. - Dai, M., Studies on thermodynamic properties of binary systems containing alcohols. VII. Temperature dependence of excess enthalpies for n-propanol + benzene an, Thermochimica Acta (1988) 285-291. doi:10.1016/0040-6031(88)80032-7

**T / K = 303.15**

**P / bar = UNKNOWN (1.0132)**

$h^M$ / J.mol$^{-1}$ $x_1$

| | |
|---|---|
| 178.20 | 0.9312 |
| 294.00 | 0.8891 |
| 397.50 | 0.8463 |
| 494.00 | 0.8028 |
| 597.70 | 0.7587 |
| 691.20 | 0.7138 |
| 793.70 | 0.6682 |
| 873.20 | 0.6218 |
| 953.20 | 0.5747 |
| 1015.2 | 0.5268 |
| 1045.1 | 0.4945 |
| 1075.7 | 0.4617 |
| 1100.1 | 0.4286 |
| 1115.2 | 0.3951 |
| 1126.6 | 0.3612 |
| 1124.1 | 0.3270 |
| 1111.1 | 0.2923 |
| 1084.0 | 0.2573 |
| 1047.5 | 0.2218 |
| 992.90 | 0.1859 |
| 917.00 | 0.1496 |
| 818.50 | 0.1129 |
| 676.20 | 0.0757 |

Chao, J.P. - Dai, M., Studies on thermodynamic properties of binary systems containing alcohols. VII. Temperature dependence of excess enthalpies for n-propanol + benzene an, Thermochimica Acta (1988) 285-291. doi:10.1016/0040-6031(88)80032-7

**T / K = 313.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 215.30 | 0.9312 |
| 344.80 | 0.8891 |
| 473.80 | 0.8463 |
| 600.10 | 0.8028 |
| 721.50 | 0.7587 |
| 833.70 | 0.7138 |
| 937.70 | 0.6682 |
| 1030.4 | 0.6218 |
| 1115.9 | 0.5747 |
| 1187.3 | 0.5268 |
| 1219.3 | 0.4945 |
| 1255.7 | 0.4617 |
| 1265.9 | 0.4286 |
| 1276.1 | 0.3951 |
| 1276.8 | 0.3612 |
| 1263.6 | 0.3270 |
| 1238.7 | 0.2923 |
| 1204.2 | 0.2573 |
| 1147.7 | 0.2218 |
| 1082.2 | 0.1859 |
| 986.60 | 0.1496 |
| 880.30 | 0.1129 |
| 710.20 | 0.0757 |

Chao, J.P. - Dai, M., Studies on thermodynamic properties of binary systems containing alcohols. VII. Temperature dependence of excess enthalpies for n-propanol + benzene an, Thermochimica Acta (1988) 285-291. doi:10.1016/0040-6031(88)80032-7

**T / K = 323.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 263.10 | 0.9312 |
| 422.60 | 0.8891 |
| 571.00 | 0.8463 |
| 721.70 | 0.8028 |
| 859.20 | 0.7587 |
| 983.10 | 0.7138 |
| 1093.0 | 0.6682 |
| 1195.1 | 0.6218 |
| 1282.7 | 0.5747 |
| 1352.2 | 0.5268 |
| 1386.0 | 0.4945 |
| 1410.3 | 0.4617 |
| 1427.6 | 0.4286 |
| 1433.0 | 0.3951 |
| 1426.4 | 0.3612 |
| 1410.3 | 0.3270 |
| 1381.0 | 0.2923 |
| 1336.4 | 0.2573 |
| 1273.4 | 0.2218 |
| 1193.7 | 0.1859 |
| 1087.4 | 0.1496 |
| 951.10 | 0.1129 |
| 776.50 | 0.0757 |

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**Heat capacity of mixing**

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Recko, W.M., Excess heat capacity of the binary systems formed by n-propyl alcohol with benzene, mesitylene, and cyclohexane, Bull. Acad. Pol. Sci. Ser. Sci. Chim. 10 (1968) 549-552.

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|

| | |
|---|---|
| 9.800 | 0.8123 |
| 11.00 | 0.6602 |
| 14.20 | 0.5012 |
| 14.80 | 0.3570 |
| 13.10 | 0.2100 |

Recko, W.M., Excess heat capacity of the binary systems formed by n-propyl alcohol with benzene, mesitylene, and cyclohexane, Bull. Acad. Pol. Sci. Ser. Sci. Chim. 10 (1968) 549-552.

**T / K =** **303.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / $J.mol^{-1}.K^{-1}$ | $x_1$ |
|---|---|
| 10.30 | 0.8123 |
| 12.20 | 0.6602 |
| 15.20 | 0.5012 |
| 15.80 | 0.3570 |
| 13.60 | 0.2100 |

Recko, W.M., Excess heat capacity of the binary systems formed by n-propyl alcohol with benzene, mesitylene, and cyclohexane, Bull. Acad. Pol. Sci. Ser. Sci. Chim. 10 (1968) 549-552.

**T / K =** **308.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / $J.mol^{-1}.K^{-1}$ | $x_1$ |
|---|---|
| 11.00 | 0.8123 |
| 12.60 | 0.6602 |
| 15.50 | 0.5012 |
| 16.00 | 0.3570 |
| 13.60 | 0.2100 |

Recko, W.M., Excess heat capacity of the binary systems formed by n-propyl alcohol with benzene, mesitylene, and cyclohexane, Bull. Acad. Pol. Sci. Ser. Sci. Chim. 10 (1968) 549-552.

**T / K =** **313.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / $J.mol^{-1}.K^{-1}$ | $x_1$ |
|---|---|
| 11.80 | 0.8123 |
| 12.20 | 0.6602 |
| 15.20 | 0.5012 |
| 15.40 | 0.3570 |
| 13.20 | 0.2100 |

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**Critical point**

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Skaates, J.M. - Kay, W.B., The phase relations of binary systems that form azeotropes, Chemical Engineering Science 7 (1964) 431-444. doi:10.1016/0009-2509(64)85070-3

| T / K | P / bar | $x_1$ |
|---|---|---|
| 556.71 | 49.86 | 0.1010 |
| 548.07 | 50.72 | 0.2984 |
| 541.79 | 51.10 | 0.4963 |
| 537.90 | 51.39 | 0.6912 |
| 536.60 | 51.57 | 0.8894 |
| 536.57 | 51.69 | 0.9381 |
| 536.62 | 51.61 | 0.9848 |

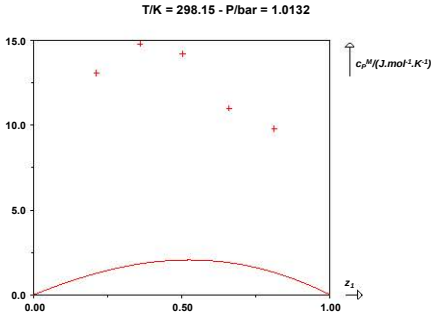
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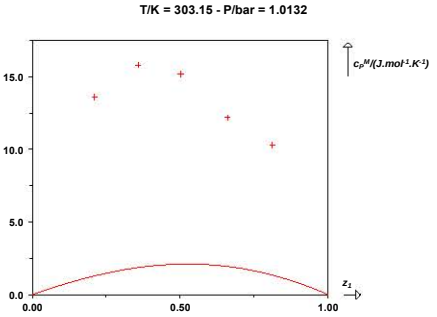
**Azeotropic point**

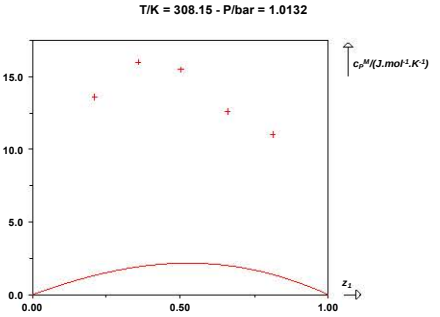
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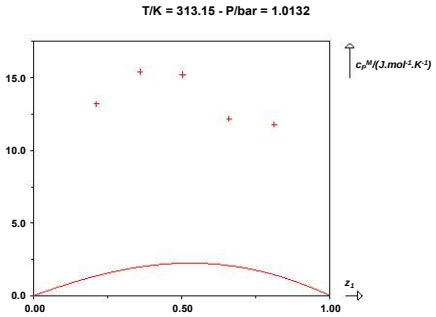
Hiaki, Toshihiko - Tochigi, Katsumi - Kojima, Kazuo, Measurement of vapor-liquid equilibria and determination of azeotropic point, Fluid Phase Equilibria 1 (1986) 83-102. doi:10.1016/0378-3812(86)85006-3

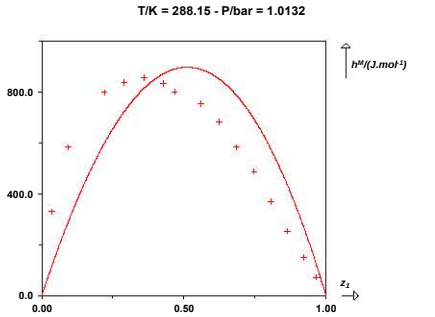
| T / K | P / bar | $x_1$ |
|---|---|---|
| 350.05 | 1.013 | 0.2060 |

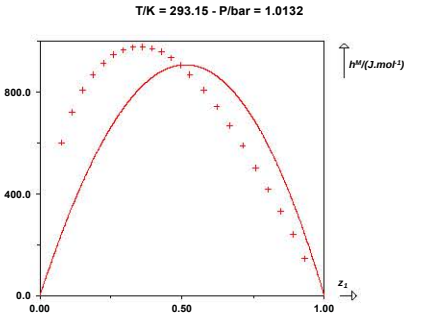

T/K = 298.15 - P/bar = 1.0132
$c_p^M/(J.mol^{-1}.K^{-1})$
$z_1$

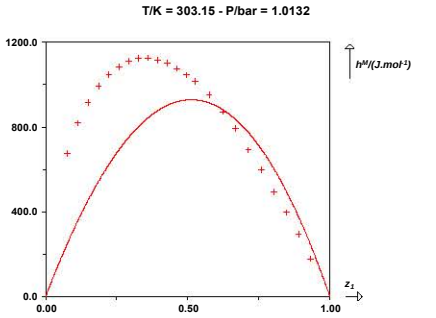

T/K = 303.15 - P/bar = 1.0132
$c_p^M/(J.mol^{-1}.K^{-1})$
$z_1$

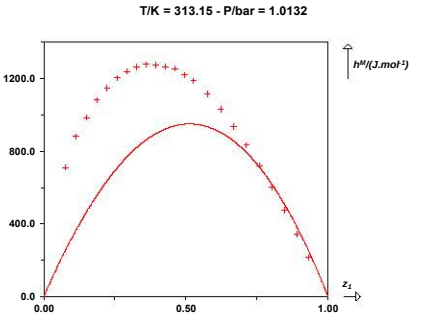

T/K = 308.15 - P/bar = 1.0132
$c_p^M/(J.mol^{-1}.K^{-1})$
$z_1$

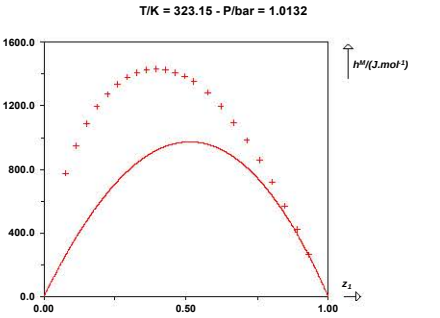

T/K = 313.15 - P/bar = 1.0132
$c_p^M/(J.mol^{-1}.K^{-1})$
$z_1$

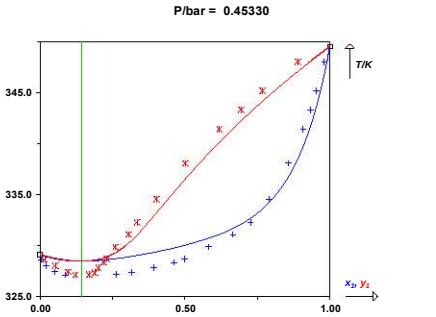

T/K = 288.15 - P/bar = 1.0132
$h^M/(J.mol^{-1})$
$z_1$

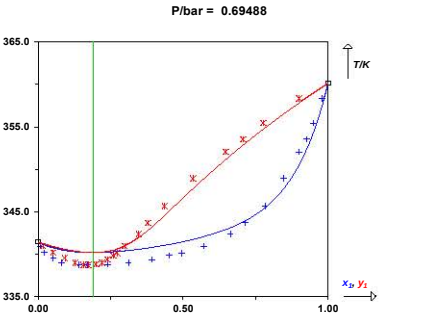

T/K = 293.15 - P/bar = 1.0132
$h^M/(J.mol^{-1})$
$z_1$

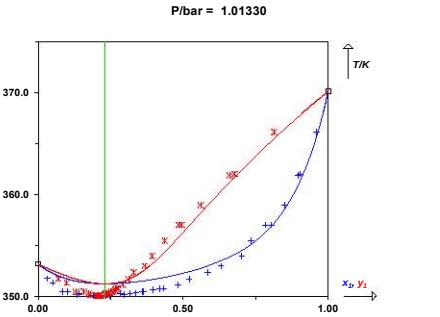

T/K = 303.15 - P/bar = 1.0132
$h^M/(J.mol^{-1})$
$z_1$

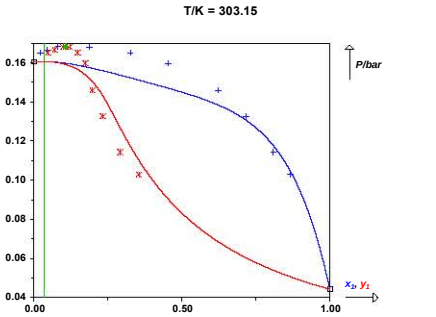

T/K = 313.15 - P/bar = 1.0132
$h^M/(J.mol^{-1})$
$z_1$

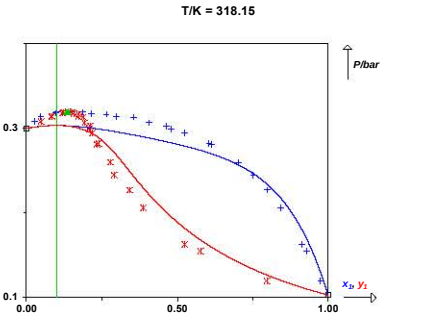

T/K = 323.15 - P/bar = 1.0132
$h^M/(J.mol^{-1})$
$z_1$

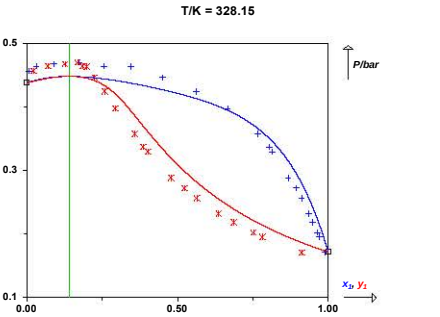

P/bar = 0.45330
T/K
$x_1, y_1$


P/bar = 0.69488
T/K
$x_1, y_1$

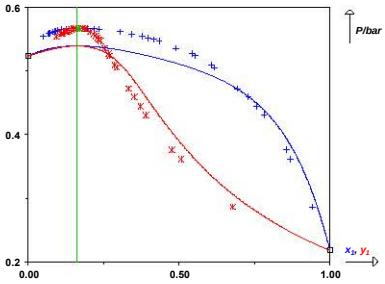

P/bar = 1.01330
T/K
$x_1, y_1$


T/K = 303.15
P/bar
$x_1, y_1$

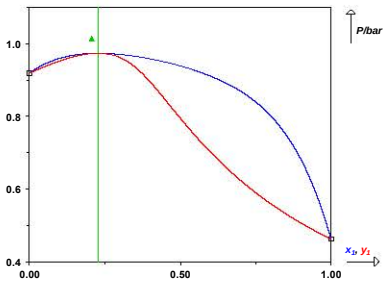

T/K = 318.15
P/bar
$x_1, y_1$


T/K = 328.15
P/bar
$x_1, y_1$

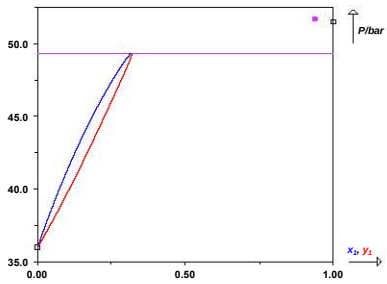
T/K = 333.15



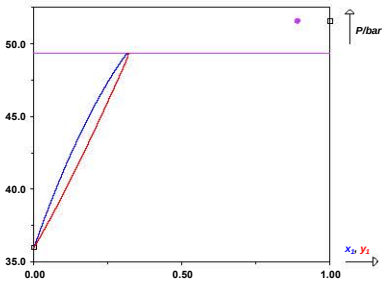

T/K = 350.05



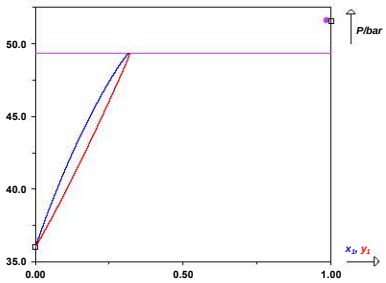

T/K = 536.57



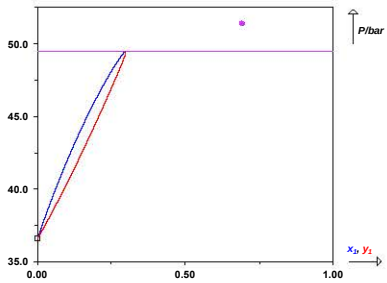

T/K = 536.60



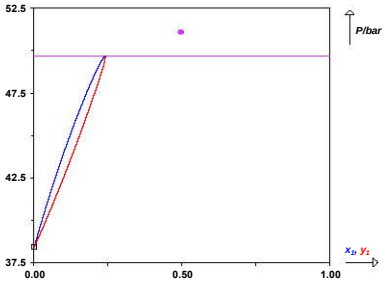

T/K = 536.62



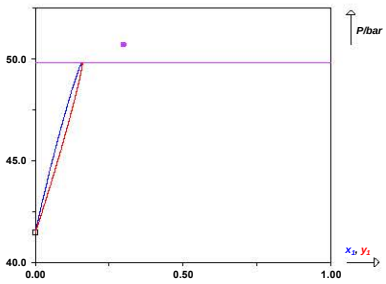

T/K = 537.90



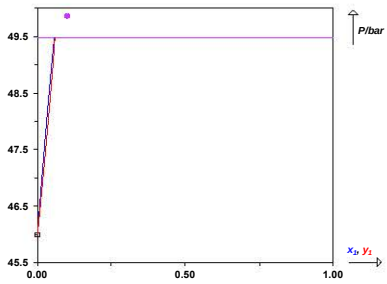

T/K = 541.79




T/K = 548.07




T/K = 556.71



## ETHANOL (1) + BENZENE (2)

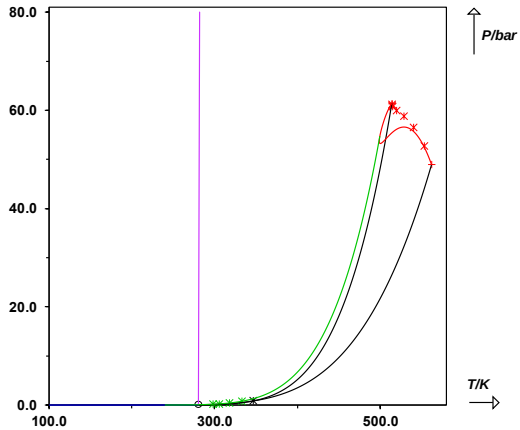
| | | |
|---|---|---|
| **CAS** | 64-17-5 | 71-43-2 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | UHOVQNZJYSORNB-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 562.05 |
| **$P_c$ / bar** | 61.37 | 48.95 |
| **ω** | 0.644 | 0.210 |

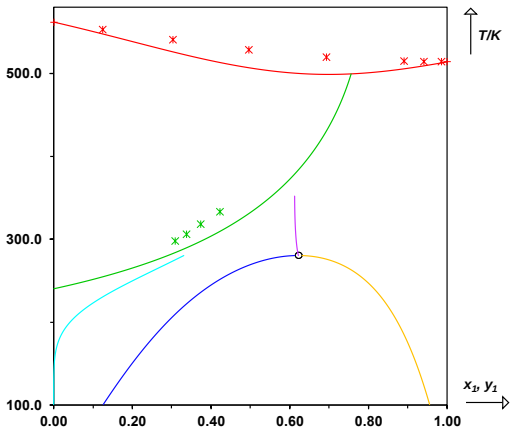
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 401
B/MPa = 112

*Deviations*
MAPE on x = 34 %
MAPE on y = 12 %
MAPE on $x_c$ = 430 %
MAPE on $P_c$ = 5.7 %
MAPE on $x_{az}$ = 19 %
MAPE on $P_{az}$ = 1.8 %
MAPE on $h^M$ = 50 %
MAPE on $c_P^M$ = 110 %



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**Isothermal phase equilibrium data**

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Iguchi, A., Vapor-liquid equilibriums at 25°C for binary systems between alcohols and hydrocarbons, Kagaku Sochi 3 (1978) 66-68.

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1605 | 0.1000 | 0.2490 | |
| 0.1640 | 0.2000 | 0.2830 | |
| 0.1647 | 0.3000 | 0.3100 | |
| 0.1647 | 0.3090 | 0.3090 | AZEO |
| 0.1643 | 0.4000 | 0.3360 | |
| 0.1627 | 0.5000 | 0.3570 | |
| 0.1597 | 0.6000 | 0.3800 | |
| 0.1533 | 0.7000 | 0.4190 | |
| 0.1432 | 0.8000 | 0.4740 | |
| 0.1237 | 0.9000 | 0.5830 | |

Smith, Vinson C. - Robinson, Robert Louis, Vapor-Liquid Equilibria at 25°C in the Binary Mixtures Formed by Hexane, Benzene, and Ethanol, Journal of Chemical & Engineering Data 3 (1970) 391-395. doi:10.1021/je60046a005

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1616 | 0.1000 | 0.2600 |
| 0.1660 | 0.2000 | 0.3000 |
| 0.1665 | 0.3000 | 0.3120 |
| 0.1659 | 0.4000 | 0.3280 |
| 0.1647 | 0.5000 | 0.3420 |
| 0.1611 | 0.6000 | 0.3680 |
| 0.1543 | 0.7000 | 0.4060 |
| 0.1420 | 0.8000 | 0.4700 |
| 0.1193 | 0.9000 | 0.6030 |

Tamir, Abraham - Apelblat, Alexander - Wagner, Moshe, A new device for measuring isothermal vapor - liquid equilibria, Fluid Phase Equilibria 3-4 (1981) 237-259. doi:10.1016/0378-3812(81)85007-8

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.3522 | 0.0240 | 0.1250 | |
| 0.3950 | 0.0940 | 0.2650 | |
| 0.4113 | 0.2400 | 0.3450 | |
| 0.4129 | 0.3200 | 0.3560 | |
| 0.4134 | 0.3730 | 0.3730 | AZEO |
| 0.4125 | 0.4200 | 0.3780 | |
| 0.4080 | 0.5460 | 0.4150 | |
| 0.3962 | 0.6650 | 0.4510 | |
| 0.3813 | 0.7370 | 0.4850 | |
| 0.3400 | 0.8470 | 0.5850 | |
| 0.2557 | 0.9760 | 0.9100 | |

Zharov, V.T. - Morachevskii, A.G., Liquid-vapor equilibrium in the ethyl alcohol-benzene system and the verification of the thermodynamic data, Zh. Prikl. Khim 11 (1963) 2397-2402.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4140 | 0.0210 | 0.1360 |
| 0.4453 | 0.0480 | 0.2090 |
| 0.4746 | 0.0850 | 0.2730 |
| 0.4973 | 0.1550 | 0.3260 |
| 0.5046 | 0.2010 | 0.3430 |
| 0.5113 | 0.5000 | 0.4210 |
| 0.5026 | 0.5940 | 0.4480 |
| 0.4853 | 0.7000 | 0.4870 |
| 0.4546 | 0.8010 | 0.5570 |
| 0.4346 | 0.8450 | 0.6040 |
| 0.3973 | 0.9000 | 0.6860 |
| 0.3533 | 0.9490 | 0.8000 |

Fu, H. - Mo, X. - Han, S. - Li, H., Study on Isothermal Vapor-Liquid Equilibrium for Ethanol - Benzene, Chloroform - Benzene and Ethanol - Chloroform Binary Systems, Shiyou Xuebao Shiyou Jiagong 1 (1995) 87-92.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4426 | 0.0013 | 0.0166 |
| 0.5597 | 0.0775 | 0.2677 |
| 0.6015 | 0.1849 | 0.3449 |
| 0.6127 | 0.2731 | 0.3610 |
| 0.6169 | 0.2897 | 0.3804 |
| 0.6202 | 0.4842 | 0.4305 |
| 0.6132 | 0.5976 | 0.4529 |
| 0.6092 | 0.5997 | 0.4659 |
| 0.5930 | 0.7000 | 0.4954 |
| 0.5756 | 0.7624 | 0.5343 |
| 0.5583 | 0.8080 | 0.5687 |
| 0.5146 | 0.8791 | 0.6490 |
| 0.4903 | 0.9023 | 0.6940 |
| 0.4668 | 0.9277 | 0.7471 |
| 0.4184 | 0.9695 | 0.8608 |
| 0.3748 | 0.9973 | 0.9899 |
| 0.3737 | 0.9976 | 0.9940 |

Fu, H. - Mo, X. - Han, S. - Li, H., Study on Isothermal Vapor-Liquid Equilibrium for Ethanol - Benzene,

Chloroform - Benzene and Ethanol - Chloroform Binary Systems, Shiyou Xuebao Shiyou Jiagong 1 (1995) 87-92.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5696 | 0.0144 | 0.0969 |
| 0.6791 | 0.0786 | 0.2712 |
| 0.7069 | 0.1144 | 0.3100 |
| 0.7334 | 0.1866 | 0.3522 |
| 0.7469 | 0.2496 | 0.3747 |
| 0.7542 | 0.3691 | 0.4032 |
| 0.7534 | 0.4110 | 0.4114 |
| 0.7508 | 0.5105 | 0.4426 |
| 0.7320 | 0.6531 | 0.4880 |
| 0.7070 | 0.7401 | 0.5372 |
| 0.6871 | 0.7866 | 0.5680 |
| 0.6320 | 0.8697 | 0.6600 |
| 0.6089 | 0.8986 | 0.6960 |
| 0.5755 | 0.9272 | 0.7638 |
| 0.5577 | 0.9413 | 0.7963 |
| 0.4923 | 0.9858 | 0.9387 |
| 0.4802 | 0.9927 | 0.9675 |

Udovenko, V.V. - Fatkulina, L.G., Vapor pressure of three-component systems. I. The system ethyl alcohol-1,2-dichloroethane-benzene, Zh. Fiz. Khim. 5 (1952) 719-730.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.6036 | 0.0260 | 0.1610 | |
| 0.6909 | 0.0800 | 0.3100 | |
| 0.7382 | 0.1850 | 0.3750 | |
| 0.7533 | 0.3220 | 0.4080 | |
| 0.7573 | 0.3980 | 0.4200 | |
| 0.7575 | 0.4230 | 0.4230 | AZEO |
| 0.7554 | 0.4840 | 0.4360 | |
| 0.7501 | 0.5680 | 0.4550 | |
| 0.7315 | 0.6800 | 0.4900 | |
| 0.6989 | 0.7710 | 0.5370 | |
| 0.6466 | 0.8590 | 0.6250 | |
| 0.5754 | 0.9290 | 0.7470 | |
| 0.5032 | 0.9810 | 0.9040 | |

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**Isobaric phase equilibrium data**

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Nielsen, R. L. - Weber, J. H., Vapor-Liquid Equilibria at Subatmospheric Pressures. Binary and Ternary Systems Containing Ethyl Alcohol, Benzene, and n-Heptane., Journal of Chemical & Engineering Data 2 (1959) 145-151. doi:10.1021/je60002a011

**P / bar = 0.2400**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 306.75 | 0.1000 | 0.2770 |
| 305.95 | 0.2000 | 0.3140 |
| 305.75 | 0.4000 | 0.3490 |
| 306.05 | 0.5000 | 0.3700 |
| 306.45 | 0.6000 | 0.3990 |
| 307.15 | 0.7000 | 0.4340 |
| 308.65 | 0.8000 | 0.5000 |
| 312.45 | 0.9000 | 0.6520 |

Zharov, V.T. - Morachevskii, A.G., Liquid-vapor equilibrium in the ethyl alcohol-benzene system and the verification of the thermodynamic data, Zh. Prikl. Khim 11 (1963) 2397-2402.

**P / bar = 0.5999**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 328.15 | 0.1550 | 0.3340 |
| 327.25 | 0.3000 | 0.3900 |
| 327.35 | 0.5000 | 0.4300 |
| 328.55 | 0.7000 | 0.5070 |
| 331.15 | 0.8450 | 0.6250 |

Zharov, V.T. - Morachevskii, A.G., Liquid-vapor equilibrium in the ethyl alcohol-benzene system and the verification of the thermodynamic data, Zh. Prikl. Khim 11 (1963) 2397-2402.

**P / bar = 0.7999**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 335.85 | 0.1550 | 0.3450 |
| 334.75 | 0.3000 | 0.4010 |
| 334.77 | 0.5000 | 0.4490 |
| 335.85 | 0.7000 | 0.5260 |
| 338.50 | 0.8450 | 0.6520 |

Kao, Chien-Ping Chai - Miller, Ralph N. - Sturgis, James F., Double Azeotropy in Binary Mixtures 1,1,1,2,3,4,4,5,5,5-Decafluoropentane + Tetrahydrofuran, Journal of Chemical & Engineering Data 2 (2001) 229-233. doi:10.1021/je000212b

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 352.25 | 0.0029 | 0.0256 |
| 349.79 | 0.0177 | 0.1070 |
| 347.31 | 0.0440 | 0.1837 |
| 343.65 | 0.1061 | 0.2973 |
| 341.64 | 0.2124 | 0.3720 |
| 340.97 | 0.3661 | 0.4252 |
| 340.92 | 0.4641 | 0.4511 |

| | | |
|---|---|---|
| 340.97 | 0.5666 | 0.4836 |
| 341.26 | 0.6394 | 0.5091 |
| 342.34 | 0.7536 | 0.5753 |
| 343.52 | 0.8095 | 0.6216 |
| 346.33 | 0.9111 | 0.7555 |
| 348.53 | 0.9570 | 0.8639 |
| 349.42 | 0.9729 | 0.9053 |
| 350.76 | 0.9907 | 0.9714 |

Kao, Chien-Ping Chai - Miller, Ralph N. - Sturgis, James F., Double Azeotropy in Binary Mixtures 1,1,1,2,3,4,4,5,5,5-Decafluoropentane + Tetrahydrofuran, Journal of Chemical & Engineering Data 2 (2001) 229-233. doi:10.1021/je000212b

**P / bar = 3.025**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 389.39 | 0.0256 | 0.0922 |
| 386.85 | 0.0495 | 0.1447 |
| 383.66 | 0.0800 | 0.2170 |
| 379.53 | 0.1427 | 0.3340 |
| 375.93 | 0.2845 | 0.4434 |
| 375.15 | 0.3501 | 0.4747 |
| 374.56 | 0.4434 | 0.5091 |
| 374.30 | 0.5551 | 0.5587 |
| 374.44 | 0.6312 | 0.5932 |
| 375.38 | 0.7686 | 0.6764 |

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**Enthalpy of mixing**

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Cen, P. - Zhu, Z., The Measurement of Mixing Heat and the Prediction of Vapor-Liquid Equilibrium Data for Hydrocarbon - Alcohol Systems, Huagong Xuebao 1 (1984) 51-65.

**T / K = 283.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 387.70 | 0.0616 |
| 499.70 | 0.1304 |
| 569.50 | 0.2006 |
| 602.60 | 0.2629 |
| 609.70 | 0.3225 |
| 600.60 | 0.3794 |
| 570.20 | 0.4361 |
| 525.90 | 0.5033 |
| 482.20 | 0.5688 |
| 426.30 | 0.6319 |
| 366.20 | 0.6900 |
| 307.30 | 0.7460 |
| 254.50 | 0.7862 |
| 210.30 | 0.8350 |
| 163.00 | 0.8625 |
| 75.40 | 0.9356 |

Stokes, R.H. - Burfitt, Carol, Enthalpies of dilution and transfer of ethanol in non-polar solvents, The Journal of Chemical Thermodynamics 5 (1973) 623-631. doi:10.1016/S0021-9614(73)80003-5

**T / K = 283.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 5.401 | 0.0003 |
| 10.70 | 0.0007 |
| 15.77 | 0.0010 |
| 20.84 | 0.0013 |
| 25.70 | 0.0017 |
| 30.53 | 0.0020 |
| 39.81 | 0.0026 |
| 48.71 | 0.0032 |
| 57.20 | 0.0038 |
| 65.29 | 0.0043 |
| 80.59 | 0.0054 |
| 94.55 | 0.0064 |
| 107.25 | 0.0074 |
| 115.81 | 0.0082 |
| 119.13 | 0.0083 |
| 129.78 | 0.0091 |
| 189.33 | 0.0146 |
| 241.80 | 0.0204 |
| 310.09 | 0.0304 |
| 361.92 | 0.0402 |

Cen, P. - Zhu, Z., The Measurement of Mixing Heat and the Prediction of Vapor-Liquid Equilibrium Data for Hydrocarbon - Alcohol Systems, Huagong Xuebao 1 (1984) 51-65.

**T / K = 288.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 427.80 | 0.0616 |
| 572.80 | 0.1304 |
| 650.70 | 0.2006 |
| 693.10 | 0.2629 |
| 706.60 | 0.3225 |
| 701.70 | 0.3794 |
| 661.00 | 0.4361 |
| 606.10 | 0.5033 |
| 556.10 | 0.5688 |
| 490.40 | 0.6319 |
| 422.60 | 0.6900 |

| | |
|---|---|
| 349.60 | 0.7460 |
| 295.40 | 0.7862 |
| 238.10 | 0.8350 |
| 193.20 | 0.8625 |
| 89.10 | 0.9356 |

Zhao, J. - Dai, M., Studies on Thermodynamic Properties of Binary Systems containing Alcohols. I. Excess Enthalpies of C1 to C5 Normal Alcohols + Benzene, Wuli Huaxue Xuebao 2 (1986) 141-145.

**T / K =** **298.15**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 703.50 | 0.0889 |
| 773.50 | 0.1144 |
| 851.40 | 0.1630 |
| 875.90 | 0.1869 |
| 887.00 | 0.2103 |
| 900.70 | 0.2560 |
| 901.40 | 0.2782 |
| 901.40 | 0.3001 |
| 897.70 | 0.3217 |
| 883.70 | 0.3637 |
| 857.90 | 0.4044 |
| 831.90 | 0.4438 |
| 782.40 | 0.5006 |
| 728.10 | 0.5549 |
| 664.50 | 0.6068 |
| 598.10 | 0.6565 |
| 526.70 | 0.7041 |
| 459.40 | 0.7497 |
| 389.20 | 0.7935 |
| 320.50 | 0.8355 |
| 250.20 | 0.8759 |
| 179.60 | 0.9148 |

Yan, Wei-Dong - Lin, Rui-Sen - Yen, Wen-Hsing, Excess enthalpies of seven binary liquid systems, Thermochimica Acta (1990) 171-184. doi:10.1016/0040-6031(90)80143-M

**T / K =** **303.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 228.85 | 0.0110 |
| 641.20 | 0.0793 |
| 841.36 | 0.1618 |
| 906.66 | 0.2349 |
| 927.63 | 0.2961 |
| 919.71 | 0.3483 |
| 900.44 | 0.3954 |
| 875.32 | 0.4339 |
| 847.22 | 0.4677 |
| 702.66 | 0.6089 |
| 684.40 | 0.6213 |
| 654.28 | 0.6406 |
| 621.34 | 0.6606 |
| 579.55 | 0.6845 |
| 546.60 | 0.7058 |
| 502.31 | 0.7307 |
| 454.93 | 0.7576 |
| 402.34 | 0.7860 |
| 347.07 | 0.8155 |
| 280.57 | 0.8501 |
| 214.27 | 0.8840 |
| 144.04 | 0.9214 |
| 60.77 | 0.9650 |

Missopolinou, Doukeni - Tsivintzelis, Ioannis - Panayiotou, Costas, Excess enthalpies of binary mixtures of 2-ethoxyethanol with four hydrocarbons at 298.15, 308.15, and 318.15K, Fluid Phase Equilibria 2 (2006) 89-101. doi:10.1016/j.fluid.2006.04.016

**T / K =** **308.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 585.20 | 0.0640 |
| 771.40 | 0.1049 |
| 843.60 | 0.1248 |
| 868.20 | 0.1542 |
| 959.10 | 0.1828 |
| 1003.1 | 0.2381 |
| 1013.8 | 0.2908 |
| 1021.8 | 0.3413 |
| 1001.9 | 0.3895 |
| 958.20 | 0.4357 |
| 960.40 | 0.4357 |
| 958.10 | 0.4506 |
| 931.60 | 0.4799 |
| 871.70 | 0.5224 |
| 833.20 | 0.5631 |
| 769.30 | 0.6023 |
| 640.80 | 0.6761 |
| 519.70 | 0.7447 |
| 396.00 | 0.8084 |
| 277.10 | 0.8678 |

Stokes, R.H. - Burfitt, Carol, Enthalpies of dilution and transfer of ethanol in non-polar solvents, The Journal of Chemical Thermodynamics 5 (1973) 623-631. doi:10.1016/S0021-9614(73)80003-5

**T / K =** **318.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 6.418 | 0.0004 |
| 11.73 | 0.0008 |
| 17.02 | 0.0011 |
| 22.12 | 0.0014 |
| 27.05 | 0.0017 |
| 31.95 | 0.0021 |
| 42.27 | 0.0027 |
| 51.40 | 0.0033 |
| 68.68 | 0.0045 |
| 84.87 | 0.0056 |
| 99.80 | 0.0066 |
| 113.74 | 0.0075 |
| 124.51 | 0.0082 |
| 126.81 | 0.0084 |
| 139.01 | 0.0093 |
| 209.91 | 0.0144 |
| 288.14 | 0.0205 |
| 402.54 | 0.0306 |
| 496.62 | 0.0404 |

Missopolinou, Doukeni - Tsivintzelis, Ioannis - Panayiotou, Costas, Excess enthalpies of binary mixtures of 2-ethoxyethanol with four hydrocarbons at 298.15, 308.15, and 318.15K, Fluid Phase Equilibria 2 (2006) 89-101. doi:10.1016/j.fluid.2006.04.016

**T / K =** **318.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 628.50 | 0.0640 |
| 932.70 | 0.1248 |
| 1077.9 | 0.1828 |
| 1134.6 | 0.2381 |
| 1176.6 | 0.2908 |
| 1174.2 | 0.3413 |
| 1160.3 | 0.3895 |
| 1080.9 | 0.4799 |
| 967.40 | 0.5631 |
| 902.50 | 0.6023 |
| 771.90 | 0.6761 |
| 629.60 | 0.7447 |
| 484.10 | 0.8084 |
| 337.70 | 0.8678 |
| 185.20 | 0.9233 |

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**Heat capacity of mixing**

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Tamura, K. - Sonoda, T. - Murakami, S., Thermodynamic properties of aqueous solution of 2-isopropoxyethanol at 25 °C, J. Solution Chem. 6 (1999) 777-789. doi:10.1023/A:1021728430543

**T / K =** **293.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 12.28 | 0.1759 |
| 12.90 | 0.2977 |
| 12.50 | 0.4222 |
| 11.34 | 0.5229 |
| 9.000 | 0.6409 |
| 7.601 | 0.7178 |
| 6.040 | 0.7982 |
| 4.197 | 0.8755 |
| 3.917 | 0.9097 |

Tanaka, Reiji - Toyama, Satoru, Excess Molar Volumes and Excess Molar Heat Capacities for Binary Mixtures of (Ethanol + Benzene, or Toluene, or o-Xylene, or Chlorobenzene) at a Temperature of 298.15 K, Journal of Chemical & Engineering Data 5 (1997) 871-874. doi:10.1021/je9700479

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.0083 | 0.0021 |
| 0.0039 | 0.0041 |
| 0.0856 | 0.0060 |
| 0.1410 | 0.0076 |
| 0.2157 | 0.0092 |
| 0.3620 | 0.0117 |
| 1.640 | 0.0233 |
| 3.360 | 0.0355 |
| 3.950 | 0.0400 |
| 5.930 | 0.0573 |
| 7.590 | 0.0767 |
| 9.110 | 0.0996 |
| 10.59 | 0.1303 |
| 11.53 | 0.1557 |
| 13.97 | 0.2903 |
| 14.51 | 0.3659 |
| 13.80 | 0.4797 |
| 12.27 | 0.5826 |
| 9.770 | 0.6959 |
| 7.170 | 0.7891 |
| 3.600 | 0.8988 |

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**Critical point**

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Skaates, J.M. - Kay, W.B., The phase relations of binary systems that form azeotropes, Chemical Engineering Science 7 (1964) 431-444. doi:10.1016/0009-2509(64)85070-3

| T / K | P / bar | $x_1$ |
|---|---|---|
| 553.13 | 52.73 | 0.1250 |
| 540.46 | 56.49 | 0.3025 |
| 528.71 | 58.83 | 0.4954 |
| 519.55 | 59.93 | 0.6932 |
| 514.86 | 60.74 | 0.8900 |
| 514.31 | 60.94 | 0.9410 |
| 514.03 | 61.16 | 0.9860 |

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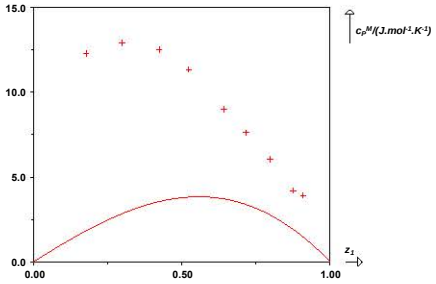
**Azeotropic point**

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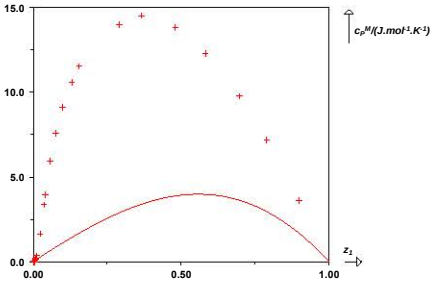
Nielsen, R. L. - Weber, J. H., Vapor-Liquid Equilibria at Subatmospheric Pressures. Binary and Ternary Systems Containing Ethyl Alcohol, Benzene, and n-Heptane., Journal of Chemical & Engineering Data 2 (1959) 145-151. doi:10.1021/je60002a011

| T / K | P / bar | $x_1$ |
|---|---|---|
| 305.65 | 0.2400 | 0.3380 |

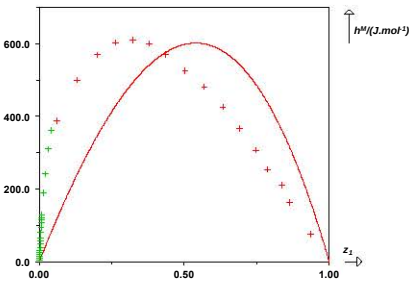
T/K = 293.15 - P/bar = 1.0132



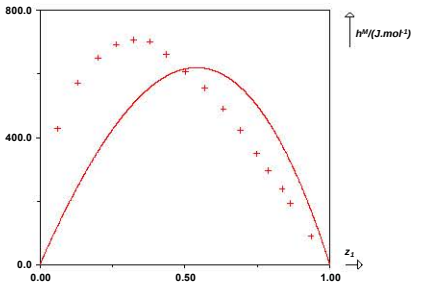

T/K = 298.15 - P/bar = 1.0132



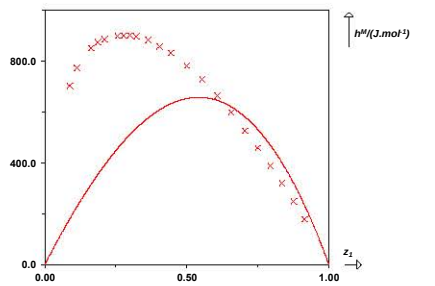

T/K = 283.15 - P/bar = 1.0132 1.0132



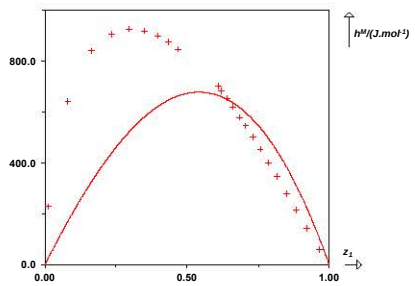

T/K = 288.15 - P/bar = 1.0132



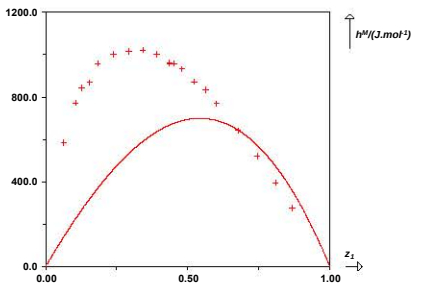

T/K = 298.15 - P/bar = 1.0132



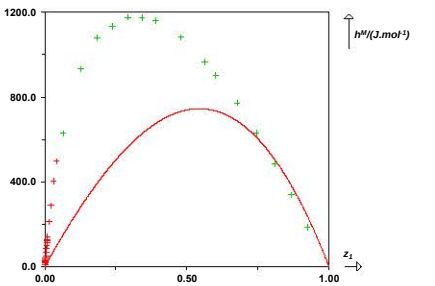

T/K = 303.15 - P/bar = 1.0132



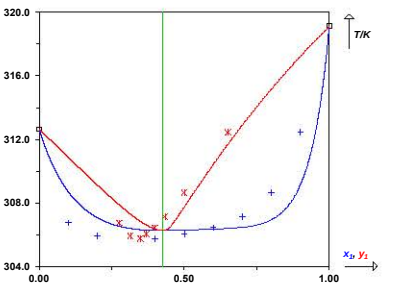

T/K = 308.15 - P/bar = 1.0132



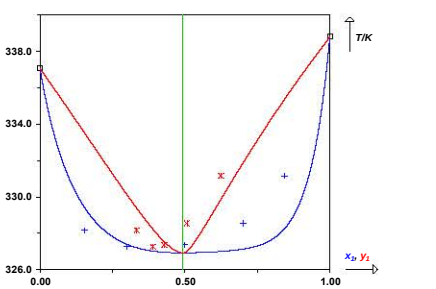

T/K = 318.15 - P/bar = 1.0132 1.0132



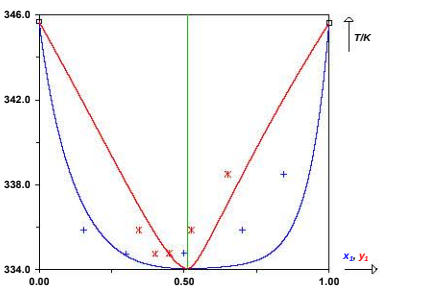

P/bar = 0.23998



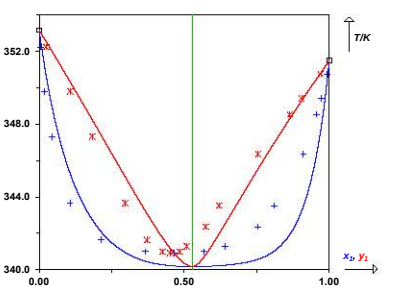

P/bar = 0.59995



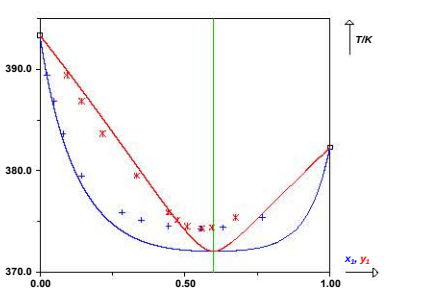

P/bar = 0.79993



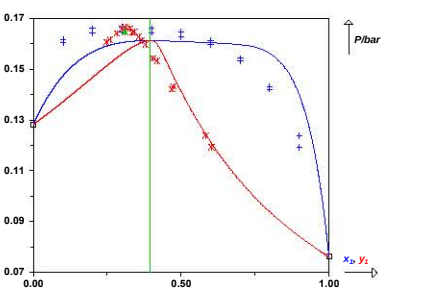

P/bar = 1.01300



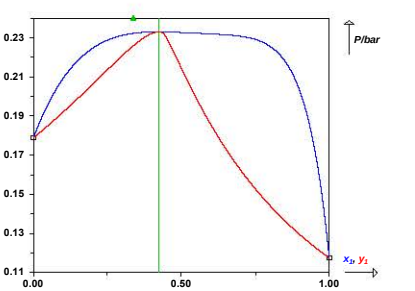

P/bar = 3.02500



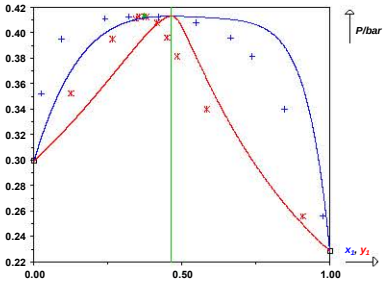

T/K = 298.15



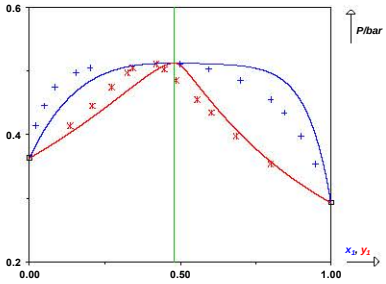

T/K = 305.65



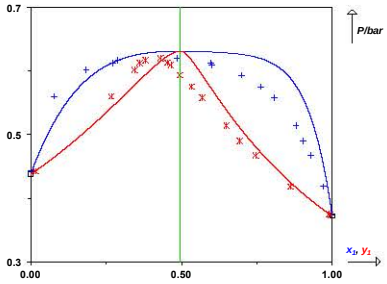
T/K = 318.15



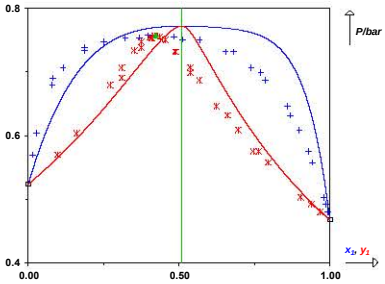

T/K = 323.15



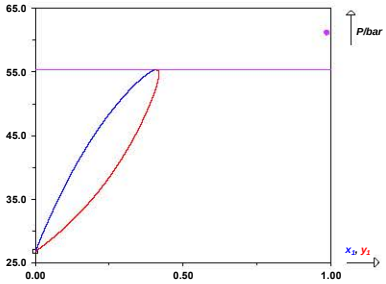

T/K = 328.15



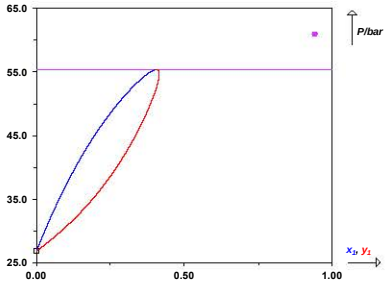

T/K = 333.15



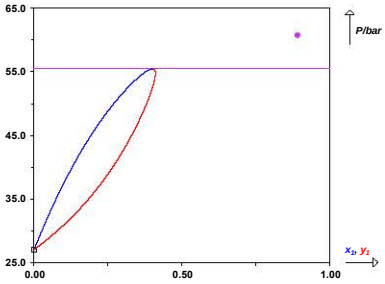

T/K = 514.03



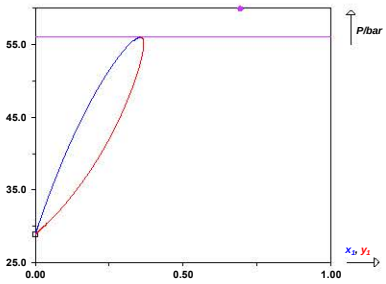

T/K = 514.31



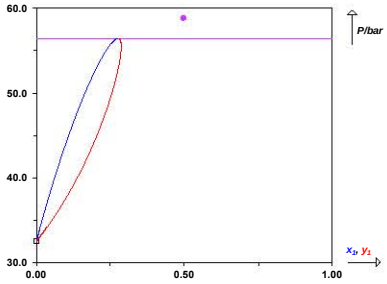

T/K = 514.86



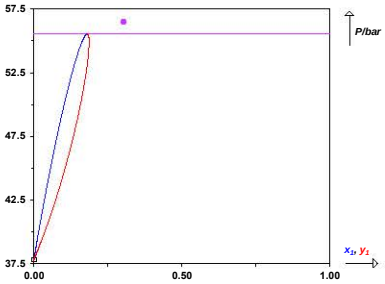

T/K = 519.55



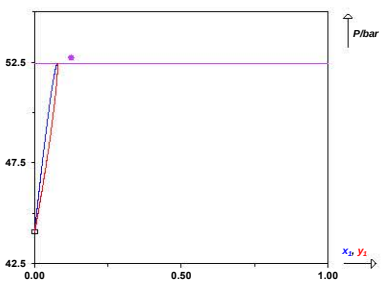

T/K = 528.71




T/K = 540.46




T/K = 553.13



## ISOPROPANOL (1) + 2,2,4-TRIMETHYLPENTANE (2)

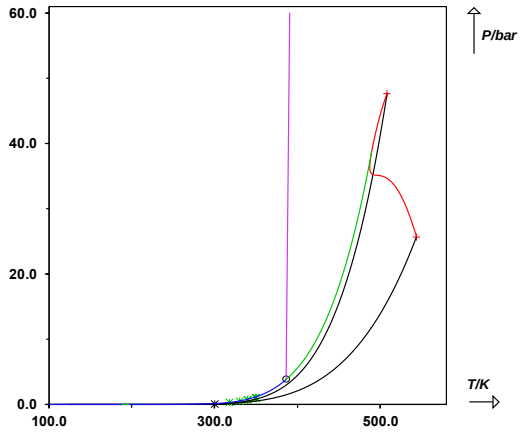
| | | |
|---|---|---|
| **CAS** | 67-63-0 | 540-84-1 |
| **InChiKey** | KFZMGEQAYNKOFK-UHFFFAOYSA-N | NHTMVDHEPJAVLT-UHFFFAOYSA-N |
| **$T_c$ / K** | 508.30 | 543.80 |
| **$P_c$ / bar** | 47.65 | 25.70 |
| **ω** | 0.663 | 0.303 |

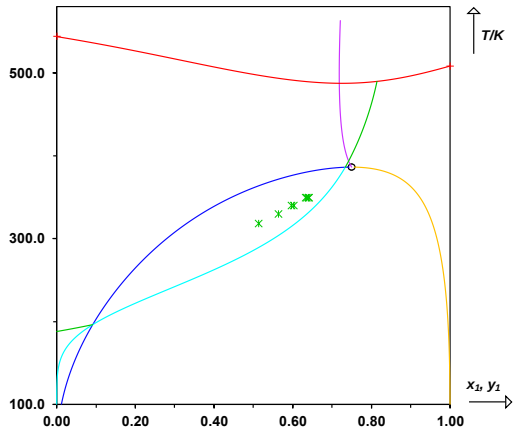
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 375
B/MPa = 259

*Deviations*
MAPE on x = 45 %
MAPE on y = 15 %
MAPE on $h^M$ = 29 %



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**Isothermal phase equilibrium data**

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Neau, Evelyne - Blanc, Claude - Bares, Daniel, Les fonctions thermodynamiques d'excès du binaire 2 propanol-isooctane, Journal de Chimie Physique (1973) 843-849. doi:10.1051/jcp/1973700843

**T / K = 318.10**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2061 | 0.0180 | 0.2270 | |
| 0.2290 | 0.0430 | 0.3130 | |
| 0.2554 | 0.1400 | 0.4000 | |
| 0.2557 | 0.1520 | 0.4060 | |
| 0.2717 | 0.3328 | 0.4810 | |
| 0.2756 | 0.4150 | 0.4950 | |
| 0.2766 | 0.4920 | 0.5090 | |
| 0.2761 | 0.5125 | 0.5125 | AZEO |
| 0.2761 | 0.5140 | 0.5130 | |
| 0.2748 | 0.6200 | 0.5370 | |
| 0.2734 | 0.6580 | 0.5470 | |
| 0.2730 | 0.6660 | 0.5540 | |
| 0.2716 | 0.7030 | 0.5600 | |
| 0.2694 | 0.7300 | 0.5790 | |
| 0.2661 | 0.7740 | 0.5890 | |
| 0.2525 | 0.8540 | 0.6540 | |
| 0.2492 | 0.8740 | 0.6700 | |
| 0.2401 | 0.9020 | 0.7070 | |
| 0.2336 | 0.9220 | 0.7330 | |
| 0.2161 | 0.9550 | 0.8110 | |

Zhang, Lianzhong - Han, Jianzhi - Wang, Rongjie - Qiu, Xingying - Ji, Jianbing, Isobaric Vapor−Liquid Equilibria for Three Ternary Systems: Water + 2-Propanol + 1-Ethyl-3-methylimidazolium Tetrafluoroborate, Water + 1-Propanol + 1-Ethyl-3-methylimidazolium Tetrafluoroborate, and Water + 1-Propanol + 1-Butyl-3-methylimidazolium Tetrafluoroborate, Journal of Chemical & Engineering Data 4 (2007) 1401-1407. doi:10.1021/je700092d

**T / K = 330.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2817 | 0.0066 | 0.1004 |
| 0.3415 | 0.0259 | 0.2692 |
| 0.3982 | 0.0797 | 0.3897 |
| 0.4320 | 0.1739 | 0.4458 |
| 0.4496 | 0.2737 | 0.4834 |
| 0.4593 | 0.3859 | 0.5189 |
| 0.4595 | 0.7036 | 0.6005 |
| 0.4496 | 0.7922 | 0.6336 |
| 0.4321 | 0.8649 | 0.6921 |
| 0.4314 | 0.8665 | 0.6944 |
| 0.4158 | 0.9051 | 0.7387 |
| 0.3973 | 0.9365 | 0.7871 |
| 0.3779 | 0.9586 | 0.8465 |
| 0.3608 | 0.9754 | 0.8953 |
| 0.3463 | 0.9883 | 0.9397 |
| 0.3362 | 0.9958 | 0.9799 |

Wichterle, I., Isothermal vapor-liquid equilibria in the ternary system propan-2-ol + diisopropyl ether + 2,2,4-trimethylpentane and the three binary subsystems at 330 K and 340 K, ELDATA Int. Electron. J. Phys. Chem. Data 4 (1999) 179-189.

**T / K = 330.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.3261 | 0.0142 | 0.2363 | |
| 0.3937 | 0.0673 | 0.3826 | |
| 0.4121 | 0.0994 | 0.4139 | |
| 0.4317 | 0.1585 | 0.4508 | |
| 0.4391 | 0.1924 | 0.4652 | |
| 0.4504 | 0.2640 | 0.4901 | |
| 0.4567 | 0.3257 | 0.5074 | |
| 0.4614 | 0.3810 | 0.5213 | |
| 0.4642 | 0.4346 | 0.5335 | |
| 0.4654 | 0.4863 | 0.5456 | |
| 0.4664 | 0.5630 | 0.5630 | AZEO |
| 0.4664 | 0.5699 | 0.5643 | |
| 0.4657 | 0.6144 | 0.5744 | |
| 0.4652 | 0.6559 | 0.5853 | |
| 0.4599 | 0.7327 | 0.6111 | |
| 0.4401 | 0.8472 | 0.6768 | |
| 0.4297 | 0.8770 | 0.7054 | |
| 0.4182 | 0.9036 | 0.7372 | |
| 0.4036 | 0.9288 | 0.7760 | |
| 0.3910 | 0.9465 | 0.8128 | |
| 0.3768 | 0.9623 | 0.8587 | |
| 0.3613 | 0.9789 | 0.9033 | |
| 0.3463 | 0.9907 | 0.9529 | |
| 0.3373 | 0.9977 | 0.9840 | |

Zhang, Lianzhong - Han, Jianzhi - Wang, Rongjie - Qiu, Xingying - Ji, Jianbing, Isobaric Vapor−Liquid Equilibria for Three Ternary Systems: Water + 2-Propanol + 1-Ethyl-3-methylimidazolium Tetrafluoroborate, Water + 1-Propanol + 1-Ethyl-3-methylimidazolium Tetrafluoroborate, and Water + 1-Propanol + 1-Butyl-3-methylimidazolium Tetrafluoroborate, Journal of Chemical & Engineering Data 4 (2007) 1401-1407. doi:10.1021/je700092d

**T / K = 340.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4057 | 0.0080 | 0.1065 |

| | | | |
|---|---|---|---|
| 0.5792 | 0.0873 | 0.3920 | |
| 0.6375 | 0.1646 | 0.4641 | |
| 0.6679 | 0.2636 | 0.5048 | |
| 0.6863 | 0.3782 | 0.5358 | |
| 0.6953 | 0.4823 | 0.5642 | |
| 0.6984 | 0.5955 | 0.5963 | |
| 0.6984 | 0.5967 | 0.5967 | AZEO |
| 0.6952 | 0.6949 | 0.6224 | |
| 0.6843 | 0.7882 | 0.6624 | |
| 0.6422 | 0.8960 | 0.7543 | |
| 0.6185 | 0.9299 | 0.7998 | |
| 0.5936 | 0.9510 | 0.8537 | |
| 0.5697 | 0.9721 | 0.9054 | |
| 0.5495 | 0.9860 | 0.9498 | |
| 0.5346 | 0.9956 | 0.9804 | |

Wichterle, I., Isothermal vapor-liquid equilibria in the ternary system propan-2-ol + diisopropyl ether + 2,2, 4-trimethylpentane and the three binary subsystems at 330 K and 340 K, ELDATA Int. Electron. J. Phys. Chem. Data 4 (1999) 179-189.

**T / K = 340.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.5866 | 0.0808 | 0.4087 | |
| 0.6104 | 0.1113 | 0.4372 | |
| 0.6411 | 0.1706 | 0.4741 | |
| 0.6524 | 0.2012 | 0.4881 | |
| 0.6707 | 0.2698 | 0.5172 | |
| 0.6823 | 0.3281 | 0.5368 | |
| 0.6895 | 0.3796 | 0.5552 | |
| 0.6958 | 0.4338 | 0.5586 | |
| 0.6989 | 0.4830 | 0.5714 | |
| 0.7014 | 0.5297 | 0.5822 | |
| 0.7023 | 0.5628 | 0.5912 | |
| 0.7026 | 0.6020 | 0.6020 | AZEO |
| 0.7027 | 0.6054 | 0.6011 | |
| 0.7018 | 0.6447 | 0.6150 | |
| 0.7003 | 0.6852 | 0.6243 | |
| 0.6616 | 0.8662 | 0.7193 | |
| 0.6482 | 0.8937 | 0.7522 | |
| 0.6314 | 0.9179 | 0.7835 | |
| 0.6142 | 0.9383 | 0.8199 | |
| 0.5950 | 0.9567 | 0.8600 | |
| 0.5510 | 0.9892 | 0.9528 | |

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**Isobaric phase equilibrium data**

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Lin, Dun-Yi - Tu, Chein-Hsiun, (Vapour+liquid) equilibria for binary and ternary mixtures of 2-propanol, tetrahydropyran, and 2,2,4-trimethylpentane at P=101.3kPa, The Journal of Chemical Thermodynamics (2012) 260-266. doi:10.1016/j.jct.2011.10.025

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 361.23 | 0.0530 | 0.3100 |
| 358.96 | 0.0730 | 0.3600 |
| 356.86 | 0.0980 | 0.4160 |
| 354.77 | 0.1380 | 0.4680 |
| 353.35 | 0.1750 | 0.4990 |
| 351.80 | 0.2460 | 0.5490 |
| 350.57 | 0.3660 | 0.5810 |
| 350.23 | 0.4320 | 0.5970 |
| 349.99 | 0.5210 | 0.6090 |
| 349.96 | 0.5330 | 0.6130 |
| 349.93 | 0.5490 | 0.6170 |
| 349.65 | 0.6080 | 0.6270 |
| 349.69 | 0.6400 | 0.6340 |
| 349.85 | 0.6930 | 0.6480 |
| 349.95 | 0.7350 | 0.6680 |
| 350.17 | 0.7870 | 0.6920 |
| 350.39 | 0.8050 | 0.7150 |
| 351.74 | 0.9110 | 0.7930 |
| 353.17 | 0.9530 | 0.8750 |

Hiaki, Toshihiko - Takahashi, Kenji - Tsuji, Tomoya - Hongo, Masaru - Kojima, Kazuo, Vapor-Liquid Equilibria of 1-Propanol or 2-Propanol with 2,2,4-Trimethylpentane at 101.3 kPa, Journal of Chemical & Engineering Data 3 (1994) 602-604. doi:10.1021/je00015a047

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 357.85 | 0.0737 | 0.3824 |
| 354.74 | 0.1209 | 0.4529 |
| 353.44 | 0.1573 | 0.4847 |
| 352.09 | 0.2155 | 0.5135 |
| 351.64 | 0.2393 | 0.5234 |
| 351.12 | 0.2900 | 0.5479 |
| 350.54 | 0.3575 | 0.5685 |
| 350.04 | 0.4553 | 0.5910 |
| 349.80 | 0.4953 | 0.5994 |
| 349.75 | 0.5370 | 0.6039 |
| 349.58 | 0.5994 | 0.6226 |
| 349.63 | 0.6518 | 0.6415 |
| 349.74 | 0.6913 | 0.6538 |
| 349.81 | 0.7311 | 0.6632 |

| | | |
|---|---|---|
| 349.90 | 0.7651 | 0.6773 |
| 350.10 | 0.7970 | 0.6981 |
| 350.54 | 0.8444 | 0.7358 |
| 351.52 | 0.9010 | 0.7999 |
| 352.84 | 0.9469 | 0.8725 |

Huang, Tzu-Te - Tu, Chein-Hsiun, Vapor–Liquid Equilibria for Binary and Ternary Mixtures of 1,3-Dioxolane, 2-Propanol, and 2,2,4-Trimethylpentane at 101.3 kPa, Journal of Chemical & Engineering Data 1 (2010) 513-518. doi:10.1021/je900327x

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 360.65 | 0.0580 | 0.3190 |
| 358.30 | 0.0810 | 0.3820 |
| 356.27 | 0.1050 | 0.4230 |
| 354.65 | 0.1320 | 0.4570 |
| 353.44 | 0.1670 | 0.4850 |
| 352.14 | 0.2320 | 0.5270 |
| 350.80 | 0.3530 | 0.5650 |
| 350.27 | 0.4120 | 0.5800 |
| 350.06 | 0.5140 | 0.6060 |
| 349.99 | 0.5230 | 0.6120 |
| 349.94 | 0.5450 | 0.6140 |
| 349.47 | 0.6130 | 0.6280 |
| 349.67 | 0.6370 | 0.6390 |
| 349.73 | 0.6840 | 0.6530 |
| 349.82 | 0.7280 | 0.6600 |
| 350.00 | 0.7800 | 0.6820 |
| 350.31 | 0.8160 | 0.7020 |
| 351.36 | 0.8940 | 0.7940 |
| 352.94 | 0.9460 | 0.8780 |

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**Enthalpy of mixing**

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Heintz, A., The Pressure Dependence of the Excess Enthalpy of Mixtures of Isopropanol with Heptane and Isooctane up to 553 bar, Berichte der Bunsengesellschaft für physikalische Chemie 9 (1981) 632-635. doi:10.1002/bbpc.19810850905

**T / K = 298.15**

**P / bar = 1.0000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 678.00 | 0.1640 |
| 807.00 | 0.3010 |
| 819.00 | 0.4180 |
| 778.00 | 0.5190 |
| 727.00 | 0.5900 |
| 708.00 | 0.6060 |
| 620.00 | 0.6830 |
| 522.00 | 0.7510 |
| 507.00 | 0.7640 |
| 424.00 | 0.8120 |
| 314.00 | 0.8660 |
| 208.00 | 0.9150 |
| 103.00 | 0.9600 |

Heintz, A., The Pressure Dependence of the Excess Enthalpy of Mixtures of Isopropanol with Heptane and Isooctane up to 553 bar, Berichte der Bunsengesellschaft für physikalische Chemie 9 (1981) 632-635. doi:10.1002/bbpc.19810850905

**T / K = 298.15**

**P / bar = 42.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 669.00 | 0.1640 |
| 791.00 | 0.3010 |
| 811.00 | 0.4180 |
| 765.00 | 0.5190 |
| 714.00 | 0.5900 |
| 693.00 | 0.6060 |
| 607.00 | 0.6830 |
| 511.00 | 0.7510 |
| 494.00 | 0.7640 |
| 412.00 | 0.8120 |
| 308.00 | 0.8660 |
| 203.00 | 0.9150 |
| 101.00 | 0.9600 |

Heintz, A., The Pressure Dependence of the Excess Enthalpy of Mixtures of Isopropanol with Heptane and Isooctane up to 553 bar, Berichte der Bunsengesellschaft für physikalische Chemie 9 (1981) 632-635. doi:10.1002/bbpc.19810850905

**T / K = 298.15**

**P / bar = 196.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 640.00 | 0.1620 |
| 751.00 | 0.2990 |
| 758.00 | 0.4160 |
| 716.00 | 0.5170 |
| 678.00 | 0.5880 |
| 652.00 | 0.6050 |
| 576.00 | 0.6820 |
| 488.00 | 0.7500 |
| 467.00 | 0.7630 |
| 385.00 | 0.8110 |
| 292.00 | 0.8660 |
| 189.00 | 0.9150 |

| | |
|---|---|
| 88.00 | 0.9600 |

Heintz, A., The Pressure Dependence of the Excess Enthalpy of Mixtures of Isopropanol with Heptane and Isooctane up to 553 bar, Berichte der Bunsengesellschaft für physikalische Chemie 9 (1981) 632-635. doi:10.1002/bbpc.19810850905

**T / K = 298.15**

**P / bar = 361.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 608.00 | 0.1600 |
| 718.00 | 0.2980 |
| 720.00 | 0.4150 |
| 674.00 | 0.5160 |
| 637.00 | 0.5870 |
| 609.00 | 0.6040 |
| 543.00 | 0.6810 |
| 453.00 | 0.7500 |
| 437.00 | 0.7630 |
| 368.00 | 0.8110 |
| 275.00 | 0.8660 |
| 176.00 | 0.9150 |
| 83.00 | 0.9600 |

Heintz, A., The Pressure Dependence of the Excess Enthalpy of Mixtures of Isopropanol with Heptane and Isooctane up to 553 bar, Berichte der Bunsengesellschaft für physikalische Chemie 9 (1981) 632-635. doi:10.1002/bbpc.19810850905

**T / K = 298.15**

**P / bar = 542.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 582.00 | 0.1560 |
| 673.00 | 0.2950 |
| 677.00 | 0.4130 |
| 639.00 | 0.5140 |
| 596.00 | 0.5860 |
| 570.00 | 0.6030 |
| 507.00 | 0.6810 |
| 424.00 | 0.7500 |
| 411.00 | 0.7630 |
| 337.00 | 0.8110 |
| 253.00 | 0.8660 |
| 161.00 | 0.9160 |
| 70.00 | 0.9610 |

Neau, Evelyne - Blanc, Claude - Bares, Daniel, Les fonctions thermodynamiques d'excès du binaire 2 propanol-isooctane, Journal de Chimie Physique (1973) 843-849. doi:10.1051/jcp/1973700843

**T / K = 318.14**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 239.90 | 0.0116 |
| 319.87 | 0.0165 |
| 405.70 | 0.0228 |
| 644.35 | 0.0502 |
| 711.34 | 0.0610 |
| 771.21 | 0.0792 |
| 869.18 | 0.1058 |
| 962.55 | 0.1425 |
| 1033.3 | 0.1768 |
| 1067.2 | 0.2066 |
| 1129.2 | 0.2406 |
| 1145.1 | 0.2574 |
| 1135.9 | 0.2815 |
| 1188.6 | 0.3049 |
| 1168.5 | 0.3252 |
| 1202.9 | 0.3589 |
| 1213.8 | 0.3805 |
| 1225.1 | 0.4018 |
| 1213.3 | 0.4564 |
| 1192.8 | 0.4927 |
| 1201.2 | 0.5061 |
| 1165.6 | 0.5460 |
| 1164.3 | 0.5478 |
| 1099.5 | 0.5767 |
| 1073.1 | 0.5921 |
| 1055.1 | 0.5970 |
| 1057.2 | 0.6086 |
| 1048.0 | 0.6476 |
| 1003.6 | 0.6482 |
| 998.13 | 0.6548 |
| 920.68 | 0.6914 |
| 904.35 | 0.7013 |
| 757.81 | 0.7680 |
| 679.52 | 0.7992 |
| 484.83 | 0.8640 |
| 344.99 | 0.9066 |
| 195.94 | 0.9483 |

Neau, Evelyne - Blanc, Claude - Bares, Daniel, Les fonctions thermodynamiques d'excès du binaire 2 propanol-isooctane, Journal de Chimie Physique (1973) 843-849. doi:10.1051/jcp/1973700843

**T / K = 338.10**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 216.88 | 0.0102 |
| 276.75 | 0.0135 |

| | |
|---|---|
| 282.61 | 0.0136 |
| 458.45 | 0.0236 |
| 473.11 | 0.0244 |
| 736.04 | 0.0493 |
| 978.46 | 0.0753 |
| 1158.1 | 0.1055 |
| 1288.3 | 0.1440 |
| 1395.0 | 0.1771 |
| 1501.0 | 0.2145 |
| 1506.4 | 0.2424 |
| 1554.6 | 0.2591 |
| 1568.0 | 0.2778 |
| 1592.7 | 0.3036 |
| 1611.5 | 0.3374 |
| 1613.6 | 0.3713 |
| 1620.7 | 0.4112 |
| 1609.8 | 0.4214 |
| 1596.8 | 0.4554 |
| 1573.8 | 0.5028 |
| 1550.0 | 0.5460 |
| 1446.1 | 0.6013 |
| 1353.6 | 0.6529 |
| 1187.4 | 0.7105 |
| 1015.3 | 0.7637 |
| 910.63 | 0.7912 |
| 667.38 | 0.8592 |
| 460.55 | 0.9091 |
| 278.84 | 0.9472 |
| 254.98 | 0.9515 |

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**Azeotropic point**

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Huang, Tzu-Te - Tu, Chein-Hsiun, Vapor−Liquid Equilibria for Binary and Ternary Mixtures of 1,3-Dioxolane, 2-Propanol, and 2,2,4-Trimethylpentane at 101.3 kPa, Journal of Chemical & Engineering Data 1 (2010) 513-518. doi:10.1021/je900327x

| T / K | P / bar | $x_1$ |
|---|---|---|
| 349.67 | 1.013 | 0.6400 |

Hiaki, Toshihiko - Takahashi, Kenji - Tsuji, Tomoya - Hongo, Masaru - Kojima, Kazuo, Vapor-Liquid Equilibria of 1-Propanol or 2-Propanol with 2,2,4-Trimethylpentane at 101.3 kPa, Journal of Chemical & Engineering Data 3 (1994) 602-604. doi:10.1021/je00015a047

| T / K | P / bar | $x_1$ |
|---|---|---|
| 349.58 | 1.013 | 0.6350 |

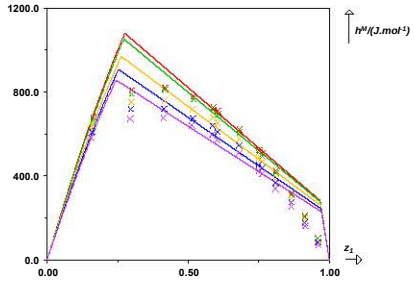
Huang, Tzu-Te - Tu, Chein-Hsiun, Vapor−Liquid Equilibria for Binary and Ternary Mixtures of 1,3-Dioxolane, 2-Propanol, and 2,2,4-Trimethylpentane at 101.3 kPa, Journal of Chemical & Engineering Data 1 (2010) 513-518. doi:10.1021/je900327x

| T / K | P / bar | $x_1$ |
|---|---|---|
| 349.66 | 1.013 | 0.6420 |

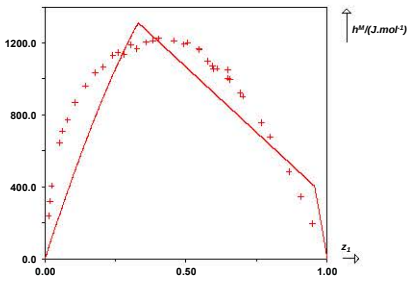
Lin, Dun-Yi - Tu, Chein-Hsiun, (Vapour+liquid) equilibria for binary and ternary mixtures of 2-propanol, tetrahydropyran, and 2,2,4-trimethylpentane at P=101.3kPa, The Journal of Chemical Thermodynamics (2012) 260-266. doi:10.1016/j.jct.2011.10.025

| T / K | P / bar | $x_1$ |
|---|---|---|
| 349.66 | 1.013 | 0.6320 |

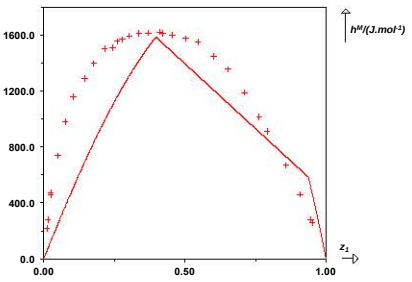
T/K = 298.15 - P/bar = 1.00 42.00 196.00 361.00 542.00



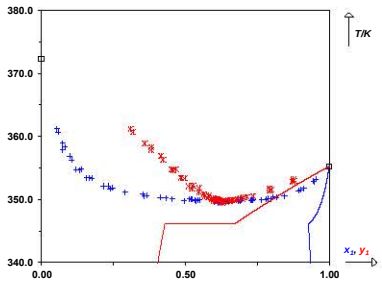

T/K = 318.14 - P/bar = 1.0132



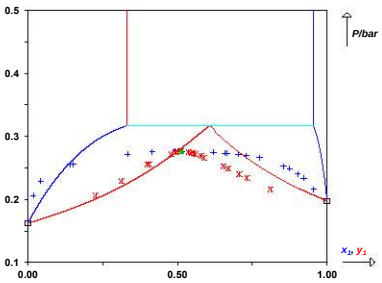

T/K = 338.10 - P/bar = 1.0132



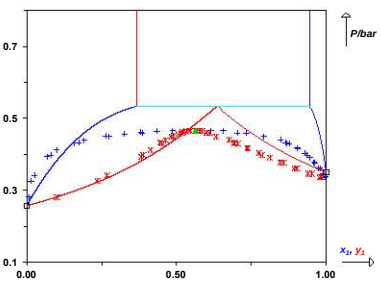

P/bar = 1.01300



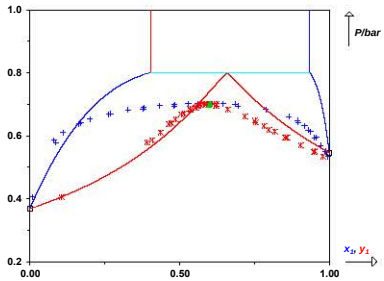

T/K = 318.10



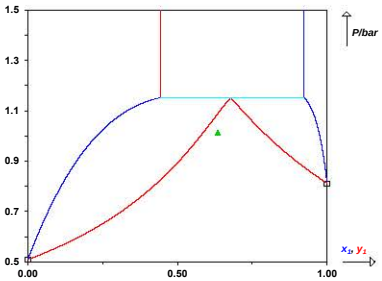

T/K = 330.00



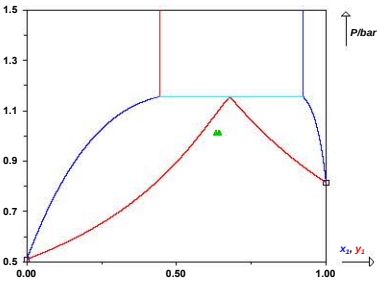

T/K = 340.00



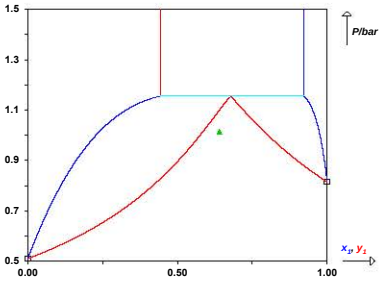

T/K = 349.58




T/K = 349.66




T/K = 349.67



## 2-BUTANOL (1) + CYCLOHEXANE (2)

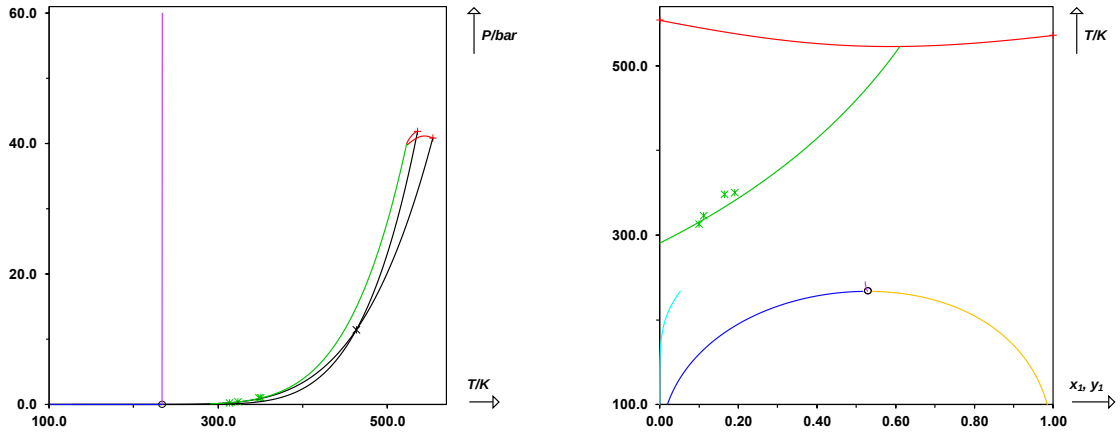
| | | |
|---|---|---|
| **CAS** | 78-92-2 | 110-82-7 |
| **InChiKey** | BTANRVKWQNVYAZ-UHFFFAOYSA-N | XDTMQSROBMDMFD-UHFFFAOYSA-N |
| **$T_c$ / K** | 535.90 | 553.80 |
| **$P_c$ / bar** | 41.89 | 40.80 |
| **ω** | 0.581 | 0.208 |

Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 238
B/MPa = 192

*Deviations*
MAPE on x = 16 %
MAPE on y = 14 %
MAPE on $x_{az}$ = 10 %
MAPE on $P_{az}$ = 3.7 %
MAPE on $h^M$ = 32 %



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**Isothermal phase equilibrium data**

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Belabbaci, Aouicha - Villamañán, Rosa M. - Negadi, Latifa - Martín, M. Carmen, Vapor–Liquid Equilibria of Binary Mixtures Containing 2-Butanol and Hydrocarbons at 313.15 K, Journal of Chemical & Engineering Data 3 (2012) 982-987. doi:10.1021/je201284y

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1022 | 0.9497 | 0.5665 | |
| 0.1350 | 0.9001 | 0.4102 | |
| 0.1609 | 0.8504 | 0.3305 | |
| 0.1811 | 0.8007 | 0.2826 | |
| 0.1972 | 0.7508 | 0.2503 | |
| 0.2100 | 0.7009 | 0.2270 | |
| 0.2203 | 0.6508 | 0.2093 | |
| 0.2530 | 0.3500 | 0.1492 | |
| 0.2559 | 0.3002 | 0.1411 | |
| 0.2584 | 0.2499 | 0.1329 | |
| 0.2602 | 0.2002 | 0.1248 | |
| 0.2613 | 0.1501 | 0.1166 | |
| 0.2603 | 0.0999 | 0.0999 | AZEO |
| 0.2617 | 0.0999 | 0.1063 | |
| 0.2601 | 0.0498 | 0.0844 | |

Araujo, M.E. - Maciel, M.R.W. - Francesconi, A.Z., Excess Gibbs free energies of (hexane + butan-2-ol) and of (cyclohexane + butan-2-ol) at the temperatures (323.15, 338.15, and 348.15) K, The Journal of Chemical Thermodynamics 11 (1993) 1295-1299. doi:10.1006/jcht.1993.1129

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2698 | 0.8020 | 0.3550 | |
| 0.2879 | 0.7560 | 0.3220 | |
| 0.3091 | 0.7130 | 0.2880 | |
| 0.3340 | 0.6720 | 0.2560 | |
| 0.3409 | 0.6330 | 0.2450 | |
| 0.3549 | 0.5960 | 0.2250 | |
| 0.3591 | 0.5590 | 0.2150 | |
| 0.3713 | 0.4900 | 0.1940 | |
| 0.3775 | 0.4550 | 0.1830 | |
| 0.3812 | 0.4220 | 0.1650 | |
| 0.3879 | 0.2880 | 0.1380 | |
| 0.3946 | 0.1110 | 0.1110 | AZEO |
| 0.3930 | 0.0360 | 0.0860 | |

Araujo, M.E. - Maciel, M.R.W. - Francesconi, A.Z., Excess Gibbs free energies of (hexane + butan-2-ol) and of (cyclohexane + butan-2-ol) at the temperatures (323.15, 338.15, and 348.15) K, The Journal of Chemical Thermodynamics 11 (1993) 1295-1299. doi:10.1006/jcht.1993.1129

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.5026 | 0.9440 | 0.8490 | |
| 0.6045 | 0.8970 | 0.7130 | |
| 0.7677 | 0.8020 | 0.5240 | |
| 0.7927 | 0.7800 | 0.4880 | |
| 0.8629 | 0.7130 | 0.3880 | |
| 0.8894 | 0.6720 | 0.3550 | |
| 0.9192 | 0.5960 | 0.3220 | |
| 0.9383 | 0.5240 | 0.2880 | |
| 0.9823 | 0.2880 | 0.1940 | |
| 0.9866 | 0.1650 | 0.1650 | AZEO |
| 0.9813 | 0.0860 | 0.1380 | |
| 0.9749 | 0.0610 | 0.1110 | |
| 0.9405 | 0.0360 | 0.0860 | |

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**Isobaric phase equilibrium data**

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GascÓn, I. - Artigas, H. - Cea, P. - DomÍnguez, M. - Royo, F.M., Isobaric Vapour-Liquid Equilibrium of Ternary Mixtures Cyclohexane (or n -Hexane) Plus 1,3-Dioxolane Plus 2-Butanol at 40.0 and 101.3 kPa, Physics and Chemistry of Liquids 1 (2003) 1-13. doi:10.1080/00319100290032703

**P / bar = 0.4000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 338.05 | 0.8910 | 0.5300 |
| 336.00 | 0.8530 | 0.4670 |
| 332.40 | 0.7930 | 0.3710 |
| 331.12 | 0.7510 | 0.3440 |
| 329.16 | 0.6840 | 0.2950 |
| 327.17 | 0.5600 | 0.2500 |
| 326.18 | 0.4900 | 0.2280 |
| 325.79 | 0.4420 | 0.2200 |
| 325.20 | 0.3650 | 0.1970 |
| 324.77 | 0.2820 | 0.1830 |
| 324.40 | 0.1940 | 0.1590 |
| 324.38 | 0.1340 | 0.1480 |

Feng, Li-Chia - Chou, Chih-Hao - Tang, Muoi - Chen, Yan-Ping, Vapor−Liquid Equilibria of Binary Mixtures 2-Butanol + Butyl Acetate, Hexane + Butyl Acetate, and Cyclohexane + 2-Butanol at 101.3 kPa, Journal of Chemical & Engineering Data 4 (1998) 658-661. doi:10.1021/je9800205

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 368.41 | 0.9636 | 0.8385 |
| 366.76 | 0.9457 | 0.7787 |
| 362.48 | 0.8905 | 0.6249 |
| 358.49 | 0.8204 | 0.5050 |
| 356.27 | 0.7567 | 0.4294 |
| 353.10 | 0.6328 | 0.3411 |
| 352.45 | 0.5905 | 0.3198 |
| 351.94 | 0.5544 | 0.3145 |
| 351.53 | 0.5192 | 0.2903 |
| 350.93 | 0.4442 | 0.2659 |
| 350.68 | 0.4038 | 0.2543 |
| 350.59 | 0.3861 | 0.2493 |
| 350.34 | 0.3338 | 0.2331 |
| 350.24 | 0.2858 | 0.2206 |
| 350.17 | 0.2537 | 0.2107 |
| 350.14 | 0.2172 | 0.2002 |
| 350.13 | 0.1942 | 0.1927 |
| 350.12 | 0.1923 | 0.1912 |
| 350.14 | 0.1891 | 0.1901 |
| 350.18 | 0.1780 | 0.1863 |
| 350.27 | 0.1429 | 0.1725 |
| 350.44 | 0.1064 | 0.1551 |
| 350.73 | 0.0771 | 0.1363 |
| 351.28 | 0.0498 | 0.1089 |

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**Enthalpy of mixing**

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French, Han T., Thermodynamic functions for the systems 1-butanol, 2-butanol, andt-butanol + cyclohexane, Journal of Solution Chemistry 12 (1983) 869-887. doi:10.1007/BF00643927

**T / K = 288.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 23.34 | 0.9900 |
| 46.37 | 0.9800 |
| 113.90 | 0.9500 |
| 221.76 | 0.9000 |
| 419.52 | 0.8000 |
| 591.15 | 0.7000 |
| 726.24 | 0.6000 |
| 815.25 | 0.5000 |
| 840.72 | 0.4000 |
| 792.33 | 0.3000 |
| 670.40 | 0.2000 |
| 638.81 | 0.1800 |
| 605.20 | 0.1600 |
| 568.77 | 0.1400 |
| 529.16 | 0.1200 |
| 485.91 | 0.1000 |
| 450.94 | 0.0850 |
| 413.19 | 0.0700 |
| 354.02 | 0.0500 |
| 319.56 | 0.0400 |
| 281.66 | 0.0300 |
| 229.32 | 0.0200 |
| 202.12 | 0.0150 |
| 161.67 | 0.0100 |
| 130.12 | 0.0070 |
| 102.09 | 0.0050 |
| 85.34 | 0.0040 |
| 66.43 | 0.0030 |
| 45.51 | 0.0020 |
| 23.12 | 0.0010 |

Veselý, František - Dohnal, Vladimír - Valentová, Miriam - Pick, Jiří, Concentration and temperature dependence of heats of mixing of 1-butanol, 2-butanol, and 2-methyl-2-propanol with cyclohexane, Collection of Czechoslovak Chemical Communications 12 (1983) 3482-3494. doi:10.1135/cccc19833482

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 162.60 | 0.9377 |
| 357.90 | 0.8595 |
| 501.90 | 0.7940 |
| 579.60 | 0.7568 |
| 651.40 | 0.7208 |
| 730.10 | 0.6742 |
| 755.10 | 0.6610 |
| 815.80 | 0.6154 |
| 846.60 | 0.5890 |
| 877.10 | 0.5584 |
| 908.00 | 0.5321 |
| 928.40 | 0.5037 |
| 950.80 | 0.4626 |
| 958.30 | 0.4163 |
| 954.10 | 0.3870 |
| 943.30 | 0.3597 |
| 903.70 | 0.3087 |
| 880.70 | 0.2798 |
| 832.30 | 0.2390 |
| 781.10 | 0.2025 |
| 703.70 | 0.1569 |
| 607.50 | 0.1111 |

| | |
|---|---|
| 462.30 | 0.0591 |

French, Han T., Thermodynamic functions for the systems 1-butanol, 2-butanol, andt-butanol + cyclohexane, Journal of Solution Chemistry 12 (1983) 869-887. doi:10.1007/BF00643927

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 31.91 | 0.9900 |
| 63.56 | 0.9800 |
| 156.94 | 0.9500 |
| 306.09 | 0.9000 |
| 576.48 | 0.8000 |
| 800.31 | 0.7000 |
| 966.96 | 0.6000 |
| 1064.5 | 0.5000 |
| 1088.2 | 0.4000 |
| 1035.1 | 0.3000 |
| 910.08 | 0.2000 |
| 876.01 | 0.1800 |
| 837.85 | 0.1600 |
| 796.08 | 0.1400 |
| 749.55 | 0.1200 |
| 696.69 | 0.1000 |
| 650.82 | 0.0850 |
| 598.99 | 0.0700 |
| 514.90 | 0.0500 |
| 463.49 | 0.0400 |
| 400.42 | 0.0300 |
| 325.16 | 0.0200 |
| 260.78 | 0.0150 |
| 195.72 | 0.0100 |
| 145.62 | 0.0070 |
| 107.26 | 0.0050 |
| 86.89 | 0.0040 |
| 65.86 | 0.0030 |
| 44.27 | 0.0020 |
| 22.28 | 0.0010 |

Veselý, František - Dohnal, Vladimír - Valentová, Miriam - Pick, Jiří, Concentration and temperature dependence of heats of mixing of 1-butanol, 2-butanol, and 2-methyl-2-propanol with cyclohexane, Collection of Czechoslovak Chemical Communications 12 (1983) 3482-3494. doi:10.1135/cccc19833482

**T / K = 313.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 263.60 | 0.9203 |
| 477.50 | 0.8508 |
| 619.20 | 0.7928 |
| 729.70 | 0.7535 |
| 828.00 | 0.7125 |
| 913.60 | 0.6612 |
| 931.80 | 0.6575 |
| 1000.7 | 0.6137 |
| 1036.8 | 0.5880 |
| 1073.4 | 0.5592 |
| 1103.7 | 0.5295 |
| 1129.4 | 0.4986 |
| 1148.2 | 0.4650 |
| 1157.5 | 0.4172 |
| 1153.7 | 0.3918 |
| 1146.2 | 0.3691 |
| 1132.3 | 0.3402 |
| 1112.6 | 0.3197 |
| 1085.7 | 0.2861 |
| 1062.6 | 0.2660 |
| 1021.7 | 0.2345 |
| 982.40 | 0.2084 |
| 935.10 | 0.1808 |
| 885.00 | 0.1561 |
| 766.00 | 0.1063 |
| 605.90 | 0.0605 |

Veselý, František - Dohnal, Vladimír - Valentová, Miriam - Pick, Jiří, Concentration and temperature dependence of heats of mixing of 1-butanol, 2-butanol, and 2-methyl-2-propanol with cyclohexane, Collection of Czechoslovak Chemical Communications 12 (1983) 3482-3494. doi:10.1135/cccc19833482

**T / K = 318.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 252.10 | 0.9300 |
| 502.00 | 0.8533 |
| 659.90 | 0.7953 |
| 772.30 | 0.7542 |
| 850.30 | 0.7203 |
| 895.00 | 0.7058 |
| 969.80 | 0.6614 |
| 983.00 | 0.6579 |
| 1046.7 | 0.6213 |
| 1107.8 | 0.5800 |
| 1133.8 | 0.5620 |
| 1167.0 | 0.5362 |
| 1194.9 | 0.5018 |
| 1201.8 | 0.4883 |

| | |
|---|---|
| 1217.0 | 0.4604 |
| 1221.0 | 0.4302 |
| 1227.3 | 0.4204 |
| 1222.4 | 0.4003 |
| 1215.0 | 0.3758 |
| 1190.9 | 0.3320 |
| 1170.3 | 0.3018 |
| 1140.4 | 0.2691 |
| 1102.4 | 0.2347 |
| 1065.8 | 0.2168 |
| 1033.0 | 0.1982 |
| 951.30 | 0.1542 |
| 832.40 | 0.1105 |
| 654.50 | 0.0612 |

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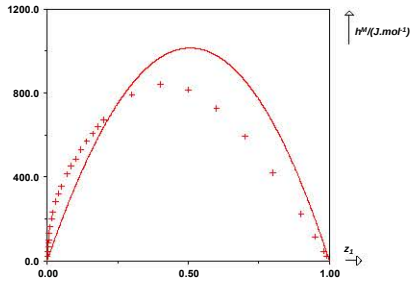
**Azeotropic point**

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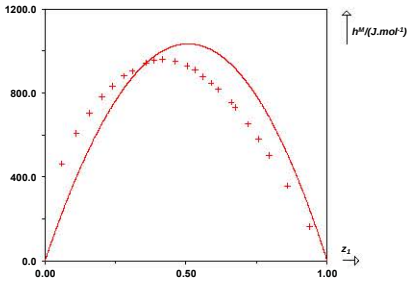
Feng, Li-Chia - Chou, Chih-Hao - Tang, Muoi - Chen, Yan-Ping, Vapor–Liquid Equilibria of Binary Mixtures 2-Butanol + Butyl Acetate, Hexane + Butyl Acetate, and Cyclohexane + 2-Butanol at 101.3 kPa, Journal of Chemical & Engineering Data 4 (1998) 658-661. doi:10.1021/je9800205

| T / K | P / bar | $x_1$ |
|---|---|---|
| 350.12 | 1.013 | 0.1910 |

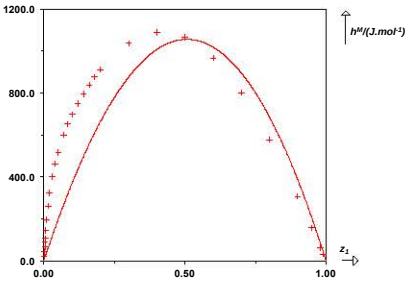
T/K = 288.15 - P/bar = 1.0132



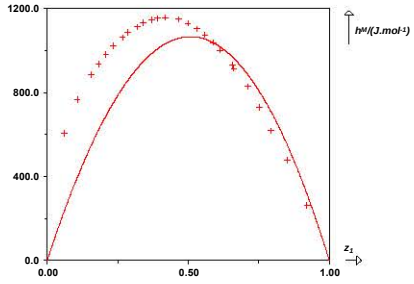

T/K = 298.15 - P/bar = 1.0132



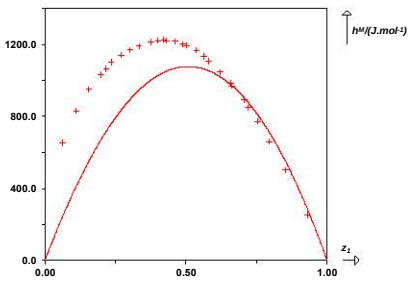

T/K = 308.15 - P/bar = 1.0132



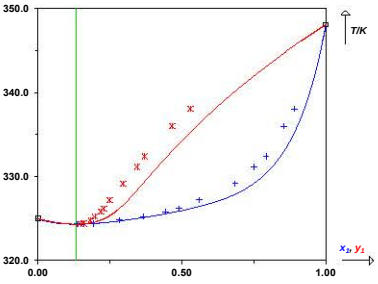

T/K = 313.15 - P/bar = 1.0132



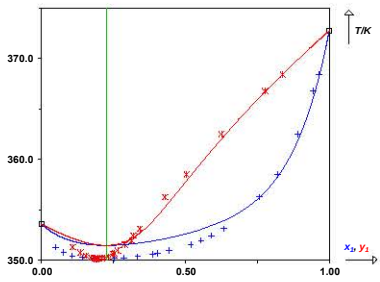

T/K = 318.15 - P/bar = 1.0132



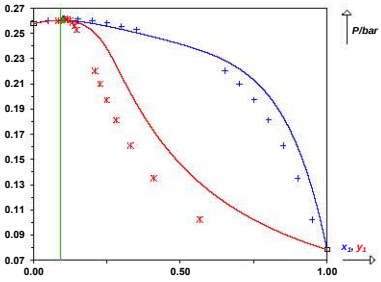

P/bar = 0.39999



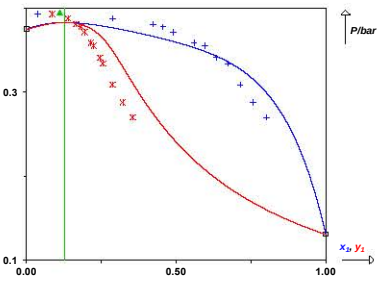

P/bar = 1.01300



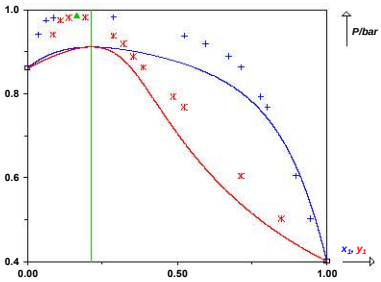

T/K = 313.15



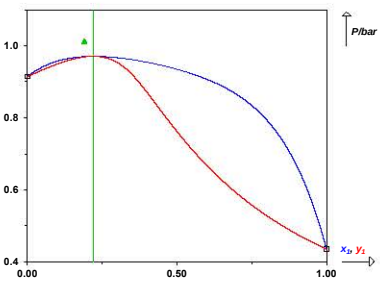

T/K = 323.15




T/K = 348.15




T/K = 350.12



## n-HEXANE (1) + 1-PROPANOL (2)

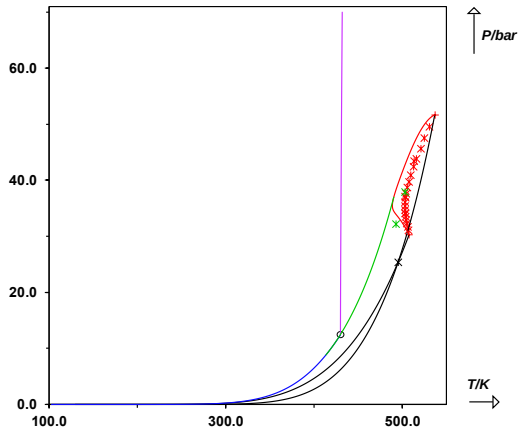
| | | |
|---|---|---|
| **CAS** | 110-54-3 | 71-23-8 |
| **InChiKey** | VLKZOEOYAKHREP-UHFFFAOYSA-N | BDERNNFJNOPAEC-UHFFFAOYSA-N |
| **$T_c$ / K** | 507.60 | 536.80 |
| **$P_c$ / bar** | 30.25 | 51.69 |
| **ω** | 0.301 | 0.621 |

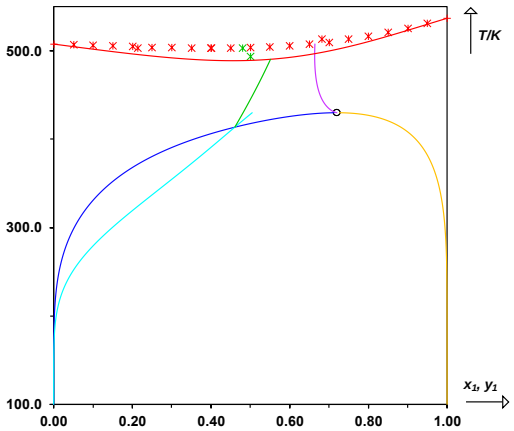
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 645
B/MPa = 989

*Deviations*
MAPE on x = 66 %
MAPE on y = 22 %
MAPE on $h^M$ = 24 %



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**Isothermal phase equilibrium data**

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Diaz Pena, M. - Rodriguez Cheda, D.R., Liquid-vapor equilibrium. III. Systems of n-propanol-n-hexane at 50. deg. and n-propanol-n-heptane at 60. deg, An. Quim. (1970) 747-755.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2375 | 0.0426 | 0.5019 |
| 0.2591 | 0.0528 | 0.5482 |
| 0.2753 | 0.0606 | 0.5764 |
| 0.3210 | 0.0848 | 0.6423 |
| 0.3407 | 0.0976 | 0.6649 |
| 0.3696 | 0.1175 | 0.6960 |
| 0.4374 | 0.1802 | 0.7513 |
| 0.4463 | 0.1898 | 0.7576 |
| 0.4774 | 0.2327 | 0.7787 |
| 0.5043 | 0.2795 | 0.7940 |
| 0.5100 | 0.2924 | 0.7988 |
| 0.5375 | 0.3698 | 0.8140 |
| 0.5482 | 0.4125 | 0.8220 |
| 0.5494 | 0.4178 | 0.8218 |
| 0.5581 | 0.4613 | 0.8265 |
| 0.5692 | 0.5787 | 0.8361 |
| 0.5702 | 0.6003 | 0.8375 |
| 0.5760 | 0.8497 | 0.8536 |
| 0.5706 | 0.9325 | 0.8951 |
| 0.5508 | 0.9825 | 0.9630 |

Maciel, Maria Regina W - Francesconi, A.Z, Excess Gibbs free energies of (n-hexane + propan-1-ol) at 338.15 and 348.15 K and of (n-hexane + propan-2-ol) at 323.15, 338.15, and 348.15 K, The Journal of Chemical Thermodynamics 5 (1988) 539-544. doi:10.1016/0021-9614(88)90081-X

**T / K = 338.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2773 | 0.0010 | 0.0500 |
| 0.2978 | 0.0040 | 0.1140 |
| 0.3588 | 0.0160 | 0.2490 |
| 0.4442 | 0.0250 | 0.4140 |
| 0.5826 | 0.0730 | 0.5740 |
| 0.7349 | 0.1430 | 0.6790 |
| 0.7892 | 0.1680 | 0.6950 |
| 0.8349 | 0.2200 | 0.7210 |
| 0.8717 | 0.2660 | 0.7370 |
| 0.9297 | 0.3710 | 0.7670 |
| 0.9666 | 0.4860 | 0.7820 |
| 0.9726 | 0.5330 | 0.7900 |
| 0.9753 | 0.5850 | 0.7950 |
| 0.9846 | 0.6120 | 0.7880 |
| 0.9928 | 0.6590 | 0.8040 |
| 0.9964 | 0.7050 | 0.8100 |
| 1.001 | 0.7760 | 0.8180 |
| 0.9971 | 0.8820 | 0.8400 |
| 0.9981 | 0.9080 | 0.8550 |
| 0.9948 | 0.9240 | 0.8600 |
| 0.9838 | 0.9430 | 0.8810 |
| 0.9813 | 0.9530 | 0.8890 |
| 0.9797 | 0.9590 | 0.8970 |
| 0.9682 | 0.9680 | 0.9050 |

Maciel, Maria Regina W - Francesconi, A.Z, Excess Gibbs free energies of (n-hexane + propan-1-ol) at 338.15 and 348.15 K and of (n-hexane + propan-2-ol) at 323.15, 338.15, and 348.15 K, The Journal of Chemical Thermodynamics 5 (1988) 539-544. doi:10.1016/0021-9614(88)90081-X

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4669 | 0.0070 | 0.1110 |
| 0.5805 | 0.0250 | 0.2970 |
| 0.6397 | 0.0340 | 0.3610 |
| 0.7456 | 0.0590 | 0.4630 |
| 0.8403 | 0.0800 | 0.5280 |
| 0.9444 | 0.1110 | 0.5910 |
| 1.079 | 0.1780 | 0.6590 |
| 1.202 | 0.2640 | 0.7170 |
| 1.254 | 0.3320 | 0.7290 |
| 1.305 | 0.4280 | 0.7500 |
| 1.348 | 0.5600 | 0.7650 |
| 1.353 | 0.6030 | 0.7720 |
| 1.363 | 0.6490 | 0.7750 |
| 1.375 | 0.7920 | 0.7980 |
| 1.379 | 0.8150 | 0.8030 |
| 1.356 | 0.9330 | 0.8550 |
| 1.254 | 0.9910 | 0.9760 |

Oh, Byung Chul - Kim, Youngdae - Shin, Hun Yong - Kim, Hwayong, Vapor–liquid equilibria for the system 1-propanol+n-hexane near the critical region, Fluid Phase Equilibria 1 (2004) 41-46. doi:10.1016/j.fluid.2003.12.004

**T / K = 493.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 26.00 | 0.0290 | 0.0540 | |
| 28.00 | 0.0960 | 0.1550 | |
| 32.15 | 0.5000 | 0.5000 | AZEO |
| 29.87 | 0.7590 | 0.7270 | |

| | | |
|---|---|---|
| 29.25 | 0.8070 | 0.7560 |
| 28.22 | 0.8520 | 0.8080 |
| 26.20 | 0.9420 | 0.9130 |

Oh, Byung Chul - Kim, Youngdae - Shin, Hun Yong - Kim, Hwayong, Vapor–liquid equilibria for the system 1-propanol+n-hexane near the critical region, Fluid Phase Equilibria 1 (2004) 41-46. doi:10.1016/j.fluid.2003.12.004

**T / K = 493.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 30.82 | 0.2470 | 0.3190 | |
| 31.81 | 0.3540 | 0.4060 | |
| 32.12 | 0.4210 | 0.4410 | |
| 32.15 | 0.4730 | 0.4940 | |
| 32.15 | 0.5000 | 0.5000 | AZEO |
| 31.60 | 0.6190 | 0.5920 | |
| 31.06 | 0.6840 | 0.6470 | |

Oh, Byung Chul - Kim, Youngdae - Shin, Hun Yong - Kim, Hwayong, Vapor–liquid equilibria for the system 1-propanol+n-hexane near the critical region, Fluid Phase Equilibria 1 (2004) 41-46. doi:10.1016/j.fluid.2003.12.004

**T / K = 503.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 29.64 | 0.9540 | 0.9350 | |
| 37.05 | 0.5990 | 0.5990 | CRIT |

Oh, Byung Chul - Kim, Youngdae - Shin, Hun Yong - Kim, Hwayong, Vapor–liquid equilibria for the system 1-propanol+n-hexane near the critical region, Fluid Phase Equilibria 1 (2004) 41-46. doi:10.1016/j.fluid.2003.12.004

**T / K = 503.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 31.97 | 0.0610 | 0.1030 | |
| 34.47 | 0.1790 | 0.2240 | |
| 36.34 | 0.2910 | 0.3250 | |
| 37.18 | 0.3620 | 0.3850 | |
| 37.54 | 0.4040 | 0.4210 | |
| 37.75 | 0.4320 | 0.4490 | |
| 37.88 | 0.4950 | 0.5020 | |
| 37.58 | 0.5410 | 0.5330 | |
| 37.05 | 0.5990 | 0.5990 | CRIT |
| 33.33 | 0.8290 | 0.8140 | |
| 32.74 | 0.8530 | 0.8350 | |
| 31.90 | 0.8880 | 0.8640 | |

Oh, Byung Chul - Kim, Youngdae - Shin, Hun Yong - Kim, Hwayong, Vapor–liquid equilibria for the system 1-propanol+n-hexane near the critical region, Fluid Phase Equilibria 1 (2004) 41-46. doi:10.1016/j.fluid.2003.12.004

**T / K = 513.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 37.14 | 0.0340 | 0.0640 | |
| 40.40 | 0.1340 | 0.1810 | |
| 42.12 | 0.2380 | 0.2650 | |
| 43.13 | 0.3000 | 0.3070 | |
| 43.32 | 0.3120 | 0.3170 | |
| 43.40 | 0.3190 | 0.3190 | CRIT |

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**Enthalpy of mixing**

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Gmehling, J. - Meents, B., Excess enthalpy. 1-Propanol - hexane system, Int. Data Ser. Sel. Data Mixtures Ser. A 3 (1992)

**T / K = 273.15**

**P / bar = 6.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 63.01 | 0.0600 |
| 63.10 | 0.0600 |
| 92.34 | 0.0920 |
| 120.13 | 0.1256 |
| 173.20 | 0.1976 |
| 224.62 | 0.2769 |
| 270.39 | 0.3648 |
| 311.56 | 0.4628 |
| 342.77 | 0.5727 |
| 351.68 | 0.6328 |
| 349.88 | 0.6968 |
| 336.74 | 0.7650 |
| 299.01 | 0.8379 |
| 272.92 | 0.8763 |
| 232.38 | 0.9161 |
| 177.66 | 0.9573 |

Mato, M. M. - Cebreiro, S. M. - Verdes, P. V. - Legido, J. L. - Paz Andrade, M. I., Thermodynamic properties of the ternary system MTBE+1-propanol+hexane: Application of different group contribution models and empirical methods, Journal of Thermal Analysis and Calorimetry 2 (2005) 303-309. doi:10.1007/s10973-005-0651-4

**T / K = 298.15**

**P / bar = 1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 461.60 | 0.9013 |
| 579.30 | 0.8016 |
| 598.50 | 0.7316 |

| | |
|---|---|
| 594.30 | 0.6365 |
| 573.20 | 0.5658 |
| 542.30 | 0.4966 |
| 504.90 | 0.4298 |
| 462.20 | 0.3573 |
| 425.30 | 0.3165 |
| 351.00 | 0.2490 |
| 299.50 | 0.2033 |
| 236.70 | 0.1582 |
| 181.50 | 0.1159 |
| 173.20 | 0.1087 |
| 114.20 | 0.0674 |
| 59.90 | 0.0341 |

Brown, I - Fock, W - Smith, F, Heats of mixing. V. Systems of n-alcohols with n-hexane, Australian Journal of Chemistry 10 (1964) doi:10.1071/CH9641106

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 561.00 | 0.3537 |
| 565.00 | 0.3562 |
| 567.00 | 0.3590 |
| 743.00 | 0.6190 |
| 746.00 | 0.6429 |
| 700.00 | 0.7889 |
| 680.00 | 0.8102 |
| 582.00 | 0.8874 |

Brown, I - Fock, W - Smith, F, Heats of mixing. V. Systems of n-alcohols with n-hexane, Australian Journal of Chemistry 10 (1964) doi:10.1071/CH9641106

**T / K = 318.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 340.00 | 0.1523 |
| 680.00 | 0.3528 |
| 683.00 | 0.3533 |
| 703.00 | 0.3720 |
| 906.00 | 0.6185 |
| 905.00 | 0.6433 |
| 858.00 | 0.7885 |
| 830.00 | 0.8106 |
| 678.00 | 0.9034 |

Gmehling, J. - Meents, B., Excess enthalpy. 1-Propanol - hexane system, Int. Data Ser. Sel. Data Mixtures Ser. A 3 (1992)

**T / K = 363.15**

**P / bar = 8.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 292.84 | 0.0600 |
| 614.18 | 0.1256 |
| 615.36 | 0.1256 |
| 772.89 | 0.1607 |
| 917.57 | 0.1976 |
| 917.15 | 0.1976 |
| 1220.0 | 0.2769 |
| 1364.7 | 0.3197 |
| 1500.0 | 0.3648 |
| 1731.2 | 0.4628 |
| 1832.2 | 0.5162 |
| 1884.6 | 0.5727 |
| 1890.5 | 0.5727 |
| 1943.3 | 0.6328 |
| 1939.8 | 0.6328 |
| 1932.4 | 0.6968 |
| 1855.7 | 0.7650 |
| 1783.6 | 0.8008 |
| 1666.3 | 0.8379 |
| 1501.5 | 0.8763 |
| 1241.4 | 0.9161 |
| 1043.3 | 0.9365 |
| 794.04 | 0.9573 |
| 431.35 | 0.9784 |

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**Critical point**

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Gil, Laura - Blanco, Sofía T. - Rivas, Clara - Laga, Eduardo - Fernández, Javier - Artal, Manuela - Velasco, Inmaculada, Experimental determination of the critical loci for {n-C6H14 or CO2+alkan-1-ol} mixtures. Evaluation of their critical and subcritical behavior using PC-SAFT EoS, The Journal of Supercritical Fluids (2012) 26-44. doi:10.1016/j.supflu.2012.07.008

| T / K | P / bar | $x_1$ |
|---|---|---|
| 530.79 | 49.55 | 0.0500 |
| 525.23 | 47.56 | 0.0999 |
| 520.83 | 45.62 | 0.1501 |
| 516.21 | 43.84 | 0.2000 |
| 512.88 | 42.45 | 0.2500 |
| 509.56 | 40.92 | 0.3001 |
| 507.59 | 39.75 | 0.3498 |
| 505.50 | 38.67 | 0.4000 |
| 504.28 | 37.64 | 0.4501 |
| 503.52 | 36.89 | 0.4999 |

| | | |
|---|---|---|
| 502.90 | 36.12 | 0.5506 |
| 502.81 | 35.41 | 0.6001 |
| 502.87 | 34.73 | 0.6497 |
| 503.64 | 34.12 | 0.7001 |
| 503.82 | 33.46 | 0.7497 |
| 504.58 | 32.87 | 0.7998 |
| 505.24 | 32.26 | 0.8501 |
| 506.11 | 31.63 | 0.9002 |
| 507.02 | 31.05 | 0.9498 |

Oh, Byung Chul - Kim, Youngdae - Shin, Hun Yong - Kim, Hwayong, Vapor–liquid equilibria for the system 1-propanol+n-hexane near the critical region, Fluid Phase Equilibria 1 (2004) 41-46. doi:10.1016/j.fluid.2003.12.004

| T / K | P / bar | $x_1$ |
|---|---|---|
| 503.15 | 34.07 | 0.7860 |

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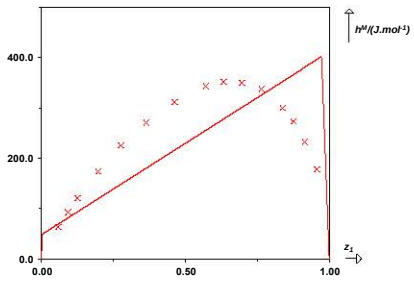
**Azeotropic point**

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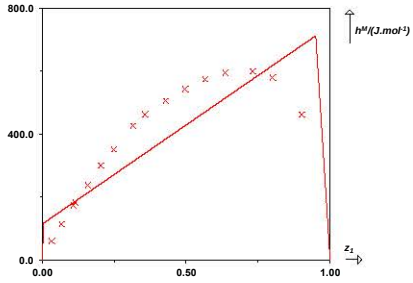
Oh, Byung Chul - Kim, Youngdae - Shin, Hun Yong - Kim, Hwayong, Vapor–liquid equilibria for the system 1-propanol+n-hexane near the critical region, Fluid Phase Equilibria 1 (2004) 41-46. doi:10.1016/j.fluid.2003.12.004

| T / K | P / bar | $x_1$ |
|---|---|---|
| 503.15 | 37.88 | 0.52 |

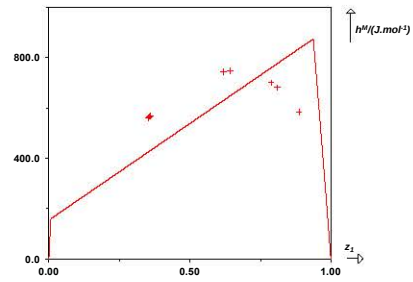
T/K = 273.15 - P/bar = 6.00



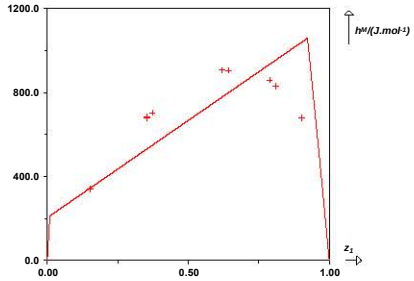

T/K = 298.15 - P/bar = 1.0132



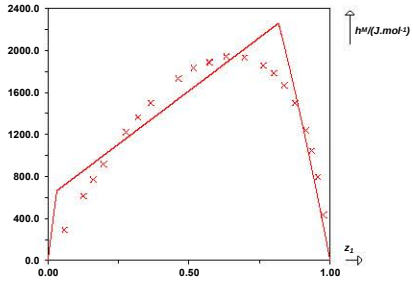

T/K = 308.15 - P/bar = 1.0132



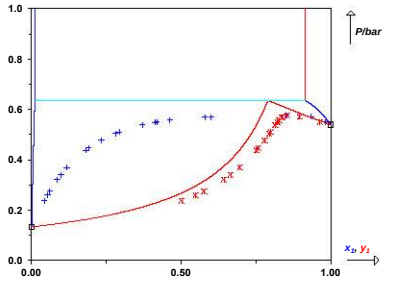

T/K = 318.15 - P/bar = 1.0132



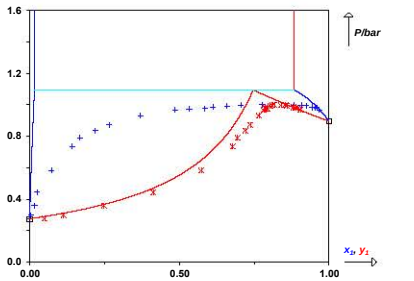

T/K = 363.15 - P/bar = 8.00



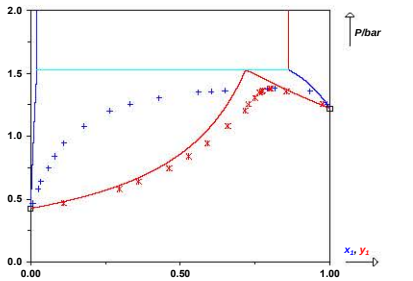

T/K = 323.15



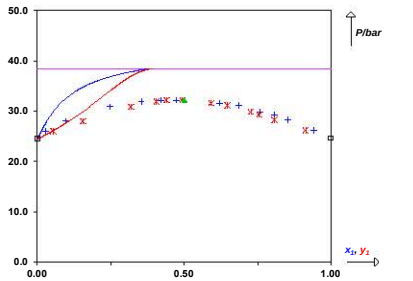

T/K = 338.15



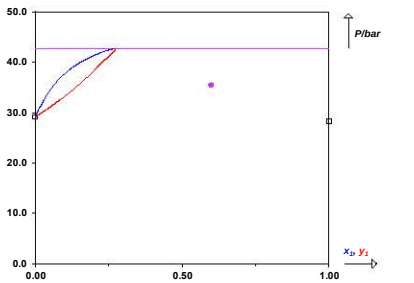

T/K = 348.15



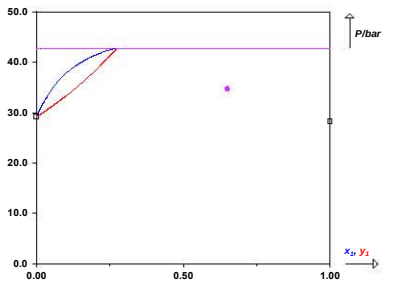

T/K = 493.15



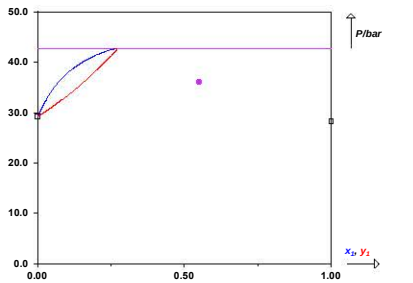

T/K = 502.81



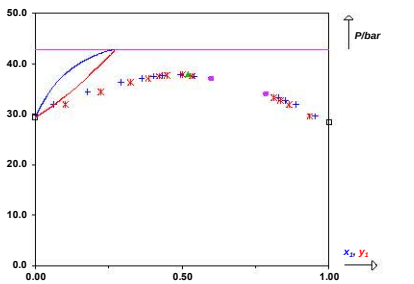

T/K = 502.87



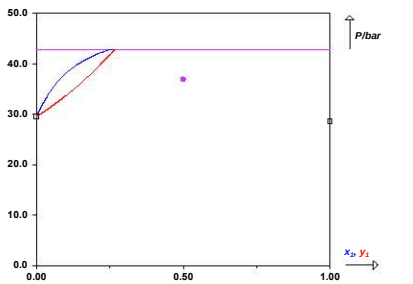

T/K = 502.90



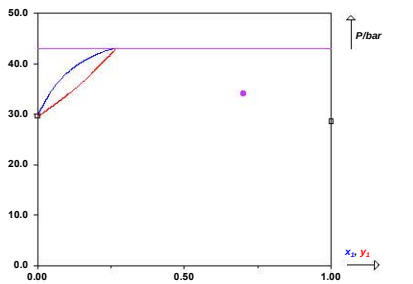

T/K = 503.15



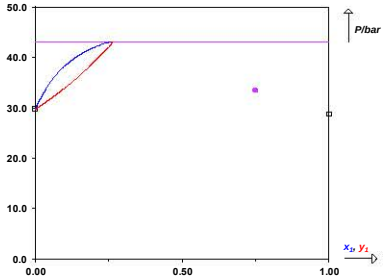

T/K = 503.52



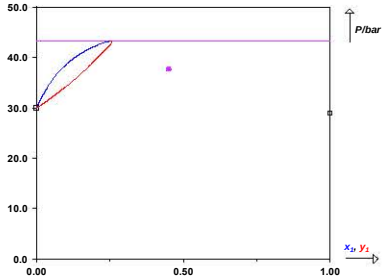

T/K = 503.64



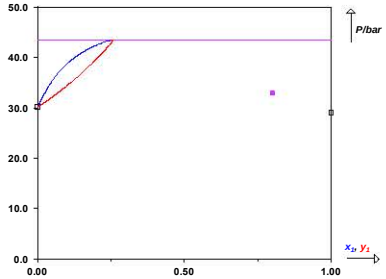
T/K = 503.82



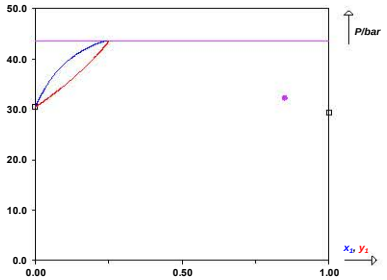

T/K = 504.28



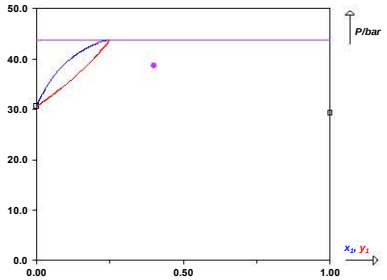

T/K = 504.58



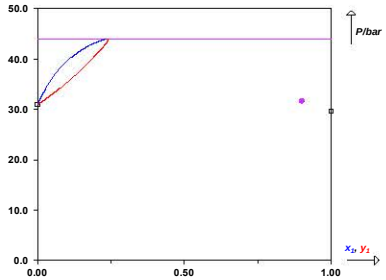

T/K = 505.24



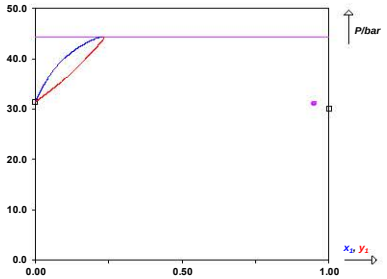

T/K = 505.50



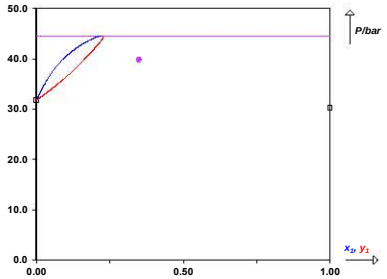

T/K = 506.11



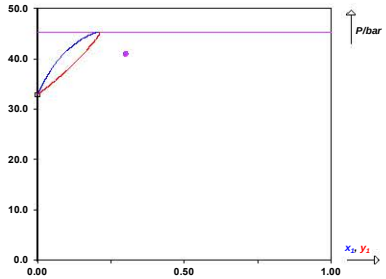

T/K = 507.02



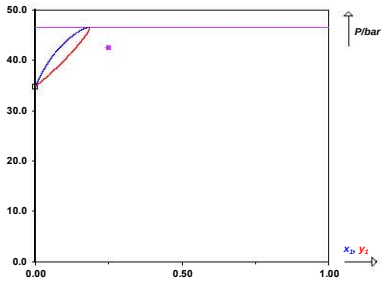

T/K = 507.59



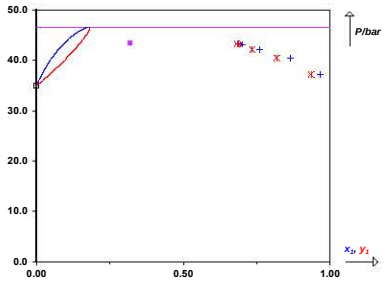

T/K = 509.56



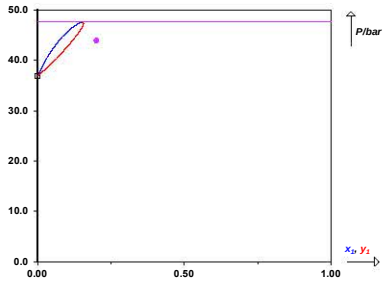

T/K = 512.88



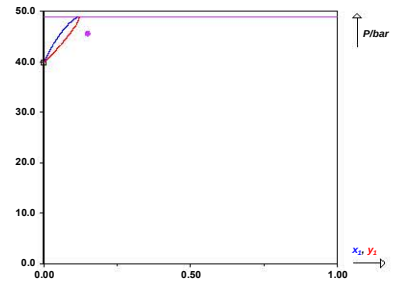

T/K = 513.15



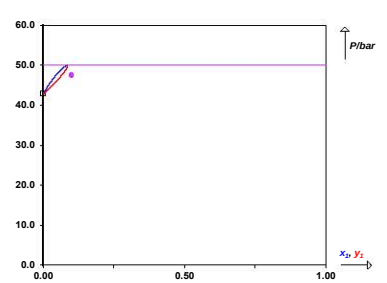

T/K = 516.21



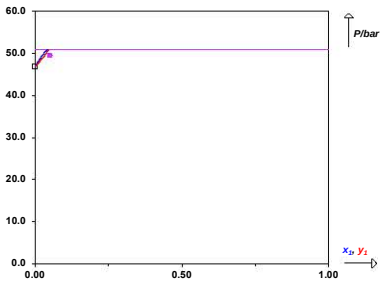

T/K = 520.83




T/K = 525.23




T/K = 530.79



## ETHANOL (1) + n-HEPTANE (2)

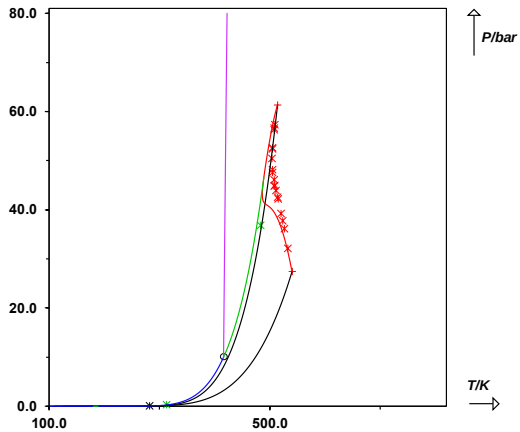
| | | |
|---|---|---|
| **CAS** | 64-17-5 | 142-82-5 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | IMNFDUFMRHMDMM-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 540.20 |
| **$P_c$ / bar** | 61.37 | 27.40 |
| **ω** | 0.644 | 0.349 |

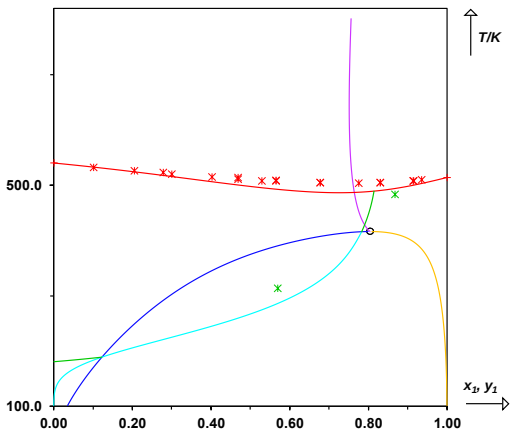
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 468
B/MPa = 238

*Deviations*
MAPE on x = 44 %
MAPE on y = 12 %
MAPE on $x_{az}$ = 24 %
MAPE on $P_{az}$ = 13 %
MAPE on $h^M$ = 30 %
MAPE on $c_P^M$ = 88 %



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**Isothermal phase equilibrium data**

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Berro, Charles - Rogalski, Marek - Péneloux, André, A new ebulliometric technique. Vapour-liquid equilibria in the binary systems ethanol-n-heptane and ethanol-n-nonane, Fluid Phase Equilibria 1 (1982) 55-73. doi:10.1016/0378-3812(82)80005-8

**T / K = 303.27**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1398 | 0.0383 | 0.4488 |
| 0.1428 | 0.0472 | 0.4622 |
| 0.1447 | 0.0542 | 0.4699 |
| 0.1465 | 0.0614 | 0.4763 |
| 0.1492 | 0.0776 | 0.4879 |
| 0.1534 | 0.1087 | 0.5048 |
| 0.1561 | 0.1385 | 0.5169 |
| 0.1578 | 0.1577 | 0.5228 |
| 0.1587 | 0.1749 | 0.5268 |
| 0.1593 | 0.1900 | 0.5296 |
| 0.1600 | 0.2212 | 0.5337 |
| 0.1606 | 0.2435 | 0.5357 |
| 0.1610 | 0.2733 | 0.5379 |
| 0.1612 | 0.3032 | 0.5399 |
| 0.1614 | 0.3206 | 0.5411 |
| 0.1615 | 0.3292 | 0.5417 |
| 0.1617 | 0.3422 | 0.5426 |
| 0.1616 | 0.3589 | 0.5437 |
| 0.1621 | 0.3858 | 0.5455 |
| 0.1620 | 0.3947 | 0.5461 |
| 0.1622 | 0.4287 | 0.5482 |
| 0.1624 | 0.4646 | 0.5501 |
| 0.1626 | 0.5127 | 0.5526 |
| 0.1627 | 0.5476 | 0.5546 |
| 0.1626 | 0.5688 | 0.5561 |
| 0.1624 | 0.5767 | 0.5567 |
| 0.1623 | 0.5998 | 0.5586 |
| 0.1623 | 0.6178 | 0.5602 |
| 0.1624 | 0.6199 | 0.5604 |
| 0.1623 | 0.6361 | 0.5621 |
| 0.1622 | 0.6554 | 0.5643 |
| 0.1618 | 0.7008 | 0.5703 |
| 0.1615 | 0.7122 | 0.5721 |
| 0.1606 | 0.7558 | 0.5804 |
| 0.1587 | 0.8086 | 0.5959 |
| 0.1561 | 0.8467 | 0.6142 |
| 0.1497 | 0.8950 | 0.6538 |
| 0.1418 | 0.9288 | 0.7023 |
| 0.1389 | 0.9389 | 0.7226 |
| 0.1317 | 0.9581 | 0.7731 |
| 0.1264 | 0.9693 | 0.8131 |
| 0.1215 | 0.9774 | 0.8489 |
| 0.1192 | 0.9814 | 0.8694 |
| 0.1146 | 0.9880 | 0.9081 |
| 0.1108 | 0.9932 | 0.9440 |
| 0.1088 | 0.9956 | 0.9624 |
| 0.1072 | 0.9979 | 0.9814 |
| 0.1064 | 0.9988 | 0.9892 |
| 0.1056 | 0.9996 | 0.9964 |

Ratcliff, G. A. - Chao, K. C., Prediction of thermodynamic properties of polar mixtures by a group solution model, The Canadian Journal of Chemical Engineering 2 (1969) 148-153. doi:10.1002/cjce.5450470208

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2128 | 0.0352 | 0.4392 | |
| 0.2324 | 0.0717 | 0.4744 | |
| 0.2488 | 0.1451 | 0.5235 | |
| 0.2612 | 0.3327 | 0.5524 | |
| 0.2639 | 0.5620 | 0.5680 | |
| 0.2640 | 0.5700 | 0.5700 | AZEO |
| 0.2615 | 0.7262 | 0.5885 | |
| 0.2611 | 0.7586 | 0.5986 | |
| 0.2420 | 0.8786 | 0.6553 | |
| 0.2275 | 0.9175 | 0.7082 | |
| 0.2080 | 0.9615 | 0.8017 | |

Diaz Pena, M. - Rodriguez Cheda, D.R., Liquid-vapor equilibrium. II. Ethanol-n-heptane system at 40 and 60.deg., An. Quim. (1970) 737-745.

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2054 | 0.0277 | 0.4079 |
| 0.2619 | 0.2905 | 0.5314 |
| 0.2615 | 0.3809 | 0.5410 |
| 0.2632 | 0.5052 | 0.5607 |
| 0.2643 | 0.5565 | 0.5740 |
| 0.2641 | 0.6413 | 0.5967 |
| 0.2636 | 0.7055 | 0.6055 |
| 0.2604 | 0.7943 | 0.6296 |
| 0.2571 | 0.8357 | 0.6424 |
| 0.2529 | 0.8802 | 0.6615 |
| 0.2443 | 0.9191 | 0.6925 |
| 0.2125 | 0.9724 | 0.8143 |
| 0.1857 | 0.9949 | 0.9563 |

Diaz Pena, M. - Rodriguez Cheda, D.R., Liquid-vapor equilibrium. II. Ethanol-n-heptane system at 40 and 60.deg., An. Quim. (1970) 737-745.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4472 | 0.0302 | 0.3741 |
| 0.6236 | 0.1564 | 0.5686 |
| 0.6320 | 0.2817 | 0.5819 |
| 0.6383 | 0.3835 | 0.5875 |
| 0.6454 | 0.5405 | 0.6152 |
| 0.6476 | 0.6356 | 0.6253 |
| 0.6451 | 0.7060 | 0.6395 |
| 0.6403 | 0.7719 | 0.6558 |
| 0.6300 | 0.8390 | 0.6799 |
| 0.6183 | 0.8750 | 0.7001 |
| 0.5988 | 0.9116 | 0.7369 |
| 0.5767 | 0.9401 | 0.7802 |
| 0.5382 | 0.9672 | 0.8464 |
| 0.5060 | 0.9847 | 0.9150 |

Berro, Charles - Rogalski, Marek - Péneloux, André, A new ebulliometric technique. Vapour-liquid equilibria in the binary systems ethanol-n-heptane and ethanol-n-nonane, Fluid Phase Equilibria 1 (1982) 55-73. doi:10.1016/0378-3812(82)80005-8

**T / K = 343.17**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.8387 | 0.0976 | 0.5344 |
| 0.8443 | 0.1013 | 0.5371 |
| 0.8877 | 0.1510 | 0.5655 |
| 0.8964 | 0.1666 | 0.5710 |
| 0.9104 | 0.1957 | 0.5807 |
| 0.9237 | 0.2344 | 0.5898 |
| 0.9294 | 0.2547 | 0.5943 |
| 0.9393 | 0.3003 | 0.6018 |
| 0.9415 | 0.3161 | 0.6043 |
| 0.9463 | 0.3419 | 0.6078 |
| 0.9467 | 0.3483 | 0.6089 |
| 0.9552 | 0.4248 | 0.6173 |
| 0.9561 | 0.4303 | 0.6182 |
| 0.9590 | 0.4698 | 0.6227 |
| 0.9599 | 0.4904 | 0.6241 |
| 0.9607 | 0.5046 | 0.6264 |
| 0.9618 | 0.5288 | 0.6282 |
| 0.9621 | 0.5356 | 0.6298 |
| 0.9633 | 0.5671 | 0.6326 |
| 0.9650 | 0.6116 | 0.6381 |
| 0.9643 | 0.6524 | 0.6436 |
| 0.9628 | 0.7116 | 0.6542 |
| 0.9607 | 0.7420 | 0.6613 |
| 0.9554 | 0.7835 | 0.6735 |
| 0.9498 | 0.8101 | 0.6833 |
| 0.9418 | 0.8403 | 0.6985 |
| 0.9209 | 0.8815 | 0.7267 |
| 0.8825 | 0.9259 | 0.7767 |
| 0.8083 | 0.9710 | 0.8742 |
| 0.7909 | 0.9788 | 0.9001 |
| 0.7517 | 0.9922 | 0.9569 |
| 0.7422 | 0.9950 | 0.9713 |
| 0.7351 | 0.9968 | 0.9812 |

Seo, Jungha - Lee, Jongcheon - Kim, Hwayong, Measurement and Correlation of Vapor–Liquid Equilibria for the 2-Propanol + n-Hexane System near the Critical Region, Journal of Chemical & Engineering Data 4 (2003) 856-859. doi:10.1021/je025604s

**T / K = 483.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 17.20 | 0.1040 | 0.2070 | |
| 22.39 | 0.2150 | 0.3560 | |
| 25.99 | 0.3150 | 0.4540 | |
| 36.77 | 0.8670 | 0.8670 | AZEO |

Seo, Jungha - Lee, Jongcheon - Kim, Hwayong, Measurement and Correlation of Vapor–Liquid Equilibria for the 2-Propanol + n-Hexane System near the Critical Region, Journal of Chemical & Engineering Data 4 (2003) 856-859. doi:10.1021/je025604s

**T / K = 483.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 30.80 | 0.4670 | 0.5890 | |
| 34.21 | 0.6180 | 0.6860 | |
| 35.72 | 0.7350 | 0.7730 | |
| 36.47 | 0.8220 | 0.8250 | |
| 36.77 | 0.8670 | 0.8670 | AZEO |
| 36.55 | 0.9490 | 0.9410 | |

Seo, Jungha - Lee, Jongcheon - Kim, Hwayong, Measurement and Correlation of Vapor–Liquid Equilibria for the 2-Propanol + n-Hexane System near the Critical Region, Journal of Chemical & Engineering Data 4 (2003) 856-859. doi:10.1021/je025604s

**T / K = 508.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 26.17 | 0.1410 | 0.2470 | |
| 56.58 | 0.9150 | 0.9150 | CRIT |

Seo, Jungha - Lee, Jongcheon - Kim, Hwayong, Measurement and Correlation of Vapor–Liquid Equilibria for the 2-Propanol + n-Hexane System near the Critical Region, Journal of Chemical & Engineering Data 4 (2003) 856-859. doi:10.1021/je025604s

**T / K = 508.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 34.21 | 0.2870 | 0.4090 | |
| 38.71 | 0.3790 | 0.4760 | |
| 40.83 | 0.4220 | 0.5080 | |
| 43.84 | 0.5000 | 0.5350 | |
| 44.64 | 0.5250 | 0.5380 | |
| 56.58 | 0.9150 | 0.9150 | CRIT |
| 56.55 | 0.9190 | 0.9160 | |
| 56.49 | 0.9270 | 0.9240 | |
| 56.10 | 0.9730 | 0.9700 | |

Seo, Jungha - Lee, Jongcheon - Kim, Hwayong, Measurement and Correlation of Vapor−Liquid Equilibria for the 2-Propanol + n-Hexane System near the Critical Region, Journal of Chemical & Engineering Data 4 (2003) 856-859. doi:10.1021/je025604s

**T / K = 523.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 27.95 | 0.0900 | 0.1480 | |
| 34.90 | 0.2020 | 0.2700 | |
| 37.72 | 0.2790 | 0.2790 | CRIT |

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**Isobaric phase equilibrium data**

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Van Ness, Hendrick C. - Soczek, C. A. - Kochar, Nand K., Thermodynamic excess properties for ethanol-n-heptane, Journal of Chemical & Engineering Data 3 (1967) 346-351. doi:10.1021/je60034a015

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 365.22 | 0.0100 | 0.1669 |
| 358.19 | 0.0250 | 0.3371 |
| 351.96 | 0.0500 | 0.4667 |
| 349.45 | 0.0750 | 0.5110 |
| 348.16 | 0.1000 | 0.5396 |
| 345.77 | 0.2000 | 0.5853 |
| 344.99 | 0.3000 | 0.6029 |
| 344.64 | 0.4000 | 0.6140 |
| 344.43 | 0.5000 | 0.6250 |
| 344.37 | 0.6000 | 0.6302 |
| 344.40 | 0.7000 | 0.6495 |
| 344.72 | 0.8000 | 0.6834 |
| 345.80 | 0.9000 | 0.7449 |
| 347.46 | 0.9500 | 0.8214 |
| 348.93 | 0.9750 | 0.8869 |

Kao, Chien-Ping Chai - Miller, Ralph N. - Sturgis, James F., Double Azeotropy in Binary Mixtures 1,1,1,2,3,4,4,5,5,5-Decafluoropentane + Tetrahydrofuran, Journal of Chemical & Engineering Data 2 (2001) 229-233. doi:10.1021/je000212b

**P / bar = 5.068**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 428.16 | 0.0258 | 0.1679 |
| 421.91 | 0.0557 | 0.2715 |
| 417.70 | 0.0724 | 0.3349 |
| 408.72 | 0.1235 | 0.4695 |
| 400.80 | 0.2103 | 0.5773 |
| 396.65 | 0.3343 | 0.6373 |
| 394.58 | 0.4640 | 0.6717 |
| 394.27 | 0.5285 | 0.6930 |
| 393.72 | 0.6612 | 0.7201 |
| 393.53 | 0.7139 | 0.7363 |
| 393.56 | 0.7818 | 0.7601 |
| 394.93 | 0.9202 | 0.8568 |
| 395.83 | 0.9488 | 0.8978 |
| 398.09 | 0.9906 | 0.9783 |

Kao, Chien-Ping Chai - Miller, Ralph N. - Sturgis, James F., Double Azeotropy in Binary Mixtures 1,1,1,2,3,4,4,5,5,5-Decafluoropentane + Tetrahydrofuran, Journal of Chemical & Engineering Data 2 (2001) 229-233. doi:10.1021/je000212b

**P / bar = 7.093**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 424.66 | 0.1348 | 0.4599 |
| 417.16 | 0.1960 | 0.5599 |
| 414.06 | 0.2402 | 0.6040 |
| 409.33 | 0.3596 | 0.6585 |
| 408.46 | 0.4136 | 0.6782 |
| 406.66 | 0.5668 | 0.7099 |
| 406.35 | 0.6108 | 0.7216 |
| 405.97 | 0.7262 | 0.7512 |
| 406.03 | 0.8311 | 0.7982 |
| 407.46 | 0.9288 | 0.8800 |

Kao, Chien-Ping Chai - Miller, Ralph N. - Sturgis, James F., Double Azeotropy in Binary Mixtures 1,1,1,2,3,4,4,5,5,5-Decafluoropentane + Tetrahydrofuran, Journal of Chemical & Engineering Data 2 (2001) 229-233. doi:10.1021/je000212b

**P / bar = 8.106**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 452.07 | 0.0314 | 0.1646 |
| 442.38 | 0.0751 | 0.3059 |
| 433.65 | 0.1292 | 0.4198 |
| 426.44 | 0.1990 | 0.5288 |
| 420.63 | 0.2732 | 0.6012 |
| 416.97 | 0.3347 | 0.6499 |

| | | |
|---|---|---|
| 414.28 | 0.4245 | 0.6815 |
| 412.10 | 0.5640 | 0.7090 |
| 411.62 | 0.6369 | 0.7315 |
| 411.12 | 0.7528 | 0.7688 |
| 411.15 | 0.8084 | 0.7917 |
| 411.85 | 0.8992 | 0.8571 |
| 412.59 | 0.9356 | 0.8940 |
| 414.23 | 0.9714 | 0.9464 |

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**Enthalpy of mixing**

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Lietzmann, Andreas - Loewen, Burkhard - Schulz, Siegfried, Excess Molar Enthalpies of Propanone + Heptane, Propanone + Ethanol, Ethanol + Heptane, and 2-Propanol + Water at 283.15, 298.15, 323.15, 343.15, and 363.15 K, Journal of Chemical & Engineering Data 4 (1994) 785-788. doi:10.1021/je00016a033

**T / K = 283.15**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 225.50 | 0.0530 |
| 289.60 | 0.1020 |
| 351.80 | 0.1520 |
| 381.60 | 0.1930 |
| 412.20 | 0.2470 |
| 433.50 | 0.2950 |
| 446.80 | 0.3530 |
| 451.20 | 0.3960 |
| 453.40 | 0.4440 |
| 456.20 | 0.5010 |
| 434.30 | 0.5560 |
| 420.60 | 0.6130 |
| 410.30 | 0.6530 |
| 386.00 | 0.7010 |
| 364.80 | 0.7530 |
| 321.90 | 0.8070 |
| 275.90 | 0.8520 |
| 212.90 | 0.9000 |
| 122.40 | 0.9500 |

Grosse-Wortmann, H. - Jost, W. - Wagner, H. Gg., Kalorimetrische Messungen am System Äthanol - Cyclohexan - n-Heptan, Zeitschrift für Physikalische Chemie 1_2 (1966) 74-93. doi:10.1524/zpch.1966.49.1_2.074

**T / K = 293.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 408.96 | 0.1085 |
| 532.68 | 0.2619 |
| 557.70 | 0.3301 |
| 553.46 | 0.4932 |
| 457.35 | 0.7020 |

van Ness, H.C. - Abbott, M.M., Excess enthalpy. Ethanol (ethyl alcohol)-n-hexane system, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1976)

**T / K = 303.15**

**P / bar = 2.100**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 186.40 | 0.0102 |
| 225.60 | 0.0141 |
| 267.60 | 0.0199 |
| 312.40 | 0.0281 |
| 398.40 | 0.0530 |
| 478.70 | 0.0894 |
| 547.50 | 0.1351 |
| 603.00 | 0.1882 |
| 639.60 | 0.2409 |
| 663.40 | 0.2974 |
| 674.20 | 0.3615 |
| 672.10 | 0.4243 |
| 659.70 | 0.4807 |
| 638.70 | 0.5373 |
| 613.90 | 0.5858 |
| 565.80 | 0.6562 |
| 443.70 | 0.7779 |
| 348.10 | 0.8468 |
| 253.40 | 0.8998 |
| 131.60 | 0.9540 |
| 25.60 | 0.9916 |

Mier, W. - Oswald, G. - Tusel-Langer, E. - Lichtenthaler, R.N., Excess Enthalpy HE of Binary Mixtures Containing Alkanes, Ethanol and Ethyl-Tert. Butyl Ether (ETBE), Berichte der Bunsengesellschaft für physikalische Chemie 9 (1995) 1123-1130. doi:10.1002/bbpc.199500043

**T / K = 313.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 404.00 | 0.0410 |
| 650.00 | 0.1170 |
| 772.00 | 0.2190 |
| 828.00 | 0.3070 |
| 833.00 | 0.3860 |
| 809.00 | 0.4560 |
| 788.00 | 0.5180 |

| | |
|---|---|
| 685.00 | 0.6260 |
| 585.00 | 0.7150 |
| 485.00 | 0.7900 |
| 433.00 | 0.8230 |
| 171.00 | 0.9460 |

Lietzmann, Andreas - Loewen, Burkhard - Schulz, Siegfried, Excess Molar Enthalpies of Propanone + Heptane, Propanone + Ethanol, Ethanol + Heptane, and 2-Propanol + Water at 283.15, 298.15, 323.15, 343.15, and 363.15 K, Journal of Chemical & Engineering Data 4 (1994) 785-788. doi:10.1021/je00016a033

**T / K = 323.15**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 803.70 | 0.1020 |
| 884.40 | 0.1520 |
| 933.80 | 0.1930 |
| 993.60 | 0.2470 |
| 1005.9 | 0.2950 |
| 1021.4 | 0.3530 |
| 1017.7 | 0.3960 |
| 1001.5 | 0.4440 |
| 959.00 | 0.5010 |
| 914.60 | 0.5560 |
| 855.80 | 0.6130 |
| 799.70 | 0.6530 |
| 734.70 | 0.7010 |
| 665.20 | 0.7530 |
| 560.20 | 0.8070 |
| 455.10 | 0.8520 |
| 327.30 | 0.9000 |

Lietzmann, Andreas - Loewen, Burkhard - Schulz, Siegfried, Excess Molar Enthalpies of Propanone + Heptane, Propanone + Ethanol, Ethanol + Heptane, and 2-Propanol + Water at 283.15, 298.15, 323.15, 343.15, and 363.15 K, Journal of Chemical & Engineering Data 4 (1994) 785-788. doi:10.1021/je00016a033

**T / K = 343.15**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 822.70 | 0.0480 |
| 1141.4 | 0.1020 |
| 1262.1 | 0.1520 |
| 1335.5 | 0.1930 |
| 1423.9 | 0.2470 |
| 1443.7 | 0.2950 |
| 1471.2 | 0.3530 |
| 1453.3 | 0.3960 |
| 1436.3 | 0.4440 |
| 1373.4 | 0.5010 |
| 1314.3 | 0.5560 |
| 1224.4 | 0.6130 |
| 1148.1 | 0.6530 |
| 1050.4 | 0.7010 |
| 923.50 | 0.7530 |
| 771.20 | 0.8070 |
| 624.60 | 0.8520 |
| 448.80 | 0.9000 |
| 247.00 | 0.9480 |

Lietzmann, Andreas - Loewen, Burkhard - Schulz, Siegfried, Excess Molar Enthalpies of Propanone + Heptane, Propanone + Ethanol, Ethanol + Heptane, and 2-Propanol + Water at 283.15, 298.15, 323.15, 343.15, and 363.15 K, Journal of Chemical & Engineering Data 4 (1994) 785-788. doi:10.1021/je00016a033

**T / K = 363.15**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 1373.7 | 0.1020 |
| 1572.8 | 0.1520 |
| 1676.7 | 0.1930 |
| 1818.6 | 0.2470 |
| 1852.0 | 0.2950 |
| 1883.9 | 0.3530 |
| 1882.0 | 0.3960 |
| 1843.2 | 0.4440 |
| 1773.4 | 0.5010 |
| 1680.6 | 0.5560 |
| 1565.3 | 0.6130 |
| 1459.8 | 0.6530 |
| 1323.2 | 0.7010 |
| 1174.3 | 0.7530 |
| 971.00 | 0.8070 |
| 779.70 | 0.8520 |
| 551.70 | 0.9000 |

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**Heat capacity of mixing**

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Tanaka, Reiji - Toyama, Satoru - Murakami, Sachio, Heat capacities of {xCnH2n+1OH + (1 − x)C7H16} for n = 1 to 6 at 298.15 K, The Journal of Chemical Thermodynamics 1 (1986) 63-73. doi:10.1016/0021-9614(86)90044-3

**T / K = 298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.0020 | 0.0014 |
| 0.0070 | 0.0015 |
| 0.1100 | 0.0033 |
| 0.2800 | 0.0042 |
| 0.5700 | 0.0052 |
| 1.200 | 0.0067 |
| 1.780 | 0.0080 |
| 2.700 | 0.0103 |
| 2.820 | 0.0106 |
| 3.000 | 0.0111 |
| 4.140 | 0.0148 |
| 4.860 | 0.0180 |
| 5.050 | 0.0186 |
| 5.960 | 0.0246 |
| 6.510 | 0.0288 |
| 7.870 | 0.0433 |
| 8.690 | 0.0568 |
| 8.780 | 0.0569 |
| 9.110 | 0.0654 |
| 10.29 | 0.0968 |
| 10.25 | 0.0982 |
| 11.27 | 0.1474 |
| 11.94 | 0.1975 |
| 12.25 | 0.2943 |
| 11.85 | 0.3872 |
| 9.200 | 0.5963 |
| 6.840 | 0.7177 |
| 5.460 | 0.7793 |
| 2.770 | 0.8901 |

Iguchi, A., Excess molal specific heat of nonelectrolyte solutions, Kagaku Sochi (1977) 64-65.

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 7.624 | 0.0418 |
| 10.26 | 0.1007 |
| 11.71 | 0.1875 |
| 12.09 | 0.2997 |
| 11.52 | 0.4087 |
| 10.54 | 0.5007 |
| 9.047 | 0.6008 |
| 7.104 | 0.7036 |
| 4.900 | 0.8027 |
| 2.435 | 0.9021 |

Mier, W. - Lichtenthaler, R.N. - Roux, A.H. - Grolier, J.-P.E., Excess molar heat capacities CEp,m and excess molar volumes VEm of {x1CH3(CH2)5CH3 + x2CH3C(CH3)2CH2CH(CH3)CH3 + x3CH3C(CH3)2OC2H5 + (1 - x1 - x2 - x3)C2H5OH}(l) I. Binary and quaternary mixtures, The Journal of Chemical Thermodynamics 12 (1994) 1323-1334. doi:10.1006/jcht.1994.1151

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 7.481 | 0.0409 |
| 9.019 | 0.0657 |
| 11.45 | 0.1657 |
| 12.06 | 0.2499 |
| 11.99 | 0.3365 |
| 11.54 | 0.4165 |
| 10.55 | 0.5046 |
| 9.249 | 0.5933 |
| 7.670 | 0.6811 |
| 5.774 | 0.7697 |
| 3.733 | 0.8540 |
| 1.416 | 0.9443 |

Fortier, Jean-Luc - Benson, George C, Excess heat capacities of binary liquid mixtures determined with a Picker flow calorimeter, The Journal of Chemical Thermodynamics 5 (1976) 411-423. doi:10.1016/0021-9614(76)90061-6

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 5.402 | 0.0216 |
| 7.623 | 0.0418 |
| 9.060 | 0.0661 |
| 10.26 | 0.1007 |
| 11.27 | 0.1506 |
| 11.71 | 0.1875 |
| 12.09 | 0.2997 |
| 11.52 | 0.4087 |
| 10.54 | 0.5007 |
| 9.828 | 0.5520 |
| 9.047 | 0.6008 |
| 8.252 | 0.6453 |
| 7.104 | 0.7036 |
| 4.899 | 0.8027 |
| 2.435 | 0.9021 |

Klesper, I., Messung der spezifischen Wärmen binärer Flüssigkeitsgemische, Zeitschrift für Physikalische Chemie 1_2 (1966) 1-12. doi:10.1524/zpch.1966.51.1_2.001

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 6.236 | 0.0508 |
| 13.30 | 0.1972 |
| 12.47 | 0.5105 |
| 5.986 | 0.8010 |

Klesper, I., Messung der spezifischen Wärmen binärer Flüssigkeitsgemische, Zeitschrift für Physikalische Chemie 1_2 (1966) 1-12. doi:10.1524/zpch.1966.51.1_2.001

**T / K = 318.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 7.400 | 0.0508 |
| 15.88 | 0.1972 |
| 15.22 | 0.5105 |
| 7.566 | 0.8010 |

Klesper, I., Messung der spezifischen Wärmen binärer Flüssigkeitsgemische, Zeitschrift für Physikalische Chemie 1_2 (1966) 1-12. doi:10.1524/zpch.1966.51.1_2.001

**T / K = 328.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 8.647 | 0.0508 |
| 18.46 | 0.1972 |
| 18.13 | 0.5105 |
| 9.229 | 0.8010 |

Klesper, I., Messung der spezifischen Wärmen binärer Flüssigkeitsgemische, Zeitschrift für Physikalische Chemie 1_2 (1966) 1-12. doi:10.1524/zpch.1966.51.1_2.001

**T / K = 338.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 9.977 | 0.0508 |
| 21.04 | 0.1972 |
| 21.20 | 0.5105 |
| 11.14 | 0.8010 |

Klesper, I., Messung der spezifischen Wärmen binärer Flüssigkeitsgemische, Zeitschrift für Physikalische Chemie 1_2 (1966) 1-12. doi:10.1524/zpch.1966.51.1_2.001

**T / K = 343.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 10.73 | 0.0508 |
| 22.28 | 0.1972 |
| 22.86 | 0.5105 |
| 12.06 | 0.8010 |

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**Critical point**

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Soo, Chien-Bin - Théveneau, Pascal - Coquelet, Christophe - Ramjugernath, Deresh - Richon, Dominique, Determination of critical properties of pure and multi-component mixtures using a “dynamic–synthetic” apparatus, The Journal of Supercritical Fluids 2 (2010) 545-553. doi:10.1016/j.supflu.2010.10.022

| T / K | P / bar | $x_1$ |
|---|---|---|
| 513.83 | 42.49 | 0.4679 |
| 508.59 | 44.95 | 0.5656 |
| 504.67 | 47.60 | 0.6768 |
| 503.82 | 50.50 | 0.7757 |
| 504.75 | 52.39 | 0.8303 |
| 509.28 | 57.35 | 0.9348 |

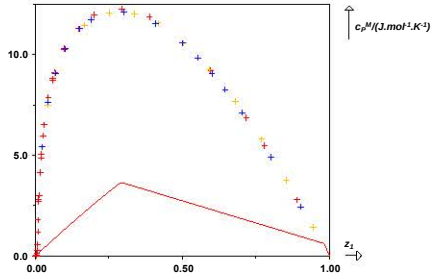
Wang, Lipu - Han, Kewei - Xia, Shuqian - Ma, Peisheng - Yan, Fangyou, Measurement and correlation of critical properties for binary mixtures and ternary mixtures containing gasoline additives, The Journal of Chemical Thermodynamics (2014) 161-168. doi:10.1016/j.jct.2014.01.025

| T / K | P / bar | $x_1$ |
|---|---|---|
| 532.40 | 32.17 | 0.1014 |
| 526.20 | 36.08 | 0.2052 |
| 520.00 | 39.22 | 0.3000 |
| 514.70 | 42.17 | 0.4018 |
| 510.60 | 43.91 | 0.4687 |
| 507.90 | 46.04 | 0.5651 |
| 504.60 | 48.17 | 0.6770 |
| 504.80 | 52.60 | 0.8305 |
| 507.40 | 56.23 | 0.9136 |

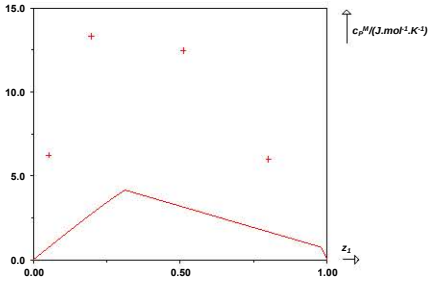
Seo, Jungha - Lee, Jongcheon - Kim, Hwayong, Measurement and Correlation of Vapor−Liquid Equilibria for the 2-Propanol + n-Hexane System near the Critical Region, Journal of Chemical & Engineering Data 4 (2003) 856-859. doi:10.1021/je025604s

| T / K | P / bar | $x_1$ |
|---|---|---|
| 508.15 | 44.80 | 0.5290 |

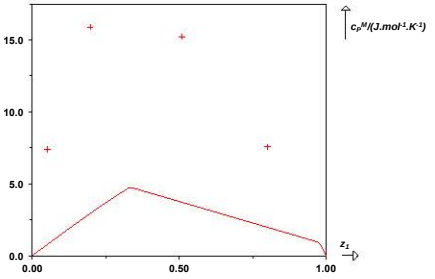
T/K = 298.15 - P/bar = 1.0132 1.0132 1.0132 1.0132



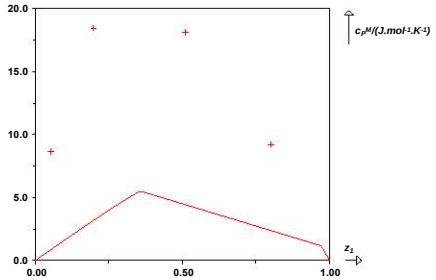

T/K = 308.15 - P/bar = 1.0132



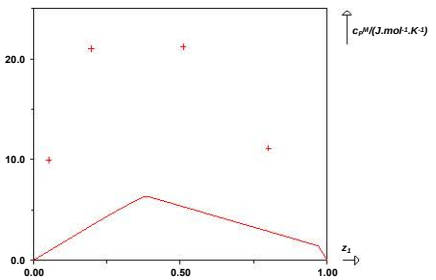

T/K = 318.15 - P/bar = 1.0132



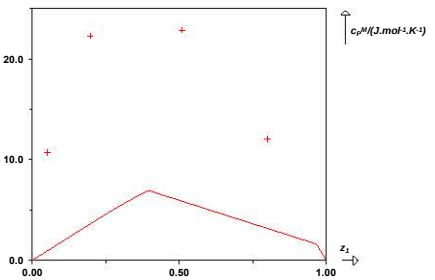

T/K = 328.15 - P/bar = 1.0132



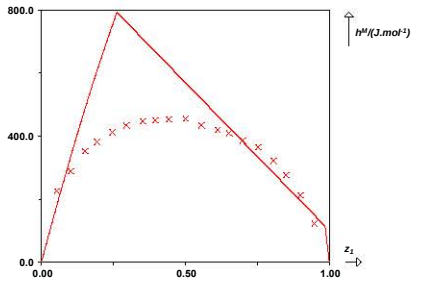

T/K = 338.15 - P/bar = 1.0132



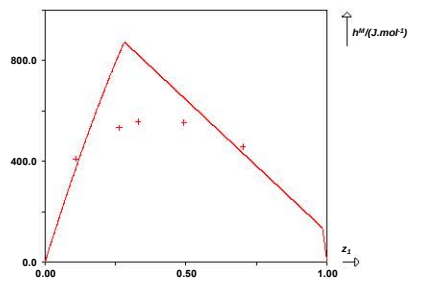

T/K = 343.15 - P/bar = 1.0132



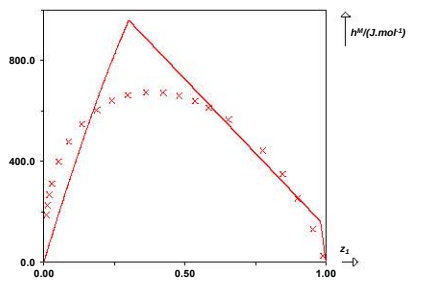

T/K = 283.15 - P/bar = 4.00



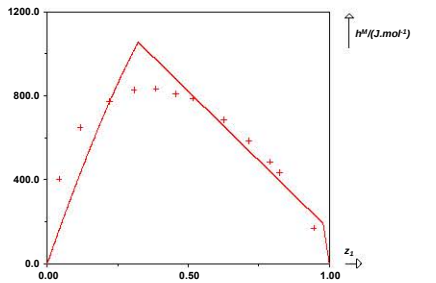

T/K = 293.15 - P/bar = 1.0132



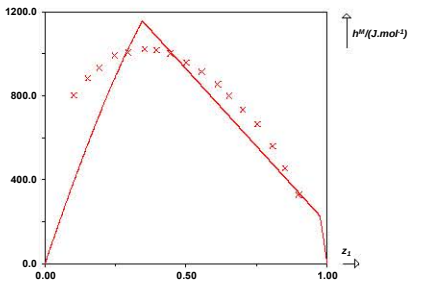

T/K = 303.15 - P/bar = 2.100



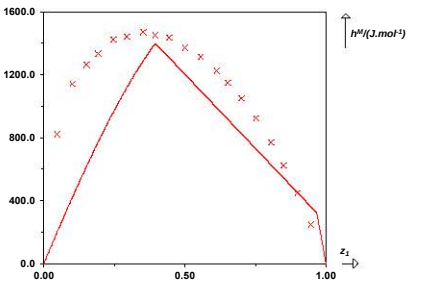

T/K = 313.15 - P/bar = 1.0132



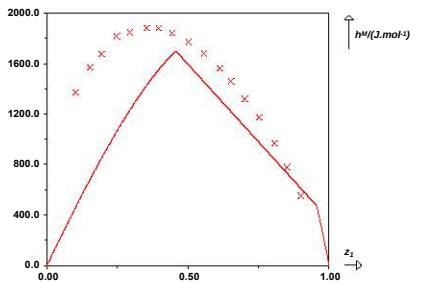

T/K = 323.15 - P/bar = 4.00



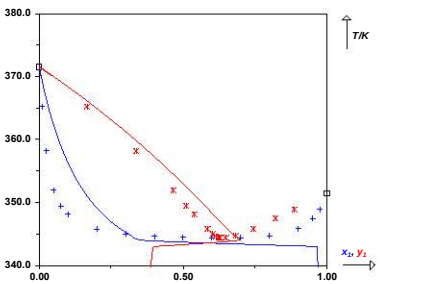

T/K = 343.15 - P/bar = 4.00



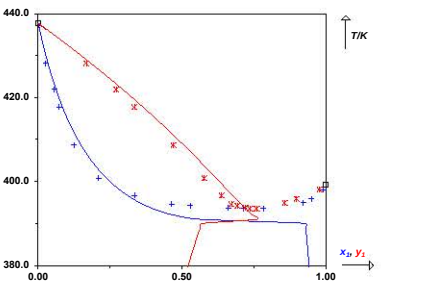

T/K = 363.15 - P/bar = 4.00



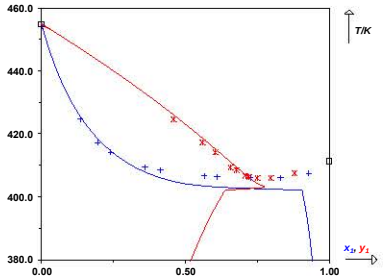

P/bar = 1.01330



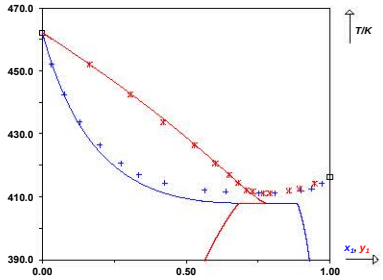

P/bar = 5.06800



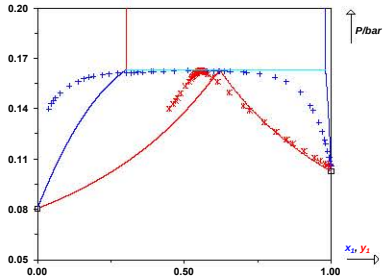
P/bar = 7.09300



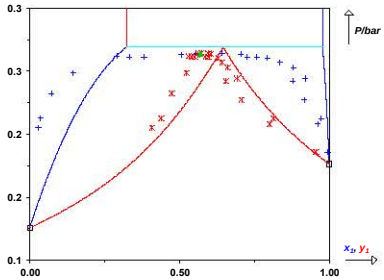

P/bar = 8.10600



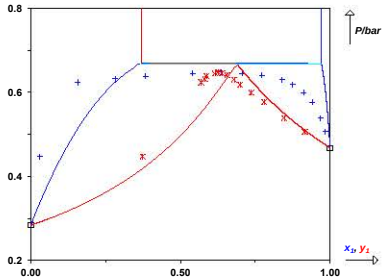

T/K = 303.27



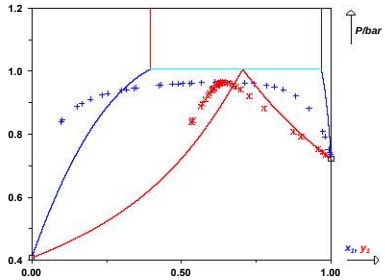

T/K = 313.15



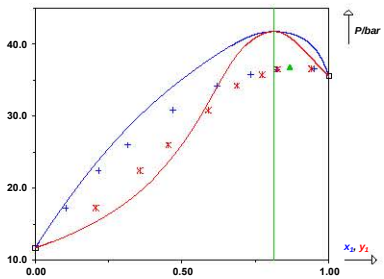

T/K = 333.15



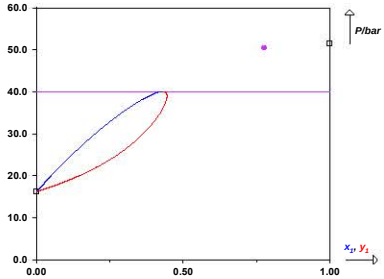

T/K = 343.17



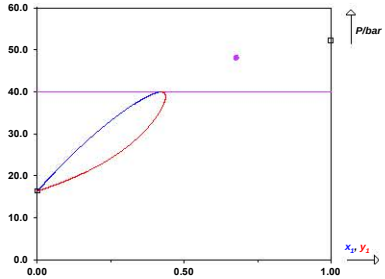

T/K = 483.15



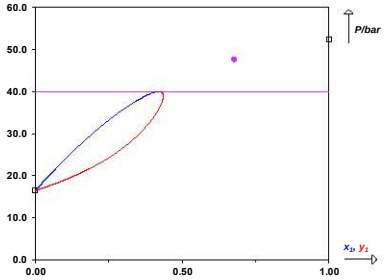

T/K = 503.82



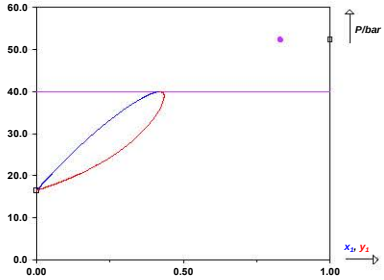

T/K = 504.60



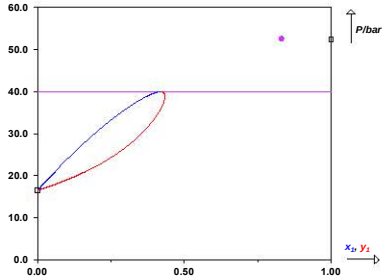

T/K = 504.67



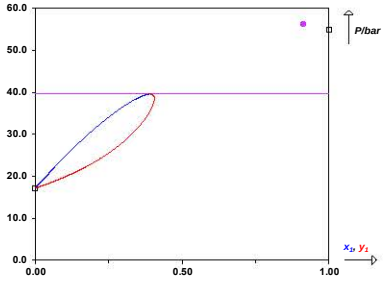

T/K = 504.75



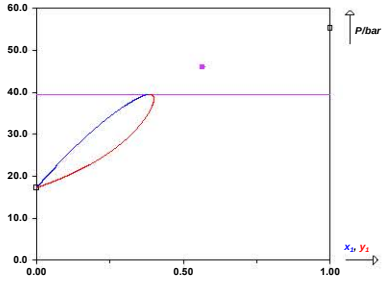

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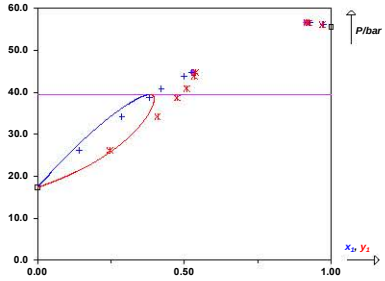

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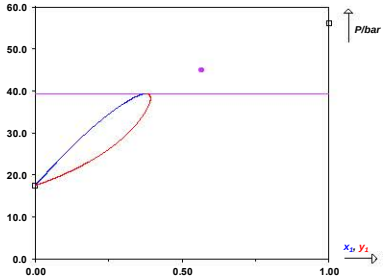

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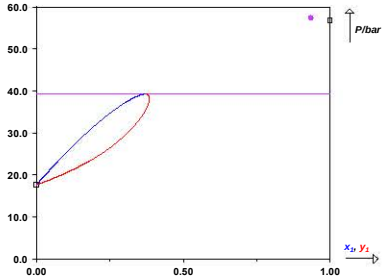

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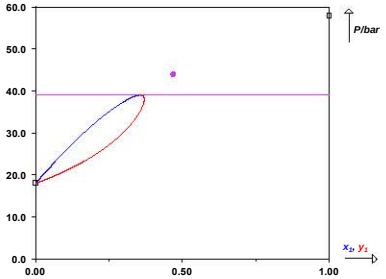
T/K = 508.59



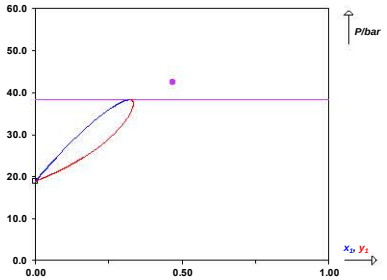

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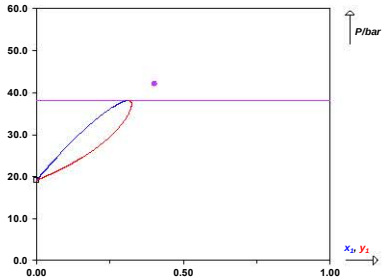

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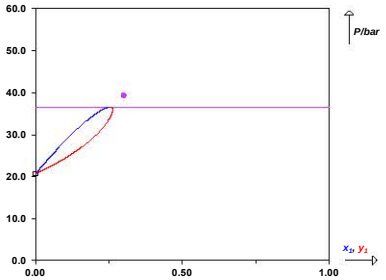

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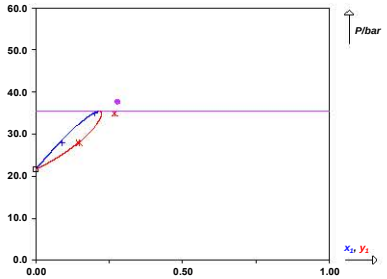

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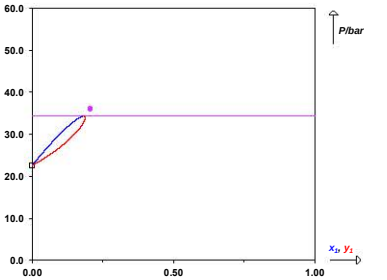

T/K = 520.00



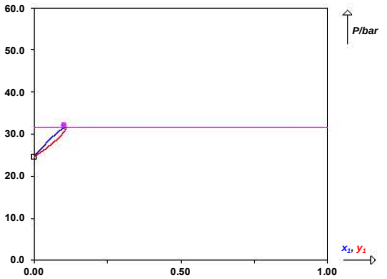

T/K = 523.15




T/K = 526.20




T/K = 532.40



## METHANOL (1) + n-HEXANE (2)

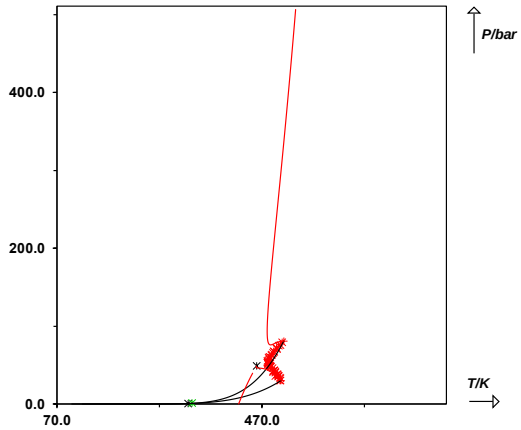
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 110-54-3 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | VLKZOEOYAKHREP-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.50 | 507.60 |
| **$P_c$ / bar** | 80.84 | 30.25 |
| **ω** | 0.566 | 0.301 |

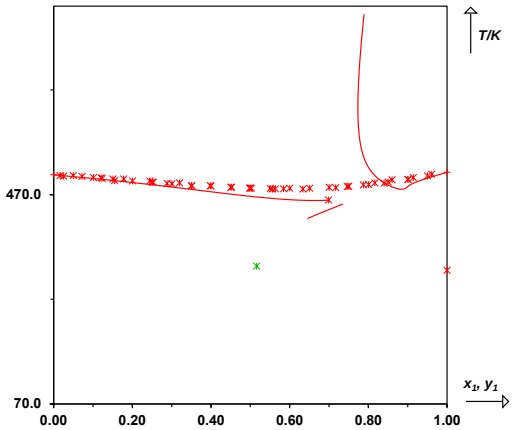
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 1160
B/MPa = 1470

*Deviations*
MAPE on x = 54 %
MAPE on y = 3.3 %
MAPE on $h^M$ = 54 %
MAPE on $c_P^M$ = 100 %



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**Isothermal phase equilibrium data**

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Scheller, M. - Schuberth, H. - Könnecke, H. G., Ergebnisse von Dampf-Flüssigkeits-Phasengleichgewichtsuntersuchungen am System n-Hexan/Methylcyclohexan/Methanol bei 60°C, Journal für Praktische Chemie 6 (1969) 974-982. doi:10.1002/prac.19693110616

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 1.075 | 0.0050 | 0.2850 | |
| 1.309 | 0.0160 | 0.4070 | |
| 1.380 | 0.0330 | 0.4380 | |
| 1.419 | 0.0600 | 0.4630 | |
| 1.435 | 0.0790 | 0.4720 | |
| 1.451 | 0.0980 | 0.4820 | |
| 1.472 | 0.1450 | 0.4880 | |
| 1.483 | 0.1750 | 0.4960 | |
| 1.490 | 0.2180 | 0.4990 | |
| 1.494 | 0.3990 | 0.5120 | |
| 1.496 | 0.4790 | 0.5160 | |
| 1.496 | 0.5160 | 0.5160 | AZEO |
| 1.496 | 0.5220 | 0.5170 | |
| 1.495 | 0.5700 | 0.5200 | |
| 1.494 | 0.6130 | 0.5210 | |
| 1.493 | 0.6570 | 0.5220 | |
| 1.493 | 0.7330 | 0.5230 | |
| 1.490 | 0.7900 | 0.5240 | |
| 1.478 | 0.8280 | 0.5330 | |
| 1.450 | 0.8770 | 0.5400 | |
| 1.442 | 0.8830 | 0.5430 | |
| 1.418 | 0.9020 | 0.5610 | |
| 1.385 | 0.9190 | 0.5740 | |
| 1.316 | 0.9380 | 0.6160 | |
| 1.265 | 0.9510 | 0.6450 | |
| 1.216 | 0.9620 | 0.6810 | |
| 1.167 | 0.9670 | 0.7140 | |
| 1.115 | 0.9790 | 0.7520 | |
| 1.105 | 0.9800 | 0.7630 | |

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**Isobaric phase equilibrium data**

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Blanco, Ana Maria - Ortega, Juan, Experimental study of miscibility, density and isobaric vapor-liquid equilibrium values for mixtures of methanol in hydrocarbons (C5, C6), Fluid Phase Equilibria 1-2 (1996) 207-222. doi:10.1016/0378-3812(96)03037-3

**P / bar = 1.413**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 346.60 | 0.0058 | 0.1815 |
| 343.75 | 0.0092 | 0.2555 |
| 340.21 | 0.0159 | 0.3334 |
| 337.17 | 0.0248 | 0.4011 |
| 335.80 | 0.0304 | 0.4289 |
| 334.24 | 0.0458 | 0.4550 |
| 332.70 | 0.0954 | 0.4813 |
| 331.83 | 0.1908 | 0.5042 |
| 331.59 | 0.2811 | 0.5091 |
| 331.53 | 0.6501 | 0.5160 |
| 331.84 | 0.8221 | 0.5282 |
| 332.15 | 0.8546 | 0.5358 |
| 333.07 | 0.9089 | 0.5704 |
| 334.37 | 0.9404 | 0.6116 |
| 338.48 | 0.9683 | 0.7183 |
| 341.23 | 0.9811 | 0.7906 |
| 343.53 | 0.9905 | 0.8826 |

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**Enthalpy of mixing**

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Kurihara, Kiyofumi - Iguchi, Takao - Banaka, Toshiaki - Ochi, Kenji - Kojima, Kazuo, Measurement and correlation of excess molar enthalpies for the partially miscible systems 2-butanone+water and methanol+hexane, Fluid Phase Equilibria 1-2 (2001) 59-69. doi:10.1016/S0378-3812(00)00510-0

**T / K = 283.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 151.40 | 0.0400 |
| 166.20 | 0.0500 |
| 201.20 | 0.0600 |
| 221.20 | 0.0700 |
| 244.30 | 0.0800 |
| 262.60 | 0.0900 |
| 278.40 | 0.1000 |
| 300.00 | 0.1100 |
| 304.20 | 0.1200 |
| 319.40 | 0.1300 |
| 329.60 | 0.2000 |
| 336.30 | 0.3000 |
| 343.00 | 0.4010 |
| 357.40 | 0.5000 |
| 366.40 | 0.6000 |
| 369.50 | 0.7000 |
| 380.30 | 0.8000 |
| 374.40 | 0.8500 |

| | |
|---|---|
| 362.70 | 0.8600 |
| 344.30 | 0.8800 |
| 300.80 | 0.9000 |
| 272.90 | 0.9200 |
| 208.50 | 0.9400 |
| 150.00 | 0.9600 |

Kurihara, Kiyofumi - Iguchi, Takao - Banaka, Toshiaki - Ochi, Kenji - Kojima, Kazuo, Measurement and correlation of excess molar enthalpies for the partially miscible systems 2-butanone+water and methanol+hexane, Fluid Phase Equilibria 1-2 (2001) 59-69. doi:10.1016/S0378-3812(00)00510-0

**T / K = 293.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 250.90 | 0.0600 |
| 324.80 | 0.1000 |
| 376.80 | 0.1400 |
| 420.00 | 0.1900 |
| 454.20 | 0.4000 |
| 458.90 | 0.5000 |
| 460.30 | 0.6000 |
| 463.50 | 0.7000 |
| 423.00 | 0.8200 |
| 332.40 | 0.9000 |
| 251.10 | 0.9300 |

van Ness, H.C. - Abbott, M.M., Excess enthalpy. Ethanol (ethyl alcohol)-n-hexane system, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1976)

**T / K = 303.15**

**P / bar = 2.100**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 176.00 | 0.0104 |
| 206.60 | 0.0141 |
| 234.50 | 0.0187 |
| 263.30 | 0.0249 |
| 288.70 | 0.0318 |
| 310.30 | 0.0388 |
| 329.80 | 0.0460 |
| 351.90 | 0.0562 |
| 430.10 | 0.1010 |
| 488.40 | 0.1503 |
| 529.20 | 0.1968 |
| 579.60 | 0.2892 |
| 583.10 | 0.3004 |
| 587.70 | 0.3143 |
| 588.00 | 0.3187 |
| 533.00 | 0.7492 |
| 525.70 | 0.7605 |
| 518.20 | 0.7701 |
| 503.70 | 0.7872 |
| 479.50 | 0.8112 |
| 449.90 | 0.8352 |
| 415.20 | 0.8587 |
| 359.90 | 0.8888 |
| 312.70 | 0.9101 |
| 256.00 | 0.9317 |
| 208.30 | 0.9474 |
| 152.50 | 0.9637 |
| 92.50 | 0.9792 |

van Ness, H.C. - Abbott, M.M., Excess enthalpy. Ethanol (ethyl alcohol)-n-hexane system, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1976)

**T / K = 313.15**

**P / bar = 2.100**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 384.20 | 0.0294 |
| 531.00 | 0.0985 |
| 656.80 | 0.2127 |
| 712.20 | 0.3515 |
| 714.90 | 0.4581 |
| 697.80 | 0.5510 |
| 676.30 | 0.6163 |
| 654.70 | 0.6629 |
| 635.40 | 0.6957 |
| 612.30 | 0.7280 |
| 592.70 | 0.7511 |
| 547.40 | 0.7945 |
| 521.90 | 0.8140 |
| 492.30 | 0.8339 |
| 452.90 | 0.8568 |
| 411.40 | 0.8775 |
| 354.20 | 0.9023 |
| 291.80 | 0.9252 |
| 231.60 | 0.9442 |
| 161.50 | 0.9636 |
| 110.00 | 0.9762 |

van Ness, H.C. - Abbott, M.M., Excess enthalpy. Ethanol (ethyl alcohol)-n-hexane system, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1976)

**T / K = 323.15**

**P / bar = 2.100**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 410.60 | 0.0284 |
| 663.70 | 0.1044 |

| | |
|---|---|
| 804.10 | 0.2272 |
| 848.70 | 0.3714 |
| 837.30 | 0.4759 |
| 806.60 | 0.5622 |
| 775.10 | 0.6206 |
| 745.10 | 0.6634 |
| 718.30 | 0.6959 |
| 691.10 | 0.7240 |
| 669.70 | 0.7438 |
| 619.30 | 0.7848 |
| 594.20 | 0.8016 |
| 559.90 | 0.8225 |
| 523.90 | 0.8418 |
| 472.00 | 0.8664 |
| 417.10 | 0.8891 |
| 348.80 | 0.9137 |
| 259.80 | 0.9408 |
| 177.30 | 0.9622 |

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**Heat capacity of mixing**

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Andreoli-Ball, Lina - Patterson, Donald - Costas, Miguel - Cáceres-Alonso, Mercedes, Heat capacity and corresponding states in alkan-1-ol–n-alkane systems, Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases 11 (1988) doi:10.1039/f19888403991

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.0123 | 0.0011 |
| 0.3033 | 0.0032 |
| 0.9583 | 0.0051 |
| 1.834 | 0.0073 |
| 4.265 | 0.0160 |
| 4.676 | 0.0194 |
| 5.467 | 0.0244 |
| 5.501 | 0.0256 |
| 7.108 | 0.0512 |
| 7.406 | 0.0529 |
| 8.588 | 0.0998 |
| 9.291 | 0.1444 |
| 9.889 | 0.2279 |

Costas, Miguel - Patterson, Donald, Self-association of alcohols in inert solvents. Apparent heat capacities and volumes of linear alcohols in hydrocarbons, Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases 3 (1985) doi:10.1039/f19858100635

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.0200 | 0.0011 |
| 0.2900 | 0.0032 |
| 0.9400 | 0.0051 |
| 1.790 | 0.0073 |
| 2.430 | 0.0099 |
| 4.180 | 0.0160 |

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**Critical point**

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Gao, Liang - Hou, Zhenshan - Zhang, Haifei - He, Jun - Liu, Zhinmin - Zhang, Xiaogang - Han, Buxing, Critical Parameters of Hexane + Carbon Monoxide + Hydrogen and Hexane + Methanol + Carbon Monoxide + Hydrogen Mixtures in the Hexane-Rich Region, Journal of Chemical & Engineering Data 6 (2001) 1635-1637. doi:10.1021/je010146t

| T / K | P / bar | $x_1$ |
|---|---|---|
| 506.20 | 30.17 | 0.0155 |
| 505.40 | 30.09 | 0.0252 |

de Loos, Th.W. - Poot, W. - de Swaan Arons, J., Vapour-liquid equilibria and critical phenomena in methanol + n-alkane systems, Fluid Phase Equilibria (1988) 209-227. doi:10.1016/0378-3812(88)80060-8

| T / K | P / bar | $x_1$ |
|---|---|---|
| 498.75 | 71.30 | 0.9000 |
| 491.50 | 65.50 | 0.8400 |
| 485.50 | 60.30 | 0.7460 |
| 481.00 | 53.20 | 0.5630 |
| 482.05 | 51.60 | 0.5020 |
| 486.60 | 48.30 | 0.3500 |
| 493.60 | 43.20 | 0.2530 |
| 501.10 | 36.90 | 0.1230 |

Gil, Laura - Blanco, Sofía T. - Rivas, Clara - Laga, Eduardo - Fernández, Javier - Artal, Manuela - Velasco, Inmaculada, Experimental determination of the critical loci for {n-C6H14 or CO2+alkan-1-ol} mixtures. Evaluation of their critical and subcritical behavior using PC-SAFT EoS, The Journal of Supercritical Fluids (2012) 26-44. doi:10.1016/j.supflu.2012.07.008

| T / K | P / bar | $x_1$ |
|---|---|---|
| 505.84 | 75.77 | 0.9501 |
| 498.87 | 70.34 | 0.9000 |
| 493.72 | 66.82 | 0.8500 |

| | | |
|---|---|---|
| 489.17 | 63.01 | 0.8000 |
| 485.92 | 60.01 | 0.7499 |
| 483.56 | 57.67 | 0.7001 |
| 482.22 | 55.71 | 0.6501 |
| 481.85 | 53.88 | 0.6002 |
| 481.72 | 52.82 | 0.5502 |
| 482.54 | 51.63 | 0.5000 |
| 483.79 | 50.28 | 0.4498 |
| 486.31 | 48.76 | 0.3999 |
| 487.67 | 47.63 | 0.3504 |
| 490.40 | 45.72 | 0.3001 |
| 493.86 | 43.21 | 0.2504 |
| 496.26 | 41.31 | 0.1999 |
| 499.99 | 38.04 | 0.1501 |
| 502.72 | 35.56 | 0.1004 |
| 506.01 | 33.31 | 0.0498 |

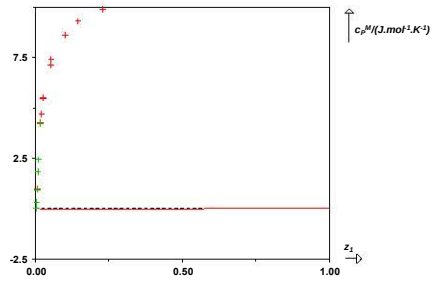
Liu, Jianguo - Qin, Zhangfeng - Wang, Guofu - Hou, Xianglin - Wang, Jianguo, Critical Properties of Binary and Ternary Mixtures of Hexane + Methanol, Hexane + Carbon Dioxide, Methanol + Carbon Dioxide, and Hexane + Carbon Dioxide + Methanol, Journal of Chemical & Engineering Data 6 (2003) 1610-1613. doi:10.1021/je034127q

| T / K | P / bar | $x_1$ |
|---|---|---|
| 504.60 | 33.50 | 0.0720 |
| 502.00 | 35.40 | 0.1200 |
| 499.80 | 37.90 | 0.1780 |
| 495.90 | 40.10 | 0.2440 |
| 492.10 | 42.00 | 0.3200 |
| 486.70 | 48.10 | 0.3980 |
| 484.30 | 49.10 | 0.4520 |
| 481.90 | 51.00 | 0.4980 |
| 480.60 | 53.20 | 0.5550 |
| 480.40 | 55.20 | 0.6330 |
| 483.30 | 59.40 | 0.7170 |
| 488.60 | 62.70 | 0.7870 |
| 492.50 | 67.50 | 0.8160 |
| 498.00 | 71.90 | 0.8600 |
| 502.50 | 75.20 | 0.9140 |
| 508.90 | 79.10 | 0.9610 |

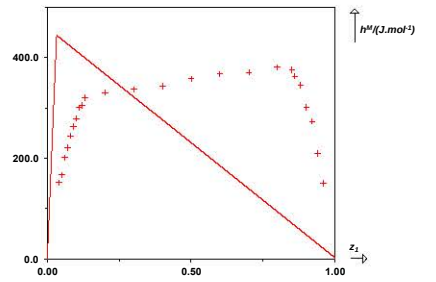
Zawisza, Andrzej, High-pressure liquid-vapour equilibria, critical state, and p(Vm, T, x) to 448.15 K and 4.053 MPa for {xC6H14 + (1−x)CH3OH}, The Journal of Chemical Thermodynamics 10 (1985) 941-947. doi:10.1016/0021-9614(85)90007-2

| T / K | P / bar | $x_1$ |
|---|---|---|
| 481.10 | 53.83 | 0.5842 |
| 491.08 | 41.01 | 0.2883 |
| 496.31 | 35.70 | 0.1547 |

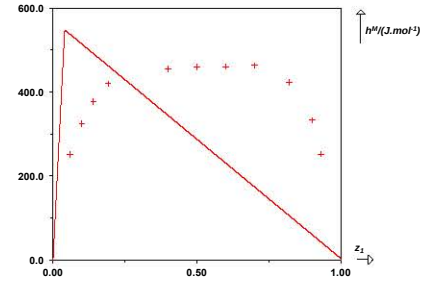
T/K = 298.15 - P/bar = 1.0132 1.0132



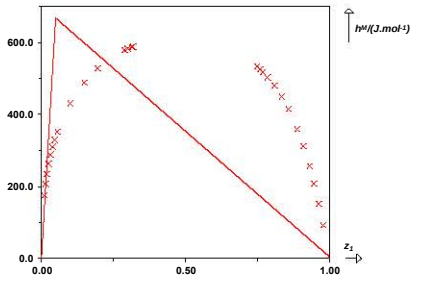

T/K = 283.15 - P/bar = 1.0132



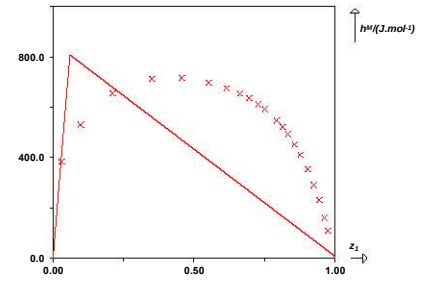

T/K = 293.15 - P/bar = 1.0132



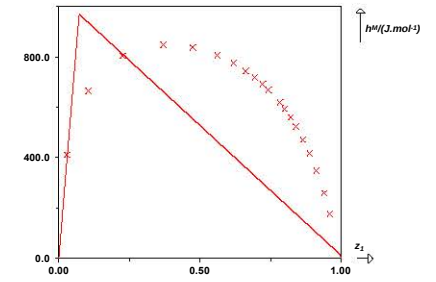

T/K = 303.15 - P/bar = 2.100



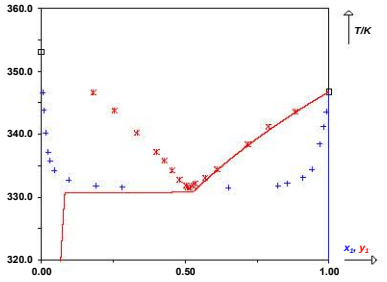

T/K = 313.15 - P/bar = 2.100



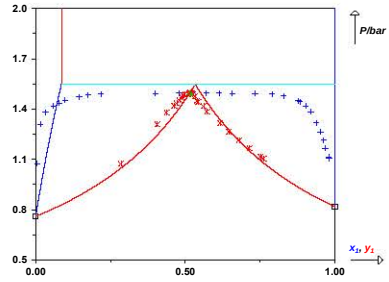

T/K = 323.15 - P/bar = 2.100



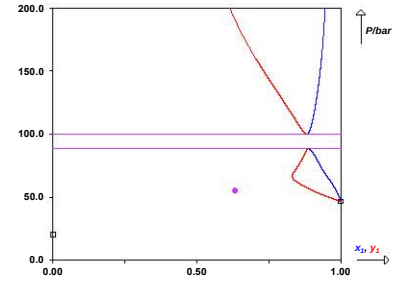

P/bar = 1.41330



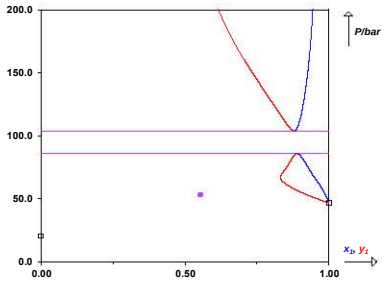

T/K = 333.15



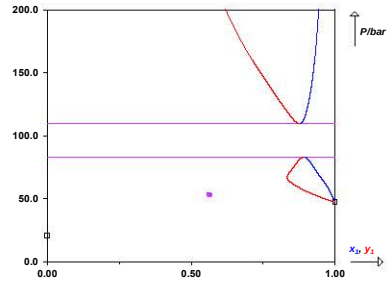

T/K = 480.40



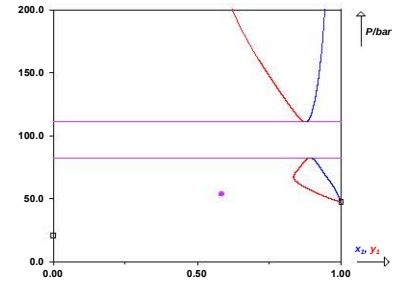

T/K = 480.60



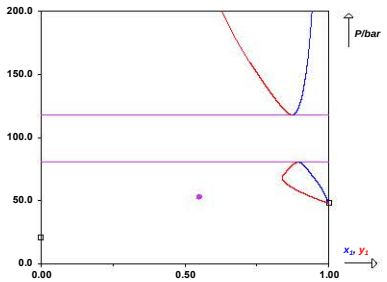

T/K = 481.00



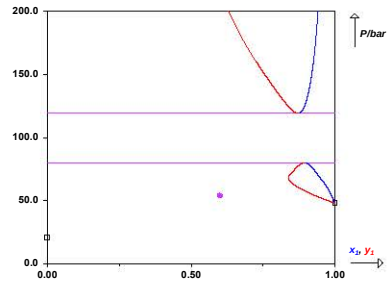

T/K = 481.10



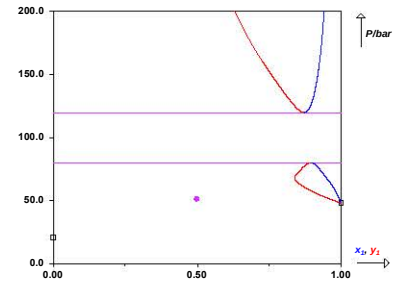

T/K = 481.72



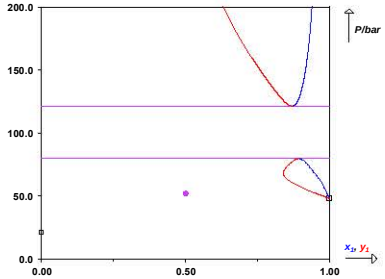

T/K = 481.85



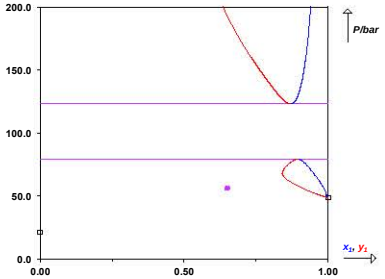

T/K = 481.90



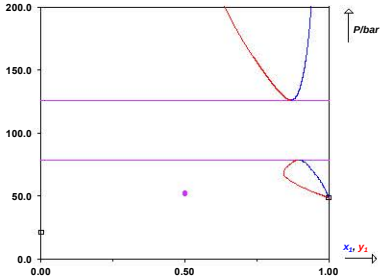
T/K = 482.05



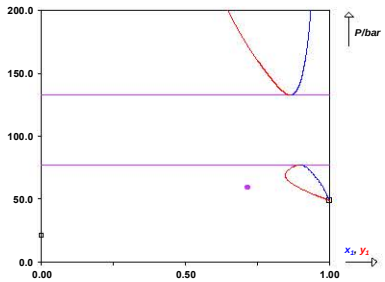

T/K = 482.22



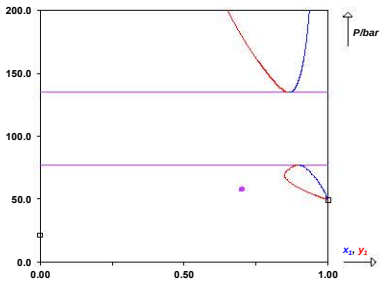

T/K = 482.54



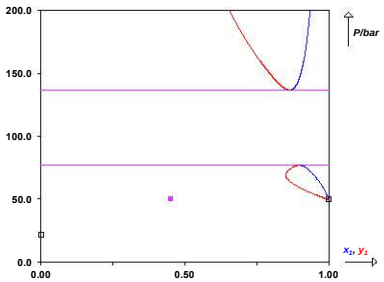

T/K = 483.30



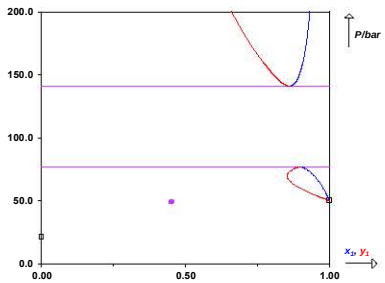

T/K = 483.56



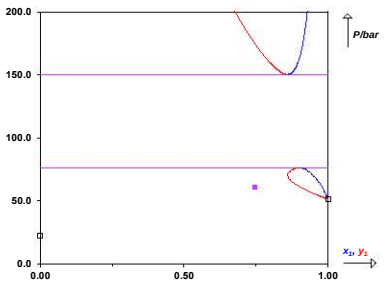

T/K = 483.79



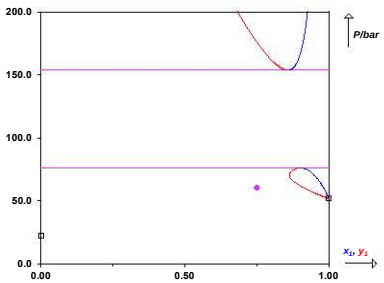

T/K = 484.30



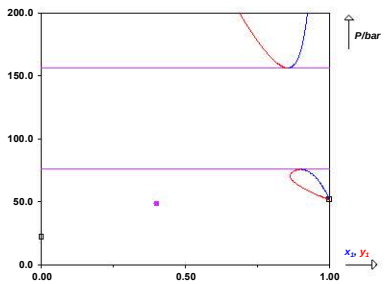

T/K = 485.50



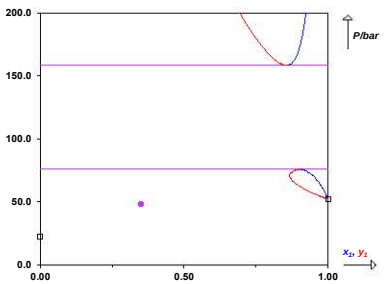

T/K = 485.92



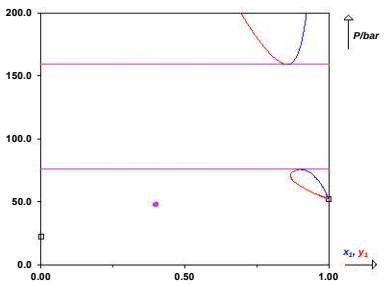

T/K = 486.31



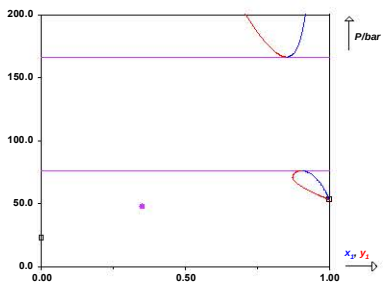

T/K = 486.60



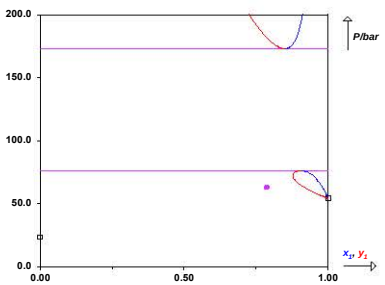

T/K = 486.70



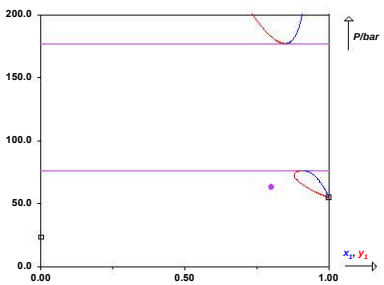

T/K = 487.67



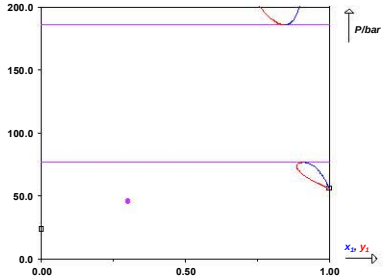

T/K = 488.60



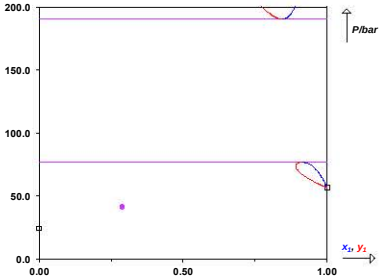

T/K = 489.17



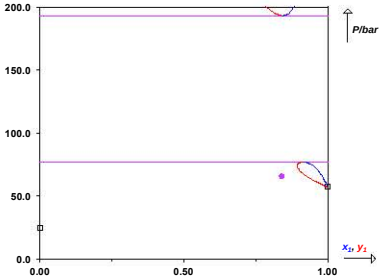
T/K = 490.40



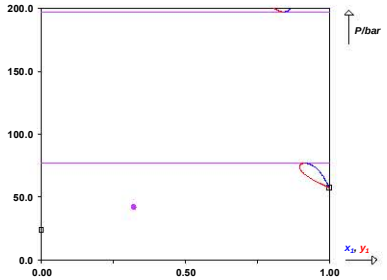

T/K = 491.08



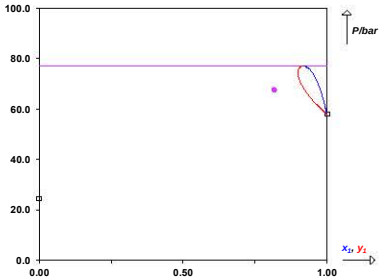

T/K = 491.50



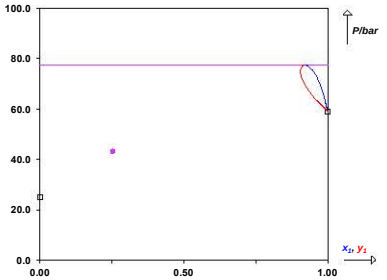

T/K = 492.10



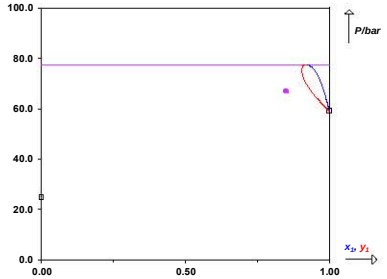

T/K = 492.50



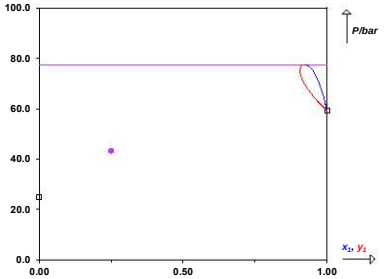

T/K = 493.60



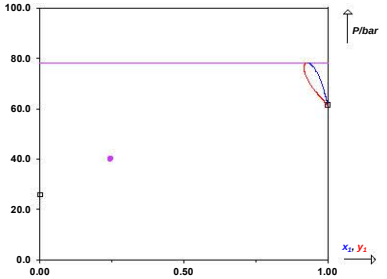

T/K = 493.72



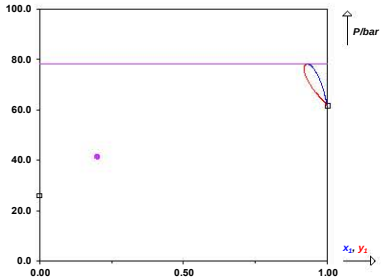

T/K = 493.86



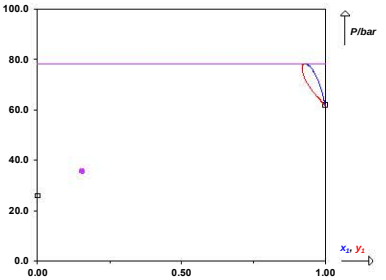

T/K = 495.90



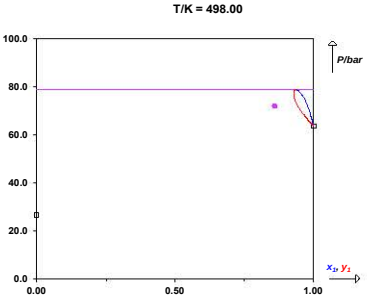

T/K = 496.26



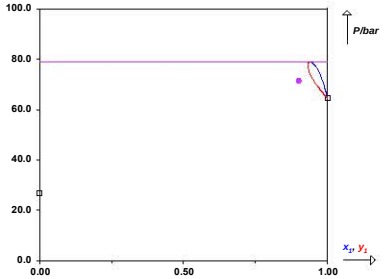

T/K = 496.31



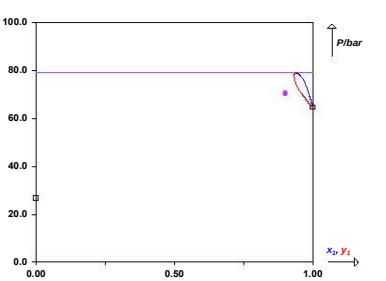

T/K = 498.00



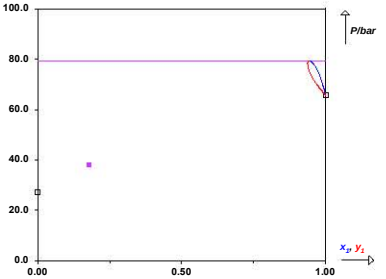

T/K = 498.75



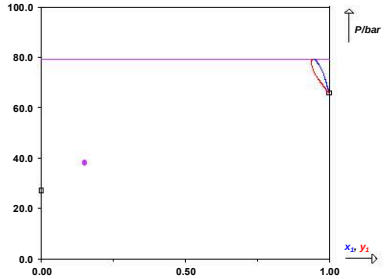

T/K = 498.87



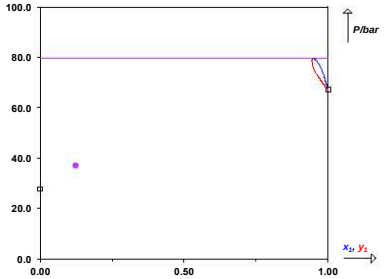

T/K = 499.80



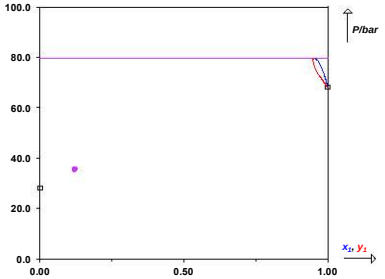
T/K = 499.99



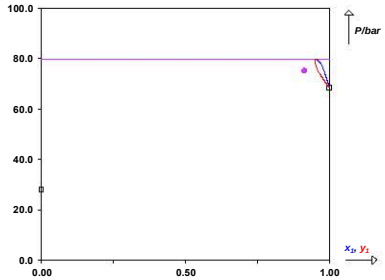

T/K = 501.10



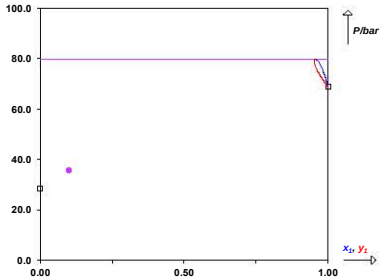

T/K = 502.00



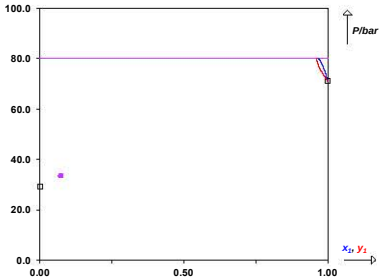

T/K = 502.50



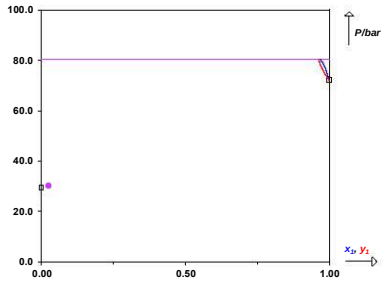

T/K = 502.72



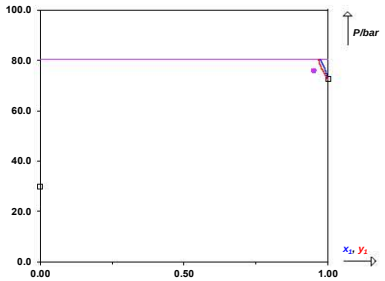

T/K = 504.60



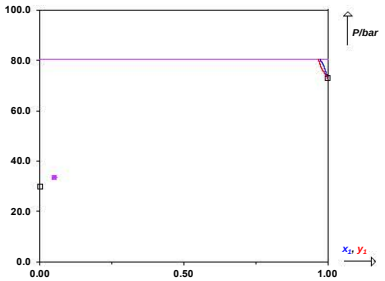

T/K = 505.40



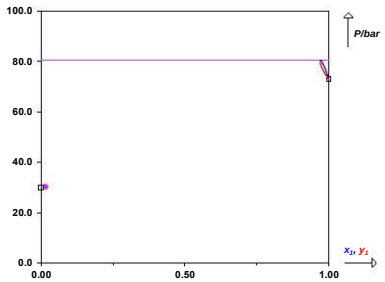

T/K = 505.84



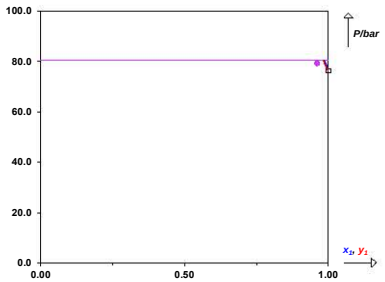

T/K = 506.01




T/K = 506.20




T/K = 508.90



## METHANOL (1) + BENZENE (2)

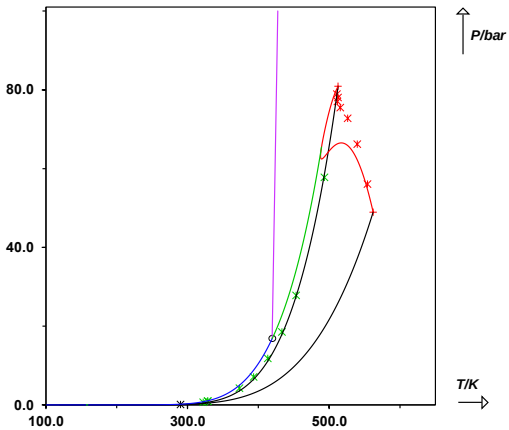
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 71-43-2 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | UHOVQNZJYSORNB-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.50 | 562.05 |
| **$P_c$ / bar** | 80.84 | 48.95 |
| **ω** | 0.566 | 0.210 |

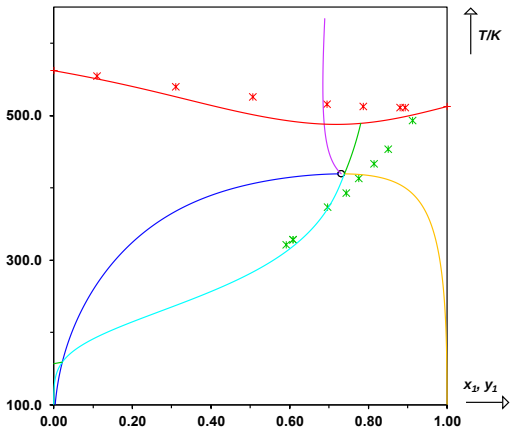
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 770
B/MPa = 542

*Deviations*
MAPE on x = 47 %
MAPE on y = 16 %
MAPE on $x_c$ = 56 %
MAPE on $P_c$ = 11 %
MAPE on $x_{az}$ = 29 %
MAPE on $P_{az}$ = 23 %
MAPE on $h^M$ = 27 %



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**Isothermal phase equilibrium data**

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Toghiani, Hossein - Toghiani, Rebecca K. - Viswanath, Dabir S., Vapor-liquid equilibria for the methanol-benzene and methanol-thiophene systems, Journal of Chemical & Engineering Data 1 (1994) 63-67. doi:10.1021/je00013a018

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3274 | 0.0037 | 0.0882 |
| 0.3536 | 0.0102 | 0.1567 |
| 0.3859 | 0.0161 | 0.2364 |
| 0.4096 | 0.0207 | 0.2794 |
| 0.4423 | 0.0314 | 0.3391 |
| 0.4683 | 0.0431 | 0.3794 |
| 0.5049 | 0.0613 | 0.4306 |
| 0.5322 | 0.0854 | 0.4642 |
| 0.5557 | 0.1263 | 0.4921 |
| 0.5745 | 0.1811 | 0.5171 |
| 0.5843 | 0.2334 | 0.5288 |
| 0.5940 | 0.3217 | 0.5450 |
| 0.5980 | 0.3805 | 0.5538 |
| 0.6002 | 0.4201 | 0.5590 |
| 0.6024 | 0.4746 | 0.5673 |
| 0.6042 | 0.5420 | 0.5783 |
| 0.6044 | 0.5716 | 0.5821 |
| 0.6042 | 0.6164 | 0.5908 |
| 0.6035 | 0.6509 | 0.5990 |
| 0.6022 | 0.6793 | 0.6067 |
| 0.5987 | 0.7259 | 0.6216 |
| 0.5948 | 0.7575 | 0.6346 |
| 0.5832 | 0.8171 | 0.6681 |
| 0.5621 | 0.8744 | 0.7181 |
| 0.5469 | 0.9033 | 0.7525 |
| 0.5304 | 0.9264 | 0.7896 |
| 0.5101 | 0.9497 | 0.8368 |
| 0.5005 | 0.9594 | 0.8599 |
| 0.4877 | 0.9707 | 0.8916 |
| 0.4754 | 0.9804 | 0.9222 |
| 0.4623 | 0.9895 | 0.9558 |

Strubl, K. - Svoboda, V. - Holub, R., Liquid-vapour equilibrium. LV. The system methanol-benzene, Collection of Czechoslovak Chemical Communications 11 (1972) 3522-3531. doi:10.1135/cccc19723522

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3168 | 0.0032 | 0.0555 |
| 0.3272 | 0.0051 | 0.0869 |
| 0.3494 | 0.0100 | 0.1527 |
| 0.3968 | 0.0227 | 0.2523 |
| 0.4149 | 0.0272 | 0.2909 |
| 0.4314 | 0.0317 | 0.3072 |
| 0.4670 | 0.0514 | 0.3775 |
| 0.4981 | 0.0634 | 0.4164 |
| 0.5160 | 0.0860 | 0.4412 |
| 0.5346 | 0.1014 | 0.4683 |
| 0.5548 | 0.1272 | 0.4899 |
| 0.5718 | 0.1538 | 0.5093 |
| 0.5894 | 0.2250 | 0.5325 |
| 0.5965 | 0.2701 | 0.5438 |
| 0.6044 | 0.3607 | 0.5588 |
| 0.6081 | 0.4721 | 0.5765 |
| 0.6110 | 0.5543 | 0.5899 |
| 0.6092 | 0.6316 | 0.6045 |
| 0.6064 | 0.7027 | 0.6249 |
| 0.6054 | 0.7245 | 0.6319 |
| 0.6038 | 0.7597 | 0.6437 |
| 0.5772 | 0.8680 | 0.7177 |
| 0.5493 | 0.9173 | 0.7786 |
| 0.4961 | 0.9730 | 0.9002 |
| 0.4737 | 0.9853 | 0.9397 |

Scatchard, George - Wood, Scott E. - Mochel, John M., Vapor-Liquid Equilibrium. VI. Benzene-Methanol Mixtures, Journal of the American Chemical Society 10 (1946) 1957-1960. doi:10.1021/ja01214a024

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.6211 | 0.0304 | 0.3019 | |
| 0.7028 | 0.0493 | 0.4051 | |
| 0.7966 | 0.1031 | 0.4841 | |
| 0.8856 | 0.3297 | 0.5540 | |
| 0.9008 | 0.4874 | 0.5845 | |
| 0.9013 | 0.4984 | 0.5858 | |
| 0.9045 | 0.6076 | 0.6078 | |
| 0.9045 | 0.6079 | 0.6079 | AZEO |
| 0.8865 | 0.7896 | 0.6716 | |
| 0.8297 | 0.9014 | 0.7697 | |

Butcher, K. L. - Medani, M. S., Thermodynamic properties of methanol-benzene mixtures at elevated temperatures, Journal of Applied Chemistry 4 (2007) 100-107. doi:10.1002/jctb.5010180402

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.123 | 0.0926 | 0.4577 |
| 3.468 | 0.1586 | 0.5324 |
| 3.834 | 0.3328 | 0.6075 |

| | | | |
|---|---|---|---|
| 4.054 | 0.4776 | 0.6422 | |
| 4.116 | 0.5940 | 0.6708 | |
| 4.178 | 0.6865 | 0.6929 | |
| 4.185 | 0.6961 | 0.6961 | AZEO |
| 4.164 | 0.7290 | 0.7084 | |
| 4.116 | 0.7747 | 0.7271 | |
| 4.027 | 0.8596 | 0.7868 | |
| 3.951 | 0.9065 | 0.8376 | |

Butcher, K. L. - Medani, M. S., Thermodynamic properties of methanol-benzene mixtures at elevated temperatures, Journal of Applied Chemistry 4 (2007) 100-107. doi:10.1002/jctb.5010180402

**T / K = 393.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 4.868 | 0.0865 | 0.4212 | |
| 5.633 | 0.1555 | 0.5162 | |
| 6.467 | 0.3253 | 0.6136 | |
| 6.819 | 0.4763 | 0.6578 | |
| 6.998 | 0.5870 | 0.6882 | |
| 7.122 | 0.6857 | 0.7167 | |
| 7.136 | 0.7430 | 0.7430 | AZEO |
| 7.109 | 0.7730 | 0.7597 | |
| 7.074 | 0.8070 | 0.7765 | |
| 7.012 | 0.8606 | 0.8171 | |
| 6.860 | 0.9148 | 0.8668 | |

Butcher, K. L. - Medani, M. S., Thermodynamic properties of methanol-benzene mixtures at elevated temperatures, Journal of Applied Chemistry 4 (2007) 100-107. doi:10.1002/jctb.5010180402

**T / K = 413.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 6.743 | 0.0619 | 0.3224 | |
| 8.446 | 0.1325 | 0.4633 | |
| 9.225 | 0.2018 | 0.5469 | |
| 10.32 | 0.3105 | 0.6127 | |
| 11.09 | 0.4560 | 0.6644 | |
| 11.45 | 0.5886 | 0.7073 | |
| 11.55 | 0.6845 | 0.7374 | |
| 11.87 | 0.7748 | 0.7748 | AZEO |
| 11.84 | 0.8095 | 0.7938 | |
| 11.72 | 0.8614 | 0.8317 | |
| 11.55 | 0.9159 | 0.8773 | |

Butcher, K. L. - Medani, M. S., Thermodynamic properties of methanol-benzene mixtures at elevated temperatures, Journal of Applied Chemistry 4 (2007) 100-107. doi:10.1002/jctb.5010180402

**T / K = 433.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 11.24 | 0.0943 | 0.3890 | |
| 13.01 | 0.1589 | 0.4873 | |
| 15.40 | 0.2967 | 0.5965 | |
| 16.86 | 0.4449 | 0.6645 | |
| 17.62 | 0.5721 | 0.7129 | |
| 18.04 | 0.6775 | 0.7487 | |
| 18.48 | 0.8140 | 0.8140 | AZEO |
| 18.44 | 0.8461 | 0.8328 | |
| 18.32 | 0.9176 | 0.8920 | |
| 17.96 | 0.9509 | 0.9287 | |

Butcher, K. L. - Medani, M. S., Thermodynamic properties of methanol-benzene mixtures at elevated temperatures, Journal of Applied Chemistry 4 (2007) 100-107. doi:10.1002/jctb.5010180402

**T / K = 453.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 15.22 | 0.0856 | 0.3361 | |
| 21.56 | 0.2790 | 0.5697 | |
| 25.75 | 0.5538 | 0.7131 | |
| 26.86 | 0.6632 | 0.7583 | |
| 27.68 | 0.8450 | 0.8555 | |
| 27.72 | 0.8500 | 0.8500 | AZEO |
| 27.61 | 0.8942 | 0.8915 | |
| 27.34 | 0.9511 | 0.9461 | |

Butcher, K. L. - Medani, M. S., Thermodynamic properties of methanol-benzene mixtures at elevated temperatures, Journal of Applied Chemistry 4 (2007) 100-107. doi:10.1002/jctb.5010180402

**T / K = 493.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 22.62 | 0.0233 | 0.1068 | |
| 27.20 | 0.0748 | 0.2626 | |
| 34.30 | 0.1778 | 0.4485 | |
| 42.71 | 0.3617 | 0.6044 | |
| 47.78 | 0.4996 | 0.6864 | |
| 57.72 | 0.9120 | 0.9120 | AZEO |

Butcher, K. L. - Medani, M. S., Thermodynamic properties of methanol-benzene mixtures at elevated temperatures, Journal of Applied Chemistry 4 (2007) 100-107. doi:10.1002/jctb.5010180402

**T / K = 493.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 52.30 | 0.6511 | 0.7606 |
| 55.19 | 0.7474 | 0.8117 |
| 56.61 | 0.8235 | 0.8569 |
| 57.64 | 0.8933 | 0.8999 |

| | | | |
|---|---|---|---|
| 57.72 | 0.9120 | 0.9120 | AZEO |
| 57.57 | 0.9521 | 0.9477 | |

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**Isobaric phase equilibrium data**

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Strubl, K. - Voňka, P. - Svoboda, V. - Holub, R., Liquid-vapour equilibrium LVI. Correlation of the benzene-methanol systems, Collection of Czechoslovak Chemical Communications 2 (1973) 468-476. doi:10.1135/cccc19730468

**P / bar = 0.3073**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 316.55 | 0.0052 | 0.0967 |
| 310.34 | 0.0257 | 0.3046 |
| 306.18 | 0.0660 | 0.4255 |
| 304.80 | 0.1116 | 0.4712 |
| 304.28 | 0.1454 | 0.4827 |
| 303.61 | 0.2005 | 0.5072 |
| 303.27 | 0.2532 | 0.5156 |
| 303.10 | 0.3214 | 0.5260 |
| 302.99 | 0.3752 | 0.5365 |
| 302.95 | 0.4278 | 0.5418 |
| 302.92 | 0.4626 | 0.5478 |
| 303.01 | 0.6510 | 0.5811 |
| 303.18 | 0.7142 | 0.5990 |
| 303.74 | 0.8104 | 0.6454 |
| 304.59 | 0.8778 | 0.7047 |
| 306.24 | 0.9371 | 0.7972 |
| 307.62 | 0.9662 | 0.8722 |
| 309.08 | 0.9847 | 0.9464 |
| 309.53 | 0.9933 | 0.9693 |
| 309.72 | 0.9956 | 0.9805 |

Toghiani, Hossein - Toghiani, Rebecca K. - Viswanath, Dabir S., Vapor-liquid equilibria for the methanol-benzene and methanol-thiophene systems, Journal of Chemical & Engineering Data 1 (1994) 63-67. doi:10.1021/je00013a018

**P / bar = 0.6952**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 340.72 | 0.0011 | 0.0274 |
| 339.75 | 0.0040 | 0.0576 |
| 336.89 | 0.0120 | 0.1504 |
| 334.34 | 0.0196 | 0.2236 |
| 332.89 | 0.0254 | 0.2698 |
| 330.84 | 0.0337 | 0.3257 |
| 329.23 | 0.0449 | 0.3650 |
| 328.07 | 0.0516 | 0.3951 |
| 327.04 | 0.0613 | 0.4201 |
| 325.94 | 0.0749 | 0.4463 |
| 324.92 | 0.0932 | 0.4694 |
| 324.01 | 0.1207 | 0.4950 |
| 323.02 | 0.1749 | 0.5177 |
| 322.38 | 0.2451 | 0.5363 |
| 321.92 | 0.3451 | 0.5540 |
| 321.65 | 0.4589 | 0.5692 |
| 321.54 | 0.5494 | 0.5839 |
| 321.53 | 0.5938 | 0.5923 |
| 321.54 | 0.6274 | 0.5993 |
| 321.58 | 0.6632 | 0.6087 |
| 321.65 | 0.7006 | 0.6198 |
| 321.84 | 0.7500 | 0.6382 |
| 322.20 | 0.8019 | 0.6651 |
| 322.82 | 0.8536 | 0.7046 |
| 323.67 | 0.8970 | 0.7532 |
| 324.23 | 0.9132 | 0.7825 |
| 325.12 | 0.9429 | 0.8296 |
| 325.83 | 0.9591 | 0.8669 |
| 326.53 | 0.9727 | 0.9035 |
| 327.20 | 0.9838 | 0.9385 |
| 327.55 | 0.9891 | 0.9568 |

Hudson, John W. - Van Winkle, Matthew, Multicomponent vapor-liquid equilibriums in systems of mixed positive and negative deviations, Journal of Chemical & Engineering Data 3 (1969) 310-318. doi:10.1021/je60042a025

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 343.82 | 0.0260 | 0.2670 |
| 339.59 | 0.0500 | 0.3710 |
| 336.02 | 0.0880 | 0.4570 |
| 333.35 | 0.1640 | 0.5260 |
| 331.79 | 0.3330 | 0.5590 |
| 331.17 | 0.5490 | 0.5950 |
| 331.25 | 0.6990 | 0.6330 |
| 331.62 | 0.7820 | 0.6650 |
| 333.05 | 0.8980 | 0.7600 |
| 335.86 | 0.9730 | 0.9070 |

Triday, J. - Andrade, A. - Aguirre Ode, F., Isobaric study of the binary systems formed by thiophene or benzene with light alcohols, Scientia Valparaiso (1978) 1-24.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 350.18 | 0.0100 | 0.1100 |
| 339.09 | 0.0540 | 0.3900 |
| 334.89 | 0.1020 | 0.4850 |
| 333.17 | 0.1650 | 0.5250 |

| | | |
|---|---|---|
| 332.01 | 0.2600 | 0.5560 |
| 331.63 | 0.3460 | 0.5680 |
| 331.45 | 0.4080 | 0.5780 |
| 331.27 | 0.4740 | 0.5880 |
| 331.20 | 0.5510 | 0.6020 |
| 331.12 | 0.6220 | 0.6120 |
| 331.14 | 0.6330 | 0.6190 |
| 331.23 | 0.7060 | 0.6400 |
| 331.30 | 0.7380 | 0.6500 |
| 331.74 | 0.8070 | 0.6850 |
| 332.77 | 0.8820 | 0.7480 |
| 333.85 | 0.9270 | 0.8060 |
| 335.01 | 0.9560 | 0.8680 |

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**Enthalpy of mixing**

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Cen, P. - Zhu, Z., The Measurement of Mixing Heat and the Prediction of Vapor-Liquid Equilibrium Data for Hydrocarbon - Alcohol Systems, Huagong Xuebao 1 (1984) 51-65.

**T / K =** **283.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 384.50 | 0.0877 |
| 451.60 | 0.1500 |
| 480.10 | 0.2076 |
| 497.20 | 0.2620 |
| 500.00 | 0.3121 |
| 497.70 | 0.3601 |
| 468.80 | 0.4468 |
| 428.10 | 0.5239 |
| 388.80 | 0.5930 |
| 344.70 | 0.6552 |
| 302.50 | 0.7115 |
| 255.90 | 0.7628 |
| 201.40 | 0.8096 |
| 155.30 | 0.8526 |
| 96.30 | 0.9108 |
| 43.80 | 0.9625 |

Cen, P. - Zhu, Z., The Measurement of Mixing Heat and the Prediction of Vapor-Liquid Equilibrium Data for Hydrocarbon - Alcohol Systems, Huagong Xuebao 1 (1984) 51-65.

**T / K =** **288.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 488.20 | 0.0877 |
| 562.10 | 0.1500 |
| 607.70 | 0.2076 |
| 620.70 | 0.2620 |
| 621.60 | 0.3121 |
| 616.30 | 0.3601 |
| 581.40 | 0.4468 |
| 538.50 | 0.5239 |
| 488.60 | 0.5930 |
| 428.60 | 0.6552 |
| 367.30 | 0.7115 |
| 305.40 | 0.7628 |
| 248.10 | 0.8096 |
| 197.00 | 0.8526 |
| 121.20 | 0.9108 |
| 53.90 | 0.9625 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K =** **293.15**

**P / bar =** **1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 229.21 | 0.0429 |
| 400.04 | 0.0839 |
| 519.12 | 0.1230 |
| 578.55 | 0.1604 |
| 609.77 | 0.1962 |
| 615.82 | 0.3545 |
| 556.50 | 0.4849 |
| 471.24 | 0.5942 |
| 381.06 | 0.6872 |
| 286.01 | 0.7672 |
| 196.51 | 0.8368 |
| 121.52 | 0.8978 |
| 52.58 | 0.9519 |

Zhao, J. - Dai, M., Studies on Thermodynamic Properties of Binary Systems containing Alcohols. I. Excess Enthalpies of C1 to C5 Normal Alcohols + Benzene, Wuli Huaxue Xuebao 2 (1986) 141-145.

**T / K =** **298.15**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 473.60 | 0.0577 |
| 594.50 | 0.0920 |
| 657.50 | 0.1250 |
| 714.20 | 0.1874 |
| 736.30 | 0.2454 |
| 744.30 | 0.2995 |

| | |
|---|---|
| 734.80 | 0.3500 |
| 693.70 | 0.4419 |
| 648.50 | 0.5037 |
| 599.40 | 0.5603 |
| 533.20 | 0.6287 |
| 462.30 | 0.6902 |
| 390.00 | 0.7458 |
| 318.70 | 0.7962 |
| 249.60 | 0.8423 |
| 187.40 | 0.8845 |
| 128.80 | 0.9232 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 303.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 253.39 | 0.0429 |
| 466.89 | 0.0839 |
| 611.74 | 0.1230 |
| 676.75 | 0.1604 |
| 713.74 | 0.1962 |
| 719.85 | 0.3545 |
| 645.35 | 0.4849 |
| 557.10 | 0.5942 |
| 445.51 | 0.6872 |
| 336.75 | 0.7672 |
| 234.25 | 0.8368 |
| 142.48 | 0.8978 |
| 59.46 | 0.9519 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 308.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 269.04 | 0.0429 |
| 497.94 | 0.0839 |
| 653.28 | 0.1230 |
| 738.16 | 0.1604 |
| 767.75 | 0.1962 |
| 767.39 | 0.3545 |
| 699.15 | 0.4849 |
| 600.26 | 0.5942 |
| 476.03 | 0.6872 |
| 366.53 | 0.7672 |
| 255.96 | 0.8368 |
| 152.54 | 0.8978 |
| 63.13 | 0.9519 |

Vesely, F. - Hynek, V. - Svoboda, V. - Holub, R., Isothermal calorimeter for measuring endothermic heats of mixing, Collect. Czech. Chem. Commun. 2 (1974) 355-365. doi:10.1135/cccc19740355

**T / K = 318.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 599.00 | 0.0628 |
| 753.00 | 0.0981 |
| 812.40 | 0.1218 |
| 925.90 | 0.1857 |
| 958.40 | 0.2275 |
| 974.10 | 0.2848 |
| 970.20 | 0.3368 |
| 940.00 | 0.4057 |
| 933.90 | 0.4169 |
| 867.60 | 0.5004 |
| 781.80 | 0.5672 |
| 626.90 | 0.6751 |
| 616.20 | 0.6816 |
| 612.00 | 0.6827 |
| 609.30 | 0.6855 |
| 475.90 | 0.7621 |
| 277.10 | 0.8667 |

Williamson, A.G. - Scott, R.L., Heats of Mixing of Non-Electrolyte Solutions. I. Ethanol + Benzene and Methanol + Benzene, J. Phys. Chem. (1960) 440-442. doi:10.1021/j100833a015

**T / K = 318.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 862.48 | 0.1790 |
| 895.98 | 0.2070 |
| 937.84 | 0.2980 |
| 942.03 | 0.3450 |
| 908.54 | 0.4190 |
| 808.05 | 0.5300 |
| 577.78 | 0.7030 |
| 397.75 | 0.8030 |
| 200.97 | 0.8990 |

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**Critical point**

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Skaates, J.M. - Kay, W.B., The phase relations of binary systems that form azeotropes, Chemical Engineering Science 7 (1964) 431-444. doi:10.1016/0009-2509(64)85070-3

| T / K | P / bar | $x_1$ |
|---|---|---|
| 511.09 | 78.83 | 0.8936 |
| 515.59 | 75.50 | 0.6944 |
| 525.74 | 72.74 | 0.5054 |
| 539.75 | 66.22 | 0.3106 |
| 554.14 | 56.10 | 0.1106 |

Krichevskii, I.R. - Khazanova, N.E. - Linshits, L.R., The liquid-vapor equilibrium in the benzene-methanol system at high pressures, Zh. Fiz. Khim. 12 (1957) 2711-2716.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 512.15 | 78.02 | 0.7869 |
| 511.15 | 77.01 | 0.8797 |

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**Azeotropic point**

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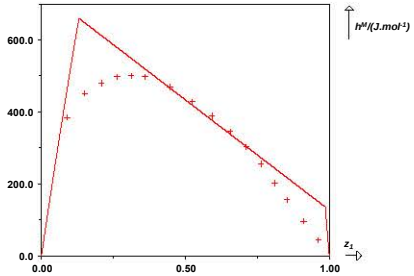
Toghiani, Hossein - Toghiani, Rebecca K. - Viswanath, Dabir S., Vapor-liquid equilibria for the methanol-benzene and methanol-thiophene systems, Journal of Chemical & Engineering Data 1 (1994) 63-67. doi:10.1021/je00013a018

| T / K | P / bar | $x_1$ |
|---|---|---|
| 321.53 | 0.6952 | 0.5916 |

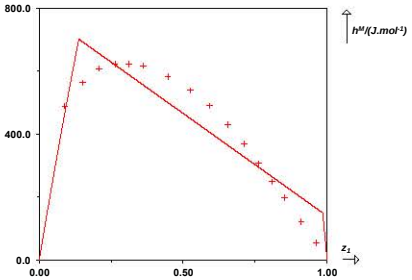
Scatchard, George - Wood, Scott E. - Mochel, John M., Vapor-Liquid Equilibrium. VI. Benzene-Methanol Mixtures, Journal of the American Chemical Society 10 (1946) 1957-1960. doi:10.1021/ja01214a024

| T / K | P / bar | $x_1$ |
|---|---|---|
| 328.15 | 0.9045 | 0.6079 |

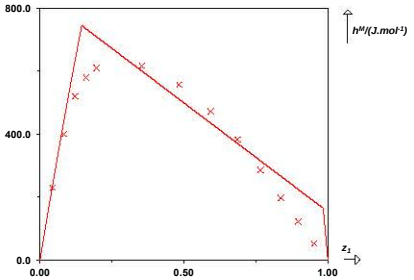
T/K = 283.15 - P/bar = 1.0132



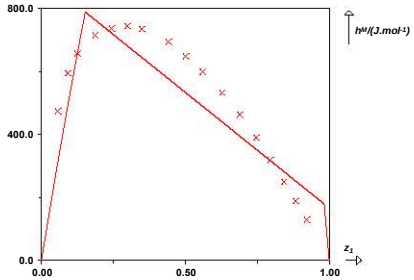

T/K = 288.15 - P/bar = 1.0132



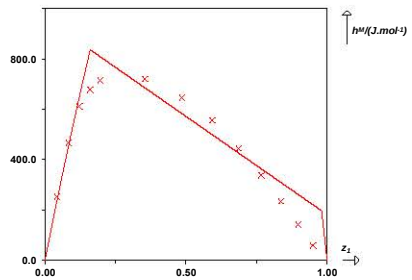

T/K = 293.15 - P/bar = 1.0100



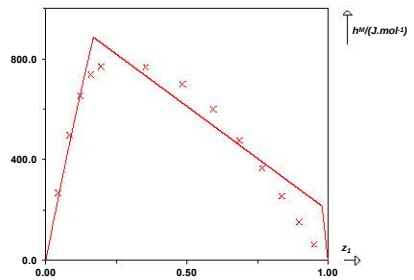

T/K = 298.15 - P/bar = 1.0132



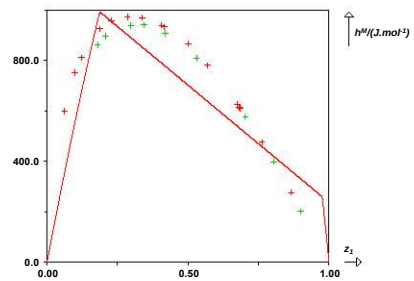

T/K = 303.15 - P/bar = 1.0100



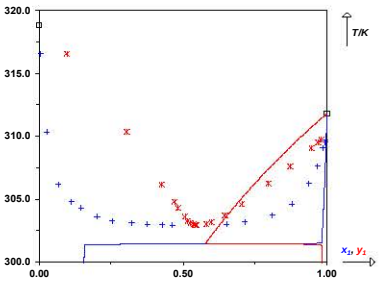

T/K = 308.15 - P/bar = 1.0100



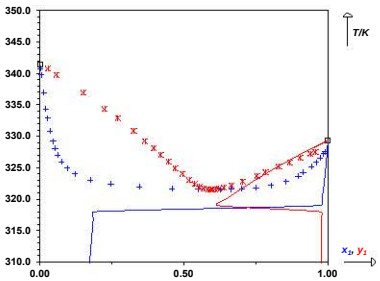

T/K = 318.15 - P/bar = 1.0132 1.0132



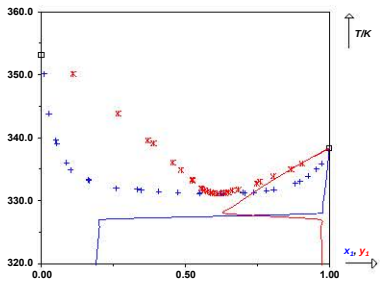

P/bar = 0.30731



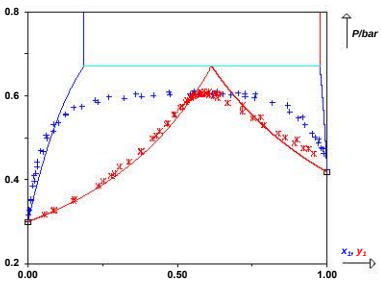

P/bar = 0.69520



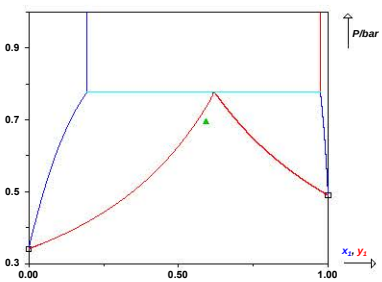

P/bar = 1.01330



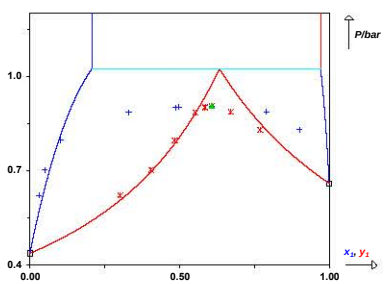

T/K = 318.15



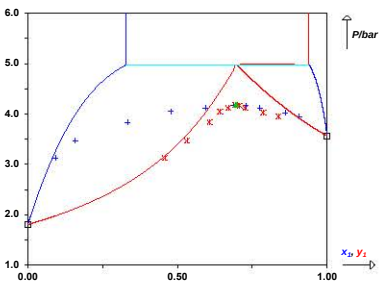

T/K = 321.53



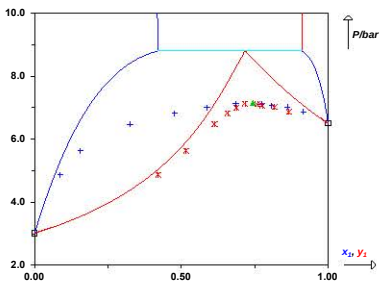

T/K = 328.15



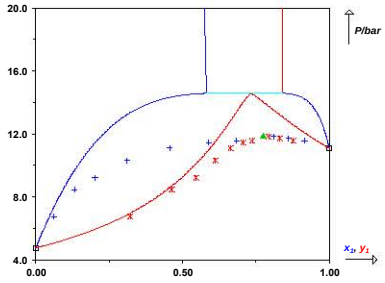

T/K = 373.15



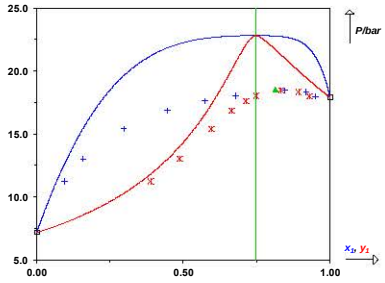

T/K = 393.15



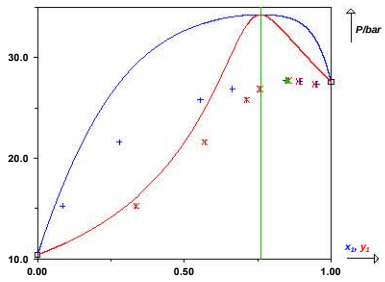
T/K = 413.15



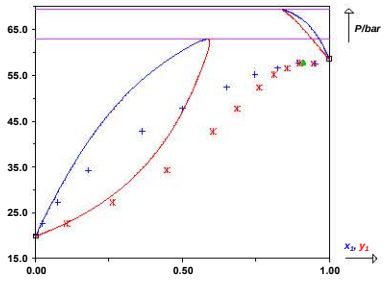

T/K = 433.15



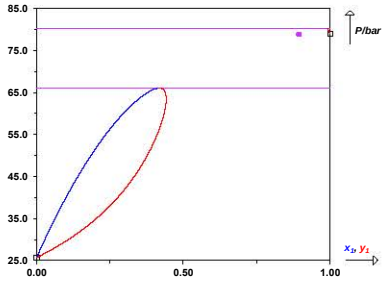

T/K = 453.15



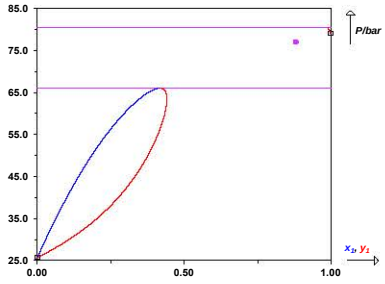

T/K = 493.15



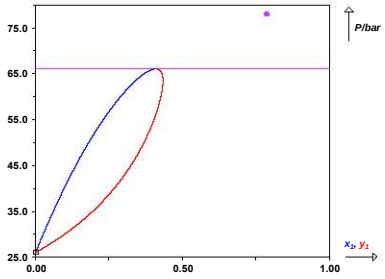

T/K = 511.09



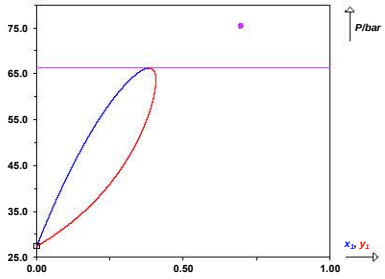

T/K = 511.15



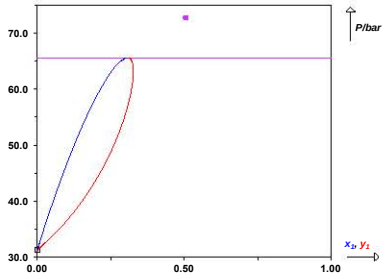

T/K = 512.15



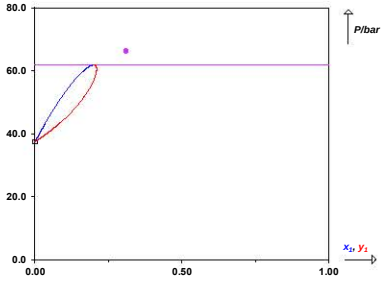

T/K = 515.59



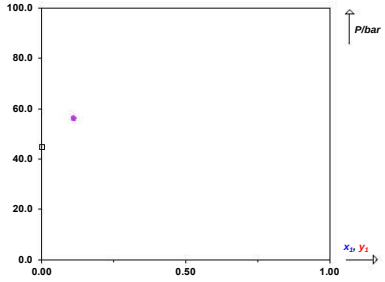

T/K = 525.74




T/K = 539.75




T/K = 554.14



# E-H systems (AC = 6)

## CARBON DIOXIDE (1) + CHLORODIFLUOROMETHANE (2)

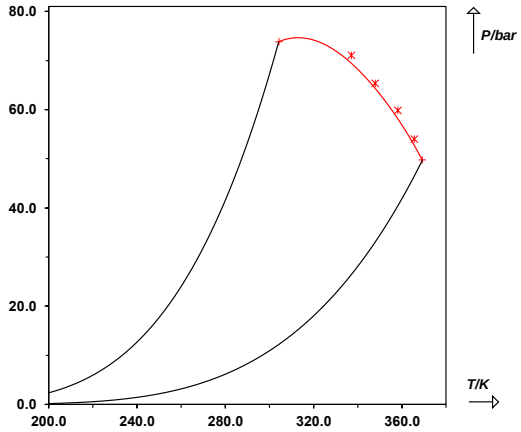
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 75-45-6 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | VOPWNXZWBYDODV-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 369.30 |
| **$P_c$ / bar** | 73.83 | 49.71 |
| **ω** | 0.2240 | 0.2190 |

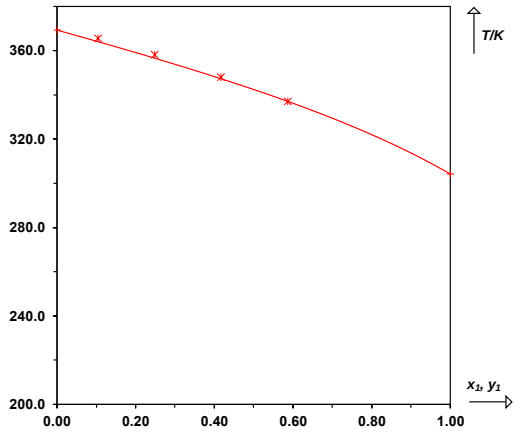
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**PPR78 results**

*Parameters*
A/MPa = 8.95
B/MPa = -120

*Deviations*
MAPE on x = 2.2 %
MAPE on y = 1.6 %
MAPE on $x_c$ = 6.2 %
MAPE on $P_c$ = 2.2 %



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**Isothermal phase equilibrium data**

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Wang, Xiaoqing - Wang, Yanru - Shi, Jun - Lu, Benjamin C. Y., Isothermal vapor-liquid equilibria at elevated pressures for the systems containing nitrogen, carbon dioxide, and chlorodifluoromethane, Journal of Chemical & Engineering Data 4 (1991) 436-439. doi:10.1021/je00004a027

**T / K = 263.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.160 | 0.0870 | 0.3670 |
| 7.070 | 0.1900 | 0.5710 |
| 8.800 | 0.2810 | 0.6830 |
| 9.900 | 0.3410 | 0.7330 |
| 11.08 | 0.3890 | 0.7760 |
| 13.08 | 0.4700 | 0.8310 |
| 15.14 | 0.5640 | 0.8740 |
| 16.81 | 0.6310 | 0.9010 |
| 18.94 | 0.7200 | 0.9280 |
| 20.67 | 0.7890 | 0.9490 |
| 22.87 | 0.8760 | 0.9700 |
| 24.14 | 0.9210 | 0.9820 |

Wang, Xiaoqing - Wang, Yanru - Shi, Jun - Lu, Benjamin C. Y., Isothermal vapor-liquid equilibria at elevated pressures for the systems containing nitrogen, carbon dioxide, and chlorodifluoromethane, Journal of Chemical & Engineering Data 4 (1991) 436-439. doi:10.1021/je00004a027

**T / K = 268.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.570 | 0.0730 | 0.2930 |
| 6.290 | 0.1120 | 0.3820 |
| 7.410 | 0.1630 | 0.4940 |
| 8.970 | 0.2280 | 0.6070 |
| 9.530 | 0.2560 | 0.6370 |
| 10.88 | 0.3160 | 0.7000 |
| 13.20 | 0.4080 | 0.7760 |
| 15.26 | 0.4820 | 0.8270 |
| 16.97 | 0.5490 | 0.8600 |
| 18.92 | 0.6150 | 0.8900 |
| 19.88 | 0.6580 | 0.9010 |
| 21.04 | 0.6970 | 0.9160 |
| 22.71 | 0.7460 | 0.9350 |
| 24.78 | 0.8180 | 0.9540 |
| 26.70 | 0.8780 | 0.9710 |
| 27.87 | 0.9170 | 0.9810 |

Wang, Xiaoqing - Wang, Yanru - Shi, Jun - Lu, Benjamin C. Y., Isothermal vapor-liquid equilibria at elevated pressures for the systems containing nitrogen, carbon dioxide, and chlorodifluoromethane, Journal of Chemical & Engineering Data 4 (1991) 436-439. doi:10.1021/je00004a027

**T / K = 273.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.050 | 0.0470 | 0.2140 |
| 7.040 | 0.0960 | 0.3430 |
| 9.040 | 0.1780 | 0.5170 |
| 9.380 | 0.1950 | 0.5440 |
| 11.13 | 0.2640 | 0.6330 |
| 13.01 | 0.3410 | 0.7060 |
| 14.27 | 0.3780 | 0.7450 |
| 15.97 | 0.4420 | 0.7880 |
| 17.38 | 0.4920 | 0.8170 |
| 20.98 | 0.6160 | 0.8760 |
| 24.93 | 0.7350 | 0.9220 |
| 25.88 | 0.7610 | 0.9300 |
| 27.96 | 0.8190 | 0.9490 |
| 30.50 | 0.8950 | 0.9700 |
| 30.83 | 0.9030 | 0.9720 |

Wang, Xiaoqing - Wang, Yanru - Shi, Jun - Lu, Benjamin C. Y., Isothermal vapor-liquid equilibria at elevated pressures for the systems containing nitrogen, carbon dioxide, and chlorodifluoromethane, Journal of Chemical & Engineering Data 4 (1991) 436-439. doi:10.1021/je00004a027

**T / K = 288.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.940 | 0.0340 | 0.1390 |
| 10.35 | 0.0830 | 0.2780 |
| 12.18 | 0.1420 | 0.4060 |
| 14.08 | 0.1990 | 0.5040 |
| 14.38 | 0.2060 | 0.5160 |
| 17.51 | 0.2960 | 0.6270 |
| 23.19 | 0.4370 | 0.7540 |
| 27.09 | 0.5380 | 0.8150 |
| 28.84 | 0.5720 | 0.8360 |
| 34.77 | 0.7020 | 0.8930 |
| 40.62 | 0.8260 | 0.9370 |
| 46.54 | 0.9330 | 0.9750 |

Nohka, Junichi - Sarashina, Eiji - Arai, Yasuhiko - Saito, Shozaburo, Correlation Of Vapor-Liquid Equilibria For Systems Containing A Polar Component By The Bwr Equation, Journal of Chemical Engineering of Japan 1 (1973) 10-17. doi:10.1252/jcej.6.10

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 28.07 | 0.1420 | 0.3180 |

| | | |
|---|---|---|
| 39.31 | 0.3170 | 0.5370 |
| 51.68 | 0.4820 | 0.6720 |
| 57.55 | 0.5600 | 0.7260 |
| 63.84 | 0.6430 | 0.7640 |
| 67.38 | 0.6860 | 0.7850 |
| 70.93 | 0.7260 | 0.7980 |
| 73.26 | 0.7490 | 0.8050 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 27.62 | 0.0964 | 0.2160 |
| 32.32 | 0.1676 | 0.3357 |
| 36.99 | 0.2423 | 0.4288 |
| 41.99 | 0.3069 | 0.5027 |
| 46.97 | 0.3745 | 0.5632 |
| 52.03 | 0.4390 | 0.6134 |
| 57.00 | 0.5003 | 0.6538 |
| 62.06 | 0.5610 | 0.6894 |
| 67.49 | 0.6218 | 0.7171 |
| 70.15 | 0.6538 | 0.7280 |

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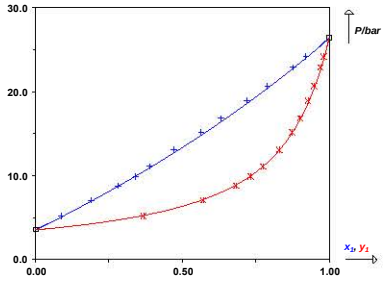
**Critical point**

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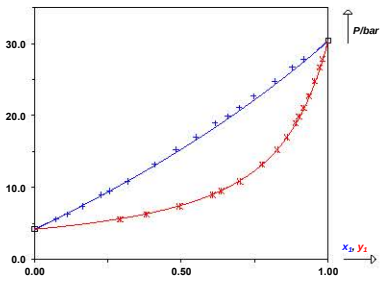
Lee, Jae Min - Lee, Byung-Chul - Cho, Chan-Hwi, Measurement of bubble point pressures and critical points of carbon dioxide and chlorodifluoromethane mixtures using the variable-volume view cell apparatus, Korean Journal of Chemical Engineering 5 (2000) 510-515. doi:10.1007/BF02707158

| T / K | P / bar | $x_1$ |
|---|---|---|
| 365.55 | 54.00 | 0.1036 |
| 358.15 | 59.80 | 0.2476 |
| 347.85 | 65.30 | 0.4160 |
| 337.15 | 71.00 | 0.5866 |

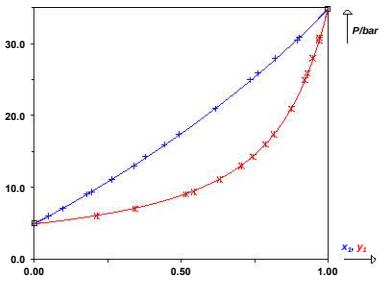
T/K = 263.20



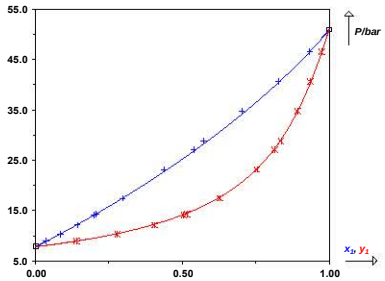

T/K = 268.20



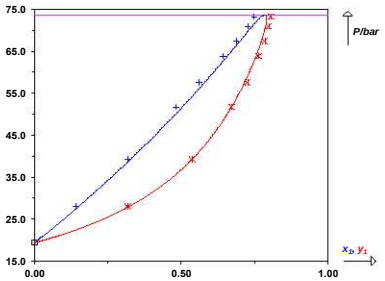

T/K = 273.20



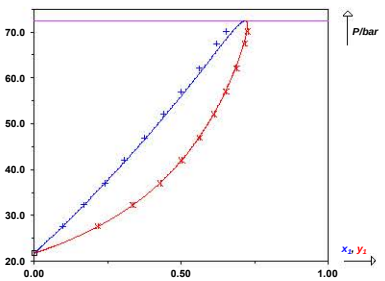

T/K = 288.20



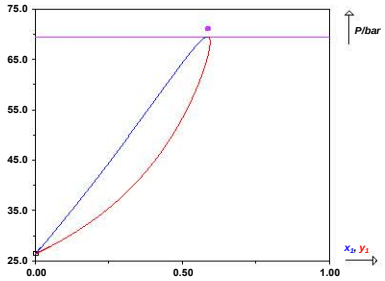

T/K = 323.15



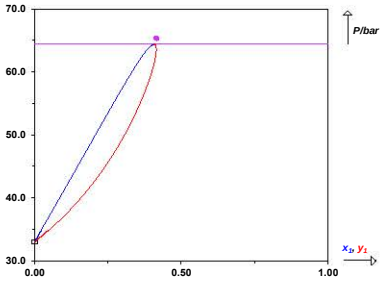

T/K = 328.15



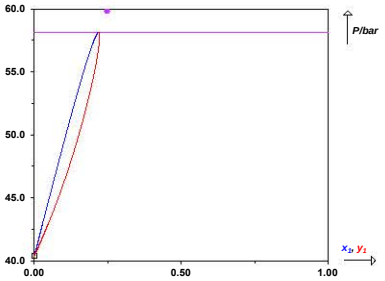

T/K = 337.15



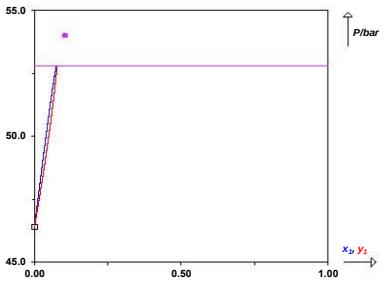

T/K = 347.85




T/K = 358.15




T/K = 365.55



## CARBON DIOXIDE (1) + 1,1,1,2-TETRAFLUOROETHANE (2)

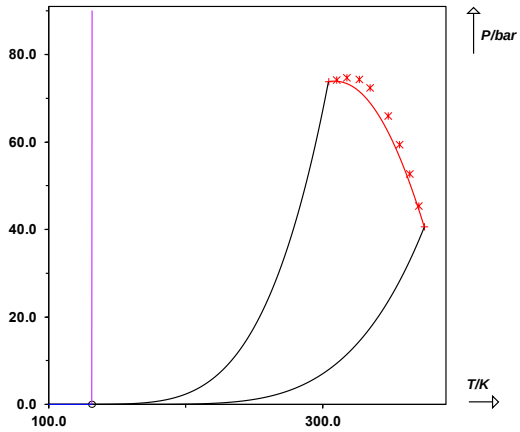
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 811-97-2 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | LVGUZGTVOIAKKC-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 374.18 |
| **$P_c$ / bar** | 73.83 | 40.56 |
| **ω** | 0.2240 | 0.3270 |

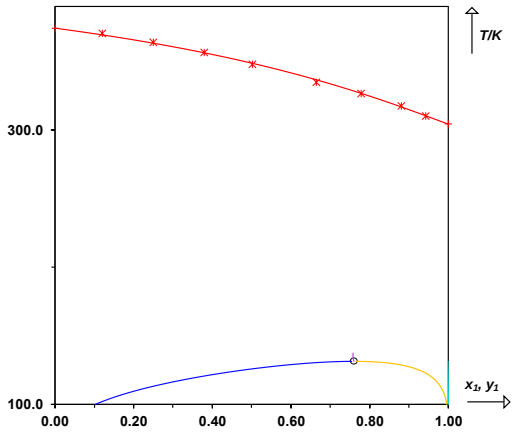
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 92.8
B/MPa = 219

*Deviations*
MAPE on x = 3.4 %
MAPE on y = 3.5 %
MAPE on $x_c$ = 3.5 %
MAPE on $P_c$ = 3.4 %



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**Isothermal phase equilibrium data**

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Duran-Valencia, C. - Pointurier, G. - Valtz, A. - Guilbot, P. - Richon, D., Vapor−Liquid Equilibrium (VLE) Data for the Carbon Dioxide (CO2) + 1,1,1,2-Tetrafluoroethane (R134a) System at Temperatures from 252.95 K to 292.95 K and Pressures up to 2 MPa, Journal of Chemical & Engineering Data 1 (2002) 59-61. doi:10.1021/je010075y

**T / K = 252.95**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.080 | 0.2230 | 0.7720 |
| 6.830 | 0.3260 | 0.8480 |
| 8.000 | 0.3930 | 0.8780 |
| 10.03 | 0.5060 | 0.9190 |
| 13.57 | 0.6970 | 0.9540 |
| 15.76 | 0.8100 | 0.9740 |
| 16.85 | 0.8670 | 0.9830 |

Duran-Valencia, C. - Pointurier, G. - Valtz, A. - Guilbot, P. - Richon, D., Vapor−Liquid Equilibrium (VLE) Data for the Carbon Dioxide (CO2) + 1,1,1,2-Tetrafluoroethane (R134a) System at Temperatures from 252.95 K to 292.95 K and Pressures up to 2 MPa, Journal of Chemical & Engineering Data 1 (2002) 59-61. doi:10.1021/je010075y

**T / K = 272.75**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.340 | 0.0870 | 0.4680 |
| 6.980 | 0.1490 | 0.6070 |
| 8.620 | 0.2130 | 0.6950 |
| 9.770 | 0.2540 | 0.7380 |
| 11.55 | 0.3140 | 0.7930 |
| 14.54 | 0.4160 | 0.8490 |
| 16.07 | 0.4660 | 0.8710 |
| 18.21 | 0.5360 | 0.8950 |
| 20.33 | 0.6060 | 0.9160 |

Silva-Oliver, G. - Galicia-Luna, L.A., Vapor−liquid equilibria for carbon dioxide + 1,1,1,2-tetrafluoroethane (R-134a) systems at temperatures from 329 to 354 K and pressures upto 7.37 MPa, Fluid Phase Equilibria 1-2 (2002) 213-222. doi:10.1016/S0378-3812(01)00816-0

**T / K = 329.60**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 19.91 | 0.0821 | 0.2412 |
| 27.85 | 0.2005 | 0.4497 |
| 34.16 | 0.2904 | 0.5566 |
| 39.44 | 0.3467 | 0.6057 |
| 46.06 | 0.4225 | 0.6570 |
| 53.73 | 0.5102 | 0.7068 |
| 59.82 | 0.5751 | 0.7363 |
| 68.13 | 0.6627 | 0.7637 |
| 71.29 | 0.7008 | 0.7693 |
| 73.69 | 0.7450 | 0.7640 |

Lim, Jong Sung - Jin, Jung Min - Yoo, Ki-Pung, VLE measurement for binary systems of CO2+1,1,1,2-tetrafluoroethane (HFC-134a) at high pressures, The Journal of Supercritical Fluids 3 (2008) 279-283. doi:10.1016/j.supflu.2007.09.025

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 24.30 | 0.1020 | 0.2410 |
| 28.30 | 0.1590 | 0.3500 |
| 35.00 | 0.2420 | 0.4540 |
| 41.00 | 0.3250 | 0.5390 |
| 50.90 | 0.4440 | 0.6290 |
| 58.90 | 0.5480 | 0.6900 |
| 68.00 | 0.6360 | 0.7120 |
| 69.90 | 0.6630 | 0.7010 |

Silva-Oliver, G. - Galicia-Luna, L.A., Vapor−liquid equilibria for carbon dioxide + 1,1,1,2-tetrafluoroethane (R-134a) systems at temperatures from 329 to 354 K and pressures upto 7.37 MPa, Fluid Phase Equilibria 1-2 (2002) 213-222. doi:10.1016/S0378-3812(01)00816-0

**T / K = 339.10**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 23.05 | 0.0666 | 0.1781 |
| 28.38 | 0.1378 | 0.3141 |
| 35.01 | 0.2223 | 0.4341 |
| 41.00 | 0.2952 | 0.5087 |
| 50.91 | 0.4042 | 0.5939 |
| 58.91 | 0.4876 | 0.6399 |
| 65.65 | 0.5564 | 0.6638 |
| 70.98 | 0.6266 | 0.6612 |

Silva-Oliver, G. - Galicia-Luna, L.A., Vapor−liquid equilibria for carbon dioxide + 1,1,1,2-tetrafluoroethane (R-134a) systems at temperatures from 329 to 354 K and pressures upto 7.37 MPa, Fluid Phase Equilibria 1-2 (2002) 213-222. doi:10.1016/S0378-3812(01)00816-0

**T / K = 354.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 32.50 | 0.0826 | 0.1733 |
| 39.00 | 0.1564 | 0.2832 |
| 46.40 | 0.2343 | 0.3735 |
| 55.63 | 0.3433 | 0.4383 |

| | | |
|---|---|---|
| 60.43 | 0.3920 | 0.4560 |

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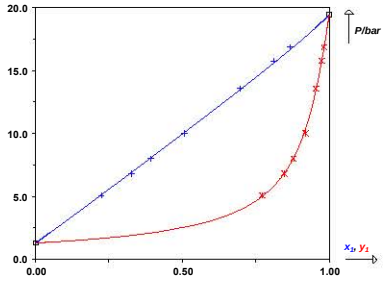
**Critical point**

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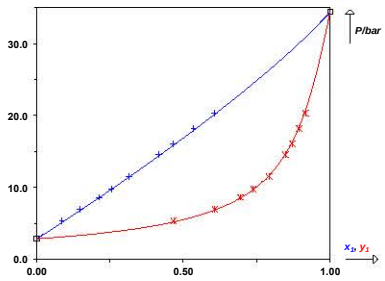
Uchida, Yuko - Yasumoto, Masahiko - Yamada, Yasufu - Ochi, Kenji - Furuya, Takeshi - Otake, Katsuto, Critical Properties of Four HFE + HFC Binary Systems: Trifluoromethoxymethane (HFE-143m) + Pentafluoroethane (HFC-125), + 1,1,1,2-Tetrafluoroethane (HFC-134a), + 1,1,1,2,3,3,3-Heptafluoropropane (HFC-227ea), and + 1,1,1,2,3,3-Hexafluoropropane (HFC-236ea), Journal of Chemical & Engineering Data 6 (2004) 1615-1621. doi:10.1021/je0499723

| T / K | P / bar | $x_1$ |
|---|---|---|
| 310.05 | 74.12 | 0.9420 |
| 317.55 | 74.74 | 0.8800 |
| 326.50 | 74.26 | 0.7780 |
| 334.60 | 72.39 | 0.6650 |
| 347.65 | 65.91 | 0.5020 |
| 356.25 | 59.43 | 0.3790 |
| 363.65 | 52.67 | 0.2490 |
| 370.25 | 45.37 | 0.1200 |

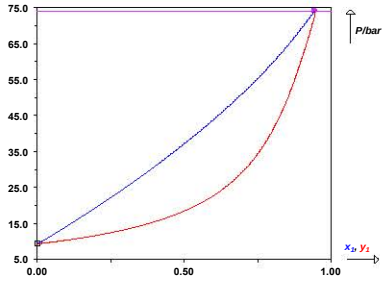
T/K = 252.95



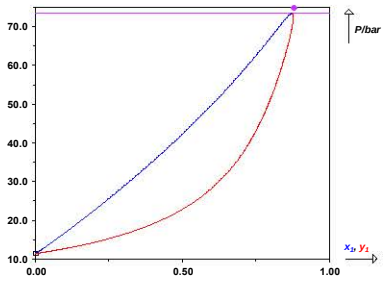

T/K = 272.75



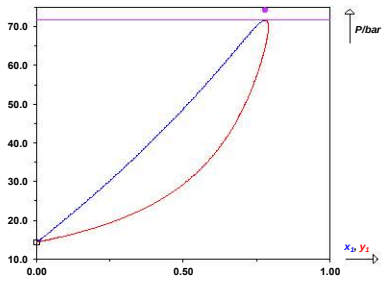

T/K = 310.05



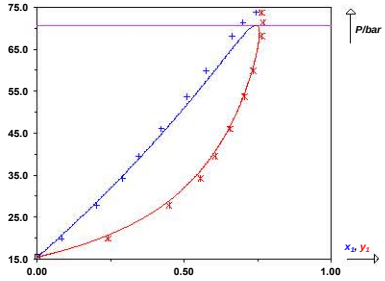

T/K = 317.55



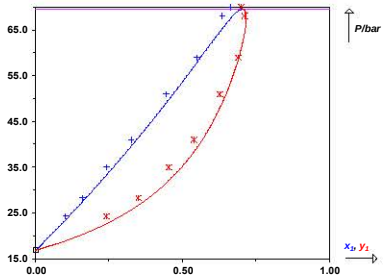

T/K = 326.50



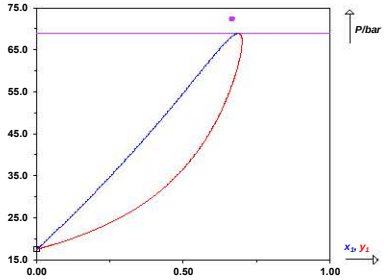

T/K = 329.60



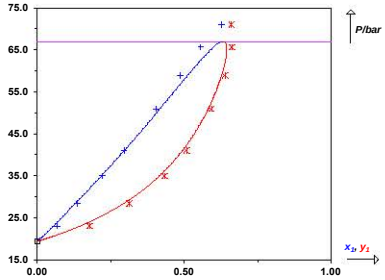

T/K = 333.15



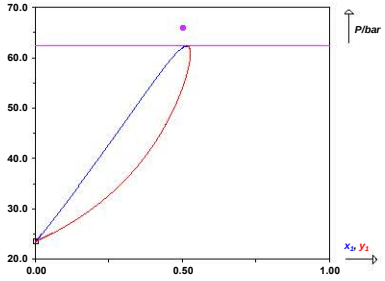

T/K = 334.60



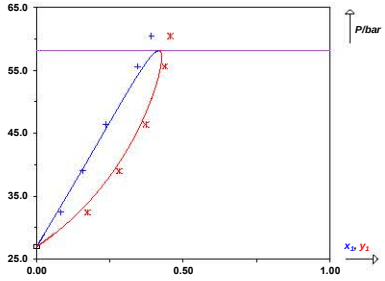

T/K = 339.10



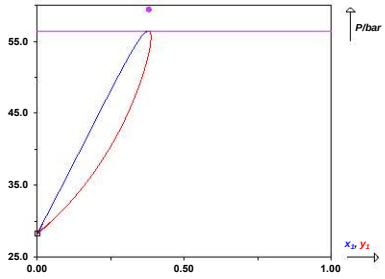

T/K = 347.65



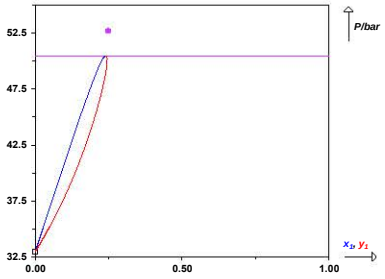

T/K = 354.00



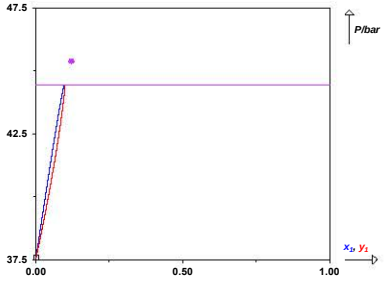

T/K = 356.25




T/K = 363.65




T/K = 370.25



## CARBON DIOXIDE (1) + 1,1,1,2,3,3,3-HEPTAFLUOROPROPANE (2)

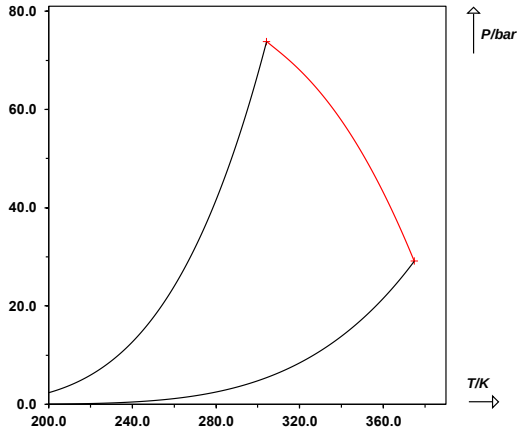
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 431-89-0 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | YFMFNYKEUDLDTL-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 374.83 |
| **$P_c$ / bar** | 73.83 | 29.116 |
| **ω** | 0.2240 | 0.3550 |

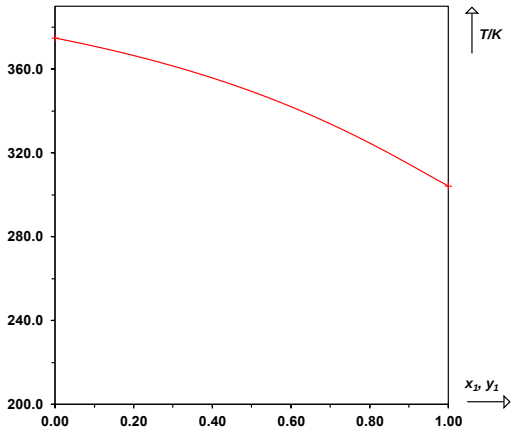
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 143
B/MPa = -54

*Deviations*
MAPE on x = 2.8 %
MAPE on y = 3.9 %



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**Isothermal phase equilibrium data**

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Valtz, A. - Coquelet, C. - Baba-Ahmed, A. - Richon, D., Vapor–liquid equilibrium data for the CO2 + 1,1,1,2,3,3,3,-heptafluoropropane (R227ea) system at temperatures from 276.01 to 367.30 K and pressures up to 7.4 MPa, Fluid Phase Equilibria 1-2 (2003) 53-67. doi:10.1016/S0378-3812(02)00326-6

**T / K = 276.01**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.566 | 0.0934 | 0.5408 |
| 6.378 | 0.1592 | 0.6822 |
| 9.358 | 0.2615 | 0.7944 |
| 13.35 | 0.3950 | 0.8680 |
| 17.43 | 0.5188 | 0.9070 |
| 21.84 | 0.6434 | 0.9366 |
| 25.85 | 0.7471 | 0.9561 |

Valtz, A. - Coquelet, C. - Baba-Ahmed, A. - Richon, D., Vapor–liquid equilibrium data for the CO2 + 1,1,1,2,3,3,3,-heptafluoropropane (R227ea) system at temperatures from 276.01 to 367.30 K and pressures up to 7.4 MPa, Fluid Phase Equilibria 1-2 (2003) 53-67. doi:10.1016/S0378-3812(02)00326-6

**T / K = 276.01**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 29.44 | 0.8335 | 0.9696 |
| 31.93 | 0.8887 | 0.9779 |
| 34.42 | 0.9400 | 0.9875 |

Souza, Alexandre T. - Corazza, Marcos L. - Cardozo-Filho, Lúcio - Guirardello, Reginaldo - Meireles, M. Angela A., Phase Equilibrium Measurements for the System Clove (Eugenia caryophyllus) Oil + CO2, Journal of Chemical & Engineering Data 2 (2004) 352-356. doi:10.1021/je034190f

**T / K = 278.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.140 | 0.0760 | 0.4330 |
| 6.430 | 0.1480 | 0.6380 |
| 11.12 | 0.3010 | 0.8100 |
| 15.27 | 0.4190 | 0.8740 |
| 20.03 | 0.5580 | 0.9200 |
| 23.51 | 0.6560 | 0.9440 |
| 27.10 | 0.7460 | 0.9610 |

Souza, Alexandre T. - Corazza, Marcos L. - Cardozo-Filho, Lúcio - Guirardello, Reginaldo - Meireles, M. Angela A., Phase Equilibrium Measurements for the System Clove (Eugenia caryophyllus) Oil + CO2, Journal of Chemical & Engineering Data 2 (2004) 352-356. doi:10.1021/je034190f

**T / K = 278.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 30.99 | 0.8340 | 0.9760 |
| 33.96 | 0.8970 | 0.9860 |
| 35.72 | 0.9280 | 0.9910 |
| 36.13 | 0.9330 | 0.9920 |

Souza, Alexandre T. - Corazza, Marcos L. - Cardozo-Filho, Lúcio - Guirardello, Reginaldo - Meireles, M. Angela A., Phase Equilibrium Measurements for the System Clove (Eugenia caryophyllus) Oil + CO2, Journal of Chemical & Engineering Data 2 (2004) 352-356. doi:10.1021/je034190f

**T / K = 288.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.650 | 0.1150 | 0.5380 |
| 13.10 | 0.2630 | 0.7480 |
| 19.10 | 0.4140 | 0.8470 |
| 23.51 | 0.5200 | 0.8860 |
| 27.58 | 0.6090 | 0.9110 |

Souza, Alexandre T. - Corazza, Marcos L. - Cardozo-Filho, Lúcio - Guirardello, Reginaldo - Meireles, M. Angela A., Phase Equilibrium Measurements for the System Clove (Eugenia caryophyllus) Oil + CO2, Journal of Chemical & Engineering Data 2 (2004) 352-356. doi:10.1021/je034190f

**T / K = 288.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 31.03 | 0.6860 | 0.9300 |
| 34.68 | 0.7570 | 0.9470 |
| 37.85 | 0.8130 | 0.9590 |
| 42.06 | 0.8830 | 0.9730 |
| 45.57 | 0.9290 | 0.9840 |

Valtz, A. - Coquelet, C. - Baba-Ahmed, A. - Richon, D., Vapor–liquid equilibrium data for the CO2 + 1,1,1,2,3,3,3,-heptafluoropropane (R227ea) system at temperatures from 276.01 to 367.30 K and pressures up to 7.4 MPa, Fluid Phase Equilibria 1-2 (2003) 53-67. doi:10.1016/S0378-3812(02)00326-6

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.341 | 0.0423 | 0.2750 |
| 6.599 | 0.0774 | 0.4153 |
| 7.964 | 0.1125 | 0.5189 |
| 11.04 | 0.1887 | 0.6622 |
| 14.51 | 0.2752 | 0.7528 |
| 20.76 | 0.4184 | 0.8385 |
| 28.93 | 0.5886 | 0.8953 |

Valtz, A. - Coquelet, C. - Baba-Ahmed, A. - Richon, D., Vapor–liquid equilibrium data for the CO2 + 1,1,1,2,3,3,3,-heptafluoropropane (R227ea) system at temperatures from 276.01 to 367.30 K and pressures up to 7.4 MPa, Fluid Phase Equilibria 1-2 (2003) 53-67. doi:10.1016/S0378-3812(02)00326-6

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 37.82 | 0.7482 | 0.9360 |
| 44.87 | 0.8539 | 0.9610 |
| 50.12 | 0.9216 | 0.9769 |
| 52.61 | 0.9518 | 0.9853 |

Souza, Alexandre T. - Corazza, Marcos L. - Cardozo-Filho, Lúcio - Guirardello, Reginaldo - Meireles, M. Angela A., Phase Equilibrium Measurements for the System Clove (Eugenia caryophyllus) Oil + CO2, Journal of Chemical & Engineering Data 2 (2004) 352-356. doi:10.1021/je034190f

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.450 | 0.1100 | 0.4700 |
| 14.48 | 0.2270 | 0.6830 |
| 18.89 | 0.3260 | 0.7800 |
| 22.82 | 0.4070 | 0.8290 |

Souza, Alexandre T. - Corazza, Marcos L. - Cardozo-Filho, Lúcio - Guirardello, Reginaldo - Meireles, M. Angela A., Phase Equilibrium Measurements for the System Clove (Eugenia caryophyllus) Oil + CO2, Journal of Chemical & Engineering Data 2 (2004) 352-356. doi:10.1021/je034190f

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 29.30 | 0.5370 | 0.8820 |
| 35.44 | 0.6490 | 0.9140 |
| 41.02 | 0.7410 | 0.9310 |
| 47.37 | 0.8300 | 0.9470 |
| 53.57 | 0.9050 | 0.9670 |
| 57.85 | 0.9480 | 0.9790 |

Valtz, A. - Coquelet, C. - Baba-Ahmed, A. - Richon, D., Vapor–liquid equilibrium data for the CO2 + 1,1,1,2,3,3,3,-heptafluoropropane (R227ea) system at temperatures from 276.01 to 367.30 K and pressures up to 7.4 MPa, Fluid Phase Equilibria 1-2 (2003) 53-67. doi:10.1016/S0378-3812(02)00326-6

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.556 | 0.0312 | 0.1894 |
| 8.491 | 0.0767 | 0.3752 |
| 11.93 | 0.1559 | 0.5598 |
| 15.95 | 0.2432 | 0.6768 |
| 21.88 | 0.3619 | 0.7744 |
| 28.91 | 0.4899 | 0.8353 |

Valtz, A. - Coquelet, C. - Baba-Ahmed, A. - Richon, D., Vapor–liquid equilibrium data for the CO2 + 1,1,1,2,3,3,3,-heptafluoropropane (R227ea) system at temperatures from 276.01 to 367.30 K and pressures up to 7.4 MPa, Fluid Phase Equilibria 1-2 (2003) 53-67. doi:10.1016/S0378-3812(02)00326-6

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 36.93 | 0.6202 | 0.8806 |
| 45.83 | 0.7460 | 0.9167 |
| 53.77 | 0.8400 | 0.9424 |
| 60.66 | 0.9103 | 0.9618 |
| 65.55 | 0.9532 | 0.9772 |
| 68.80 | 0.9779 | 0.9885 |

Valtz, A. - Coquelet, C. - Baba-Ahmed, A. - Richon, D., Vapor–liquid equilibrium data for the CO2 + 1,1,1,2,3,3,3,-heptafluoropropane (R227ea) system at temperatures from 276.01 to 367.30 K and pressures up to 7.4 MPa, Fluid Phase Equilibria 1-2 (2003) 53-67. doi:10.1016/S0378-3812(02)00326-6

**T / K = 305.17**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.14 | 0.1083 | 0.4431 |
| 20.00 | 0.3108 | 0.7310 |
| 29.98 | 0.4899 | 0.8317 |
| 39.97 | 0.6448 | 0.8848 |
| 49.86 | 0.7736 | 0.9149 |
| 58.86 | 0.8708 | 0.9453 |

Souza, Alexandre T. - Corazza, Marcos L. - Cardozo-Filho, Lúcio - Guirardello, Reginaldo - Meireles, M. Angela A., Phase Equilibrium Measurements for the System Clove (Eugenia caryophyllus) Oil + CO2, Journal of Chemical & Engineering Data 2 (2004) 352-356. doi:10.1021/je034190f

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.14 | 0.0880 | 0.4210 |
| 18.20 | 0.2420 | 0.6650 |
| 25.51 | 0.3760 | 0.7680 |
| 33.03 | 0.5060 | 0.8230 |
| 44.82 | 0.6870 | 0.8850 |
| 49.71 | 0.7450 | 0.9000 |
| 56.61 | 0.8260 | 0.9160 |
| 61.29 | 0.8730 | 0.9290 |

Valtz, A. - Coquelet, C. - Baba-Ahmed, A. - Richon, D., Vapor–liquid equilibrium data for the CO2 +

1,1,1,2,3,3,3,-heptafluoropropane (R227ea) system at temperatures from 276.01 to 367.30 K and pressures up to 7.4 MPa, Fluid Phase Equilibria 1-2 (2003) 53-67. doi:10.1016/S0378-3812(02)00326-6

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.918 | 0.0596 | 0.2760 |
| 13.02 | 0.1213 | 0.4468 |
| 17.83 | 0.2097 | 0.5982 |
| 23.86 | 0.3160 | 0.7046 |
| 29.86 | 0.4152 | 0.7693 |
| 36.83 | 0.5230 | 0.8198 |
| 43.83 | 0.6206 | 0.8551 |
| 50.91 | 0.7070 | 0.8797 |
| 56.83 | 0.7691 | 0.8988 |
| 61.12 | 0.8119 | 0.9098 |
| 64.78 | 0.8442 | 0.9186 |
| 67.88 | 0.8695 | 0.9254 |
| 69.51 | 0.8832 | 0.9285 |
| 70.74 | 0.8943 | 0.9298 |
| 71.92 | 0.9048 | 0.9303 |

Souza, Alexandre T. - Corazza, Marcos L. - Cardozo-Filho, Lúcio - Guirardello, Reginaldo - Meireles, M. Angela A., Phase Equilibrium Measurements for the System Clove (Eugenia caryophyllus) Oil + CO2, Journal of Chemical & Engineering Data 2 (2004) 352-356. doi:10.1021/je034190f

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.72 | 0.1080 | 0.3930 |
| 20.13 | 0.2140 | 0.5890 |
| 27.72 | 0.3360 | 0.7070 |
| 33.44 | 0.4200 | 0.7540 |
| 38.20 | 0.4870 | 0.7840 |
| 47.99 | 0.6170 | 0.8240 |
| 54.54 | 0.6930 | 0.8480 |
| 60.95 | 0.7640 | 0.8630 |

Souza, Alexandre T. - Corazza, Marcos L. - Cardozo-Filho, Lúcio - Guirardello, Reginaldo - Meireles, M. Angela A., Phase Equilibrium Measurements for the System Clove (Eugenia caryophyllus) Oil + CO2, Journal of Chemical & Engineering Data 2 (2004) 352-356. doi:10.1021/je034190f

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 16.55 | 0.1050 | 0.3450 |
| 23.99 | 0.2160 | 0.5420 |
| 31.03 | 0.3140 | 0.6480 |
| 37.99 | 0.4060 | 0.7160 |
| 43.85 | 0.4810 | 0.7450 |
| 49.30 | 0.5450 | 0.7600 |
| 56.61 | 0.6310 | 0.7740 |
| 62.81 | 0.6990 | 0.7800 |

Valtz, A. - Coquelet, C. - Baba-Ahmed, A. - Richon, D., Vapor–liquid equilibrium data for the CO2 + 1,1,1,2,3,3,3,-heptafluoropropane (R227ea) system at temperatures from 276.01 to 367.30 K and pressures up to 7.4 MPa, Fluid Phase Equilibria 1-2 (2003) 53-67. doi:10.1016/S0378-3812(02)00326-6

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.69 | 0.0308 | 0.1200 |
| 18.20 | 0.1010 | 0.3176 |
| 23.90 | 0.1896 | 0.4701 |
| 29.97 | 0.2740 | 0.5704 |
| 36.51 | 0.3619 | 0.6428 |
| 42.97 | 0.4417 | 0.6903 |
| 49.98 | 0.5231 | 0.7322 |
| 55.95 | 0.5899 | 0.7533 |
| 60.18 | 0.6360 | 0.7610 |
| 62.95 | 0.6670 | 0.7628 |
| 65.03 | 0.6886 | 0.7614 |
| 66.46 | 0.7118 | 0.7559 |

Valtz, A. - Coquelet, C. - Baba-Ahmed, A. - Richon, D., Vapor–liquid equilibrium data for the CO2 + 1,1,1,2,3,3,3,-heptafluoropropane (R227ea) system at temperatures from 276.01 to 367.30 K and pressures up to 7.4 MPa, Fluid Phase Equilibria 1-2 (2003) 53-67. doi:10.1016/S0378-3812(02)00326-6

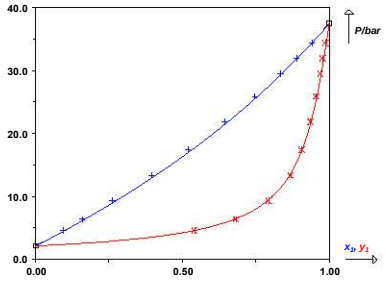
**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.98 | 0.0339 | 0.0897 |
| 24.90 | 0.0871 | 0.2023 |
| 28.95 | 0.1402 | 0.2929 |
| 33.03 | 0.1914 | 0.3588 |
| 37.35 | 0.2435 | 0.4140 |
| 40.98 | 0.2864 | 0.4497 |
| 45.03 | 0.3357 | 0.4804 |
| 48.32 | 0.3756 | 0.4972 |
| 50.14 | 0.3996 | 0.5032 |
| 52.04 | 0.4298 | 0.4985 |
| 52.73 | 0.4466 | 0.4871 |

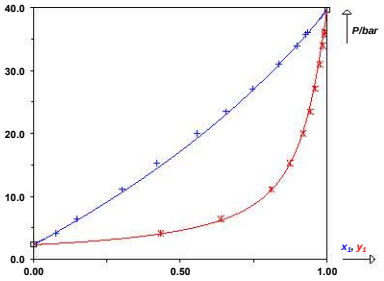
Valtz, A. - Coquelet, C. - Baba-Ahmed, A. - Richon, D., Vapor–liquid equilibrium data for the CO2 + 1,1,1,2,3,3,3,-heptafluoropropane (R227ea) system at temperatures from 276.01 to 367.30 K and pressures up to 7.4 MPa, Fluid Phase Equilibria 1-2 (2003) 53-67. doi:10.1016/S0378-3812(02)00326-6

| **T / K =** | **367.30** | |
|---|---|---|
| P / bar | $x_1$ | $y_1$ |
| 26.87 | 0.0246 | 0.0453 |
| 28.86 | 0.0506 | 0.0860 |
| 30.86 | 0.0763 | 0.1222 |
| 33.14 | 0.1058 | 0.1601 |
| 34.97 | 0.1299 | 0.1833 |
| 36.89 | 0.1571 | 0.2053 |
| 38.40 | 0.1843 | 0.2146 |

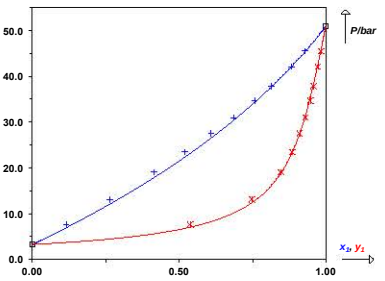
T/K = 276.01



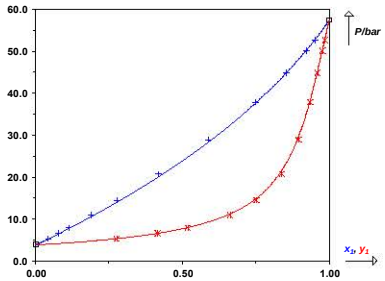

T/K = 278.15



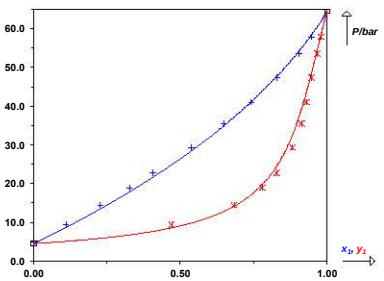

T/K = 288.15



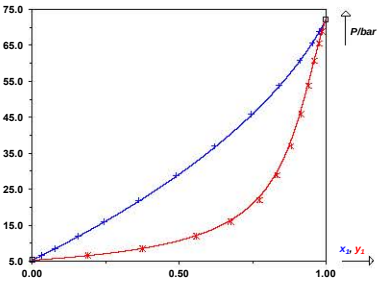

T/K = 293.15



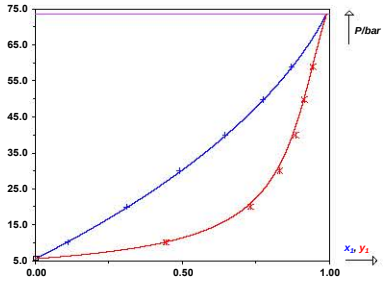

T/K = 298.15



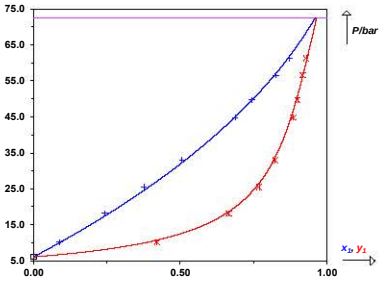

T/K = 303.15



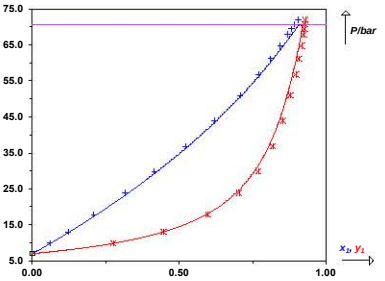

T/K = 305.17



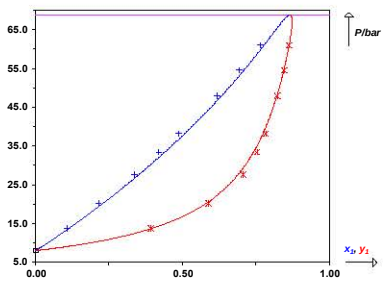

T/K = 308.15



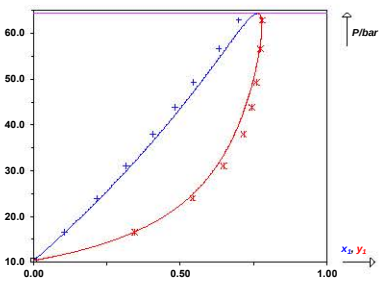

T/K = 313.15



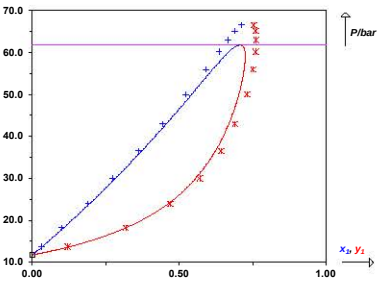

T/K = 318.15



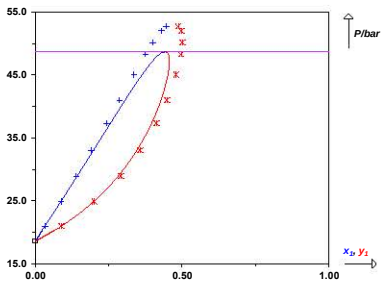

T/K = 328.15



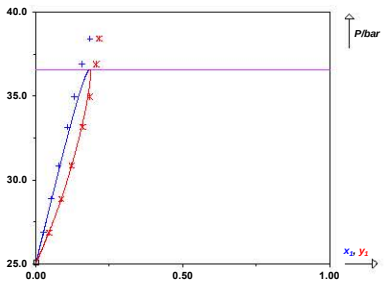

T/K = 333.15




T/K = 353.15




T/K = 367.30



## TRIFLUOROMETHANE (1) + CARBON DISULFIDE (2)

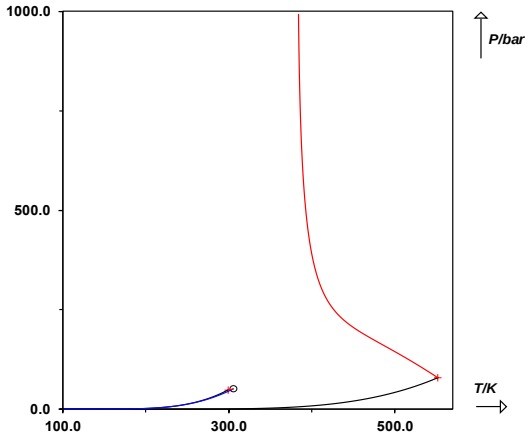
| | | |
|---|---|---|
| **CAS** | 75-46-7 | 75-15-0 |
| **InChiKey** | XPDWGBQVDMORPB-UHFFFAOYSA-N | QGJOPFRUJISHPQ-UHFFFAOYSA-N |
| **$T_c$ / K** | 299.01 | 552.00 |
| **$P_c$ / bar** | 48.16 | 79.00 |
| **ω** | 0.2640 | 0.1110 |

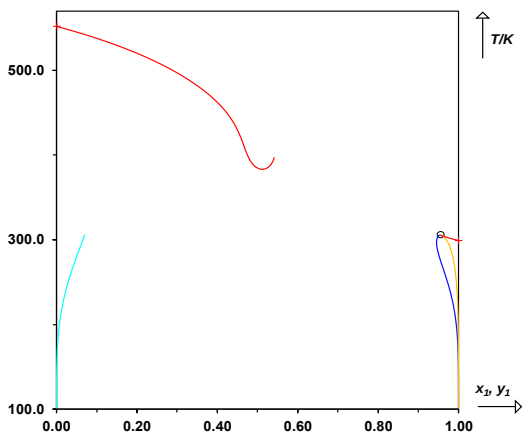
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 835
B/MPa = 1180

*Deviations*
MAPE on x = 9.0 %
MAPE on y = 6.2 %



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**Isothermal phase equilibrium data**

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Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.550 | 0.0057 | 0.9443 |
| 6.340 | 0.0090 | 0.9674 |
| 9.940 | 0.0172 | 0.9777 |
| 13.12 | 0.0215 | 0.9823 |
| 17.11 | 0.0268 | 0.9838 |
| 19.78 | 0.0288 | 0.9849 |
| 21.94 | 0.0342 | 0.9844 |
| 22.98 | 0.0353 | 0.9849 |
| 24.09 | 0.9628 | 0.9880 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.100 | 0.0057 | 0.8756 |
| 9.100 | 0.0115 | 0.9356 |
| 13.95 | 0.0180 | 0.9535 |
| 19.78 | 0.0254 | 0.9628 |
| 25.07 | 0.0321 | 0.9685 |
| 29.91 | 0.0375 | 0.9680 |
| 34.81 | 0.0431 | 0.9700 |
| 40.09 | 0.0520 | 0.9704 |
| 45.14 | 0.9699 | 0.9814 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.070 | 0.0094 | 0.8743 |
| 20.08 | 0.0263 | 0.9591 |
| 35.10 | 0.0431 | 0.9681 |
| 44.74 | 0.0566 | 0.9679 |
| 49.27 | 0.0565 | 0.9605 |
| 53.34 | 0.0595 | 0.9354 |
| 62.38 | 0.0577 | 0.9424 |
| 99.14 | 0.0600 | 0.9265 |
| 144.70 | 0.0595 | 0.9259 |
| 185.60 | 0.0592 | 0.9272 |
| 205.40 | 0.0593 | 0.9273 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.200 | 0.0102 | 0.8458 |
| 25.10 | 0.0313 | 0.9354 |
| 45.90 | 0.0537 | 0.9496 |
| 75.20 | 0.0756 | 0.9227 |
| 91.60 | 0.0802 | 0.9089 |
| 109.10 | 0.0821 | 0.9012 |
| 125.30 | 0.0824 | 0.8964 |
| 150.10 | 0.0868 | 0.8973 |
| 173.10 | 0.0855 | 0.8942 |
| 197.80 | 0.0867 | 0.8941 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.10 | 0.0105 | 0.7401 |
| 20.70 | 0.0213 | 0.8560 |
| 40.30 | 0.0490 | 0.9061 |
| 70.20 | 0.0829 | 0.9149 |
| 100.10 | 0.1052 | 0.8878 |
| 129.60 | 0.1168 | 0.8604 |
| 160.00 | 0.1246 | 0.8436 |
| 199.60 | 0.1315 | 0.8358 |
| 249.20 | 0.1370 | 0.8288 |
| 297.40 | 0.1430 | 0.8250 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.700 | 0.0065 | 0.5056 |
| 22.70 | 0.0206 | 0.7590 |
| 48.40 | 0.0527 | 0.8522 |
| 73.80 | 0.0879 | 0.8701 |
| 99.90 | 0.1189 | 0.8639 |
| 110.70 | 0.1315 | 0.8500 |
| 140.50 | 0.1581 | 0.8128 |
| 157.50 | 0.1715 | 0.7948 |
| 193.50 | 0.1918 | 0.7623 |
| 225.90 | 0.2073 | 0.7392 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 398.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.20 | 0.0089 | 0.4510 |
| 30.00 | 0.0307 | 0.6911 |
| 50.40 | 0.0547 | 0.7783 |
| 80.10 | 0.0979 | 0.8215 |
| 109.40 | 0.1405 | 0.8112 |
| 140.70 | 0.1907 | 0.7742 |
| 170.00 | 0.2394 | 0.7037 |
| 199.70 | 0.3003 | 0.6372 |
| 209.90 | 0.3265 | 0.5982 |
| 221.10 | 0.3806 | 0.5420 |
| 223.70 | 0.4037 | 0.5030 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 423.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.40 | 0.0102 | 0.3320 |
| 30.60 | 0.0250 | 0.5247 |
| 50.50 | 0.0497 | 0.6562 |
| 80.00 | 0.0942 | 0.7223 |
| 110.50 | 0.1480 | 0.7314 |
| 140.10 | 0.2086 | 0.7005 |
| 168.00 | 0.2941 | 0.6170 |
| 173.90 | 0.3224 | 0.5840 |
| 180.60 | 0.3861 | 0.5174 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 448.15**

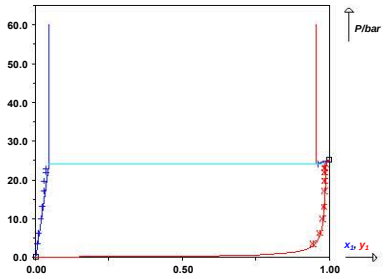
| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 22.70 | 0.0055 | 0.1403 |
| 30.50 | 0.0171 | 0.3148 |
| 45.10 | 0.0357 | 0.4728 |
| 65.00 | 0.0683 | 0.5767 |
| 85.70 | 0.0984 | 0.6171 |
| 105.50 | 0.1352 | 0.6400 |
| 125.40 | 0.1807 | 0.6260 |
| 140.40 | 0.2218 | 0.5910 |
| 150.20 | 0.2614 | 0.5626 |
| 160.00 | 0.3178 | 0.5044 |
| 163.10 | 0.3590 | 0.4503 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

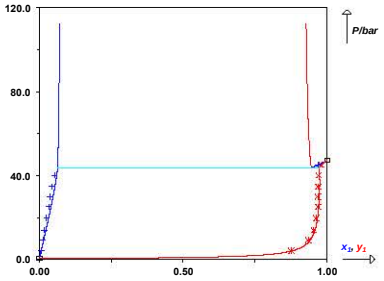
**T / K = 473.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 35.50 | 0.0112 | 0.1779 |
| 45.20 | 0.0272 | 0.3052 |
| 60.50 | 0.0490 | 0.4145 |
| 79.80 | 0.0805 | 0.4856 |
| 100.10 | 0.1202 | 0.5128 |
| 119.40 | 0.1681 | 0.5094 |
| 134.60 | 0.2203 | 0.4844 |
| 143.60 | 0.2672 | 0.4426 |
| 146.60 | 0.3043 | 0.3957 |

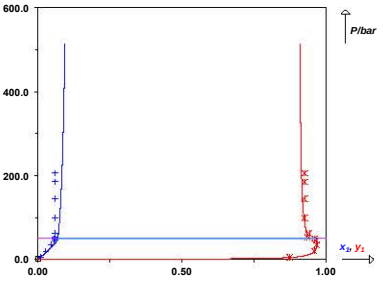
T/K = 273.15



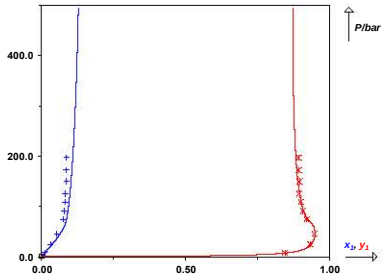

T/K = 298.15



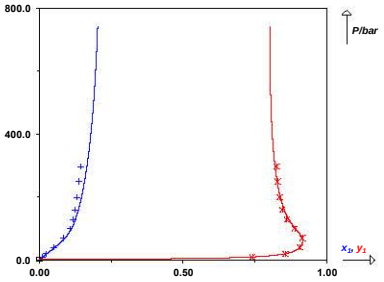

T/K = 303.15



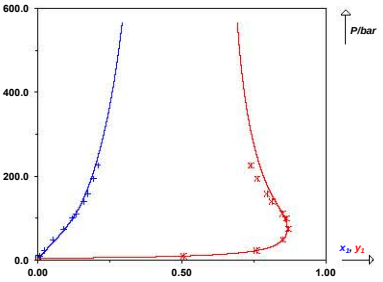

T/K = 323.15



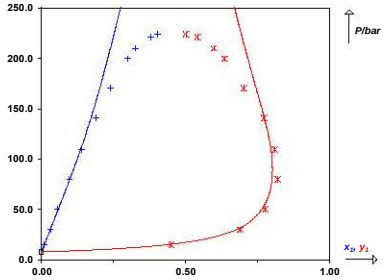

T/K = 348.15



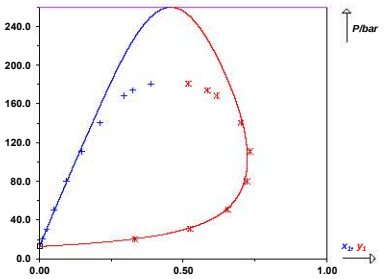

T/K = 373.15



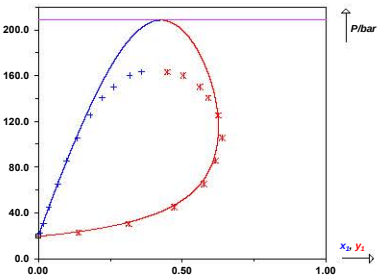

T/K = 398.15



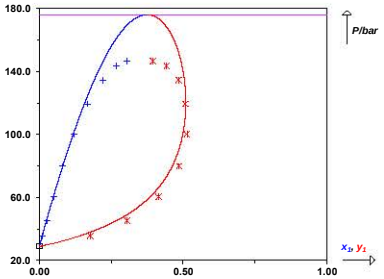

T/K = 423.15




T/K = 448.15




T/K = 473.15



## CHLOROFORM (1) + DIISOPROPYL ETHER (2)

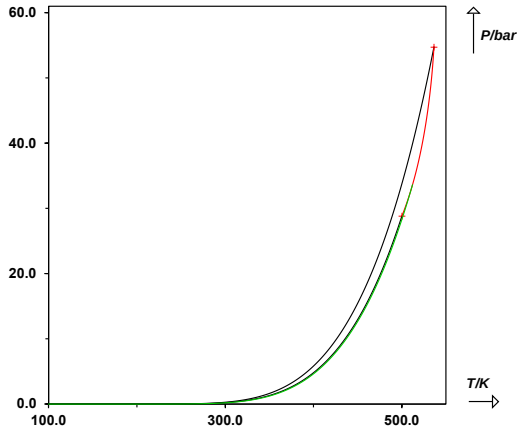
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 108-20-3 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | ZAFNJMIOTHYJRJ-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.40 | 500.05 |
| **$P_c$ / bar** | 54.72 | 28.80 |
| **ω** | 0.2220 | 0.3390 |

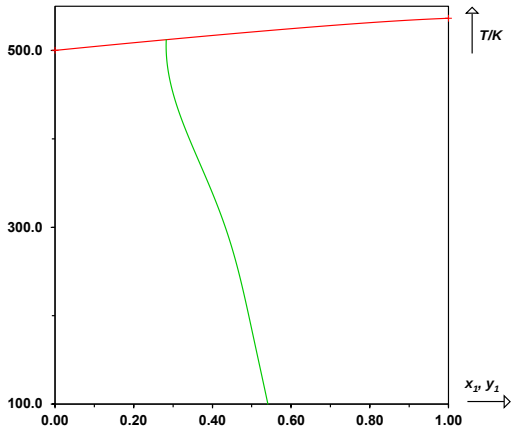
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = -145
B/MPa = -471

*Deviations*
MAPE on x = 17 %
MAPE on y = 19 %
MAPE on $h^M$ = 28 %
MAPE on $c_P^M$ = 24 %



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**Isobaric phase equilibrium data**

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Chevalier, J.L., Systèmes binaires chloroforme-éthers aliphatiques - III. — Équilibres liquide-vapeur, Journal de Chimie Physique et de Physico-Chimie Biologique (1969) 1457-1466.

**P / bar = 0.3280**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 311.00 | 0.1300 | 0.0890 |
| 311.25 | 0.1520 | 0.1130 |
| 311.50 | 0.1880 | 0.1410 |
| 311.85 | 0.2280 | 0.1810 |
| 312.25 | 0.2730 | 0.2310 |
| 312.45 | 0.3150 | 0.2750 |
| 312.65 | 0.3700 | 0.3450 |
| 312.70 | 0.4560 | 0.4690 |
| 312.60 | 0.4800 | 0.5140 |
| 312.15 | 0.5410 | 0.6030 |
| 311.80 | 0.5850 | 0.6550 |
| 310.75 | 0.6400 | 0.7350 |
| 308.65 | 0.7370 | 0.8530 |
| 307.45 | 0.7920 | 0.8980 |
| 306.45 | 0.8390 | 0.9300 |
| 304.40 | 0.9480 | 0.9820 |
| 303.80 | 0.9770 | 0.9930 |

Chevalier, J.L., Systèmes binaires chloroforme-éthers aliphatiques - III. — Équilibres liquide-vapeur, Journal de Chimie Physique et de Physico-Chimie Biologique (1969) 1457-1466.

**P / bar = 0.7693**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 333.45 | 0.1410 | 0.1000 |
| 333.70 | 0.1720 | 0.1280 |
| 333.95 | 0.2090 | 0.1660 |
| 334.45 | 0.2950 | 0.2650 |
| 334.65 | 0.3730 | 0.3620 |
| 334.40 | 0.4680 | 0.4910 |
| 333.35 | 0.5980 | 0.6620 |
| 333.15 | 0.6120 | 0.6780 |
| 333.05 | 0.6210 | 0.6940 |
| 332.95 | 0.6300 | 0.7050 |
| 332.80 | 0.6430 | 0.7210 |
| 332.65 | 0.6480 | 0.7270 |
| 332.55 | 0.6600 | 0.7400 |
| 331.75 | 0.7030 | 0.7840 |
| 330.60 | 0.7600 | 0.8500 |
| 329.45 | 0.8120 | 0.8970 |
| 327.30 | 0.9310 | 0.9750 |

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**Enthalpy of mixing**

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Becker, F. - Kiefer, M., Heat of mixing and formation of compounds in binary liquid systems. III. Ether-chloroform systems, Z. Naturforsch. Sec. A (1971) 1040-1046.

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -237.39 | 0.0250 |
| -470.60 | 0.0500 |
| -697.10 | 0.0750 |
| -917.33 | 0.1000 |
| -1130.4 | 0.1250 |
| -1336.8 | 0.1500 |
| -1539.9 | 0.1750 |
| -1724.5 | 0.2000 |
| -1904.2 | 0.2250 |
| -2077.5 | 0.2500 |
| -2229.5 | 0.2750 |
| -2373.1 | 0.3000 |
| -2504.1 | 0.3250 |
| -2619.7 | 0.3500 |
| -2719.8 | 0.3750 |
| -2803.9 | 0.4000 |
| -2870.1 | 0.4250 |
| -2917.4 | 0.4500 |
| -2945.8 | 0.4750 |
| -2955.5 | 0.5000 |
| -2945.8 | 0.5250 |
| -2916.5 | 0.5500 |
| -2868.0 | 0.5750 |
| -2800.6 | 0.6000 |
| -2716.8 | 0.6250 |
| -2608.4 | 0.6500 |
| -2467.7 | 0.6750 |
| -2322.4 | 0.7000 |
| -2173.8 | 0.7250 |
| -2014.3 | 0.7500 |
| -1844.3 | 0.7750 |
| -1665.1 | 0.8000 |
| -1477.5 | 0.8250 |
| -1281.6 | 0.8500 |
| -1080.2 | 0.8750 |
| -872.53 | 0.9000 |
| -660.68 | 0.9250 |
| -444.22 | 0.9500 |

| | |
|---|---|
| -224.41 | 0.9750 |

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**Heat capacity of mixing**

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Fenclova, D. - Dohnal, V. - Perez-Casas, S. - Frigolet, C. - Costas, M., Excess heat capacities, excess enthalpies, and excess volumes of trichloromethane + some oxygenated solvents or + the corresponding homomorphic hydrocarbons at 298.15 K, ELDATA Int. Electron. J. Phys. Chem. Data 3 (1995) 217-237.

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 4.020 | 0.1061 |
| 7.390 | 0.1924 |
| 11.61 | 0.3024 |
| 14.45 | 0.3978 |
| 15.61 | 0.4994 |
| 14.51 | 0.5935 |
| 11.37 | 0.7001 |
| 7.650 | 0.7972 |
| 3.950 | 0.8944 |

Grolier, J. -P. E. - Roux-Desgranges, G. - Berkane, M. - Wilhelm, Emmerich, Heat capacities and densities of mixtures of very polar substances. 3. Mixtures containing either trichloromethane or 1,4-dioxane or diisopropylether, Journal of Solution Chemistry 2 (1994) 153-166. doi:10.1007/BF00973543

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 1.246 | 0.0305 |
| 5.259 | 0.1231 |
| 8.067 | 0.1871 |
| 11.60 | 0.2805 |
| 13.37 | 0.3365 |
| 14.41 | 0.3709 |
| 16.19 | 0.4402 |
| 16.63 | 0.4975 |
| 15.40 | 0.5936 |
| 12.32 | 0.6840 |
| 10.23 | 0.7376 |
| 8.280 | 0.7871 |
| 5.689 | 0.8553 |
| 3.902 | 0.9062 |
| 1.796 | 0.9569 |

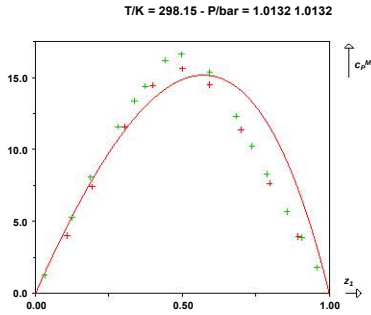
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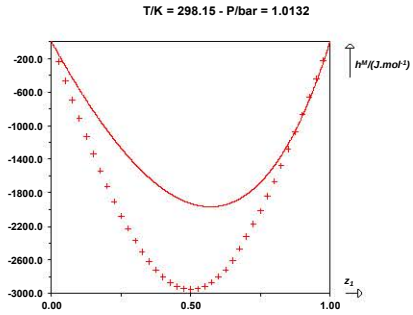
**Azeotropic point**

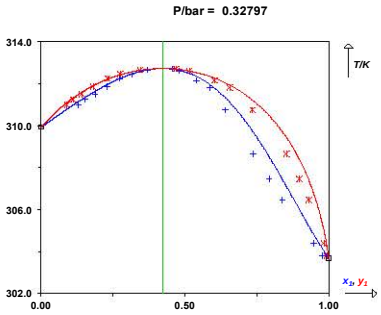
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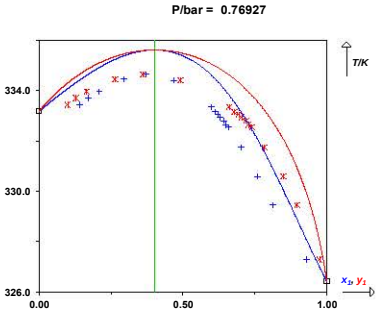
Chevalier, J.L., Systèmes binaires chloroforme-éthers aliphatiques - III. — Équilibres liquide-vapeur, Journal de Chimie Physique et de Physico-Chimie Biologique (1969) 1457-1466.

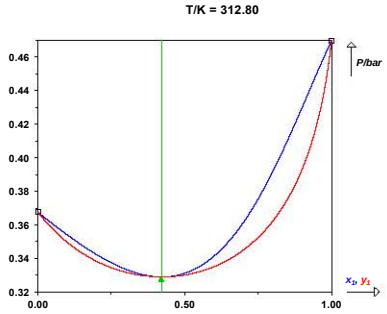
| T / K | P / bar | $x_1$ |
|---|---|---|
| 312.80 | 0.3280 | 0.4200 |


T/K = 298.15 - P/bar = 1.0132 1.0132
$c_p^M/(J.mol^{-1}.K^{-1})$
15.0
10.0
5.0
0.0
0.00
0.50
1.00
$z_1$


T/K = 298.15 - P/bar = 1.0132
$h^M/(J.mol^{-1})$
-200.0
-600.0
-1000.0
-1400.0
-1800.0
-2200.0
-2600.0
-3000.0
0.00
0.50
1.00
$z_1$


P/bar = 0.32797
T/K
314.0
310.0
306.0
302.0
0.00
0.50
1.00
$x_1, y_1$


P/bar = 0.76927
T/K
334.0
330.0
326.0
0.00
0.50
1.00
$x_1, y_1$


T/K = 312.80
P/bar
0.46
0.44
0.42
0.40
0.38
0.36
0.34
0.32
0.00
0.50
1.00
$x_1, y_1$

## 1,1,1-TRIFLUOROETHANE (1) + DIMETHYL ETHER (2)

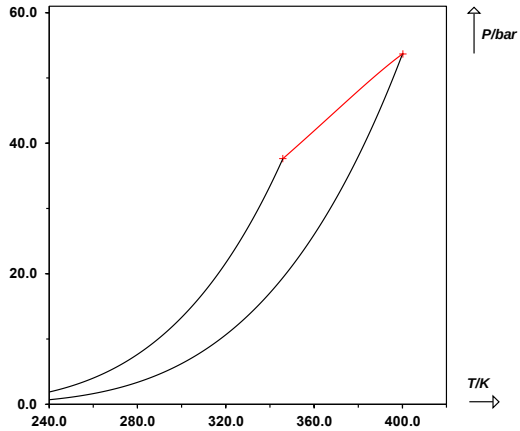
| | | |
|---|---|---|
| **CAS** | 420-46-2 | 115-10-6 |
| **InChiKey** | UJPMYEOUBPIPHQ-UHFFFAOYSA-N | LCGLNKUTAGEVQW-UHFFFAOYSA-N |
| **$T_c$ / K** | 345.88 | 400.10 |
| **$P_c$ / bar** | 37.64 | 53.70 |
| **ω** | 0.2610 | 0.2000 |

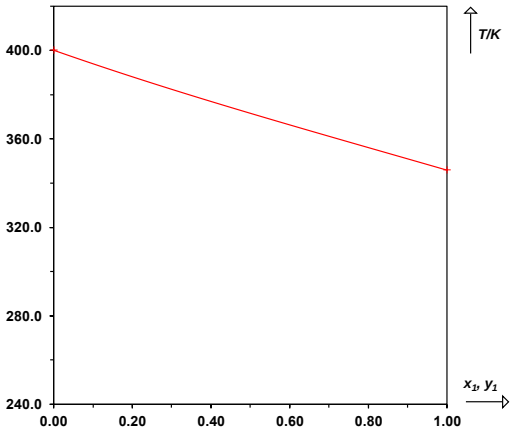
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 14.6
B/MPa = -51.9

*Deviations*
MAPE on x = 3.0 %
MAPE on y = 3.4 %



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**Isothermal phase equilibrium data**

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Im, Jihoon - Lee, Gangwon - Lee, Jongcheon - Kim, Hwayong, Vapor–liquid equilibria of the 1,1,1-trifluoroethane (HFC-143a)+dimethyl ether (DME) system, Fluid Phase Equilibria 1 (2007) 59-62. doi:10.1016/j.fluid.2006.10.017

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.010 | 0.0147 | 0.0226 |
| 9.270 | 0.0391 | 0.0618 |
| 9.840 | 0.0983 | 0.1529 |
| 10.32 | 0.1481 | 0.2236 |
| 10.90 | 0.2088 | 0.3010 |
| 11.71 | 0.2922 | 0.4012 |
| 12.53 | 0.3813 | 0.5035 |
| 13.57 | 0.4907 | 0.6043 |
| 14.57 | 0.5994 | 0.6982 |
| 15.59 | 0.7123 | 0.7898 |
| 16.72 | 0.8320 | 0.8781 |
| 17.74 | 0.9394 | 0.9581 |

Im, Jihoon - Lee, Gangwon - Lee, Jongcheon - Kim, Hwayong, Vapor–liquid equilibria of the 1,1,1-trifluoroethane (HFC-143a)+dimethyl ether (DME) system, Fluid Phase Equilibria 1 (2007) 59-62. doi:10.1016/j.fluid.2006.10.017

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.98 | 0.0453 | 0.0781 |
| 12.67 | 0.1028 | 0.1678 |
| 14.46 | 0.2531 | 0.3641 |
| 15.37 | 0.3348 | 0.4543 |
| 17.29 | 0.4972 | 0.6121 |
| 18.56 | 0.6163 | 0.7088 |
| 20.11 | 0.7491 | 0.8136 |
| 22.44 | 0.9496 | 0.9618 |

Im, Jihoon - Lee, Gangwon - Lee, Jongcheon - Kim, Hwayong, Vapor–liquid equilibria of the 1,1,1-trifluoroethane (HFC-143a)+dimethyl ether (DME) system, Fluid Phase Equilibria 1 (2007) 59-62. doi:10.1016/j.fluid.2006.10.017

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 14.97 | 0.0311 | 0.0525 |
| 15.48 | 0.0659 | 0.1081 |
| 16.30 | 0.1210 | 0.1881 |
| 17.32 | 0.1917 | 0.2826 |
| 19.08 | 0.3174 | 0.4243 |
| 20.73 | 0.4362 | 0.5409 |
| 22.58 | 0.5678 | 0.6586 |
| 24.76 | 0.7260 | 0.7845 |
| 26.61 | 0.8552 | 0.8855 |

Im, Jihoon - Lee, Gangwon - Lee, Jongcheon - Kim, Hwayong, Vapor–liquid equilibria of the 1,1,1-trifluoroethane (HFC-143a)+dimethyl ether (DME) system, Fluid Phase Equilibria 1 (2007) 59-62. doi:10.1016/j.fluid.2006.10.017

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 19.03 | 0.0524 | 0.0834 |
| 20.25 | 0.1203 | 0.1826 |
| 21.33 | 0.1826 | 0.2623 |
| 22.50 | 0.2510 | 0.3415 |
| 23.88 | 0.3336 | 0.4297 |
| 25.69 | 0.4424 | 0.5333 |
| 27.59 | 0.5532 | 0.6327 |
| 30.12 | 0.6981 | 0.7539 |
| 32.54 | 0.8392 | 0.8645 |

Im, Jihoon - Lee, Gangwon - Lee, Jongcheon - Kim, Hwayong, Vapor–liquid equilibria of the 1,1,1-trifluoroethane (HFC-143a)+dimethyl ether (DME) system, Fluid Phase Equilibria 1 (2007) 59-62. doi:10.1016/j.fluid.2006.10.017

**T / K = 353.15**

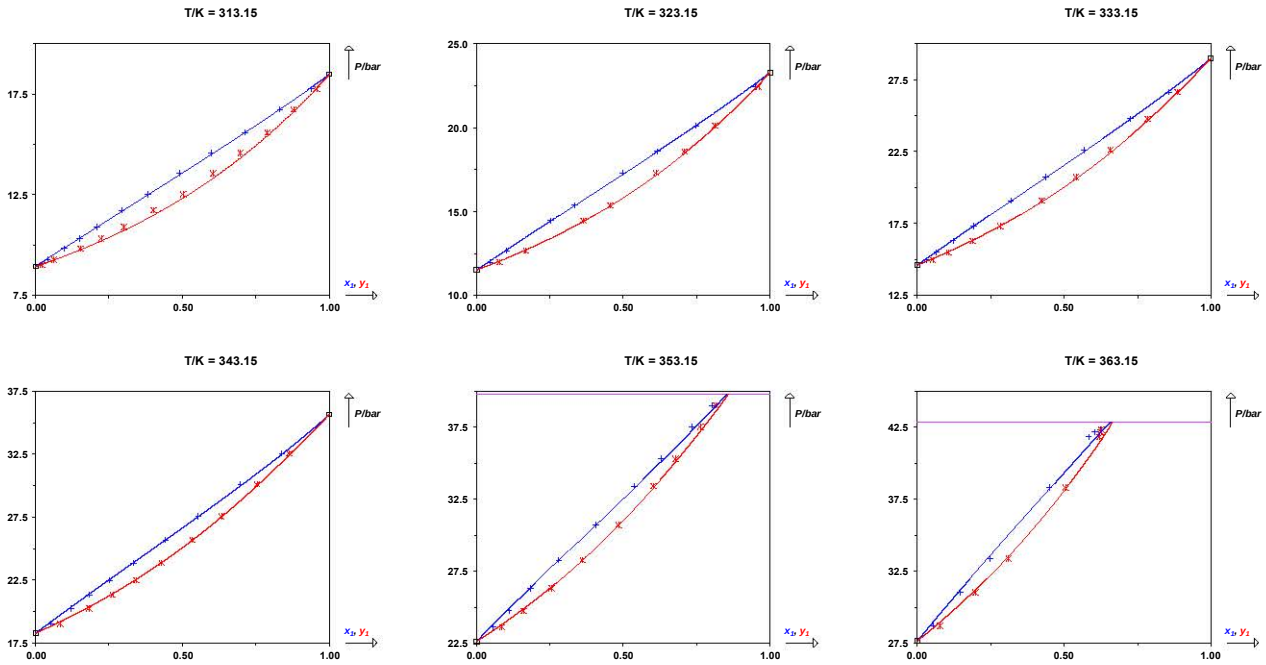
| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 23.61 | 0.0555 | 0.0860 |
| 24.73 | 0.1104 | 0.1614 |
| 26.30 | 0.1841 | 0.2559 |
| 28.26 | 0.2805 | 0.3622 |
| 30.71 | 0.4070 | 0.4848 |
| 33.40 | 0.5387 | 0.6028 |
| 35.30 | 0.6295 | 0.6779 |
| 37.53 | 0.7334 | 0.7625 |
| 39.01 | 0.8028 | 0.8161 |

Im, Jihoon - Lee, Gangwon - Lee, Jongcheon - Kim, Hwayong, Vapor–liquid equilibria of the 1,1,1-trifluoroethane (HFC-143a)+dimethyl ether (DME) system, Fluid Phase Equilibria 1 (2007) 59-62. doi:10.1016/j.fluid.2006.10.017

**T / K = 363.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 28.71 | 0.0530 | 0.0781 |
| 31.02 | 0.1456 | 0.1986 |
| 33.39 | 0.2470 | 0.3108 |
| 38.30 | 0.4486 | 0.5059 |
| 41.83 | 0.5828 | 0.6199 |

| | | |
|---|---|---|
| 42.16 | 0.6052 | 0.6262 |
| 42.33 | 0.6238 | 0.6277 |


T/K = 313.15
P/bar
17.5
12.5
7.5
0.00
0.50
1.00
x1, y1
T/K = 323.15
P/bar
25.0
20.0
15.0
10.0
0.00
0.50
1.00
x1, y1
T/K = 333.15
P/bar
27.5
22.5
17.5
12.5
0.00
0.50
1.00
x1, y1
T/K = 343.15
P/bar
37.5
32.5
27.5
22.5
17.5
0.00
0.50
1.00
x1, y1
T/K = 353.15
P/bar
37.5
32.5
27.5
22.5
0.00
0.50
1.00
x1, y1
T/K = 363.15
P/bar
42.5
37.5
32.5
27.5
0.00
0.50
1.00
x1, y1

## CHLOROFORM (1) + n-BUTYL ETHYL ETHER (2)

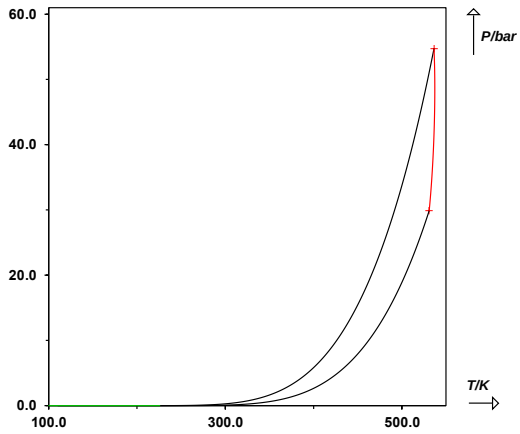
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 628-81-9 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | PZHIWRCQKBBTOW-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.40 | 531.00 |
| **$P_c$ / bar** | 54.72 | 29.90 |
| **ω** | 0.2220 | 0.3850 |

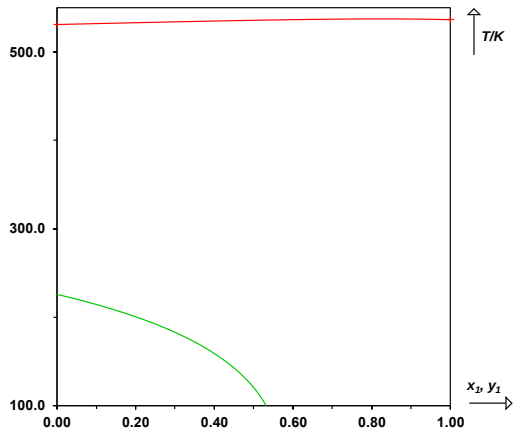
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = -112
B/MPa = -482

*Deviations*
MAPE on x = 9.2 %
MAPE on y = 8.1 %
MAPE on $h^M$ = 16 %



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**Isobaric phase equilibrium data**

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Chevalier, J.L., Systèmes binaires chloroforme-éthers aliphatiques - III. — Équilibres liquide-vapeur, Journal de Chimie Physique et de Physico-Chimie Biologique (1969) 1457-1466.

**P / bar = 0.3333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 331.05 | 0.0800 | 0.1310 |
| 329.95 | 0.1590 | 0.2330 |
| 327.55 | 0.2700 | 0.4060 |
| 326.95 | 0.2950 | 0.4350 |
| 325.75 | 0.3360 | 0.5040 |
| 323.65 | 0.4200 | 0.5950 |
| 323.45 | 0.4210 | 0.6010 |
| 319.65 | 0.5150 | 0.7400 |
| 316.45 | 0.5850 | 0.8150 |
| 313.05 | 0.6690 | 0.8890 |
| 311.65 | 0.7150 | 0.9150 |
| 309.10 | 0.7900 | 0.9470 |
| 307.35 | 0.8450 | 0.9650 |
| 305.50 | 0.9040 | 0.9850 |
| 304.50 | 0.9500 | 0.9910 |

Chevalier, J.L., Systèmes binaires chloroforme-éthers aliphatiques - III. — Équilibres liquide-vapeur, Journal de Chimie Physique et de Physico-Chimie Biologique (1969) 1457-1466.

**P / bar = 0.8666**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 358.95 | 0.0670 | 0.0840 |
| 357.25 | 0.1450 | 0.1900 |
| 356.80 | 0.1650 | 0.2070 |
| 356.25 | 0.1940 | 0.2500 |
| 355.45 | 0.2300 | 0.2920 |
| 353.35 | 0.3180 | 0.4140 |
| 349.85 | 0.4400 | 0.5870 |
| 346.65 | 0.5250 | 0.7050 |
| 343.85 | 0.5940 | 0.7850 |
| 341.05 | 0.6620 | 0.8500 |
| 339.35 | 0.7000 | 0.8840 |
| 337.35 | 0.7550 | 0.9120 |
| 336.05 | 0.7900 | 0.9300 |
| 334.30 | 0.8350 | 0.9520 |
| 332.95 | 0.8750 | 0.9660 |
| 330.65 | 0.9500 | 0.9850 |

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**Enthalpy of mixing**

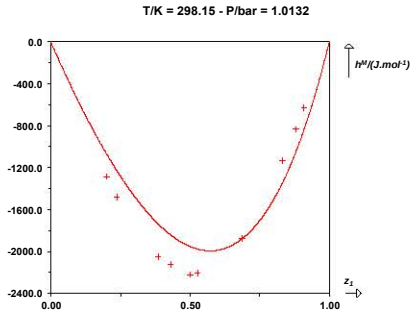
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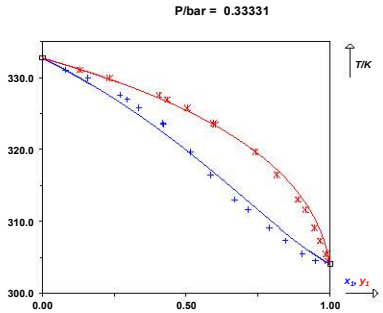
Chevalier, Jean-Louis - Bares, Daniel, Systèmes binaires chloroforme-éthers aliphatiques - I. — Chaleurs de mélange à 25 °C, Journal de Chimie Physique (1969) 1448-1452. doi:10.1051/jcp/196966s21448

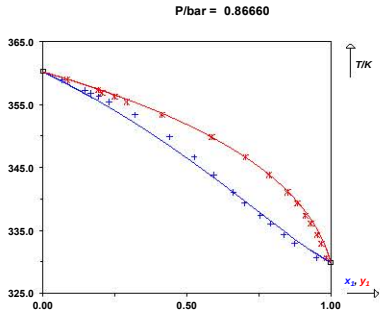
**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -1285.3 | 0.2000 |
| -1482.1 | 0.2370 |
| -2051.5 | 0.3850 |
| -2122.7 | 0.4300 |
| -2219.0 | 0.5010 |
| -2206.4 | 0.5270 |
| -1875.7 | 0.6880 |
| -1130.4 | 0.8320 |
| -837.36 | 0.8810 |
| -632.21 | 0.9090 |


T/K = 298.15 - P/bar = 1.0132
0.0
-400.0
-800.0
-1200.0
-1600.0
-2000.0
-2400.0
0.00
0.50
1.00
$h^{M}$/(J.mol$^{-1}$)
$z_1$


P/bar = 0.33331
330.0
320.0
310.0
300.0
0.00
0.50
1.00
T/K
$x_1$, $y_1$


P/bar = 0.86660
365.0
355.0
345.0
335.0
325.0
0.00
0.50
1.00
T/K
$x_1$, $y_1$

## CARBON DIOXIDE (1) + DIFLUOROMETHANE (2)

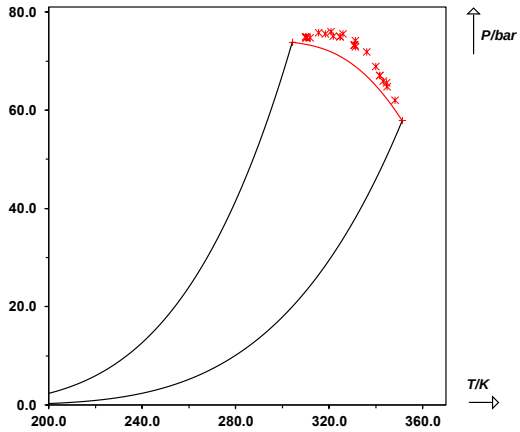
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 75-10-5 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | RWRIWBAIICGTTQ-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 351.26 |
| **$P_c$ / bar** | 73.83 | 57.84 |
| **ω** | 0.2240 | 0.2770 |

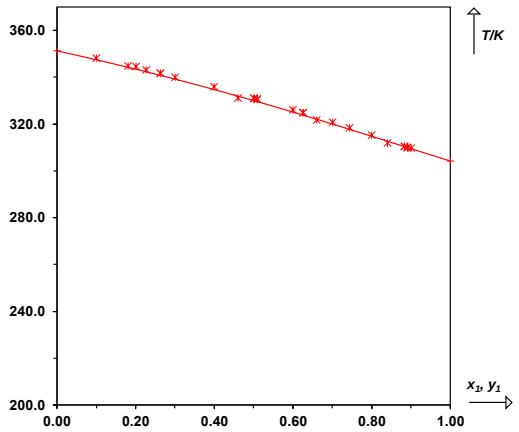
Ideal

**PPR78 results**

*Parameters*
A/MPa = 72.5
B/MPa = 49.4

*Deviations*
MAPE on x = 4.5 %
MAPE on y = 3.2 %
MAPE on $x_c$ = 3.9 %
MAPE on $P_c$ = 4.3 %



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**Isothermal phase equilibrium data**

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Stein, Fred Paul. - Adams, Robert A., Vapor-liquid equilibriums for carbon dioxide-difluoromethane system, Journal of Chemical & Engineering Data 2 (1971) 146-149. doi:10.1021/je60049a015

**T / K = 222.04**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.145 | 0.0199 | 0.1010 |
| 1.296 | 0.0440 | 0.2130 |
| 1.703 | 0.1240 | 0.4470 |
| 2.082 | 0.1990 | 0.5870 |
| 2.799 | 0.3240 | 0.7370 |
| 3.523 | 0.4580 | 0.8250 |
| 4.158 | 0.5640 | 0.8820 |
| 4.826 | 0.6880 | 0.9240 |
| 5.571 | 0.8220 | 0.9609 |
| 5.785 | 0.8640 | 0.9694 |
| 6.143 | 0.9270 | 0.9822 |

Stein, Fred Paul. - Adams, Robert A., Vapor-liquid equilibriums for carbon dioxide-difluoromethane system, Journal of Chemical & Engineering Data 2 (1971) 146-149. doi:10.1021/je60049a015

**T / K = 244.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.082 | 0.0190 | 0.0790 |
| 3.413 | 0.0480 | 0.1830 |
| 3.751 | 0.0730 | 0.2750 |
| 4.475 | 0.1350 | 0.4240 |
| 5.233 | 0.1970 | 0.5400 |
| 6.592 | 0.3130 | 0.6760 |
| 7.936 | 0.4290 | 0.7710 |
| 9.570 | 0.5600 | 0.8470 |
| 11.11 | 0.6890 | 0.9040 |
| 12.44 | 0.7980 | 0.9420 |
| 13.36 | 0.8830 | 0.9651 |
| 14.07 | 0.9440 | 0.9819 |

Stein, Fred Paul. - Adams, Robert A., Vapor-liquid equilibriums for carbon dioxide-difluoromethane system, Journal of Chemical & Engineering Data 2 (1971) 146-149. doi:10.1021/je60049a015

**T / K = 266.48**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.874 | 0.0138 | 0.0510 |
| 10.30 | 0.1730 | 0.4420 |
| 12.08 | 0.2520 | 0.5560 |
| 13.58 | 0.3200 | 0.6280 |
| 18.85 | 0.5670 | 0.8040 |
| 20.53 | 0.6330 | 0.8470 |
| 23.02 | 0.7470 | 0.8950 |
| 25.06 | 0.8310 | 0.9320 |
| 26.65 | 0.8980 | 0.9590 |
| 28.17 | 0.9605 | 0.9810 |

Rivollet, F - Chapoy, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the carbon dioxide (CO2) + difluoromethane (R32) system at temperatures from 283.12 to 343.25 K and pressures up to 7.46 MPa, Fluid Phase Equilibria 1 (2004) 95-101. doi:10.1016/j.fluid.2003.12.002

**T / K = 305.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 23.56 | 0.0720 | 0.1530 |
| 34.50 | 0.2840 | 0.4770 |
| 44.16 | 0.4680 | 0.6500 |
| 56.39 | 0.6850 | 0.7960 |
| 66.02 | 0.8540 | 0.8960 |
| 69.05 | 0.9050 | 0.9280 |

Rivollet, F - Chapoy, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the carbon dioxide (CO2) + difluoromethane (R32) system at temperatures from 283.12 to 343.25 K and pressures up to 7.46 MPa, Fluid Phase Equilibria 1 (2004) 95-101. doi:10.1016/j.fluid.2003.12.002

**T / K = 313.30**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 26.16 | 0.0250 | 0.0530 |
| 49.94 | 0.4280 | 0.5880 |
| 60.91 | 0.6020 | 0.7160 |
| 70.60 | 0.7490 | 0.8010 |
| 71.70 | 0.7660 | 0.8110 |
| 73.18 | 0.7880 | 0.8220 |

Rivollet, F - Chapoy, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the carbon dioxide (CO2) + difluoromethane (R32) system at temperatures from 283.12 to 343.25 K and pressures up to 7.46 MPa, Fluid Phase Equilibria 1 (2004) 95-101. doi:10.1016/j.fluid.2003.12.002

**T / K = 323.34**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 32.99 | 0.0250 | 0.0480 |
| 42.26 | 0.1680 | 0.2760 |
| 55.37 | 0.3630 | 0.4850 |
| 67.38 | 0.5250 | 0.6120 |
| 71.82 | 0.5820 | 0.6440 |
| 72.93 | 0.5970 | 0.6500 |
| 74.64 | 0.6250 | 0.6560 |

Rivollet, F - Chapoy, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the carbon dioxide (CO2) + difluoromethane (R32) system at temperatures from 283.12 to 343.25 K and pressures up to 7.46 MPa, Fluid Phase Equilibria 1 (2004) 95-101. doi:10.1016/j.fluid.2003.12.002

**T / K = 333.33**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 41.70 | 0.0310 | 0.0520 |
| 67.10 | 0.3690 | 0.4340 |
| 70.87 | 0.4190 | 0.4640 |
| 71.91 | 0.4330 | 0.4650 |

Rivollet, F - Chapoy, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the carbon dioxide (CO2) + difluoromethane (R32) system at temperatures from 283.12 to 343.25 K and pressures up to 7.46 MPa, Fluid Phase Equilibria 1 (2004) 95-101. doi:10.1016/j.fluid.2003.12.002

**T / K = 343.23**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 54.27 | 0.0690 | 0.0880 |
| 58.52 | 0.1190 | 0.1540 |
| 62.50 | 0.1670 | 0.2010 |
| 65.19 | 0.2040 | 0.2290 |
| 65.89 | 0.2170 | 0.2280 |

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**Critical point**

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Kordikowski, Andreas - Robertson, Duncan G. - Poliakoff, Martyn - DiNoia, Todd D. - McHugh, Mark - Aguiar-Ricardo, Ana, Acoustic Determination of the Critical Surfaces in the Ternary Systems CO2 + CH2F2 + CF3CH2F and CO + C2H4 + CH3CHCH2 and in Their Binary Subsystems, The Journal of Physical Chemistry B 30 (1997) 5853-5862. doi:10.1021/jp963061l

| T / K | P / bar | $x_1$ |
|---|---|---|
| 311.90 | 74.70 | 0.8400 |
| 321.80 | 75.00 | 0.6600 |
| 331.10 | 72.90 | 0.4600 |
| 344.80 | 64.70 | 0.1800 |

Diefenbacher, A. - Türk, M., (Vapour+liquid) Equilibria of binary mixtures of CO2, CH2F2, CHF3, and SF6, The Journal of Chemical Thermodynamics 9 (2002) 1361-1375. doi:10.1016/S0021-9614(02)00123-4

| T / K | P / bar | $x_1$ |
|---|---|---|
| 343.09 | 65.86 | 0.2260 |
| 341.63 | 67.06 | 0.2630 |
| 330.95 | 73.17 | 0.5010 |
| 330.71 | 73.27 | 0.5090 |
| 324.76 | 74.91 | 0.6260 |
| 318.29 | 75.47 | 0.7430 |
| 310.39 | 74.81 | 0.8830 |
| 309.99 | 74.75 | 0.8910 |

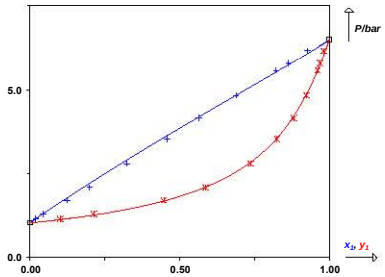
Rivollet, F - Chapoy, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the carbon dioxide (CO2) + difluoromethane (R32) system at temperatures from 283.12 to 343.25 K and pressures up to 7.46 MPa, Fluid Phase Equilibria 1 (2004) 95-101. doi:10.1016/j.fluid.2003.12.002

| T / K | P / bar | $x_1$ |
|---|---|---|
| 348.25 | 61.96 | 0.1000 |
| 344.47 | 65.53 | 0.2000 |
| 340.04 | 68.82 | 0.3000 |
| 336.00 | 71.87 | 0.4000 |
| 331.09 | 74.11 | 0.5000 |
| 325.95 | 75.48 | 0.6000 |
| 320.68 | 75.98 | 0.7000 |
| 315.33 | 75.77 | 0.8000 |
| 309.82 | 74.97 | 0.9000 |

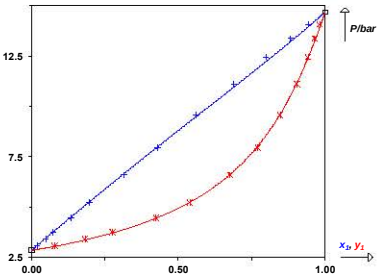
Diefenbacher, A. - Türk, M., Critical properties (pc, Tc, and ρc) and phase equilibria of binary mixtures of CO2, CHF3, CH2F2, and SF6, Fluid Phase Equilibria 1-2 (2001) 121-131. doi:10.1016/S0378-3812(01)00386-7

| T / K | P / bar | $x_1$ |
|---|---|---|
| 341.63 | 67.06 | 0.2630 |
| 330.71 | 73.27 | 0.5090 |
| 324.76 | 74.91 | 0.6260 |
| 310.39 | 74.81 | 0.8830 |
| 309.99 | 74.75 | 0.8910 |

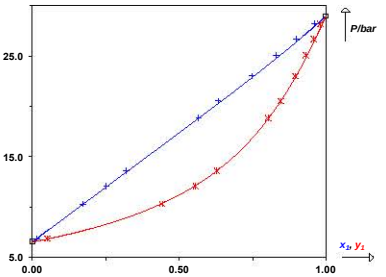
T/K = 222.04



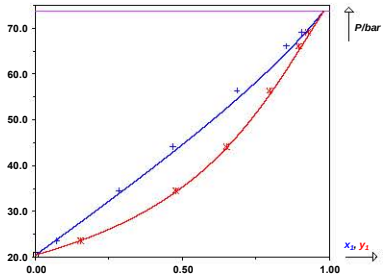

T/K = 244.26



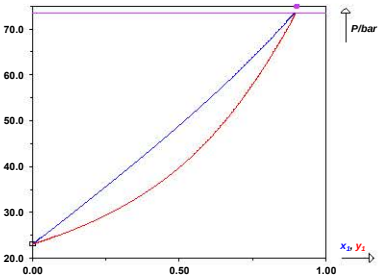

T/K = 266.48



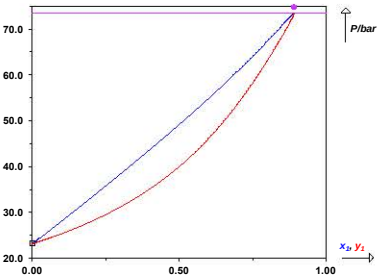

T/K = 305.15



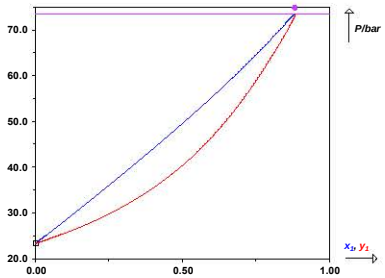

T/K = 309.82



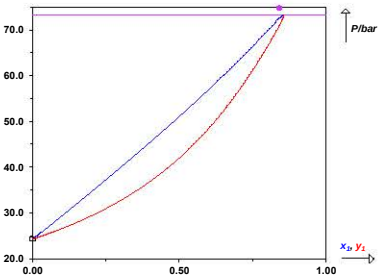

T/K = 309.99



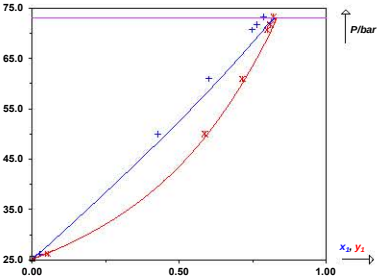

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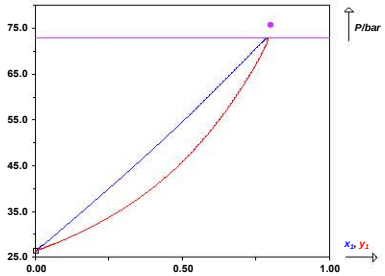

T/K = 311.90



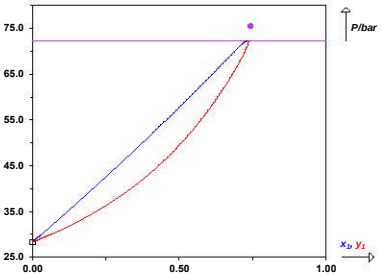

T/K = 313.30



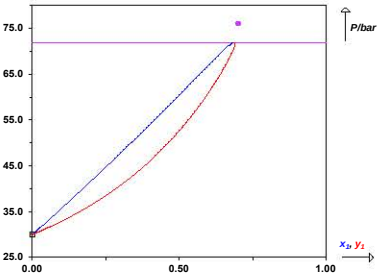

T/K = 315.33



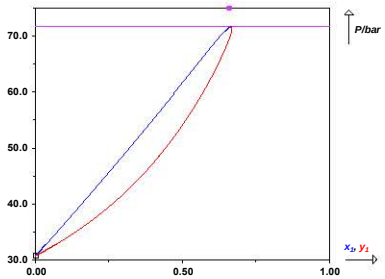

T/K = 318.29



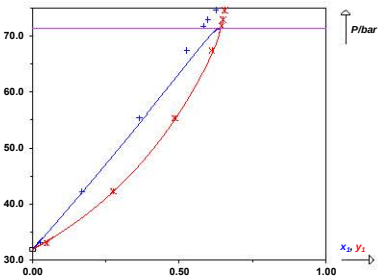

T/K = 320.68



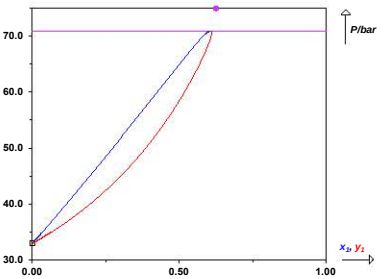

T/K = 321.80



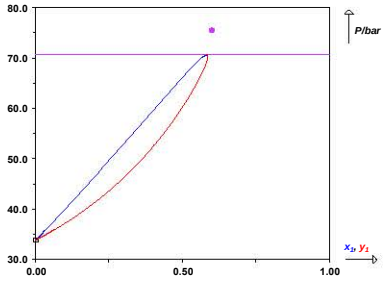

T/K = 323.34



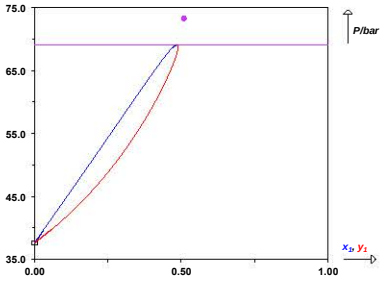

T/K = 324.76



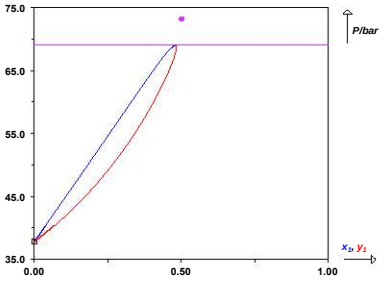
T/K = 325.95



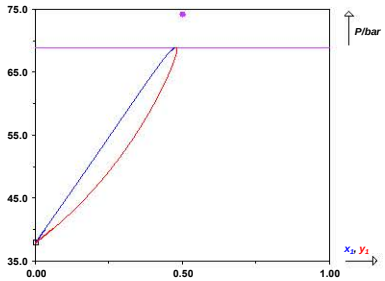

T/K = 330.71



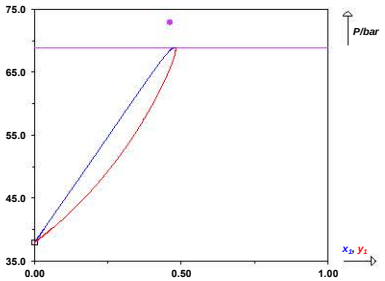

T/K = 330.95



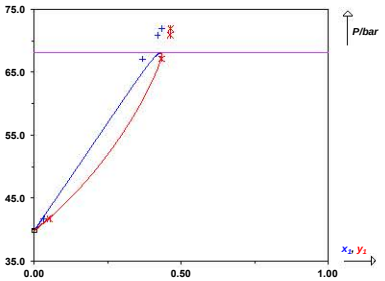

T/K = 331.09



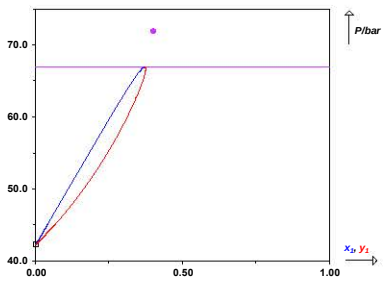

T/K = 331.10



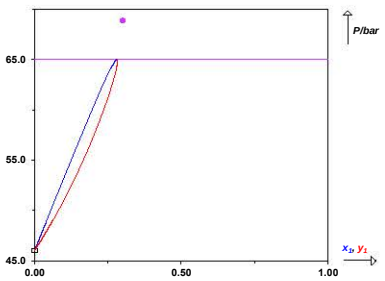

T/K = 333.33



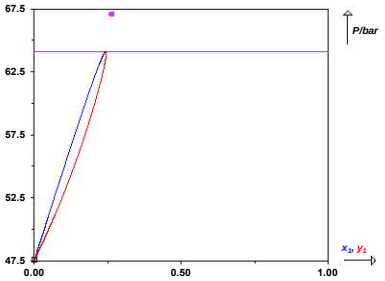

T/K = 336.00



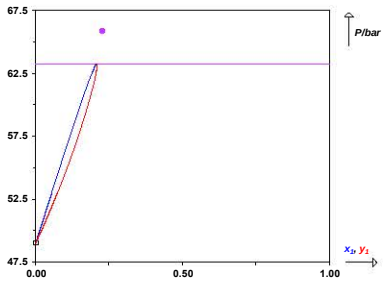

T/K = 340.04



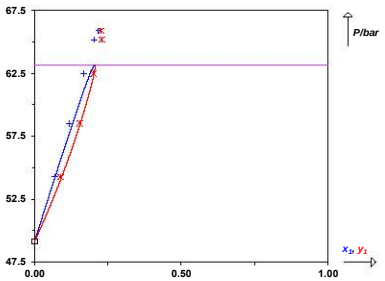

T/K = 341.63



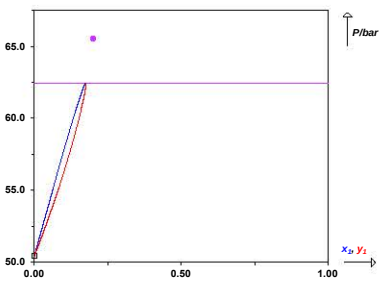

T/K = 343.09



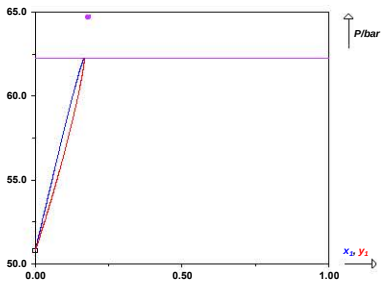

T/K = 343.23



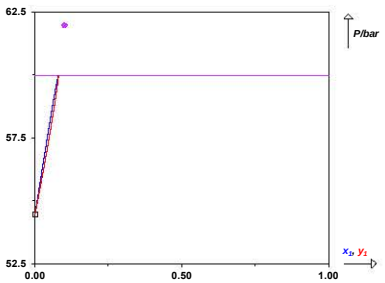

T/K = 344.47




T/K = 344.80




T/K = 348.25



## DIFLUOROMETHANE (1) + DIMETHYL ETHER (2)

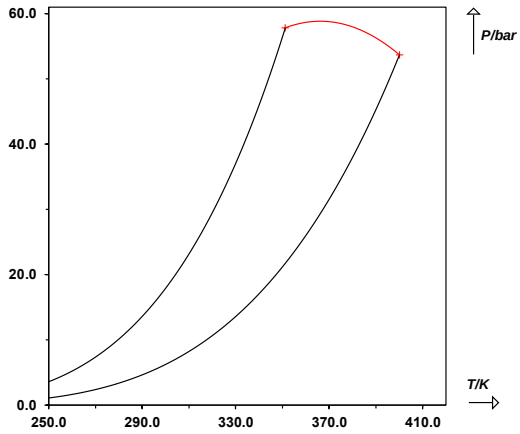
| | | |
|---|---|---|
| **CAS** | 75-10-5 | 115-10-6 |
| **InChiKey** | RWRIWBAIICGTTQ-UHFFFAOYSA-N | LCGLNKUTAGEVQW-UHFFFAOYSA-N |
| **$T_c$ / K** | 351.26 | 400.10 |
| **$P_c$ / bar** | 57.84 | 53.70 |
| **ω** | 0.2770 | 0.2000 |

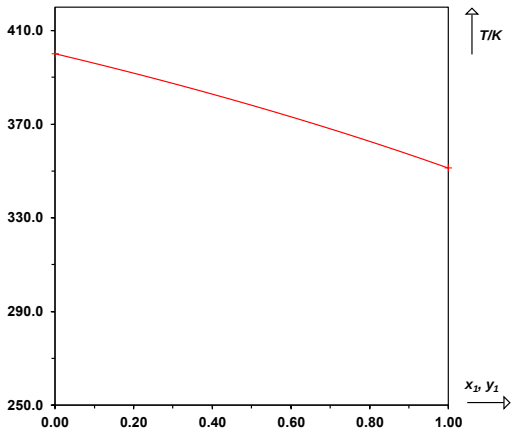
Ideal

**PPR78 results**

*Parameters*
A/MPa = -9.18
B/MPa = -20.1

*Deviations*
MAPE on x = 2.5 %
MAPE on y = 2.4 %



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**Isothermal phase equilibrium data**

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Fedele, L. - Bobbo, S. - De Stefani, V. - Camporese, R. - Stryjek, R., Isothermal VLE Measurements for Difluoromethane + Dimethyl Ether and an Evaluation of Hydrogen Bonding, J. Chem. Eng. Data 1 (2005) 128-132. doi:10.1021/je049789+

**T / K = 258.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.794 | 0.1025 | 0.2330 |
| 2.118 | 0.2160 | 0.4247 |
| 2.337 | 0.2850 | 0.5198 |
| 2.893 | 0.4423 | 0.6965 |
| 3.258 | 0.5376 | 0.7727 |
| 3.624 | 0.6386 | 0.8404 |
| 4.077 | 0.7639 | 0.9021 |
| 4.534 | 0.8983 | 0.9578 |

Fedele, L. - Bobbo, S. - De Stefani, V. - Camporese, R. - Stryjek, R., Isothermal VLE Measurements for Difluoromethane + Dimethyl Ether and an Evaluation of Hydrogen Bonding, J. Chem. Eng. Data 1 (2005) 128-132. doi:10.1021/je049789+

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.750 | 0.0181 | 0.0444 |
| 3.268 | 0.1356 | 0.2854 |
| 3.762 | 0.2378 | 0.4471 |
| 4.772 | 0.4195 | 0.6571 |
| 5.489 | 0.5405 | 0.7606 |
| 6.245 | 0.6687 | 0.8451 |
| 7.136 | 0.8258 | 0.9254 |
| 7.733 | 0.9313 | 0.9702 |

Coquelet, Christophe - Valtz, Alain - Richon, Dominique, Vapor–liquid equilibrium data for the difluoromethane (R32)–dimethyl ether (RE170) system at temperatures from 283.03 to 363.21K and pressures up to 5.5MPa, Fluid Phase Equilibria 1-2 (2005) 44-49. doi:10.1016/j.fluid.2005.02.013

**T / K = 283.03**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.998 | 0.1996 | 0.3856 |
| 5.874 | 0.3207 | 0.5513 |
| 6.794 | 0.4445 | 0.6677 |
| 7.757 | 0.5670 | 0.7688 |
| 8.959 | 0.7242 | 0.8635 |
| 9.964 | 0.8573 | 0.9324 |

Fedele, L. - Bobbo, S. - De Stefani, V. - Camporese, R. - Stryjek, R., Isothermal VLE Measurements for Difluoromethane + Dimethyl Ether and an Evaluation of Hydrogen Bonding, J. Chem. Eng. Data 1 (2005) 128-132. doi:10.1021/je049789+

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.732 | 0.0836 | 0.1749 |
| 6.547 | 0.1831 | 0.3460 |
| 7.823 | 0.3215 | 0.5310 |
| 8.988 | 0.4400 | 0.6534 |
| 10.30 | 0.5675 | 0.7580 |
| 11.72 | 0.7048 | 0.8479 |
| 12.78 | 0.8069 | 0.9046 |
| 14.16 | 0.9441 | 0.9727 |

Coquelet, Christophe - Valtz, Alain - Richon, Dominique, Vapor–liquid equilibrium data for the difluoromethane (R32)–dimethyl ether (RE170) system at temperatures from 283.03 to 363.21K and pressures up to 5.5MPa, Fluid Phase Equilibria 1-2 (2005) 44-49. doi:10.1016/j.fluid.2005.02.013

**T / K = 298.11**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.151 | 0.1357 | 0.2667 |
| 8.674 | 0.2790 | 0.4806 |
| 10.80 | 0.4702 | 0.6785 |
| 12.34 | 0.6069 | 0.7801 |
| 13.96 | 0.7509 | 0.8653 |
| 15.30 | 0.8665 | 0.9298 |

Im, Jihoon - Lee, Gangwon - Kim, Hwayong, Vapor–Liquid Equilibria of the Difluoromethane + Dimethyl Ether and 1,1,1,2-Tetrafluoroethane + Dimethyl Ether Systems, Journal of Chemical & Engineering Data 3 (2006) 1126-1129. doi:10.1021/je060028b

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.40 | 0.1186 | 0.2145 |
| 11.36 | 0.1881 | 0.3256 |
| 12.34 | 0.2555 | 0.4187 |
| 14.73 | 0.4108 | 0.5893 |
| 15.87 | 0.4815 | 0.6561 |
| 16.82 | 0.5381 | 0.6966 |
| 18.50 | 0.6370 | 0.7687 |
| 19.17 | 0.6811 | 0.8036 |
| 21.15 | 0.7964 | 0.8828 |
| 22.00 | 0.8454 | 0.9119 |
| 22.86 | 0.8936 | 0.9395 |

Im, Jihoon - Lee, Gangwon - Kim, Hwayong, Vapor–Liquid Equilibria of the Difluoromethane + Dimethyl Ether and 1,1,1,2-Tetrafluoroethane +

Dimethyl Ether Systems, Journal of Chemical & Engineering Data 3 (2006) 1126-1129. doi:10.1021/je060028b

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 12.28 | 0.0510 | 0.0849 |
| 13.23 | 0.1106 | 0.1864 |
| 14.24 | 0.1693 | 0.2850 |
| 15.26 | 0.2265 | 0.3671 |
| 16.65 | 0.3012 | 0.4624 |
| 17.83 | 0.3662 | 0.5371 |
| 20.16 | 0.4832 | 0.6476 |
| 21.46 | 0.5459 | 0.7017 |
| 23.00 | 0.6200 | 0.7569 |
| 24.35 | 0.6838 | 0.8018 |
| 25.40 | 0.7353 | 0.8367 |
| 27.32 | 0.8239 | 0.8923 |
| 28.87 | 0.8903 | 0.9326 |
| 30.28 | 0.9516 | 0.9701 |

Coquelet, Christophe - Valtz, Alain - Richon, Dominique, Vapor–liquid equilibrium data for the difluoromethane (R32)–dimethyl ether (RE170) system at temperatures from 283.03 to 363.21K and pressures up to 5.5MPa, Fluid Phase Equilibria 1-2 (2005) 44-49. doi:10.1016/j.fluid.2005.02.013

**T / K = 328.16**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.21 | 0.1253 | 0.2262 |
| 18.23 | 0.2750 | 0.4327 |
| 21.09 | 0.4077 | 0.5792 |
| 23.88 | 0.5338 | 0.6901 |
| 26.66 | 0.6556 | 0.7807 |
| 29.48 | 0.7743 | 0.8572 |
| 32.09 | 0.8786 | 0.9249 |

Im, Jihoon - Lee, Gangwon - Kim, Hwayong, Vapor–Liquid Equilibria of the Difluoromethane + Dimethyl Ether and 1,1,1,2-Tetrafluoroethane + Dimethyl Ether Systems, Journal of Chemical & Engineering Data 3 (2006) 1126-1129. doi:10.1021/je060028b

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.41 | 0.0475 | 0.0879 |
| 16.75 | 0.1139 | 0.1954 |
| 18.57 | 0.2013 | 0.3264 |
| 20.85 | 0.3037 | 0.4549 |
| 25.81 | 0.5100 | 0.6559 |
| 26.72 | 0.5434 | 0.6851 |
| 28.78 | 0.6243 | 0.7480 |
| 29.54 | 0.6546 | 0.7703 |
| 30.88 | 0.7018 | 0.8028 |
| 33.41 | 0.7984 | 0.8668 |
| 35.63 | 0.8767 | 0.9175 |
| 37.74 | 0.9501 | 0.9659 |

Im, Jihoon - Lee, Gangwon - Kim, Hwayong, Vapor–Liquid Equilibria of the Difluoromethane + Dimethyl Ether and 1,1,1,2-Tetrafluoroethane + Dimethyl Ether Systems, Journal of Chemical & Engineering Data 3 (2006) 1126-1129. doi:10.1021/je060028b

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.78 | 0.1120 | 0.1930 |
| 22.39 | 0.1765 | 0.2877 |
| 23.97 | 0.2362 | 0.3654 |
| 26.65 | 0.3339 | 0.4774 |
| 29.38 | 0.4281 | 0.5686 |
| 31.24 | 0.4919 | 0.6251 |
| 32.19 | 0.5230 | 0.6519 |
| 34.23 | 0.5870 | 0.7028 |
| 35.29 | 0.6235 | 0.7310 |
| 39.36 | 0.7470 | 0.8193 |
| 42.11 | 0.8250 | 0.8738 |
| 44.12 | 0.8777 | 0.9096 |
| 45.60 | 0.9175 | 0.9377 |
| 46.86 | 0.9548 | 0.9641 |

Coquelet, Christophe - Valtz, Alain - Richon, Dominique, Vapor–liquid equilibrium data for the difluoromethane (R32)–dimethyl ether (RE170) system at temperatures from 283.03 to 363.21K and pressures up to 5.5MPa, Fluid Phase Equilibria 1-2 (2005) 44-49. doi:10.1016/j.fluid.2005.02.013

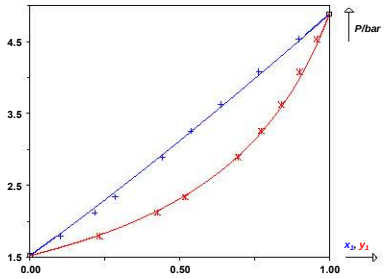
**T / K = 353.16**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 25.48 | 0.1057 | 0.1741 |
| 30.06 | 0.2494 | 0.3688 |
| 35.06 | 0.3968 | 0.5251 |
| 40.00 | 0.5349 | 0.6453 |
| 44.46 | 0.6527 | 0.7348 |
| 48.70 | 0.7569 | 0.8104 |
| 51.97 | 0.8333 | 0.8641 |
| 52.77 | 0.8525 | 0.8772 |

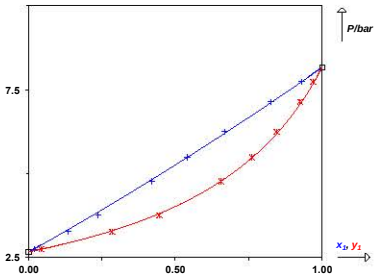
Coquelet, Christophe - Valtz, Alain - Richon, Dominique, Vapor–liquid equilibrium data for the difluoromethane (R32)–dimethyl ether (RE170) system at temperatures from 283.03 to 363.21K and pressures up to 5.5MPa, Fluid Phase Equilibria 1-2 (2005) 44-49. doi:10.1016/j.fluid.2005.02.013

| **T / K =** | **363.21** | |
|---|---|---|
| P / bar | $x_1$ | $y_1$ |
| 31.33 | 0.1163 | 0.1802 |
| 35.55 | 0.2295 | 0.3253 |
| 39.89 | 0.3381 | 0.4450 |
| 44.09 | 0.4406 | 0.5400 |
| 48.50 | 0.5430 | 0.6224 |
| 53.65 | 0.6553 | 0.7022 |
| 55.06 | 0.6859 | 0.7217 |

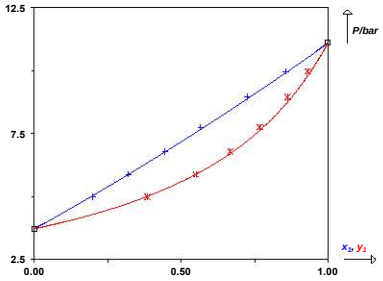
T/K = 258.15



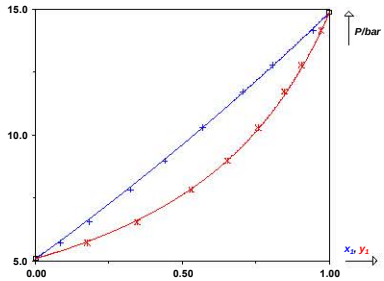

T/K = 273.15



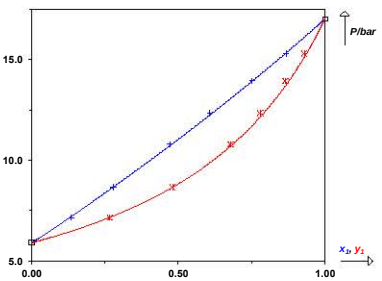

T/K = 283.03



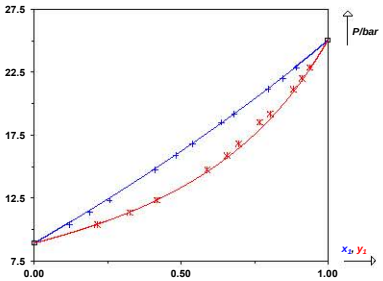

T/K = 293.15



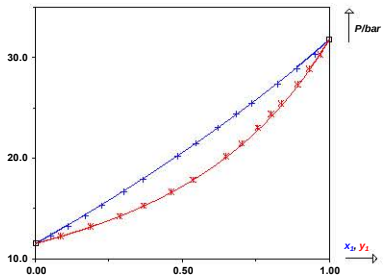

T/K = 298.11



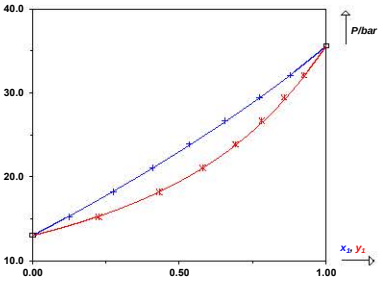

T/K = 313.15



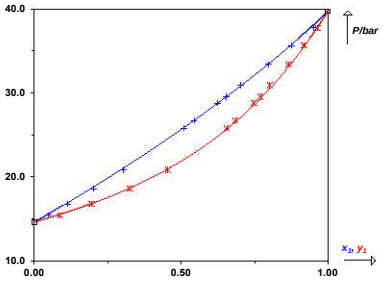

T/K = 323.15



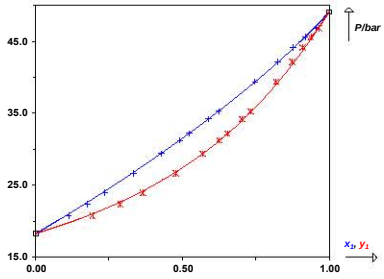

T/K = 328.16



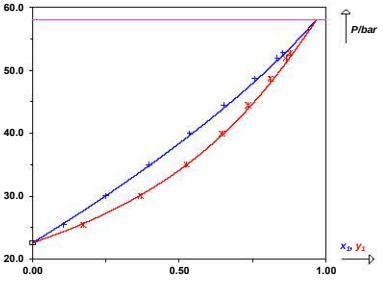

T/K = 333.15



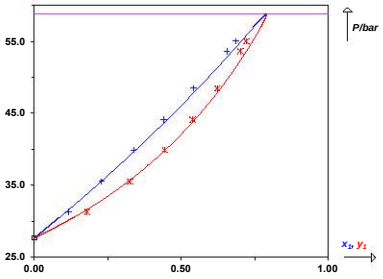

T/K = 343.15




T/K = 353.16




T/K = 363.21



## DIFLUOROMETHANE (1) + SULFUR DIOXIDE (2)

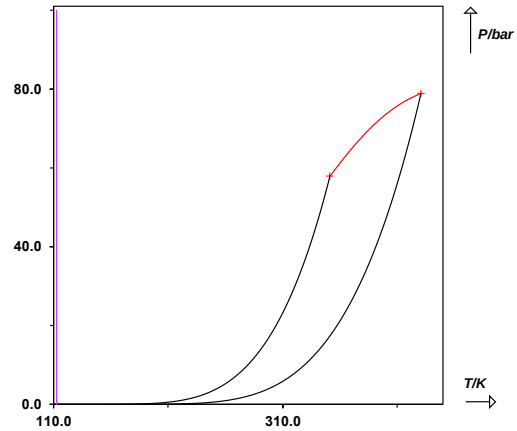
| | | |
|---|---|---|
| **CAS** | 75-10-5 | 7446-09-5 |
| **InChiKey** | RWRIWBAIICGTTQ-UHFFFAOYSA-N | RAHZWNYVWXNFOC-UHFFFAOYSA-N |
| **$T_c$ / K** | 351.26 | 430.75 |
| **$P_c$ / bar** | 57.84 | 78.84 |
| **ω** | 0.2770 | 0.2450 |

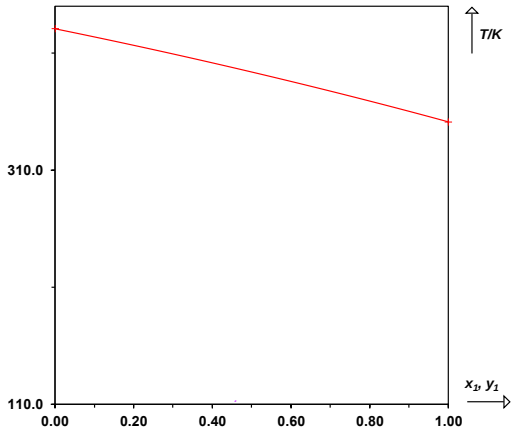
Ideal

**PPR78 results**

*Parameters*
A/MPa = 37.3
B/MPa = 109

*Deviations*
MAPE on x = 1.1 %
MAPE on y = 1.3 %



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**Isothermal phase equilibrium data**

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Valtz, A. - Coquelet, C. - Richon, D., Vapor–Liquid Equilibrium Data for the Sulfur Dioxide (SO2) + Difluoromethane (R32) System at Temperatures from 288.07 to 403.16 K and at Pressures up to 7.31 MPa, International Journal of Thermophysics 6 (2004) 1695-1711. doi:10.1007/s10765-004-7730-9

**T / K = 288.07**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.170 | 0.1350 | 0.4010 |
| 5.260 | 0.2330 | 0.5630 |
| 6.219 | 0.3330 | 0.6670 |
| 7.458 | 0.4560 | 0.7590 |
| 9.334 | 0.6510 | 0.8650 |
| 11.14 | 0.8370 | 0.9390 |

Valtz, A. - Coquelet, C. - Richon, D., Vapor–Liquid Equilibrium Data for the Sulfur Dioxide (SO2) + Difluoromethane (R32) System at Temperatures from 288.07 to 403.16 K and at Pressures up to 7.31 MPa, International Journal of Thermophysics 6 (2004) 1695-1711. doi:10.1007/s10765-004-7730-9

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.954 | 0.0840 | 0.2680 |
| 8.039 | 0.2230 | 0.5140 |
| 10.13 | 0.3700 | 0.6660 |
| 11.99 | 0.5030 | 0.7610 |
| 13.90 | 0.6380 | 0.8390 |
| 15.74 | 0.7670 | 0.8980 |
| 17.08 | 0.8560 | 0.9360 |

Valtz, A. - Coquelet, C. - Richon, D., Vapor–Liquid Equilibrium Data for the Sulfur Dioxide (SO2) + Difluoromethane (R32) System at Temperatures from 288.07 to 403.16 K and at Pressures up to 7.31 MPa, International Journal of Thermophysics 6 (2004) 1695-1711. doi:10.1007/s10765-004-7730-9

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.59 | 0.1390 | 0.3380 |
| 14.75 | 0.2780 | 0.5340 |
| 18.29 | 0.4420 | 0.6840 |
| 21.34 | 0.5840 | 0.7790 |
| 24.50 | 0.7230 | 0.8600 |
| 27.49 | 0.8480 | 0.9230 |

Valtz, A. - Coquelet, C. - Richon, D., Vapor–Liquid Equilibrium Data for the Sulfur Dioxide (SO2) + Difluoromethane (R32) System at Temperatures from 288.07 to 403.16 K and at Pressures up to 7.31 MPa, International Journal of Thermophysics 6 (2004) 1695-1711. doi:10.1007/s10765-004-7730-9

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 18.14 | 0.1230 | 0.2720 |
| 23.95 | 0.3050 | 0.5160 |
| 29.03 | 0.4660 | 0.6570 |
| 34.02 | 0.6180 | 0.7640 |
| 38.96 | 0.7590 | 0.8540 |
| 43.56 | 0.8810 | 0.9240 |

Valtz, A. - Coquelet, C. - Richon, D., Vapor–Liquid Equilibrium Data for the Sulfur Dioxide (SO2) + Difluoromethane (R32) System at Temperatures from 288.07 to 403.16 K and at Pressures up to 7.31 MPa, International Journal of Thermophysics 6 (2004) 1695-1711. doi:10.1007/s10765-004-7730-9

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 23.06 | 0.1360 | 0.2760 |
| 27.85 | 0.2630 | 0.4490 |
| 32.96 | 0.4000 | 0.5840 |
| 39.59 | 0.5710 | 0.7170 |
| 46.16 | 0.7290 | 0.8190 |
| 53.16 | 0.8800 | 0.9140 |

Valtz, A. - Coquelet, C. - Richon, D., Vapor–Liquid Equilibrium Data for the Sulfur Dioxide (SO2) + Difluoromethane (R32) System at Temperatures from 288.07 to 403.16 K and at Pressures up to 7.31 MPa, International Journal of Thermophysics 6 (2004) 1695-1711. doi:10.1007/s10765-004-7730-9

**T / K = 363.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 28.05 | 0.1290 | 0.2480 |
| 33.87 | 0.2620 | 0.4240 |
| 39.76 | 0.3970 | 0.5580 |
| 46.14 | 0.5370 | 0.6700 |
| 51.37 | 0.6460 | 0.7460 |
| 55.56 | 0.7270 | 0.7980 |
| 60.21 | 0.8140 | 0.8460 |

Valtz, A. - Coquelet, C. - Richon, D., Vapor–Liquid Equilibrium Data for the Sulfur Dioxide (SO2) + Difluoromethane (R32) System at Temperatures from 288.07 to 403.16 K and at Pressures up to 7.31 MPa, International Journal of Thermophysics 6 (2004) 1695-1711. doi:10.1007/s10765-004-7730-9

**T / K = 383.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 40.08 | 0.1070 | 0.1910 |

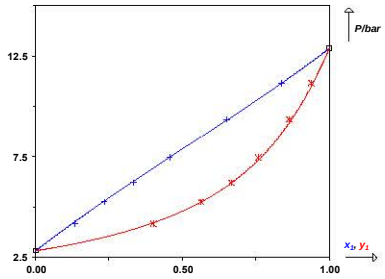
| | | |
|---|---|---|
| 44.56 | 0.1880 | 0.2980 |
| 49.52 | 0.2750 | 0.3940 |
| 54.75 | 0.3650 | 0.4800 |
| 59.81 | 0.4500 | 0.5500 |
| 65.89 | 0.5520 | 0.6130 |
| 68.45 | 0.5960 | 0.6350 |

Valtz, A. - Coquelet, C. - Richon, D., Vapor–Liquid Equilibrium Data for the Sulfur Dioxide (SO2) + Difluoromethane (R32) System at Temperatures from 288.07 to 403.16 K and at Pressures up to 7.31 MPa, International Journal of Thermophysics 6 (2004) 1695-1711. doi:10.1007/s10765-004-7730-9

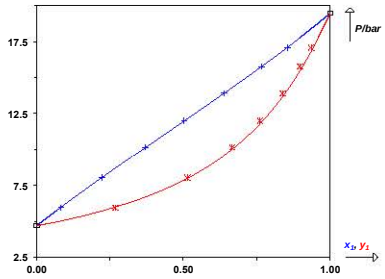
**T / K = 403.16**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 53.69 | 0.0640 | 0.1020 |
| 56.65 | 0.1050 | 0.1600 |
| 59.65 | 0.1470 | 0.2110 |
| 63.22 | 0.1960 | 0.2670 |
| 67.11 | 0.2500 | 0.3180 |
| 70.33 | 0.2960 | 0.3550 |
| 73.10 | 0.3370 | 0.3800 |

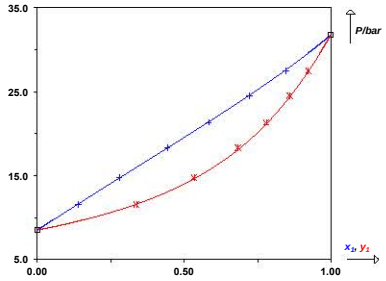
T/K = 288.07



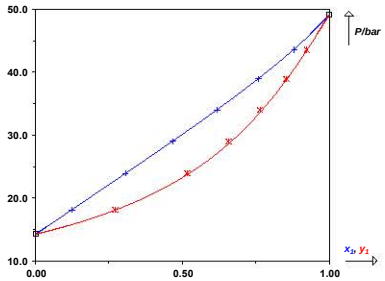

T/K = 303.15



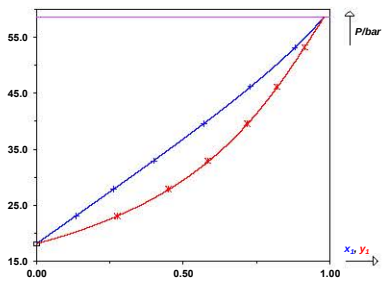

T/K = 323.15



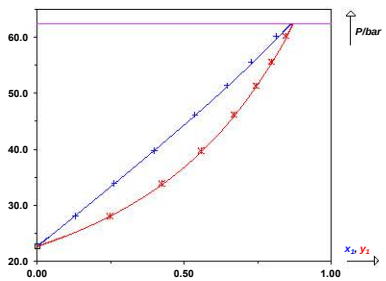

T/K = 343.15



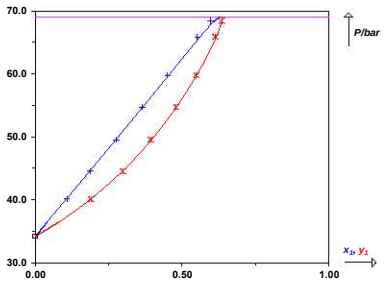

T/K = 353.15



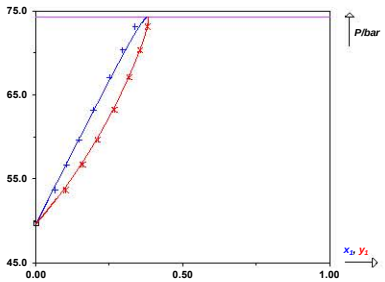

T/K = 363.15




T/K = 383.15




T/K = 403.16



## ETHYL ACETATE (1) + TRICHLOROETHYLENE (2)

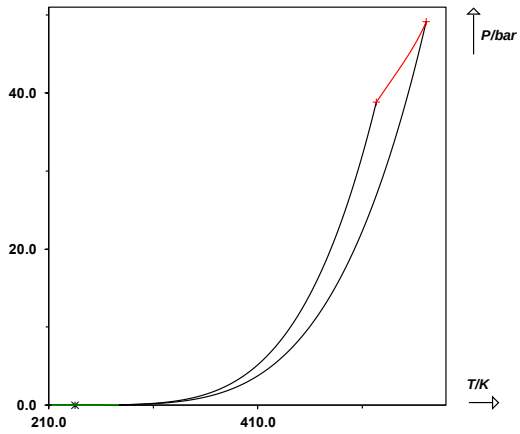
| | | |
|---|---|---|
| **CAS** | 141-78-6 | 79-01-6 |
| **InChiKey** | XEKOWRVHYACXOJ-UHFFFAOYSA-N | XSTXAVWGXDQKEL-UHFFFAOYSA-N |
| **$T_c$ / K** | 523.30 | 571.00 |
| **$P_c$ / bar** | 38.80 | 49.10 |
| **ω** | 0.3660 | 0.2170 |

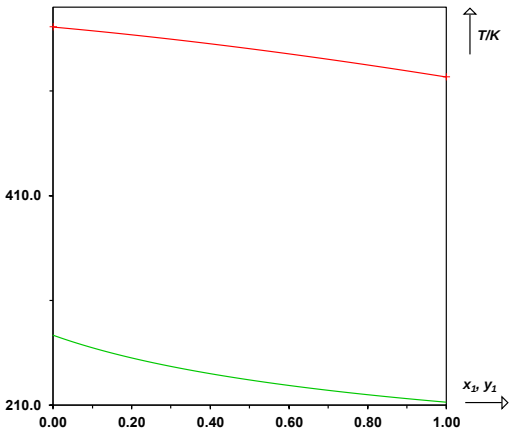
Ideal

**PPR78 results**

*Parameters*
A/MPa = -21.6
B/MPa = 6.29

*Deviations*
MAPE on x = 11 %
MAPE on y = 12 %



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**Isothermal phase equilibrium data**

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Yushina, E.A. - Fedorov, V.A. - Grinberg, E.E. - Efremov, A.A., Liquid-vapor equilibrium in binary systems based on arsenic trichloride. I. Alkyl arsenic dichloride-arsenic trichloride systems, Vysokochist. Veshchest. 4 (1993) 98-105.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4226 | 0.0230 | 0.0250 |
| 0.4240 | 0.0430 | 0.0550 |
| 0.4280 | 0.0830 | 0.0980 |
| 0.4346 | 0.1450 | 0.1800 |
| 0.4453 | 0.2350 | 0.2950 |
| 0.4826 | 0.5190 | 0.5980 |
| 0.5000 | 0.6250 | 0.7030 |
| 0.5213 | 0.7650 | 0.8200 |
| 0.5306 | 0.8230 | 0.8580 |
| 0.5400 | 0.8730 | 0.9050 |
| 0.5440 | 0.9000 | 0.9300 |
| 0.5520 | 0.9430 | 0.9680 |
| 0.5560 | 0.9680 | 0.9800 |

Yushina, E.A. - Fedorov, V.A. - Grinberg, E.E. - Efremov, A.A., Liquid-vapor equilibrium in binary systems based on arsenic trichloride. I. Alkyl arsenic dichloride-arsenic trichloride systems, Vysokochist. Veshchest. 4 (1993) 98-105.

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5920 | 0.0230 | 0.0250 |
| 0.5946 | 0.0430 | 0.0580 |
| 0.6013 | 0.0830 | 0.1050 |
| 0.6106 | 0.1380 | 0.1820 |
| 0.6266 | 0.2350 | 0.2980 |
| 0.6826 | 0.5190 | 0.6050 |
| 0.6866 | 0.5430 | 0.6280 |
| 0.7213 | 0.6980 | 0.7680 |
| 0.7373 | 0.7650 | 0.8280 |
| 0.7533 | 0.8230 | 0.8680 |
| 0.7679 | 0.8730 | 0.9050 |
| 0.7746 | 0.9000 | 0.9270 |
| 0.7879 | 0.9460 | 0.9580 |
| 0.7959 | 0.9680 | 0.9780 |

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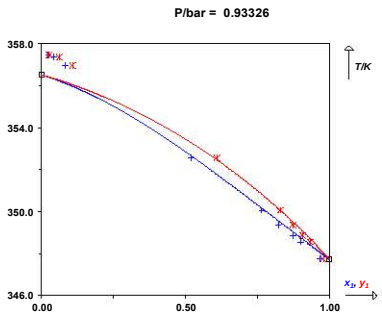
**Isobaric phase equilibrium data**

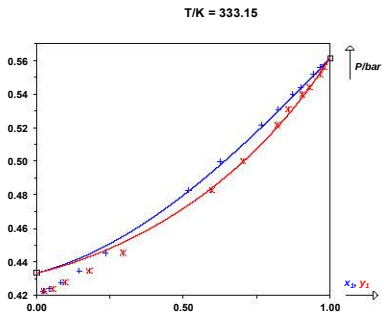
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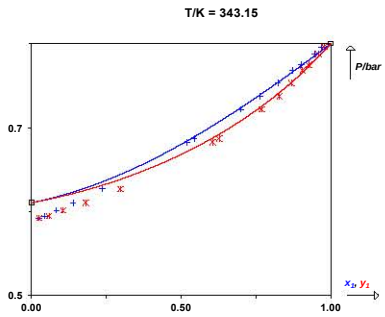
Yushina, E.A. - Fedorov, V.A. - Grinberg, E.E. - Efremov, A.A., Liquid-vapor equilibrium in binary systems based on arsenic trichloride. I. Alkyl arsenic dichloride-arsenic trichloride systems, Vysokochist. Veshchest. 4 (1993) 98-105.

**P / bar = 0.9333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 357.45 | 0.0230 | 0.0270 |
| 357.35 | 0.0430 | 0.0630 |
| 356.95 | 0.0830 | 0.1080 |
| 352.55 | 0.5190 | 0.6100 |
| 350.05 | 0.7650 | 0.8300 |
| 349.35 | 0.8230 | 0.8750 |
| 348.85 | 0.8730 | 0.9080 |
| 348.55 | 0.9000 | 0.9350 |
| 347.75 | 0.9680 | 0.9800 |


P/bar = 0.93326
358.0
354.0
350.0
346.0
T/K
0.00
0.50
1.00
x1, y1


T/K = 333.15
0.56
0.54
0.52
0.50
0.48
0.46
0.44
0.42
P/bar
0.00
0.50
1.00
x1, y1


T/K = 343.15
0.7
0.5
P/bar
0.00
0.50
1.00
x1, y1

## 1,1,1,2,3,3,3-HEPTAFLUOROPROPANE (1) + SULFUR DIOXIDE (2)

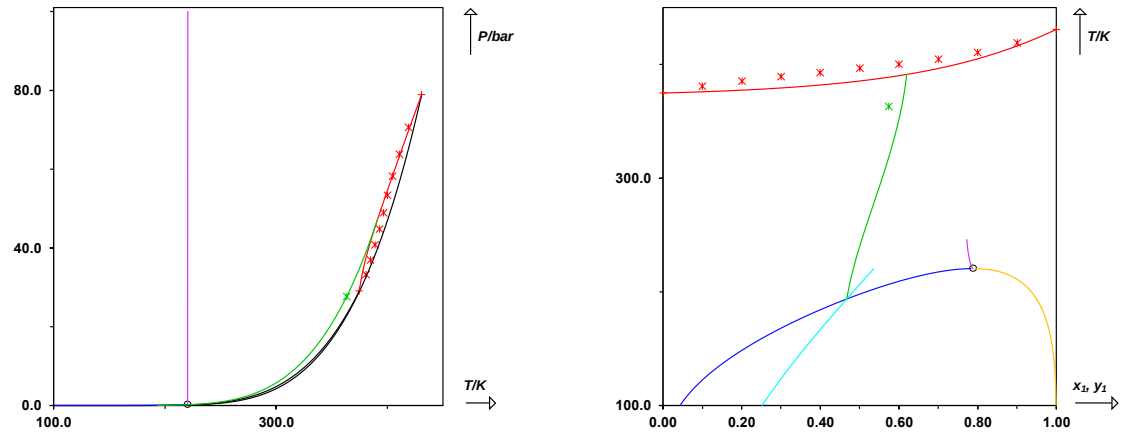
| | | |
|---|---|---|
| **CAS** | 431-89-0 | 7446-09-5 |
| **InChiKey** | YFMFNYKEUDLDTL-UHFFFAOYSA-N | RAHZWNYVWXNFOC-UHFFFAOYSA-N |
| **$T_c$ / K** | 374.83 | 430.75 |
| **$P_c$ / bar** | 29.12 | 78.84 |
| **ω** | 0.3550 | 0.2450 |

Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 359
B/MPa = 398

*Deviations*
MAPE on x = 6.4 %
MAPE on y = 4.6 %
MAPE on $x_c$ = 74 %
MAPE on $P_c$ = 6.8 %
MAPE on $x_{az}$ = 6.8 %
MAPE on $P_{az}$ = 0.26 %



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**Isothermal phase equilibrium data**

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Valtz, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the sulfur dioxide (SO2) + 1,1,1,2,3,3,3-heptafluoropropane (R227ea) system at temperatures from 288.07 to 403.19 K and pressures up to 5.38 MPa, Fluid Phase Equilibria 1 (2004) 75-82. doi:10.1016/j.fluid.2004.02.016

**T / K = 288.07**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.510 | 0.0950 | 0.2420 |
| 3.680 | 0.1590 | 0.2960 |
| 3.800 | 0.2400 | 0.3520 |
| 3.860 | 0.3080 | 0.3880 |
| 3.890 | 0.3660 | 0.4180 |
| 3.880 | 0.6150 | 0.5700 |
| 3.790 | 0.7110 | 0.6510 |
| 3.520 | 0.8930 | 0.8450 |

Valtz, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the sulfur dioxide (SO2) + 1,1,1,2,3,3,3-heptafluoropropane (R227ea) system at temperatures from 288.07 to 403.19 K and pressures up to 5.38 MPa, Fluid Phase Equilibria 1 (2004) 75-82. doi:10.1016/j.fluid.2004.02.016

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.950 | 0.0180 | 0.0740 |
| 5.290 | 0.0450 | 0.1460 |
| 5.620 | 0.0890 | 0.2160 |
| 6.010 | 0.1920 | 0.3050 |
| 6.260 | 0.3600 | 0.4030 |
| 6.280 | 0.5070 | 0.4920 |
| 6.180 | 0.6410 | 0.5900 |
| 5.920 | 0.7880 | 0.7240 |
| 5.720 | 0.8650 | 0.8110 |
| 5.570 | 0.9160 | 0.8750 |

Valtz, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the sulfur dioxide (SO2) + 1,1,1,2,3,3,3-heptafluoropropane (R227ea) system at temperatures from 288.07 to 403.19 K and pressures up to 5.38 MPa, Fluid Phase Equilibria 1 (2004) 75-82. doi:10.1016/j.fluid.2004.02.016

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.040 | 0.0270 | 0.0810 |
| 9.510 | 0.0550 | 0.1390 |
| 10.04 | 0.1060 | 0.2060 |
| 10.52 | 0.1890 | 0.2780 |
| 10.88 | 0.3150 | 0.3610 |
| 10.96 | 0.5170 | 0.4960 |
| 10.49 | 0.7290 | 0.6720 |
| 10.00 | 0.8410 | 0.7910 |
| 9.630 | 0.9160 | 0.8810 |
| 9.420 | 0.9540 | 0.9310 |

Valtz, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the sulfur dioxide (SO2) + 1,1,1,2,3,3,3-heptafluoropropane (R227ea) system at temperatures from 288.07 to 403.19 K and pressures up to 5.38 MPa, Fluid Phase Equilibria 1 (2004) 75-82. doi:10.1016/j.fluid.2004.02.016

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 14.75 | 0.0170 | 0.0450 |
| 15.42 | 0.0440 | 0.0990 |
| 16.17 | 0.0870 | 0.1610 |
| 16.87 | 0.1460 | 0.2230 |
| 17.44 | 0.2330 | 0.2900 |
| 17.70 | 0.2980 | 0.3370 |
| 17.82 | 0.5010 | 0.4810 |
| 17.31 | 0.6640 | 0.6200 |
| 16.59 | 0.7880 | 0.7410 |
| 16.04 | 0.8590 | 0.8190 |
| 15.54 | 0.9220 | 0.8960 |

Valtz, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the sulfur dioxide (SO2) + 1,1,1,2,3,3,3-heptafluoropropane (R227ea) system at temperatures from 288.07 to 403.19 K and pressures up to 5.38 MPa, Fluid Phase Equilibria 1 (2004) 75-82. doi:10.1016/j.fluid.2004.02.016

**T / K = 363.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 23.19 | 0.0160 | 0.0380 | |
| 23.96 | 0.0390 | 0.0780 | |
| 24.88 | 0.0740 | 0.1270 | |
| 25.67 | 0.1150 | 0.1740 | |
| 26.35 | 0.1660 | 0.2230 | |
| 26.82 | 0.2170 | 0.2630 | |
| 27.11 | 0.2570 | 0.2920 | |
| 27.27 | 0.2860 | 0.3170 | |
| 27.57 | 0.4260 | 0.4260 | AZEO |
| 27.57 | 0.4290 | 0.4270 | |
| 26.78 | 0.6410 | 0.6100 | |
| 26.06 | 0.7310 | 0.6970 | |
| 25.46 | 0.7930 | 0.7610 | |
| 24.75 | 0.8570 | 0.8300 | |
| 24.00 | 0.9190 | 0.9000 | |

Valtz, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the sulfur dioxide (SO2) + 1,1,1,2,3,3,3-heptafluoropropane (R227ea) system at temperatures from 288.07 to 403.19 K and pressures up to 5.38 MPa, Fluid Phase Equilibria 1 (2004) 75-82. doi:10.1016/j.fluid.2004.02.016

**T / K = 374.23**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 29.36 | 0.0210 | 0.0430 |
| 30.52 | 0.0530 | 0.0920 |
| 32.00 | 0.1130 | 0.1630 |
| 33.38 | 0.2050 | 0.2470 |
| 34.00 | 0.2750 | 0.3030 |
| 34.39 | 0.4600 | 0.4530 |
| 33.30 | 0.6510 | 0.6310 |
| 31.56 | 0.8100 | 0.7900 |

Valtz, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the sulfur dioxide (SO2) + 1,1,1,2,3,3,3-heptafluoropropane (R227ea) system at temperatures from 288.07 to 403.19 K and pressures up to 5.38 MPa, Fluid Phase Equilibria 1 (2004) 75-82. doi:10.1016/j.fluid.2004.02.016

**T / K = 383.17**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 35.04 | 0.0230 | 0.0410 |
| 37.27 | 0.0860 | 0.1240 |
| 38.93 | 0.1620 | 0.2010 |
| 40.02 | 0.2430 | 0.2710 |
| 40.39 | 0.2840 | 0.3060 |
| 40.57 | 0.3110 | 0.3260 |
| 40.74 | 0.3450 | 0.3570 |
| 40.79 | 0.4860 | 0.4830 |
| 40.75 | 0.4940 | 0.4910 |

Valtz, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the sulfur dioxide (SO2) + 1,1,1,2,3,3,3-heptafluoropropane (R227ea) system at temperatures from 288.07 to 403.19 K and pressures up to 5.38 MPa, Fluid Phase Equilibria 1 (2004) 75-82. doi:10.1016/j.fluid.2004.02.016

**T / K = 393.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 42.36 | 0.0240 | 0.0420 |
| 43.99 | 0.0610 | 0.0940 |
| 45.36 | 0.1010 | 0.1350 |
| 46.61 | 0.1520 | 0.1850 |
| 47.75 | 0.2140 | 0.2420 |
| 48.62 | 0.2830 | 0.2960 |
| 48.92 | 0.3150 | 0.3240 |

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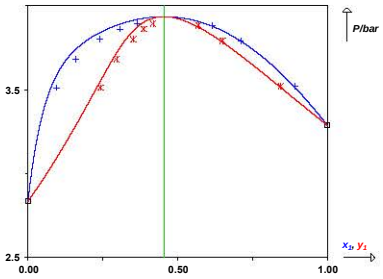
**Critical point**

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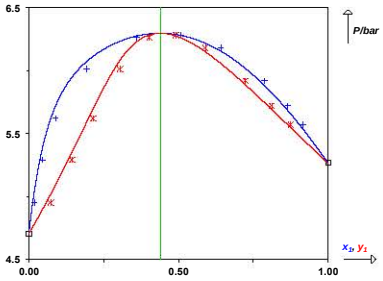
Valtz, A - Coquelet, C - Richon, D, Vapor–liquid equilibrium data for the sulfur dioxide (SO2) + 1,1,1,2,3,3,3-heptafluoropropane (R227ea) system at temperatures from 288.07 to 403.19 K and pressures up to 5.38 MPa, Fluid Phase Equilibria 1 (2004) 75-82. doi:10.1016/j.fluid.2004.02.016

| T / K | P / bar | $x_1$ |
|---|---|---|
| 419.08 | 70.61 | 0.1000 |
| 410.68 | 63.70 | 0.2000 |
| 404.76 | 58.13 | 0.3000 |
| 400.27 | 53.36 | 0.4000 |
| 396.44 | 48.97 | 0.5000 |
| 392.78 | 44.79 | 0.6000 |
| 389.03 | 40.77 | 0.7000 |
| 385.03 | 36.91 | 0.8000 |
| 380.69 | 33.25 | 0.9000 |

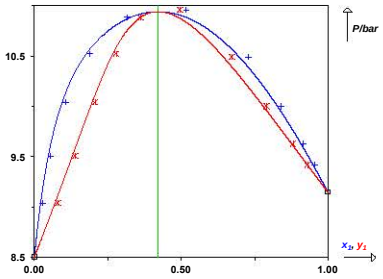
T/K = 288.07



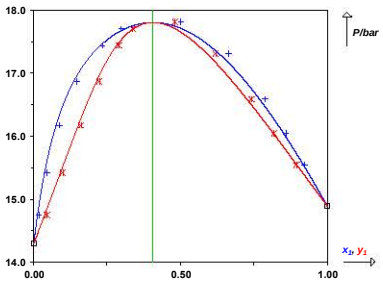

T/K = 303.15



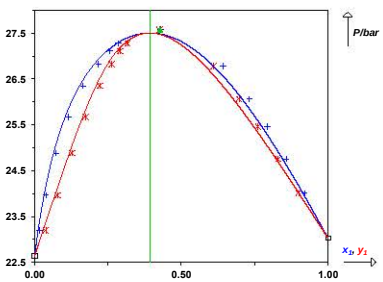

T/K = 323.15



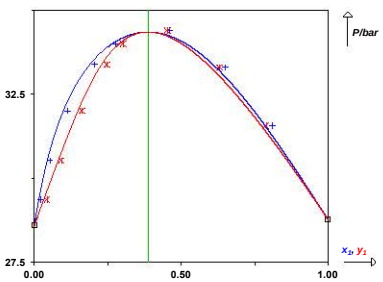

T/K = 343.15



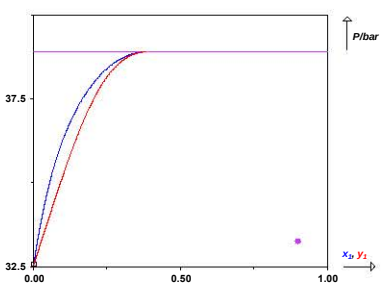

T/K = 363.15



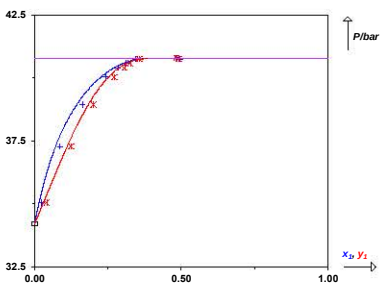

T/K = 374.23



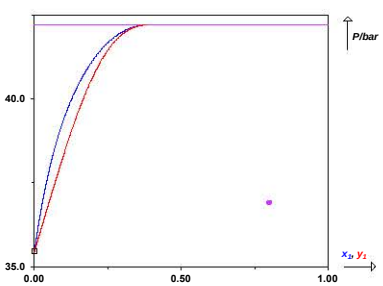

T/K = 380.69



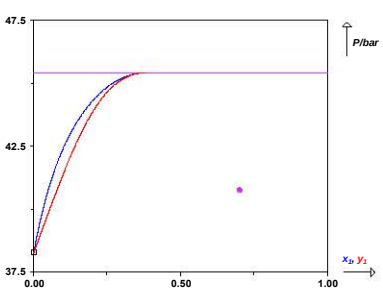

T/K = 383.17



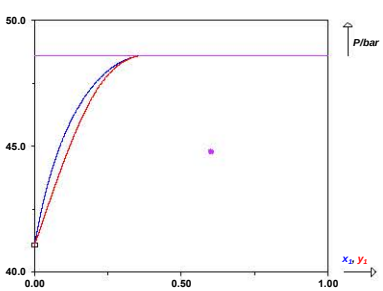

T/K = 385.03



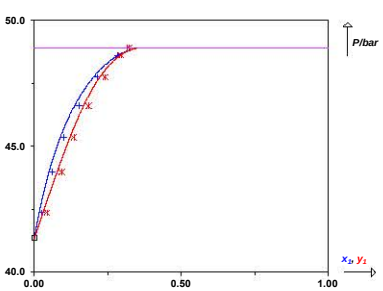

T/K = 389.03

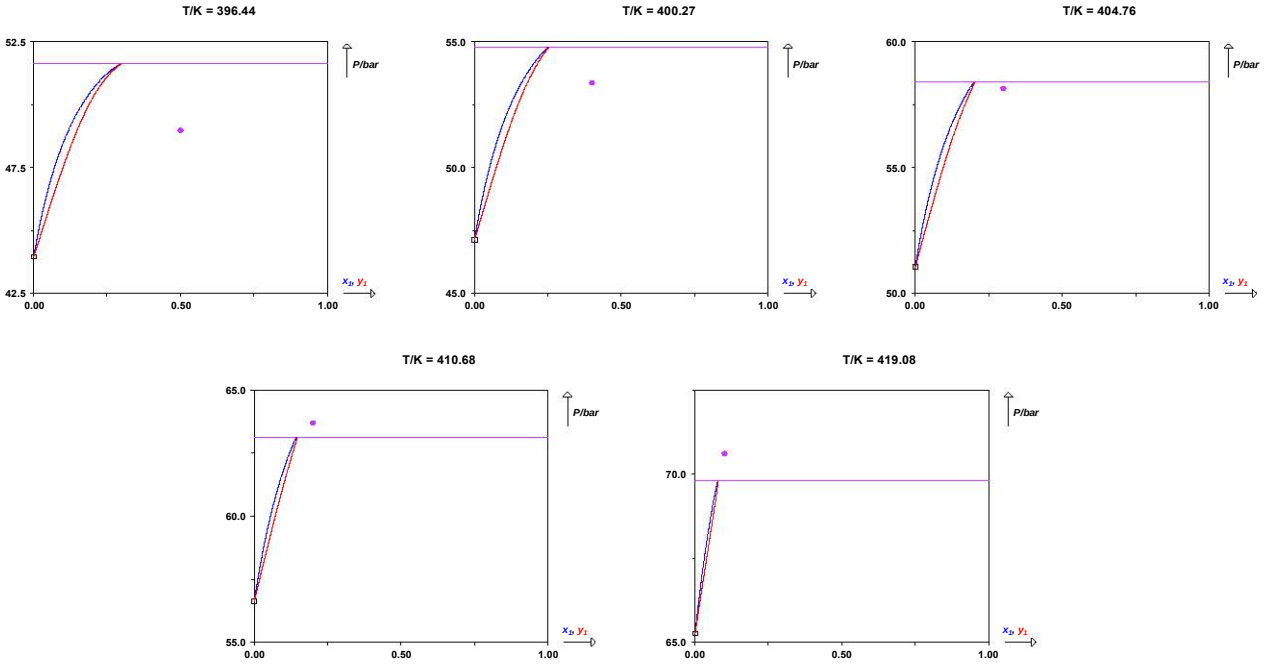



T/K = 392.78




T/K = 393.15




T/K = 396.44
52.5
47.5
42.5
P/bar
0.00
0.50
1.00
x1, y1
T/K = 400.27
55.0
50.0
45.0
P/bar
0.00
0.50
1.00
x1, y1
T/K = 404.76
60.0
55.0
50.0
P/bar
0.00
0.50
1.00
x1, y1
T/K = 410.68
65.0
60.0
55.0
P/bar
0.00
0.50
1.00
x1, y1
T/K = 419.08
70.0
65.0
P/bar
0.00
0.50
1.00
x1, y1

## CHLORODIFLUOROMETHANE (1) + DIMETHYL ETHER (2)

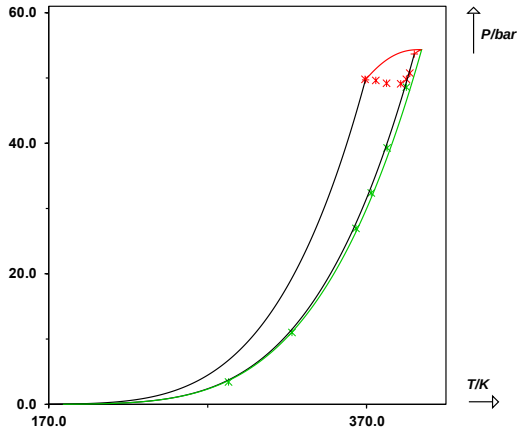
| | | |
|---|---|---|
| **CAS** | 75-45-6 | 115-10-6 |
| **InChiKey** | VOPWNXZWBYDODV-UHFFFAOYSA-N | LCGLNKUTAGEVQW-UHFFFAOYSA-N |
| **$T_c$ / K** | 369.3 | 400.1 |
| **$P_c$ / bar** | 49.71 | 53.70 |
| **ω** | 0.2190 | 0.2000 |

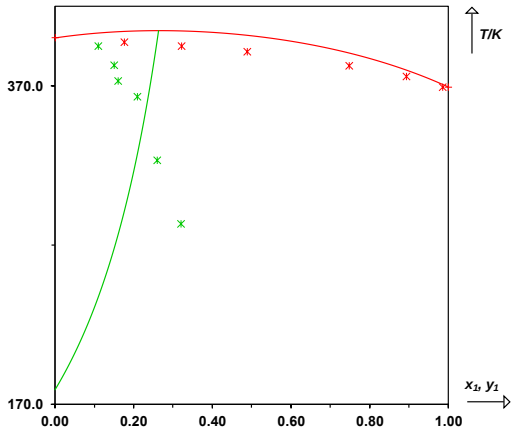
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = -251
B/MPa = -41

*Deviations*
MAPE on x = 22 %
MAPE on y = 26 %
MAPE on $x_{az}$ = 19 %
MAPE on $P_{az}$ = 3.7 %



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**Isothermal phase equilibrium data**

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Noles, Joe R. - Zollweg, John A., Vapor-liquid equilibrium for chlorodifluoromethane + dimethyl ether from 283 to 395 K at pressures to 5.0 MPa, Journal of Chemical & Engineering Data 3 (1992) 306-310. doi:10.1021/je00007a008

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.500 | 0.1630 | 0.1300 | |
| 3.410 | 0.2520 | 0.2350 | |
| 3.380 | 0.3200 | 0.3200 | AZEO |
| 3.480 | 0.4390 | 0.4930 | |
| 3.630 | 0.5050 | 0.5950 | |
| 3.820 | 0.5570 | 0.6720 | |
| 4.150 | 0.6250 | 0.7630 | |
| 4.690 | 0.7120 | 0.8520 | |
| 5.310 | 0.7980 | 0.9210 | |

Noles, Joe R. - Zollweg, John A., Vapor-liquid equilibrium for chlorodifluoromethane + dimethyl ether from 283 to 395 K at pressures to 5.0 MPa, Journal of Chemical & Engineering Data 3 (1992) 306-310. doi:10.1021/je00007a008

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 11.08 | 0.1330 | 0.1200 | |
| 10.98 | 0.2600 | 0.2600 | AZEO |
| 11.02 | 0.3140 | 0.3260 | |
| 11.12 | 0.3600 | 0.3870 | |
| 11.39 | 0.4270 | 0.4740 | |
| 11.73 | 0.4820 | 0.5500 | |
| 12.24 | 0.5470 | 0.6320 | |
| 13.23 | 0.6360 | 0.7400 | |
| 15.01 | 0.7570 | 0.8560 | |
| 17.52 | 0.8950 | 0.9510 | |

Noles, Joe R. - Zollweg, John A., Vapor-liquid equilibrium for chlorodifluoromethane + dimethyl ether from 283 to 395 K at pressures to 5.0 MPa, Journal of Chemical & Engineering Data 3 (1992) 306-310. doi:10.1021/je00007a008

**T / K = 363.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 26.90 | 0.1950 | 0.1930 | |
| 26.91 | 0.2100 | 0.2100 | AZEO |
| 27.11 | 0.3110 | 0.3300 | |
| 27.91 | 0.4210 | 0.4560 | |
| 30.23 | 0.5760 | 0.6340 | |
| 34.83 | 0.7570 | 0.8140 | |
| 37.47 | 0.8320 | 0.8780 | |
| 39.67 | 0.8910 | 0.9220 | |

Noles, Joe R. - Zollweg, John A., Vapor-liquid equilibrium for chlorodifluoromethane + dimethyl ether from 283 to 395 K at pressures to 5.0 MPa, Journal of Chemical & Engineering Data 3 (1992) 306-310. doi:10.1021/je00007a008

**T / K = 373.01**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 32.44 | 0.1180 | 0.1150 | |
| 32.41 | 0.1600 | 0.1600 | AZEO |
| 32.49 | 0.2280 | 0.2330 | |
| 34.41 | 0.4660 | 0.5040 | |
| 35.59 | 0.5330 | 0.5760 | |
| 35.93 | 0.5500 | 0.5950 | |
| 37.35 | 0.6080 | 0.6560 | |
| 37.84 | 0.6300 | 0.6790 | |
| 40.62 | 0.7220 | 0.7690 | |
| 41.75 | 0.7550 | 0.7980 | |
| 43.74 | 0.8060 | 0.8440 | |
| 44.37 | 0.8230 | 0.8560 | |
| 45.72 | 0.8550 | 0.8780 | |
| 47.90 | 0.9010 | 0.9160 | |
| 48.47 | 0.9120 | 0.9230 | |

Noles, Joe R. - Zollweg, John A., Vapor-liquid equilibrium for chlorodifluoromethane + dimethyl ether from 283 to 395 K at pressures to 5.0 MPa, Journal of Chemical & Engineering Data 3 (1992) 306-310. doi:10.1021/je00007a008

**T / K = 383.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 39.36 | 0.0650 | 0.0570 | |
| 39.28 | 0.1220 | 0.1210 | |
| 39.26 | 0.1500 | 0.1500 | AZEO |
| 39.32 | 0.2050 | 0.2100 | |
| 39.91 | 0.3180 | 0.3320 | |
| 40.81 | 0.4000 | 0.4210 | |
| 41.66 | 0.4540 | 0.4790 | |
| 46.32 | 0.6460 | 0.6730 | |
| 47.35 | 0.6780 | 0.7030 | |
| 48.13 | 0.6960 | 0.7170 | |

Noles, Joe R. - Zollweg, John A., Vapor-liquid equilibrium for chlorodifluoromethane + dimethyl ether from 283 to 395 K at pressures to 5.0 MPa, Journal of Chemical & Engineering Data 3 (1992) 306-310. doi:10.1021/je00007a008

**T / K = 395.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|

| | | | |
|---|---|---|---|
| 48.73 | 0.0200 | 0.0190 | |
| 48.58 | 0.1100 | 0.1100 | AZEO |
| 48.58 | 0.1160 | 0.1150 | |
| 48.64 | 0.1620 | 0.1640 | |
| 48.73 | 0.1940 | 0.1970 | |
| 48.81 | 0.2120 | 0.2130 | |
| 49.23 | 0.2760 | 0.2810 | |

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**Critical point**

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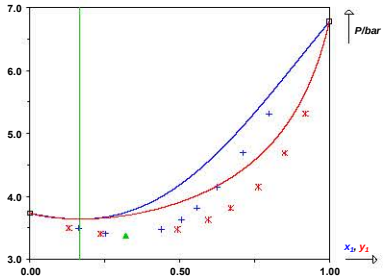
Efremova, G.D. - Kovpakova, R.F., Phase equilibriums in systems that contain ethylene and tetrachloroalkanes, Zh. Fiz. Khim. 6 (1958) 1231-1240.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 369.00 | 49.76 | 0.9850 |
| 375.78 | 49.63 | 0.8930 |
| 382.62 | 49.22 | 0.7480 |
| 391.47 | 49.08 | 0.4890 |
| 397.28 | 50.76 | 0.1760 |

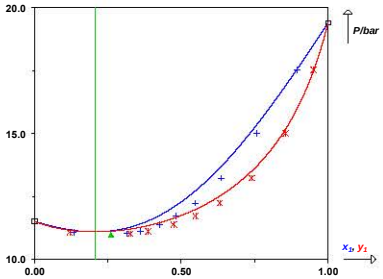
Noles, Joe R. - Zollweg, John A., Vapor-liquid equilibrium for chlorodifluoromethane + dimethyl ether from 283 to 395 K at pressures to 5.0 MPa, Journal of Chemical & Engineering Data 3 (1992) 306-310. doi:10.1021/je00007a008

| T / K | P / bar | $x_1$ |
|---|---|---|
| 395.00 | 49.79 | 0.3210 |

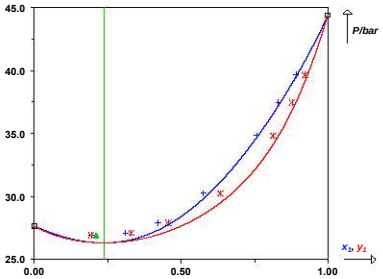
T/K = 283.15



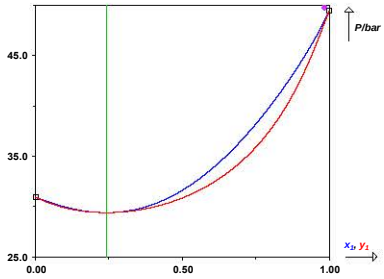

T/K = 323.15



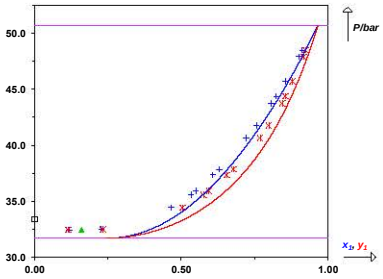

T/K = 363.15



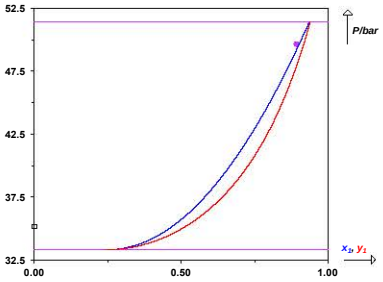

T/K = 369.00



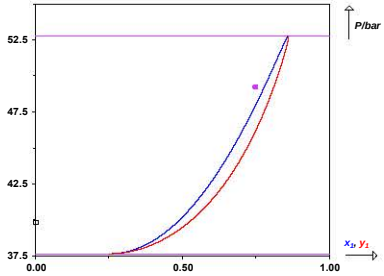

T/K = 373.01



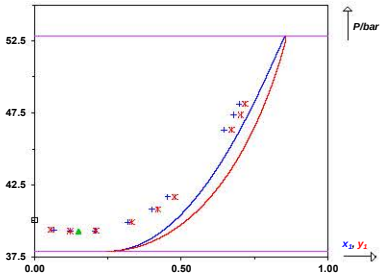

T/K = 375.78



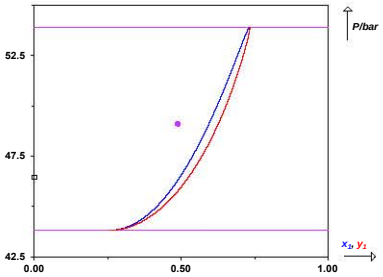

T/K = 382.62



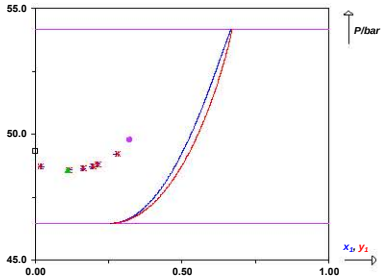

T/K = 383.00



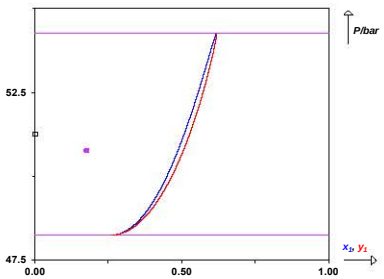

T/K = 391.47




T/K = 395.00




T/K = 397.28



## CHLORODIFLUOROMETHANE (1) + CARBON DISULFIDE (2)

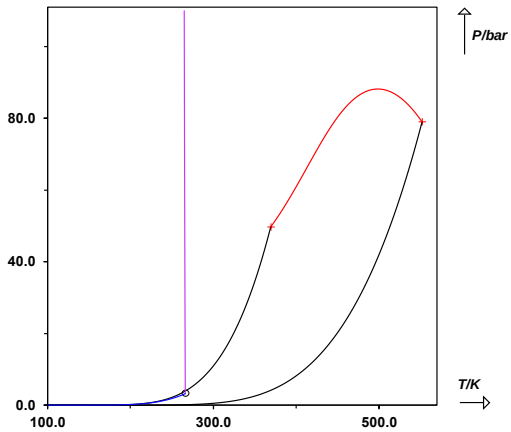
| | | |
|---|---|---|
| **CAS** | 75-45-6 | 75-15-0 |
| **InChiKey** | VOPWNXZWBYDODV-UHFFFAOYSA-N | QGJOPFRUJISHPQ-UHFFFAOYSA-N |
| **$T_c$ / K** | 369.30 | 552.00 |
| **$P_c$ / bar** | 49.71 | 79.00 |
| **ω** | 0.2190 | 0.1110 |

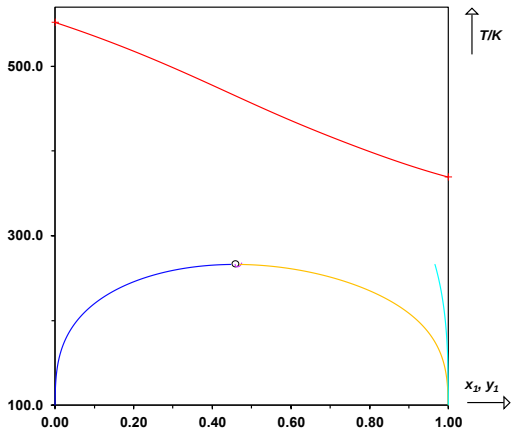
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 443
B/MPa = 657

*Deviations*
MAPE on x = 4.4 %
MAPE on y = 4.3 %



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**Isothermal phase equilibrium data**

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Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.010 | 0.0682 | 0.9117 |
| 3.070 | 0.1503 | 0.9431 |
| 3.700 | 0.2841 | 0.9531 |
| 3.830 | 0.3541 | 0.9564 |
| 3.860 | 0.3904 | 0.9556 |
| 3.930 | 0.4692 | 0.9580 |
| 4.150 | 0.7129 | 0.9637 |
| 4.220 | 0.8128 | 0.9653 |
| 4.510 | 0.8886 | 0.9724 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.260 | 0.0358 | 0.7811 |
| 3.750 | 0.0734 | 0.8670 |
| 4.980 | 0.1183 | 0.9009 |
| 6.300 | 0.2002 | 0.9204 |
| 7.010 | 0.2809 | 0.9297 |
| 7.460 | 0.3693 | 0.9354 |
| 7.810 | 0.4702 | 0.9389 |
| 8.230 | 0.6065 | 0.9452 |
| 8.950 | 0.7834 | 0.9579 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.620 | 0.0505 | 0.7445 |
| 7.680 | 0.1118 | 0.8426 |
| 9.880 | 0.1821 | 0.8768 |
| 12.38 | 0.3258 | 0.9024 |
| 14.48 | 0.5092 | 0.9225 |
| 15.85 | 0.7293 | 0.9384 |
| 16.90 | 0.8276 | 0.9526 |
| 18.43 | 0.9386 | 0.9782 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.940 | 0.0165 | 0.3884 |
| 8.320 | 0.0642 | 0.7025 |
| 9.420 | 0.0773 | 0.7341 |
| 15.83 | 0.2028 | 0.8355 |
| 20.16 | 0.3643 | 0.8713 |
| 24.17 | 0.6150 | 0.9001 |
| 28.75 | 0.8452 | 0.9419 |
| 31.39 | 0.9438 | 0.9740 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.010 | 0.0137 | 0.2565 |
| 10.33 | 0.0495 | 0.5162 |
| 14.98 | 0.0960 | 0.6802 |
| 19.10 | 0.1458 | 0.7429 |
| 24.53 | 0.2469 | 0.7928 |
| 30.45 | 0.3963 | 0.8292 |
| 35.78 | 0.5794 | 0.8570 |
| 41.42 | 0.7326 | 0.8845 |
| 45.27 | 0.8542 | 0.9179 |
| 49.65 | 0.9389 | 0.9550 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 398.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 14.99 | 0.0476 | 0.4656 |
| 21.96 | 0.1040 | 0.6209 |
| 27.90 | 0.1669 | 0.6888 |
| 34.03 | 0.2448 | 0.7296 |

| | | |
|---|---|---|
| 40.75 | 0.3540 | 0.7650 |
| 50.08 | 0.5526 | 0.7964 |
| 55.26 | 0.6725 | 0.8114 |
| 56.97 | 0.7098 | 0.8125 |
| 58.90 | 0.7492 | 0.8084 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 423.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 16.80 | 0.0249 | 0.2485 |
| 18.50 | 0.0366 | 0.3498 |
| 24.68 | 0.0749 | 0.4581 |
| 31.35 | 0.1184 | 0.5513 |
| 40.00 | 0.1914 | 0.6267 |
| 48.30 | 0.2815 | 0.6682 |
| 53.98 | 0.3534 | 0.6875 |
| 60.20 | 0.4479 | 0.7012 |
| 66.32 | 0.5556 | 0.7001 |
| 67.45 | 0.5764 | 0.6910 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

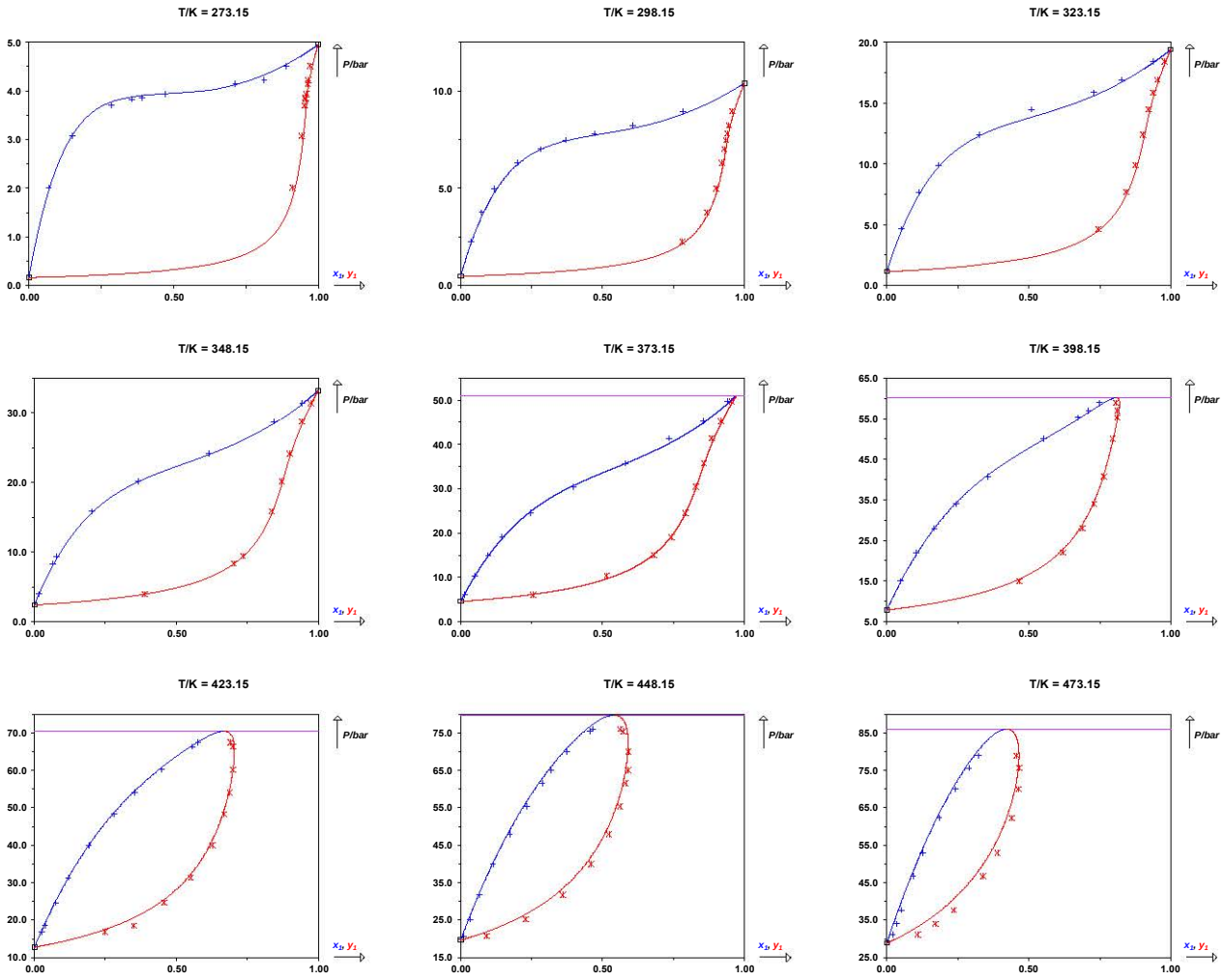
**T / K = 448.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.70 | 0.0116 | 0.0919 |
| 25.18 | 0.0333 | 0.2292 |
| 31.75 | 0.0671 | 0.3609 |
| 39.95 | 0.1131 | 0.4588 |
| 47.92 | 0.1720 | 0.5227 |
| 55.38 | 0.2328 | 0.5619 |
| 61.55 | 0.2866 | 0.5820 |
| 64.94 | 0.3192 | 0.5900 |
| 69.92 | 0.3743 | 0.5921 |
| 75.33 | 0.4563 | 0.5740 |
| 76.00 | 0.4668 | 0.5623 |

Roth, H. - Peters-Gerth, P. - Lucas, K., Experimental vapor-liquid equilibria in the systems R 22-R 23, R 22-Co2, Cs2-R 22, R 23-Co2, Cs2-R 23 and their correlation by equations of state, Fluid Phase Equilibria 1-2 (1992) 147-166. doi:10.1016/0378-3812(92)85045-A

**T / K = 473.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 31.12 | 0.0198 | 0.1091 |
| 34.05 | 0.0339 | 0.1716 |
| 37.71 | 0.0508 | 0.2361 |
| 46.72 | 0.0920 | 0.3393 |
| 53.00 | 0.1257 | 0.3906 |
| 62.20 | 0.1834 | 0.4405 |
| 70.00 | 0.2410 | 0.4646 |
| 75.58 | 0.2889 | 0.4668 |
| 78.95 | 0.3228 | 0.4582 |


T/K = 273.15
T/K = 298.15
T/K = 323.15
T/K = 348.15
T/K = 373.15
T/K = 398.15
T/K = 423.15
T/K = 448.15
T/K = 473.15
P/bar
x1, y1

## PENTAFLUOROETHANE (1) + DIMETHYL ETHER (2)

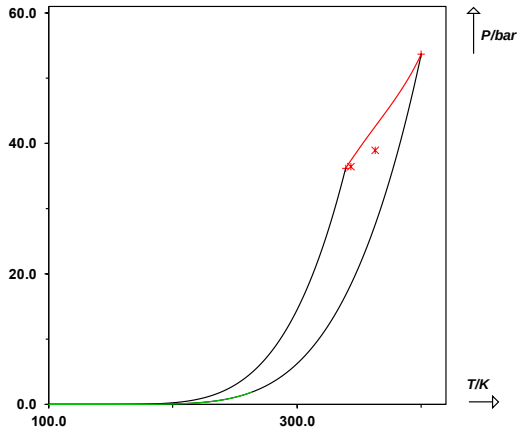
| | | |
|---|---|---|
| **CAS** | 354-33-6 | 115-10-6 |
| **InChiKey** | GTLACDSXYULKMZ-UHFFFAOYSA-N | LCGLNKUTAGEVQW-UHFFFAOYSA-N |
| **$T_c$ / K** | 339.17 | 400.10 |
| **$P_c$ / bar** | 36.2 | 53.7 |
| **ω** | 0.3050 | 0.2000 |

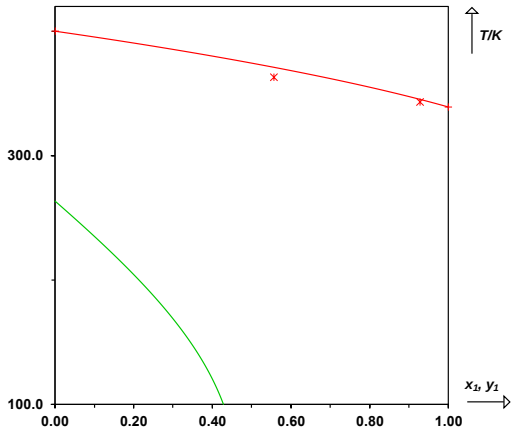
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = -135
B/MPa = -469

*Deviations*
MAPE on x = 6.9 %
MAPE on y = 5.5 %
MAPE on $x_c$ = 22 %
MAPE on $P_c$ = 6.0 %



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**Isothermal phase equilibrium data**

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Bobbo, S. - Fedele, L. - Camporese, R. - Stryjek, R., Hydrogen-bonding of HFCs with dimethyl ether: evaluation by isothermal VLE measurements, Fluid Phase Equilibria 1-2 (2002) 153-160. doi:10.1016/S0378-3812(01)00813-5

**T / K = 258.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.551 | 0.0695 | 0.0813 |
| 1.564 | 0.1153 | 0.1325 |
| 1.581 | 0.1637 | 0.1884 |
| 1.647 | 0.2843 | 0.3440 |
| 1.831 | 0.4280 | 0.5596 |
| 2.213 | 0.5654 | 0.7525 |
| 2.763 | 0.7023 | 0.8834 |
| 3.306 | 0.8220 | 0.9488 |
| 3.595 | 0.8865 | 0.9721 |

Bobbo, S. - Fedele, L. - Camporese, R. - Stryjek, R., Hydrogen-bonding of HFCs with dimethyl ether: evaluation by isothermal VLE measurements, Fluid Phase Equilibria 1-2 (2002) 153-160. doi:10.1016/S0378-3812(01)00813-5

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.760 | 0.1120 | 0.1345 |
| 2.813 | 0.1743 | 0.2094 |
| 2.953 | 0.2927 | 0.3600 |
| 3.323 | 0.4442 | 0.5775 |
| 3.971 | 0.5913 | 0.7660 |
| 4.386 | 0.6578 | 0.8283 |
| 4.947 | 0.7404 | 0.8922 |
| 5.395 | 0.8047 | 0.9299 |
| 5.904 | 0.8776 | 0.9611 |
| 6.420 | 0.9541 | 0.9874 |

Bobbo, S. - Fedele, L. - Camporese, R. - Stryjek, R., Hydrogen-bonding of HFCs with dimethyl ether: evaluation by isothermal VLE measurements, Fluid Phase Equilibria 1-2 (2002) 153-160. doi:10.1016/S0378-3812(01)00813-5

**T / K = 288.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.475 | 0.0585 | 0.0750 |
| 4.868 | 0.2668 | 0.3337 |
| 5.233 | 0.3815 | 0.4845 |
| 5.850 | 0.5007 | 0.6386 |
| 6.415 | 0.5795 | 0.7321 |
| 7.216 | 0.6716 | 0.8231 |
| 7.672 | 0.7184 | 0.8599 |
| 8.382 | 0.7911 | 0.9077 |
| 9.369 | 0.8874 | 0.9568 |
| 9.920 | 0.9398 | 0.9786 |

Bobbo, S. - Fedele, L. - Camporese, R. - Stryjek, R., Hydrogen-bonding of HFCs with dimethyl ether: evaluation by isothermal VLE measurements, Fluid Phase Equilibria 1-2 (2002) 153-160. doi:10.1016/S0378-3812(01)00813-5

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.960 | 0.0519 | 0.0695 |
| 7.523 | 0.2277 | 0.2867 |
| 8.453 | 0.4116 | 0.5162 |
| 9.825 | 0.5680 | 0.6987 |
| 11.07 | 0.6721 | 0.8025 |
| 11.14 | 0.6805 | 0.8103 |
| 12.28 | 0.7677 | 0.8756 |
| 13.21 | 0.8331 | 0.9177 |
| 14.17 | 0.8967 | 0.9526 |

Im, Jihoon - Lee, Gangwon - Lee, Jongcheon - Kim, Hwayong, (Vapour+liquid) equilibria of the {pentafluoroethane (HFC-125)+dimethyl ether (DME)} system, The Journal of Chemical Thermodynamics 12 (2006) 1510-1514. doi:10.1016/j.jct.2006.04.009

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.240 | 0.0831 | 0.1080 |
| 9.680 | 0.1790 | 0.2130 |
| 10.00 | 0.2430 | 0.2933 |
| 10.70 | 0.3558 | 0.4355 |
| 11.82 | 0.4807 | 0.5890 |
| 14.06 | 0.6569 | 0.7723 |
| 15.23 | 0.7298 | 0.8352 |
| 16.51 | 0.8050 | 0.8903 |
| 17.95 | 0.8849 | 0.9393 |
| 18.94 | 0.9391 | 0.9689 |

Im, Jihoon - Lee, Gangwon - Lee, Jongcheon - Kim, Hwayong, (Vapour+liquid) equilibria of the {pentafluoroethane (HFC-125)+dimethyl ether (DME)} system, The Journal of Chemical Thermodynamics 12 (2006) 1510-1514. doi:10.1016/j.jct.2006.04.009

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.96 | 0.0869 | 0.1131 |
| 12.38 | 0.1560 | 0.1951 |
| 12.77 | 0.2146 | 0.2679 |
| 13.26 | 0.2797 | 0.3469 |

| | | |
|---|---|---|
| 13.64 | 0.3261 | 0.4036 |
| 14.46 | 0.4079 | 0.5046 |
| 15.58 | 0.5040 | 0.6048 |
| 16.88 | 0.5920 | 0.6968 |
| 18.69 | 0.6944 | 0.7956 |
| 20.20 | 0.7688 | 0.8554 |
| 22.75 | 0.8863 | 0.9347 |

Im, Jihoon - Lee, Gangwon - Lee, Jongcheon - Kim, Hwayong, (Vapour+liquid) equilibria of the {pentafluoroethane (HFC-125)+dimethyl ether (DME)} system, The Journal of Chemical Thermodynamics 12 (2006) 1510-1514. doi:10.1016/j.jct.2006.04.009

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 14.90 | 0.0432 | 0.0580 |
| 15.33 | 0.0960 | 0.1262 |
| 15.66 | 0.1374 | 0.1748 |
| 16.26 | 0.2116 | 0.2616 |
| 16.93 | 0.2808 | 0.3408 |
| 17.66 | 0.3501 | 0.4244 |
| 19.99 | 0.5153 | 0.6089 |
| 21.29 | 0.5882 | 0.6816 |
| 22.89 | 0.6624 | 0.7508 |
| 24.91 | 0.7507 | 0.8271 |
| 26.74 | 0.8241 | 0.8796 |
| 28.49 | 0.8871 | 0.9255 |

Im, Jihoon - Lee, Gangwon - Lee, Jongcheon - Kim, Hwayong, (Vapour+liquid) equilibria of the {pentafluoroethane (HFC-125)+dimethyl ether (DME)} system, The Journal of Chemical Thermodynamics 12 (2006) 1510-1514. doi:10.1016/j.jct.2006.04.009

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 18.50 | 0.0304 | 0.0423 |
| 19.48 | 0.1222 | 0.1565 |
| 20.04 | 0.1753 | 0.2193 |
| 20.70 | 0.2373 | 0.2934 |
| 21.55 | 0.2986 | 0.3702 |
| 22.75 | 0.3882 | 0.4611 |
| 24.37 | 0.4790 | 0.5655 |
| 25.57 | 0.5411 | 0.6224 |
| 26.69 | 0.5977 | 0.6729 |
| 29.04 | 0.6889 | 0.7537 |
| 31.44 | 0.7680 | 0.8220 |
| 33.44 | 0.8378 | 0.8701 |
| 35.94 | 0.9119 | 0.9218 |
| 36.30 | 0.9224 | 0.9285 |
| 36.40 | 0.9274 | 0.9296 |
| 36.40 | 0.9285 | 0.9285 CRIT |

Im, Jihoon - Lee, Gangwon - Lee, Jongcheon - Kim, Hwayong, (Vapour+liquid) equilibria of the {pentafluoroethane (HFC-125)+dimethyl ether (DME)} system, The Journal of Chemical Thermodynamics 12 (2006) 1510-1514. doi:10.1016/j.jct.2006.04.009

**T / K = 353.15**

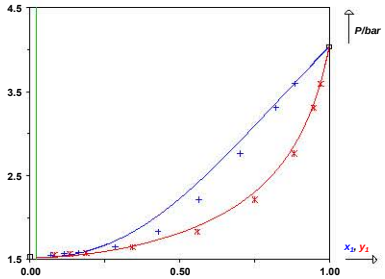
| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 23.02 | 0.0338 | 0.0490 |
| 24.25 | 0.1229 | 0.1639 |
| 25.73 | 0.2312 | 0.2860 |
| 26.90 | 0.3076 | 0.3682 |
| 29.18 | 0.4351 | 0.4968 |
| 32.31 | 0.5652 | 0.6248 |
| 34.31 | 0.6411 | 0.6864 |
| 36.69 | 0.7114 | 0.7441 |
| 37.24 | 0.7352 | 0.7510 |

Im, Jihoon - Lee, Gangwon - Lee, Jongcheon - Kim, Hwayong, (Vapour+liquid) equilibria of the {pentafluoroethane (HFC-125)+dimethyl ether (DME)} system, The Journal of Chemical Thermodynamics 12 (2006) 1510-1514. doi:10.1016/j.jct.2006.04.009

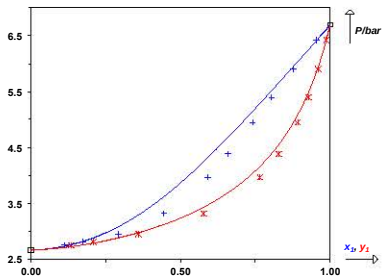
**T / K = 363.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 28.67 | 0.0705 | 0.0939 |
| 30.03 | 0.1490 | 0.1887 |
| 31.91 | 0.2561 | 0.3051 |
| 33.72 | 0.3436 | 0.3949 |
| 35.40 | 0.4174 | 0.4634 |
| 36.95 | 0.4785 | 0.5183 |
| 38.97 | 0.5548 | 0.5575 |
| 38.97 | 0.5562 | 0.5562 CRIT |

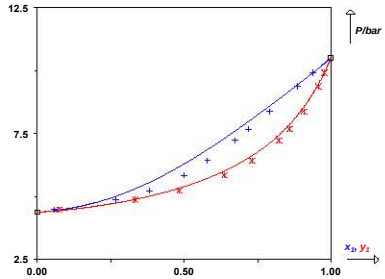
T/K = 258.15



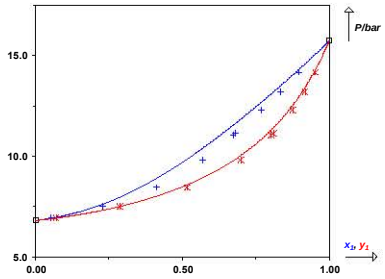

T/K = 273.15



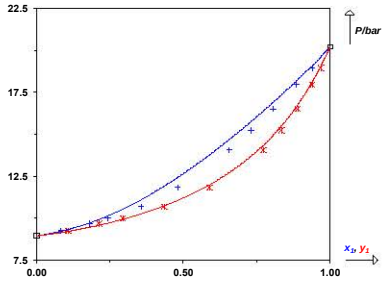

T/K = 288.15



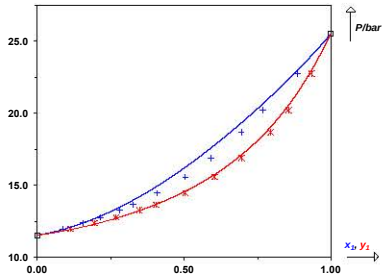

T/K = 303.15



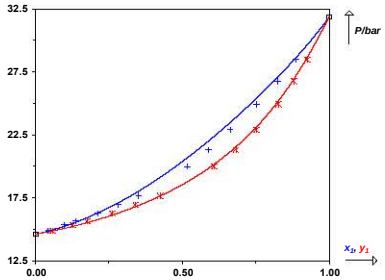

T/K = 313.15



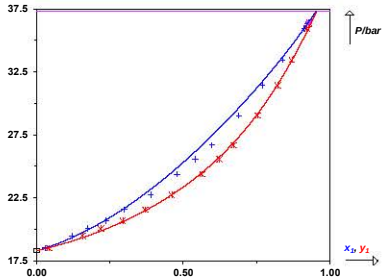

T/K = 323.15



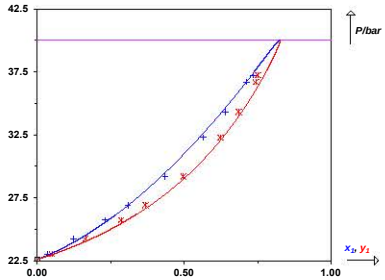

T/K = 333.15



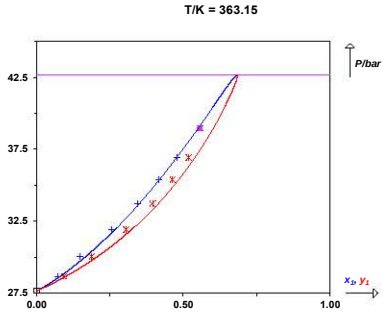

T/K = 343.15




T/K = 353.15




T/K = 363.15



## 3-PENTANONE (1) + 1,1,2,2-TETRACHLOROETHANE (2)

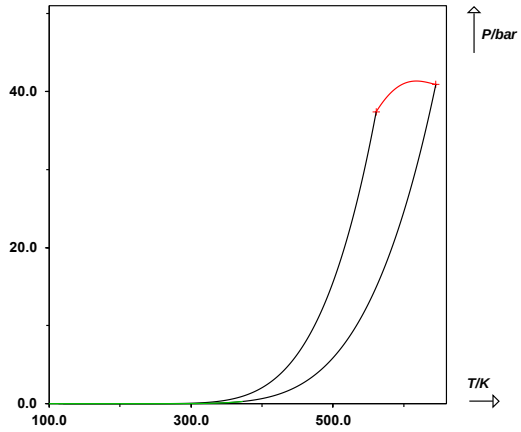
| | | |
|---|---|---|
| **CAS** | 96-22-0 | 79-34-5 |
| **InChiKey** | FDPIMTJIUBPUKL-UHFFFAOYSA-N | QPFMBZIOSGYJDE-UHFFFAOYSA-N |
| **$T_c$ / K** | 560.95 | 645.00 |
| **$P_c$ / bar** | 37.40 | 40.90 |
| **ω** | 0.3450 | 0.2470 |

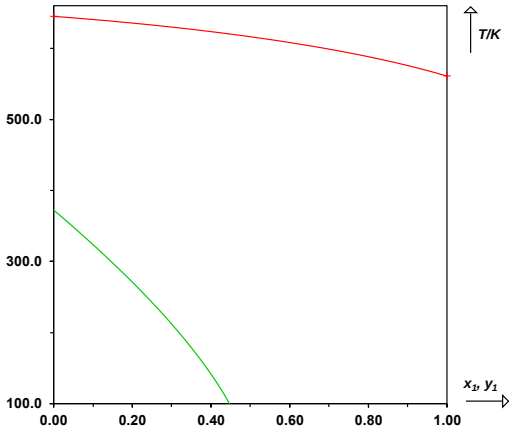
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = -273
B/MPa = -599

*Deviations*
MAPE on x = 4.6 %
MAPE on y = 8.7 %



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**Isothermal phase equilibrium data**

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Teodorescu, Mariana - Aim, Karel - Wichterle, Ivan, Isothermal vapour–liquid equilibria for pentan-3-one+1,4- dichlorobutane, +trichloromethane, +1,1,1-trichloroethane, +1,1,2,2-tetrachloroethane binary mixtures, Fluid Phase Equilibria 1-2 (1998) 215-228. doi:10.1016/S0378-3812(98)00235-0

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0765 | 0.0399 | 0.0767 |
| 0.0796 | 0.0819 | 0.1551 |
| 0.0885 | 0.1666 | 0.3231 |
| 0.0945 | 0.2122 | 0.4109 |
| 0.1044 | 0.2710 | 0.5200 |
| 0.1131 | 0.3160 | 0.5949 |
| 0.1258 | 0.3728 | 0.6765 |
| 0.1372 | 0.4220 | 0.7324 |
| 0.1512 | 0.4707 | 0.7878 |
| 0.1752 | 0.5405 | 0.8520 |
| 0.1943 | 0.5920 | 0.8889 |
| 0.2139 | 0.6459 | 0.9166 |
| 0.2204 | 0.6593 | 0.9258 |
| 0.2418 | 0.7135 | 0.9460 |
| 0.2558 | 0.7512 | 0.9597 |
| 0.2616 | 0.7653 | 0.9643 |
| 0.2790 | 0.8083 | 0.9744 |

Teodorescu, Mariana - Aim, Karel - Wichterle, Ivan, Isothermal vapour–liquid equilibria for pentan-3-one+1,4- dichlorobutane, +trichloromethane, +1,1,1-trichloroethane, +1,1,2,2-tetrachloroethane binary mixtures, Fluid Phase Equilibria 1-2 (1998) 215-228. doi:10.1016/S0378-3812(98)00235-0

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1170 | 0.0399 | 0.0788 |
| 0.1218 | 0.0819 | 0.1562 |
| 0.1357 | 0.1676 | 0.3262 |
| 0.1428 | 0.2081 | 0.3979 |
| 0.1554 | 0.2618 | 0.4924 |
| 0.1698 | 0.3139 | 0.5814 |
| 0.1854 | 0.3657 | 0.6555 |
| 0.2121 | 0.4329 | 0.7456 |
| 0.2369 | 0.4914 | 0.8055 |
| 0.2672 | 0.5581 | 0.8612 |
| 0.2949 | 0.6133 | 0.8954 |
| 0.3280 | 0.6774 | 0.9267 |
| 0.3783 | 0.7653 | 0.9616 |
| 0.4049 | 0.8148 | 0.9726 |
| 0.4618 | 0.9285 | 0.9927 |
| 0.4755 | 0.9524 | 0.9963 |

Teodorescu, Mariana - Aim, Karel - Wichterle, Ivan, Isothermal vapour–liquid equilibria for pentan-3-one+1,4- dichlorobutane, +trichloromethane, +1,1,1-trichloroethane, +1,1,2,2-tetrachloroethane binary mixtures, Fluid Phase Equilibria 1-2 (1998) 215-228. doi:10.1016/S0378-3812(98)00235-0

**T / K = 363.15**

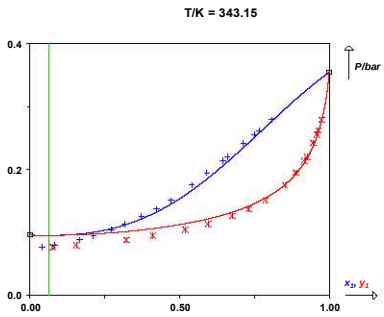
| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1736 | 0.0399 | 0.0777 |
| 0.1816 | 0.0840 | 0.1593 |
| 0.2014 | 0.1687 | 0.3231 |
| 0.2149 | 0.2164 | 0.4099 |
| 0.2313 | 0.2669 | 0.4974 |
| 0.2543 | 0.3231 | 0.5882 |
| 0.2804 | 0.3808 | 0.6717 |
| 0.3500 | 0.5337 | 0.8074 |
| 0.4300 | 0.6536 | 0.8954 |
| 0.4758 | 0.7125 | 0.9267 |
| 0.5173 | 0.7662 | 0.9469 |
| 0.5318 | 0.7784 | 0.9552 |
| 0.5368 | 0.7896 | 0.9570 |
| 0.5711 | 0.8278 | 0.9716 |
| 0.5972 | 0.8631 | 0.9799 |
| 0.6018 | 0.8705 | 0.9808 |
| 0.6493 | 0.9285 | 0.9918 |
| 0.6676 | 0.9552 | 0.9963 |

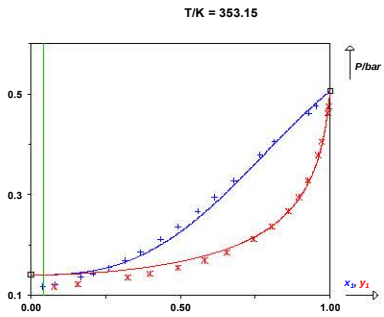
Teodorescu, Mariana - Aim, Karel - Wichterle, Ivan, Isothermal vapour–liquid equilibria for pentan-3-one+1,4- dichlorobutane, +trichloromethane, +1,1,1-trichloroethane, +1,1,2,2-tetrachloroethane binary mixtures, Fluid Phase Equilibria 1-2 (1998) 215-228. doi:10.1016/S0378-3812(98)00235-0

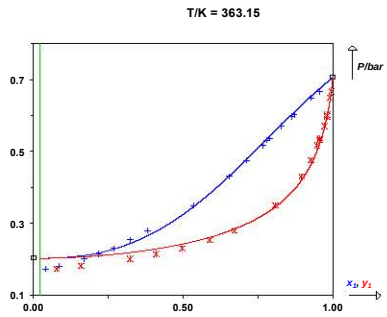
**T / K = 373.15**

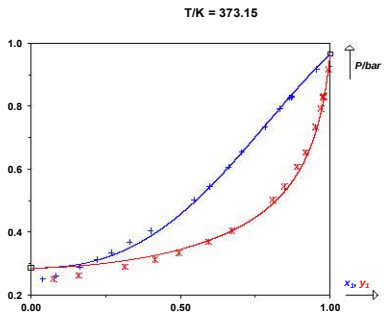
| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2513 | 0.0399 | 0.0767 |
| 0.2626 | 0.0840 | 0.1603 |
| 0.2894 | 0.1655 | 0.3139 |
| 0.3123 | 0.2212 | 0.4160 |
| 0.3337 | 0.2689 | 0.4954 |
| 0.3694 | 0.3302 | 0.5940 |
| 0.4051 | 0.4009 | 0.6736 |
| 0.5021 | 0.5464 | 0.8083 |
| 0.5444 | 0.5978 | 0.8473 |
| 0.6073 | 0.6603 | 0.8908 |
| 0.6537 | 0.7050 | 0.9175 |

| | | |
|---|---|---|
| 0.7344 | 0.7821 | 0.9515 |
| 0.7919 | 0.8325 | 0.9689 |
| 0.8268 | 0.8659 | 0.9762 |
| 0.8292 | 0.8705 | 0.9780 |
| 0.8310 | 0.8723 | 0.9790 |
| 0.9171 | 0.9561 | 0.9954 |


T/K = 343.15
P/bar
x1, y1
0.4
0.2
0.0
0.00
0.50
1.00


T/K = 353.15
P/bar
x1, y1
0.5
0.3
0.1
0.00
0.50
1.00


T/K = 363.15
P/bar
x1, y1
0.7
0.5
0.3
0.1
0.00
0.50
1.00


T/K = 373.15
P/bar
x1, y1
1.0
0.8
0.6
0.4
0.2
0.00
0.50
1.00

## DIMETHYL ETHER (1) + 1,1,1,3,3,3-HEXAFLUOROPROPANE (2)

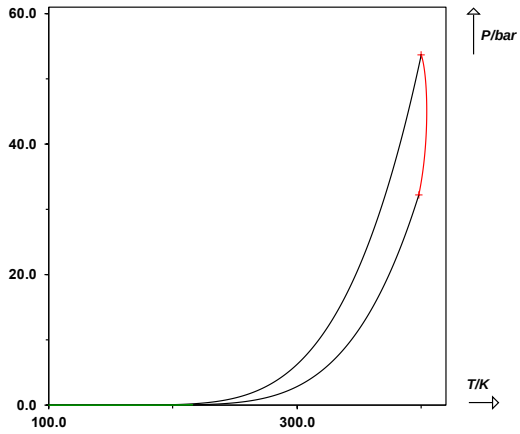
| | | |
|---|---|---|
| **CAS** | 115-10-6 | 690-39-1 |
| **InChiKey** | LCGLNKUTAGEVQW-UHFFFAOYSA-N | NSGXIBWMJZWTPY-UHFFFAOYSA-N |
| **$T_c$ / K** | 400.1 | 398.07 |
| **$P_c$ / bar** | 53.70 | 32.20 |
| **ω** | 0.2000 | 0.3900 |

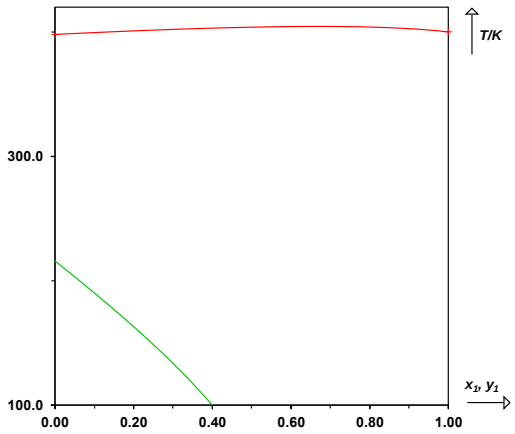
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = -138
B/MPa = -414

*Deviations*
MAPE on x = 3.2 %
MAPE on y = 4.3 %



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**Isothermal phase equilibrium data**

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Bobbo, Sergio - Fedele, Laura - Camporese, Roberto - Stryjek, Roman, Isothermal vapor–liquid equilibrium for the three binary systems 1,1,1,2,3,3-hexafluoropropane with dimethyl ether or propane, and 1,1,1,3,3,3-hexafluoropropane with dimethyl ether, Fluid Phase Equilibria 1-2 (2000) 3-12. doi:10.1016/S0378-3812(00)00413-1

**T / K = 283.12**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.620 | 0.1319 | 0.1480 |
| 1.642 | 0.1921 | 0.2265 |
| 1.710 | 0.2908 | 0.3617 |
| 2.831 | 0.7583 | 0.9073 |
| 3.225 | 0.8588 | 0.9594 |
| 3.600 | 0.9645 | 0.9918 |

Bobbo, Sergio - Camporese, Roberto - Stryjek, Roman, (Vapour + liquid) equilibrium measurements and correlations of the refrigerant mixture {dimethyl ether (RE170) + 1,1,1,3,3,3-hexafluoropropane (R236fa)} at the temperatures (303.68 and 323.75) K, The Journal of Chemical Thermodynamics 8 (1998) 1041-1046. doi:10.1006/jcht.1998.0369

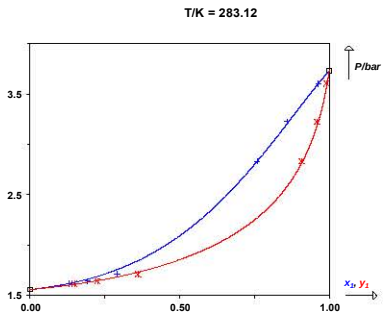
**T / K = 303.68**

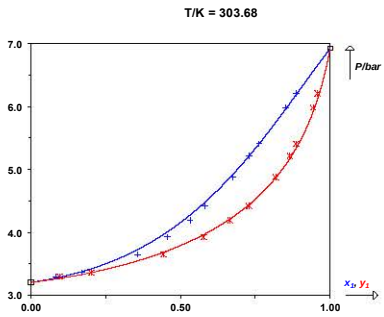
| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.296 | 0.0829 | 0.0970 |
| 3.364 | 0.1708 | 0.2016 |
| 3.649 | 0.3558 | 0.4428 |
| 3.925 | 0.4553 | 0.5774 |
| 4.195 | 0.5315 | 0.6664 |
| 4.418 | 0.5820 | 0.7298 |
| 4.881 | 0.6743 | 0.8184 |
| 5.218 | 0.7305 | 0.8656 |
| 5.409 | 0.7624 | 0.8877 |
| 5.986 | 0.8517 | 0.9426 |
| 6.207 | 0.8859 | 0.9588 |

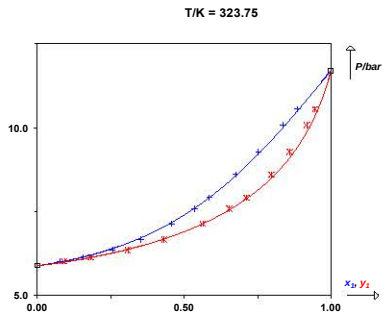
Bobbo, Sergio - Camporese, Roberto - Stryjek, Roman, (Vapour + liquid) equilibrium measurements and correlations of the refrigerant mixture {dimethyl ether (RE170) + 1,1,1,3,3,3-hexafluoropropane (R236fa)} at the temperatures (303.68 and 323.75) K, The Journal of Chemical Thermodynamics 8 (1998) 1041-1046. doi:10.1006/jcht.1998.0369

**T / K = 323.75**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.013 | 0.0779 | 0.0922 |
| 6.132 | 0.1563 | 0.1830 |
| 6.357 | 0.2557 | 0.3087 |
| 6.672 | 0.3533 | 0.4322 |
| 7.130 | 0.4557 | 0.5631 |
| 7.574 | 0.5348 | 0.6534 |
| 7.916 | 0.5864 | 0.7116 |
| 8.602 | 0.6754 | 0.7980 |
| 9.276 | 0.7527 | 0.8606 |
| 10.07 | 0.8371 | 0.9175 |
| 10.55 | 0.8860 | 0.9458 |


T/K = 283.12
P/bar
3.5
2.5
1.5
0.00
0.50
1.00
x1, y1


T/K = 303.68
P/bar
7.0
6.0
5.0
4.0
3.0
0.00
0.50
1.00
x1, y1


T/K = 323.75
P/bar
10.0
5.0
0.00
0.50
1.00
x1, y1

## DICHLOROMETHANE (1) + CARBON DISULFIDE (2)

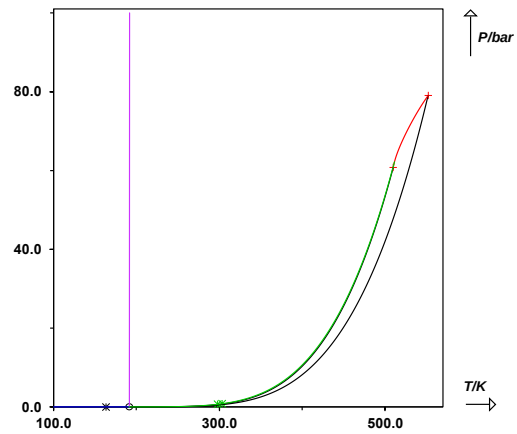
| | | |
|---|---|---|
| **CAS** | 75-09-2 | 75-15-0 |
| **InChiKey** | YMWUJEATGCHHMB-UHFFFAOYSA-N | QGJOPFRUJISHPQ-UHFFFAOYSA-N |
| **$T_c$ / K** | 510.00 | 552.00 |
| **$P_c$ / bar** | 60.80 | 79.00 |
| **ω** | 0.1990 | 0.1110 |

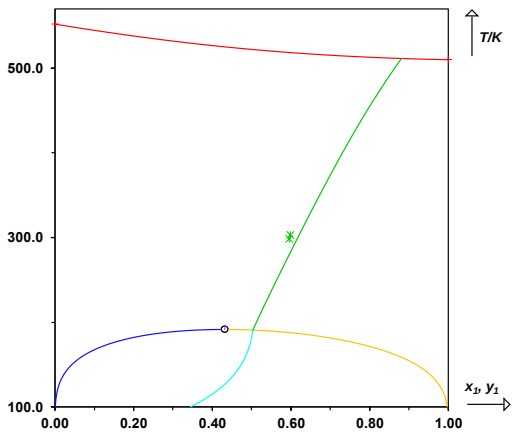
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 234
B/MPa = 407

*Deviations*
MAPE on x = 5.9 %
MAPE on y = 4.9 %
MAPE on $x_{az}$ = 4.4 %
MAPE on $P_{az}$ = 0.19 %
MAPE on $h^M$ = 7.4 %



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**Isothermal phase equilibrium data**

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Mozzhukhin, A.S. - Serafimov, I.A. - Zetkin, V.I. - Raskina, A.D. - Mitropol'skaya, V.A., Liquid-vapor equilibrium in a sulfur monochloride-perchloromethyl mercaptan system at low pressures, J. Appl. Chem. USSR 12 (1968) 2764-2766.

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.6102 | 0.2171 | 0.3306 | |
| 0.6332 | 0.3102 | 0.4081 | |
| 0.6420 | 0.3606 | 0.4457 | |
| 0.6428 | 0.3642 | 0.4483 | |
| 0.6531 | 0.4500 | 0.5051 | |
| 0.6570 | 0.4992 | 0.5352 | |
| 0.6582 | 0.5205 | 0.5481 | |
| 0.6590 | 0.5430 | 0.5617 | |
| 0.6598 | 0.5897 | 0.5908 | |
| 0.6600 | 0.5952 | 0.5952 | AZEO |
| 0.6600 | 0.5982 | 0.5962 | |
| 0.6587 | 0.6487 | 0.6302 | |
| 0.6556 | 0.7010 | 0.6688 | |
| 0.6507 | 0.7548 | 0.7126 | |
| 0.6439 | 0.8055 | 0.7577 | |
| 0.6301 | 0.8761 | 0.8266 | |
| 0.6257 | 0.8935 | 0.8451 | |

Mozzhukhin, A.S. - Serafimov, I.A. - Zetkin, V.I. - Raskina, A.D. - Mitropol'skaya, V.A., Liquid-vapor equilibrium in a sulfur monochloride-perchloromethyl mercaptan system at low pressures, J. Appl. Chem. USSR 12 (1968) 2764-2766.

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.7339 | 0.2170 | 0.3570 | |
| 0.7636 | 0.3100 | 0.4268 | |
| 0.7733 | 0.3584 | 0.4558 | |
| 0.7746 | 0.3641 | 0.4591 | |
| 0.7860 | 0.4498 | 0.5067 | |
| 0.7903 | 0.4992 | 0.5350 | |
| 0.7916 | 0.5201 | 0.5475 | |
| 0.7926 | 0.5430 | 0.5617 | |
| 0.7937 | 0.5897 | 0.5923 | |
| 0.7938 | 0.5986 | 0.5986 | AZEO |
| 0.7938 | 0.5992 | 0.5988 | |
| 0.7929 | 0.6485 | 0.6343 | |
| 0.7899 | 0.7006 | 0.6745 | |
| 0.7848 | 0.7512 | 0.7161 | |
| 0.7773 | 0.8055 | 0.7633 | |
| 0.7625 | 0.8761 | 0.8299 | |
| 0.7578 | 0.8935 | 0.8480 | |

Mozzhukhin, A.S. - Serafimov, I.A. - Zetkin, V.I. - Raskina, A.D. - Mitropol'skaya, V.A., Liquid-vapor equilibrium in a sulfur monochloride-perchloromethyl mercaptan system at low pressures, J. Appl. Chem. USSR 12 (1968) 2764-2766.

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.8742 | 0.2170 | 0.3526 |
| 0.9104 | 0.3098 | 0.4255 |
| 0.9247 | 0.3639 | 0.4603 |
| 0.9400 | 0.4498 | 0.5116 |
| 0.9462 | 0.4991 | 0.5411 |
| 0.9479 | 0.5195 | 0.5536 |
| 0.9497 | 0.5429 | 0.5683 |
| 0.9520 | 0.5896 | 0.5986 |
| 0.9521 | 0.5987 | 0.6048 |
| 0.9520 | 0.6481 | 0.6391 |
| 0.9492 | 0.7005 | 0.6780 |
| 0.9434 | 0.7545 | 0.7207 |
| 0.9351 | 0.8054 | 0.7638 |
| 0.9173 | 0.8761 | 0.8306 |
| 0.9116 | 0.8935 | 0.8490 |

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**Enthalpy of mixing**

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Siddiqi, M.A. - Lucas, K., The excess enthalpy of methyliodide + carbon disulphide, methyliodide + dichloromethane and dichloromethane + carbon disulphide over a range of temperatures and pressures, Fluid Phase Equilibria (1985) 297-304. doi:10.1016/0378-3812(85)90048-2

**T / K = 283.15**

**P / bar = 1.0000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 748.70 | 0.1930 |
| 954.20 | 0.2900 |
| 1074.5 | 0.3820 |
| 1106.3 | 0.4830 |
| 1053.3 | 0.5850 |
| 973.90 | 0.6570 |
| 815.80 | 0.7420 |
| 611.40 | 0.8280 |

Siddiqi, M.A. - Lucas, K., The excess enthalpy of methyliodide + carbon disulphide, methyliodide + dichloromethane and dichloromethane + carbon disulphide over a range of temperatures and pressures,

Fluid Phase Equilibria (1985) 297-304. doi:10.1016/0378-3812(85)90048-2

**T / K = 293.15**

**P / bar = 1.0000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 602.70 | 0.1560 |
| 802.00 | 0.2370 |
| 953.60 | 0.3200 |
| 1038.6 | 0.4020 |
| 1063.8 | 0.4870 |
| 1013.6 | 0.5710 |
| 916.50 | 0.6570 |
| 766.20 | 0.7420 |
| 568.60 | 0.8260 |

Siddiqi, M.A. - Lucas, K., The excess enthalpy of methyliodide + carbon disulphide, methyliodide + dichloromethane and dichloromethane + carbon disulphide over a range of temperatures and pressures, Fluid Phase Equilibria (1985) 297-304. doi:10.1016/0378-3812(85)90048-2

**T / K = 293.15**

**P / bar = 150.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 662.10 | 0.1470 |
| 715.60 | 0.1640 |
| 1018.0 | 0.3030 |
| 1116.5 | 0.4050 |
| 1130.3 | 0.4850 |
| 1091.2 | 0.5880 |
| 1001.8 | 0.6650 |
| 906.60 | 0.7290 |
| 662.20 | 0.8340 |

Siddiqi, M.A. - Lucas, K., The excess enthalpy of methyliodide + carbon disulphide, methyliodide + dichloromethane and dichloromethane + carbon disulphide over a range of temperatures and pressures, Fluid Phase Equilibria (1985) 297-304. doi:10.1016/0378-3812(85)90048-2

**T / K = 293.15**

**P / bar = 300.00**

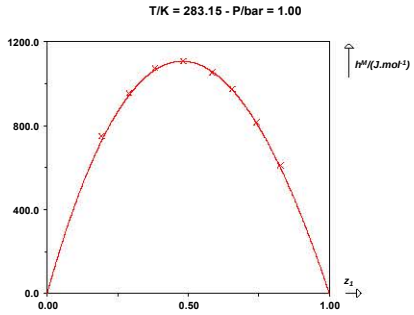
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 647.80 | 0.1270 |
| 834.80 | 0.1830 |
| 1085.2 | 0.2850 |
| 1116.4 | 0.2990 |
| 1230.0 | 0.3890 |
| 1277.2 | 0.5100 |
| 1222.0 | 0.5860 |
| 1095.7 | 0.6990 |
| 859.90 | 0.8030 |

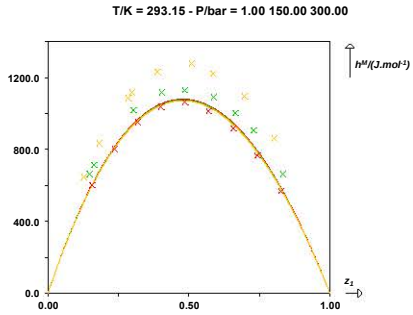
Siddiqi, M.A. - Lucas, K., The excess enthalpy of methyliodide + carbon disulphide, methyliodide + dichloromethane and dichloromethane + carbon disulphide over a range of temperatures and pressures, Fluid Phase Equilibria (1985) 297-304. doi:10.1016/0378-3812(85)90048-2

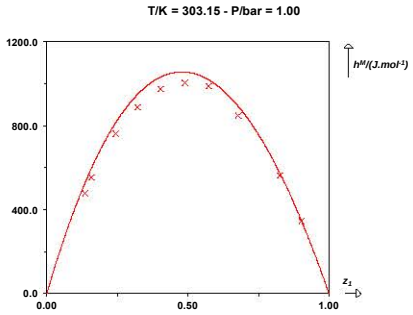
**T / K = 303.15**

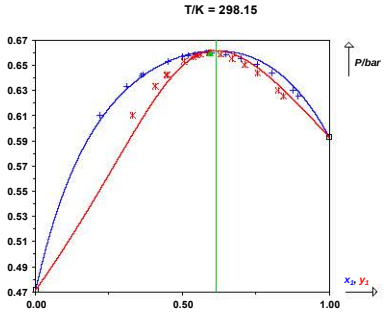
**P / bar = 1.0000**

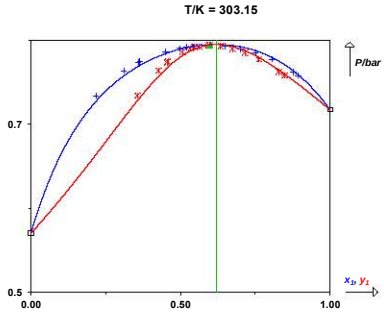
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 476.00 | 0.1360 |
| 553.40 | 0.1590 |
| 760.10 | 0.2440 |
| 887.60 | 0.3220 |
| 974.00 | 0.4030 |
| 1003.8 | 0.4900 |
| 986.90 | 0.5750 |
| 847.40 | 0.6800 |
| 563.20 | 0.8260 |
| 345.30 | 0.9030 |

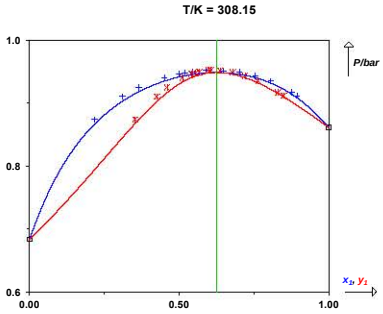

T/K = 283.15 - P/bar = 1.00
1200.0
800.0
400.0
0.0
0.00
0.50
1.00
$h^M$/(J.mol$^{-1}$)
$z_1$


T/K = 293.15 - P/bar = 1.00 150.00 300.00
1200.0
800.0
400.0
0.0
0.00
0.50
1.00
$h^M$/(J.mol$^{-1}$)
$z_1$


T/K = 303.15 - P/bar = 1.00
1200.0
800.0
400.0
0.0
0.00
0.50
1.00
$h^M$/(J.mol$^{-1}$)
$z_1$


T/K = 298.15
0.67
0.65
0.63
0.61
0.59
0.57
0.55
0.53
0.51
0.49
0.47
0.00
0.50
1.00
P/bar
$x_1$, $y_1$


T/K = 303.15
0.7
0.5
0.00
0.50
1.00
P/bar
$x_1$, $y_1$


T/K = 308.15
1.0
0.8
0.6
0.00
0.50
1.00
P/bar
$x_1$, $y_1$

## ACETONE (1) + CHLOROFORM (2)

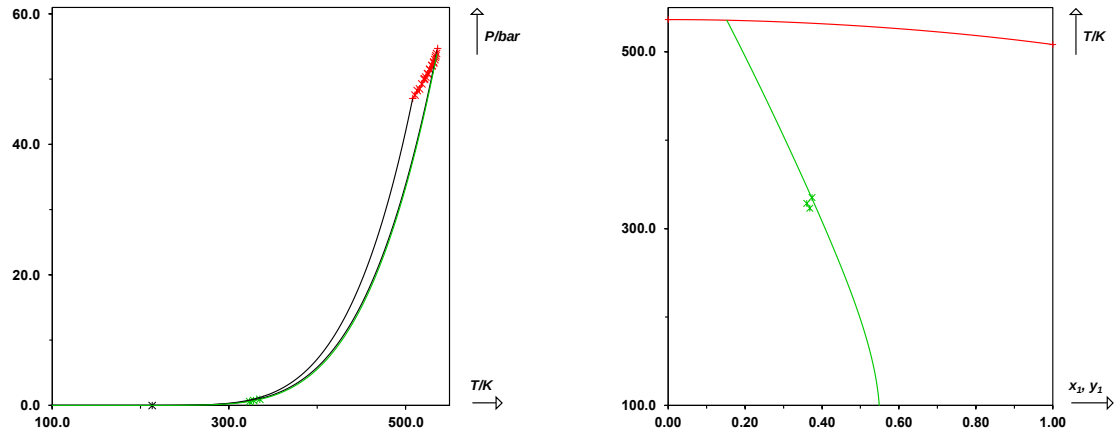
| | | |
|---|---|---|
| **CAS** | 67-64-1 | 67-66-3 |
| **InChiKey** | CSCPPACGZOOCGX-UHFFFAOYSA-N | HEDRZPFGACZZDS-UHFFFAOYSA-N |
| **$T_c$ / K** | 508.20 | 536.40 |
| **$P_c$ / bar** | 47.01 | 54.72 |
| **ω** | 0.3070 | 0.2220 |

Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = -188
B/MPa = -375

*Deviations*
MAPE on x = 12 %
MAPE on y = 13 %
MAPE on $x_c$ = 35 %
MAPE on $P_c$ = 1.7 %
MAPE on $x_{az}$ = 2.6 %
MAPE on $P_{az}$ = 1.6 %
MAPE on $h^M$ = 27 %
MAPE on $c_P^M$ = 66 %



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**Isothermal phase equilibrium data**

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Röck, H. - Schröder, W., Dampf-Flüssigkeits-Gleichgewichtsmessungen im System Azeton-Chloroform, Z. Phys. Chem. NF (1957) 41-55. doi:10.1524/zpch.1957.11.1_2.041

**T / K = 288.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1559 | 0.1050 | 0.0500 |
| 0.1441 | 0.2140 | 0.1410 |
| 0.1380 | 0.3010 | 0.2470 |
| 0.1347 | 0.4050 | 0.4100 |
| 0.1377 | 0.5070 | 0.5730 |
| 0.1447 | 0.5950 | 0.6930 |
| 0.1557 | 0.6860 | 0.8030 |
| 0.1693 | 0.7970 | 0.8960 |
| 0.1821 | 0.8920 | 0.9520 |

Röck, H. - Schröder, W., Dampf-Flüssigkeits-Gleichgewichtsmessungen im System Azeton-Chloroform, Z. Phys. Chem. NF (1957) 41-55. doi:10.1524/zpch.1957.11.1_2.041

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1971 | 0.1050 | 0.0530 |
| 0.1832 | 0.2140 | 0.1410 |
| 0.1749 | 0.3020 | 0.2520 |
| 0.1720 | 0.4050 | 0.4100 |
| 0.1756 | 0.5070 | 0.5690 |
| 0.1844 | 0.5950 | 0.6870 |
| 0.1971 | 0.6850 | 0.7960 |
| 0.2140 | 0.7970 | 0.8930 |
| 0.2291 | 0.8930 | 0.9520 |

Röck, H. - Schröder, W., Dampf-Flüssigkeits-Gleichgewichtsmessungen im System Azeton-Chloroform, Z. Phys. Chem. NF (1957) 41-55. doi:10.1524/zpch.1957.11.1_2.041

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3041 | 0.1050 | 0.0560 |
| 0.2870 | 0.1970 | 0.1360 |
| 0.2738 | 0.2990 | 0.2550 |
| 0.2694 | 0.4000 | 0.4090 |
| 0.2764 | 0.5030 | 0.5670 |
| 0.2890 | 0.5910 | 0.6890 |
| 0.3093 | 0.6970 | 0.8060 |
| 0.3320 | 0.8010 | 0.8890 |
| 0.3558 | 0.8990 | 0.9530 |

Kudryavtseva, L.S. - Susarev, M.P., Liquid-vapor equilibrium in systems chloroform-hexane and acetone-chloroform, J. Appl. Chem. USSR 6 (1963) 1231-1237.

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3729 | 0.1007 | 0.0590 |
| 0.3528 | 0.2007 | 0.1440 |
| 0.3389 | 0.3018 | 0.2700 |
| 0.3352 | 0.3982 | 0.4100 |
| 0.3441 | 0.4987 | 0.5580 |
| 0.3589 | 0.5905 | 0.6800 |
| 0.3842 | 0.6972 | 0.8050 |
| 0.4100 | 0.7961 | 0.8880 |
| 0.4361 | 0.8921 | 0.9510 |

Kudryavtseva, L.S. - Susarev, M.P., Liquid-vapor equilibrium in systems chloroform-hexane and acetone-chloroform, J. Appl. Chem. USSR 6 (1963) 1231-1237.

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5537 | 0.1005 | 0.0610 |
| 0.5265 | 0.2005 | 0.1430 |
| 0.5089 | 0.3013 | 0.2670 |
| 0.5066 | 0.3967 | 0.4080 |
| 0.5204 | 0.4880 | 0.5450 |
| 0.5384 | 0.5915 | 0.6760 |
| 0.5722 | 0.6945 | 0.8000 |
| 0.6074 | 0.7941 | 0.8830 |
| 0.6465 | 0.8936 | 0.9490 |

Vilim, O. - Hala, E. - Fried, V. - Pick, J., Liquid-vapor equilibria. XII. Fractional steam distillation of the system o-nitroethylbenzene-p-nitroethylbenzene, Chem. Listy (1954) 1109-1113.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.6850 | 0.0230 | 0.0086 |
| 0.6763 | 0.0500 | 0.0201 |
| 0.6638 | 0.0900 | 0.0408 |
| 0.6605 | 0.1000 | 0.0464 |
| 0.6493 | 0.1350 | 0.0719 |
| 0.6442 | 0.1520 | 0.0863 |
| 0.6416 | 0.1600 | 0.0935 |
| 0.6277 | 0.2040 | 0.1383 |
| 0.6190 | 0.2360 | 0.1760 |
| 0.6149 | 0.2500 | 0.1930 |
| 0.6088 | 0.3000 | 0.2582 |

| | | | |
|---|---|---|---|
| 0.6056 | 0.3500 | 0.3382 | |
| 0.6053 | 0.3640 | 0.3608 | |
| 0.6054 | 0.3680 | 0.3675 | |
| 0.6054 | 0.3683 | 0.3683 | AZEO |
| 0.6057 | 0.3900 | 0.4032 | |
| 0.6065 | 0.4200 | 0.4511 | |
| 0.6104 | 0.4500 | 0.4963 | |
| 0.6142 | 0.4690 | 0.5240 | |
| 0.6217 | 0.5000 | 0.5670 | |
| 0.6317 | 0.5390 | 0.6211 | |
| 0.6346 | 0.5500 | 0.6370 | |
| 0.6485 | 0.6000 | 0.6978 | |
| 0.6521 | 0.6120 | 0.7113 | |
| 0.6550 | 0.6220 | 0.7222 | |
| 0.6638 | 0.6500 | 0.7528 | |
| 0.6823 | 0.7000 | 0.8028 | |
| 0.7029 | 0.7500 | 0.8515 | |
| 0.7249 | 0.8000 | 0.8955 | |
| 0.7479 | 0.8500 | 0.9319 | |
| 0.7710 | 0.9000 | 0.9614 | |
| 0.7943 | 0.9500 | 0.9829 | |

Beckmann, E. - Faust, O., Die Dampfspannung der Aceton-Chloroformgemische in Abhängigkeit von der Temperatur, Zeitschrift für Physikalische Chemie 1 (1914) doi:10.1515/zpch-1914-8917

**T / K = 328.25**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.8013 | 0.1180 | 0.0910 | |
| 0.7699 | 0.2340 | 0.1900 | |
| 0.7469 | 0.3600 | 0.3600 | AZEO |
| 0.7487 | 0.3850 | 0.4000 | |
| 0.7698 | 0.5080 | 0.5570 | |
| 0.7966 | 0.5820 | 0.6770 | |
| 0.8175 | 0.6450 | 0.7380 | |
| 0.8527 | 0.7210 | 0.8120 | |
| 0.9265 | 0.9000 | 0.9440 | |

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**Isobaric phase equilibrium data**

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Segura, Hugo - Mejía, Andrés - Reich, Ricardo - Wisniak, Jaime - Loras, Sonia, Isobaric Vapor-Liquid Equilibria and Densities for the Binary Systems Oxolane + Ethyl 1,1-Dimethylethyl Ether, Oxolane + 2-Propanol and Propan-2-One + Trichloromethane, Physics and Chemistry of Liquids 3 (2003) 283-301. doi:10.1080/0031910021000044456

**P / bar = 0.9400**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 332.47 | 0.0420 | 0.0240 |
| 333.16 | 0.1020 | 0.0650 |
| 333.66 | 0.1510 | 0.1070 |
| 334.05 | 0.1830 | 0.1380 |
| 334.58 | 0.2340 | 0.1900 |
| 334.94 | 0.2740 | 0.2380 |
| 335.15 | 0.3210 | 0.2970 |
| 335.22 | 0.3500 | 0.3450 |
| 335.13 | 0.3900 | 0.4000 |
| 335.00 | 0.4170 | 0.4330 |
| 334.88 | 0.4410 | 0.4710 |
| 334.83 | 0.4510 | 0.4820 |
| 334.42 | 0.5070 | 0.5600 |
| 333.90 | 0.5600 | 0.6290 |
| 333.27 | 0.6090 | 0.6910 |
| 332.70 | 0.6470 | 0.7390 |
| 331.81 | 0.7060 | 0.8000 |
| 331.05 | 0.7550 | 0.8450 |
| 330.40 | 0.7940 | 0.8760 |
| 329.60 | 0.8430 | 0.9120 |
| 328.85 | 0.8890 | 0.9430 |
| 328.06 | 0.9390 | 0.9720 |

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**Enthalpy of mixing**

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Sabinin, V.E. - Belousov, V.P. - Morachevskii, A.G., Heats of mixing and evaporation in the acetonechloroform system, Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol. (1967) 34-38.

**T / K = 283.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -1243.5 | 0.1670 |
| -1871.5 | 0.3330 |
| -1946.9 | 0.3770 |
| -1972.0 | 0.3900 |
| -1984.5 | 0.4590 |
| -1967.8 | 0.5230 |
| -1310.5 | 0.7270 |
| -937.84 | 0.8110 |

Kulanek, M. - Bittrich, H.J., Heat of solution of the system acetone-chloroform, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg 2 (1962) 139-141.

**T / K = 287.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -1477.9 | 0.1860 |

| | |
|---|---|
| -2089.2 | 0.3400 |
| -2202.3 | 0.4690 |
| -2106.0 | 0.5780 |
| -1829.6 | 0.6730 |
| -1461.2 | 0.7550 |
| -979.71 | 0.8270 |
| -632.21 | 0.8910 |

Akamatsu, Yutaka - Ogawa, Hideo - Murakami, Sachio, Molar excess enthalpies, molar excess volumes and molar isentropic compressions of mixtures of 2-propanone with heptane, benzene and trichloromethane at 298.15 K, Thermochimica Acta (1987) 141-150. doi:10.1016/0040-6031(87)88317-X

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -402.10 | 0.0500 |
| -764.60 | 0.1001 |
| -1091.4 | 0.1501 |
| -1362.4 | 0.2001 |
| -1588.7 | 0.2501 |
| -1756.8 | 0.3001 |
| -1870.7 | 0.3501 |
| -1933.5 | 0.4001 |
| -1941.0 | 0.4502 |
| -1904.4 | 0.5002 |
| -1822.0 | 0.5501 |
| -1705.7 | 0.6001 |
| -1554.0 | 0.6501 |
| -1381.6 | 0.7001 |
| -1179.2 | 0.7501 |
| -970.50 | 0.8001 |
| -741.60 | 0.8501 |
| -501.20 | 0.9000 |
| -227.70 | 0.9500 |

Nagata, Isamu - Tamura, Kazuhiro - Tokuriki, Shinji, Excess enthalpies and complex formation of acetonitrile with acetone, chloroform, and benzene, Thermochimica Acta 3 (1981) 315-331. doi:10.1016/0040-6031(81)80110-4

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -174.60 | 0.0218 |
| -588.20 | 0.0762 |
| -940.30 | 0.1273 |
| -1228.1 | 0.1757 |
| -1475.8 | 0.2249 |
| -1657.9 | 0.2706 |
| -1811.2 | 0.3251 |
| -1899.8 | 0.3812 |
| -1929.5 | 0.4395 |
| -1903.8 | 0.4871 |
| -1840.5 | 0.5321 |
| -1756.3 | 0.5744 |
| -1676.2 | 0.6060 |
| -1517.1 | 0.6579 |
| -1327.8 | 0.7113 |
| -1108.6 | 0.7648 |
| -891.50 | 0.8149 |
| -662.60 | 0.8645 |
| -451.20 | 0.9088 |
| -226.90 | 0.9547 |
| -78.20 | 0.9844 |

Morris, John W. - Mulvey, Patrick J. - Abbott, Michael M. - Van Ness, Hendrick C., Excess thermodynamic functions for ternary systems. I. Acetone-chloroform-methanol at 50.deg., Journal of Chemical & Engineering Data 4 (1975) 403-405. doi:10.1021/je60067a019

**T / K =** **323.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -137.60 | 0.0185 |
| -382.90 | 0.0527 |
| -670.80 | 0.0961 |
| -1041.9 | 0.1601 |
| -1378.2 | 0.2331 |
| -1602.2 | 0.3017 |
| -1713.9 | 0.3555 |
| -1771.7 | 0.4114 |
| -1772.5 | 0.4672 |
| -1746.7 | 0.5021 |
| -1703.4 | 0.5361 |
| -1433.5 | 0.6583 |
| -1261.4 | 0.7110 |
| -1058.6 | 0.7654 |
| -784.40 | 0.8318 |
| -447.40 | 0.9067 |
| -226.80 | 0.9532 |

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**Heat capacity of mixing**

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Fenclova, D. - Dohnal, V. - Perez-Casas, S. - Frigolet, C. - Costas, M., Excess heat capacities, excess enthalpies, and excess volumes of trichloromethane + some oxygenated solvents or + the corresponding

homomorphic hydrocarbons at 298.15 K, ELDATA Int. Electron. J. Phys. Chem. Data 3 (1995) 217-237.

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 2.210 | 0.1008 |
| 3.800 | 0.2041 |
| 4.630 | 0.3010 |
| 4.650 | 0.4021 |
| 4.130 | 0.5086 |
| 3.060 | 0.6072 |
| 1.920 | 0.7080 |
| 1.150 | 0.7948 |
| 0.4000 | 0.9006 |

Yamanaka, Katsuhiko - Ogawa, Hideo - Murakami, Sachio, Excess molar isobaric heat capacities of mixtures of 2-propanone with heptane, benzene, and trichloromethane at 298.15 K, Thermochimica Acta (1990) 193-201. doi:10.1016/0040-6031(90)80145-O

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 1.290 | 0.0500 |
| 2.402 | 0.1001 |
| 4.262 | 0.2001 |
| 5.410 | 0.3001 |
| 5.601 | 0.4002 |
| 4.941 | 0.5002 |
| 3.824 | 0.6002 |
| 2.541 | 0.7001 |
| 1.364 | 0.8001 |
| 0.4800 | 0.9001 |
| 0.2000 | 0.9500 |

Grolier, J. -P. E. - Roux-Desgranges, G. - Berkane, M. - Wilhelm, Emmerich, Heat capacities and densities of mixtures of very polar substances. 3. Mixtures containing either trichloromethane or 1,4-dioxane or diisopropylether, Journal of Solution Chemistry 2 (1994) 153-166. doi:10.1007/BF00973543

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 1.855 | 0.0653 |
| 3.195 | 0.1398 |
| 4.184 | 0.2143 |
| 5.179 | 0.3182 |
| 5.275 | 0.4047 |
| 5.037 | 0.4562 |
| 4.143 | 0.5541 |
| 3.101 | 0.6340 |
| 1.763 | 0.7492 |
| 1.143 | 0.8201 |
| 0.6340 | 0.8836 |
| 0.2190 | 0.9517 |

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**Critical point**

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Jaubert, Jean-Noël - Privat, Romain - Juntarachat, Niramol, General reflection on critical negative azeotropy and upgrade of the Bancroft's rule with application to the acetone+chloroform binary system, The Journal of Supercritical Fluids (2014) 17-29. doi:10.1016/j.supflu.2014.06.014

| T / K | P / bar | $x_1$ |
|---|---|---|
| 510.68 | 47.60 | 0.9215 |
| 513.52 | 48.25 | 0.8486 |
| 515.78 | 48.54 | 0.7852 |
| 518.63 | 49.26 | 0.7001 |
| 521.04 | 49.99 | 0.6195 |
| 521.86 | 50.07 | 0.6009 |
| 523.15 | 50.35 | 0.5455 |
| 524.86 | 50.84 | 0.5053 |
| 525.56 | 50.82 | 0.4834 |
| 527.52 | 51.54 | 0.4174 |
| 527.64 | 51.48 | 0.3895 |
| 529.98 | 52.13 | 0.3082 |
| 530.31 | 52.05 | 0.3050 |
| 531.80 | 52.62 | 0.2015 |
| 532.19 | 52.51 | 0.2006 |
| 532.96 | 52.95 | 0.1597 |
| 533.90 | 53.32 | 0.1086 |
| 534.54 | 53.57 | 0.0998 |
| 535.26 | 53.98 | 0.0608 |

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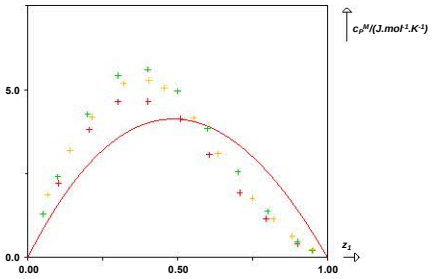
**Azeotropic point**

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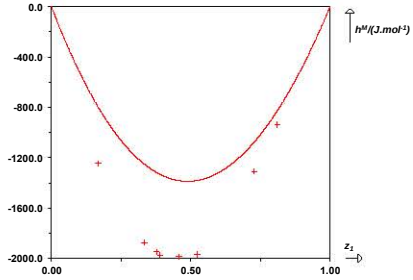
Segura, Hugo - Mejía, Andrés - Reich, Ricardo - Wisniak, Jaime - Loras, Sonia, Isobaric Vapor-Liquid Equilibria and Densities for the Binary Systems Oxolane + Ethyl 1,1-Dimethylethyl Ether, Oxolane + 2-Propanol and Propan-2-One + Trichloromethane, Physics and Chemistry of Liquids 3 (2003) 283-301. doi:10.1080/0031910021000044456

| T / K | P / bar | $x_1$ |
|---|---|---|
| 335.16 | 0.9400 | 0.3740 |

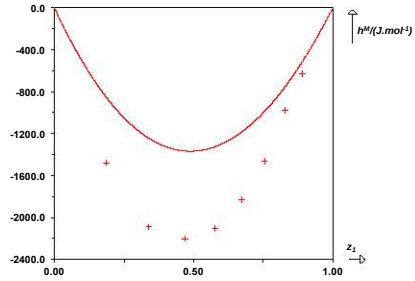
T/K = 298.15 - P/bar = 1.0132 1.0132 1.0132



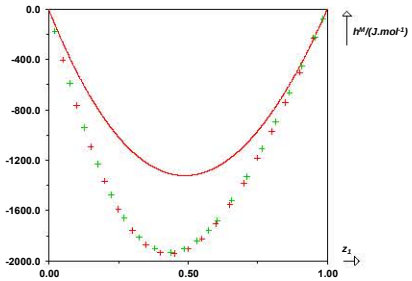

T/K = 283.15 - P/bar = 1.0132



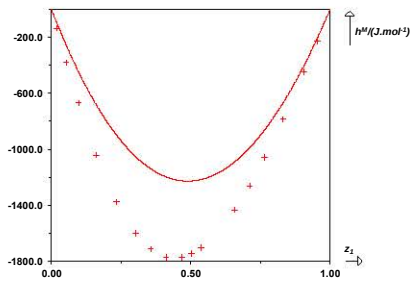

T/K = 287.15 - P/bar = 1.0132



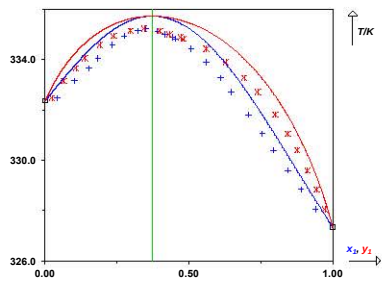

T/K = 298.15 - P/bar = 1.0132 1.0132



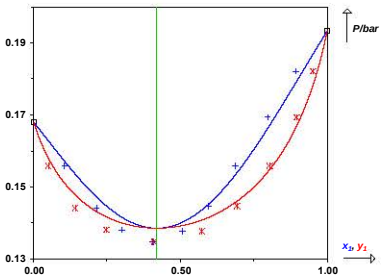

T/K = 323.15 - P/bar = 1.0132



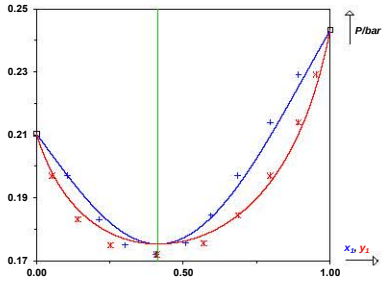

P/bar = 0.94000



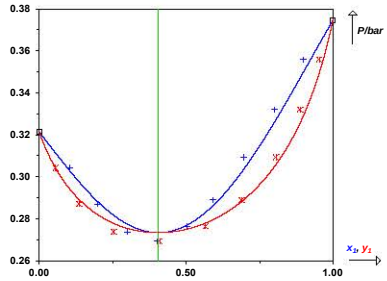

T/K = 288.15



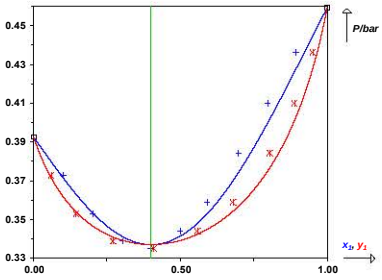

T/K = 293.15



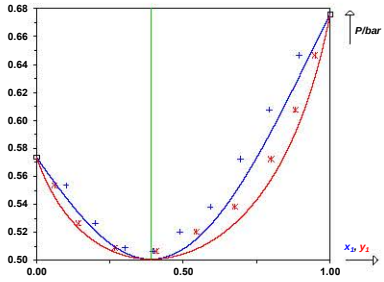

T/K = 303.15



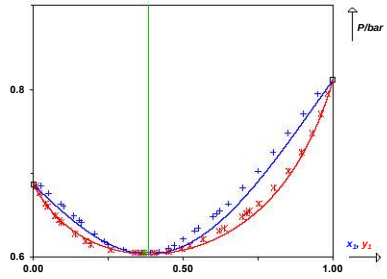

T/K = 308.15



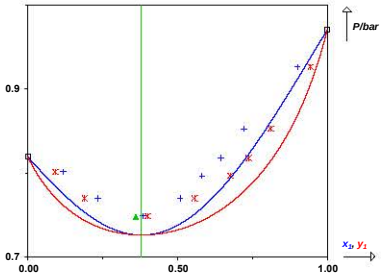

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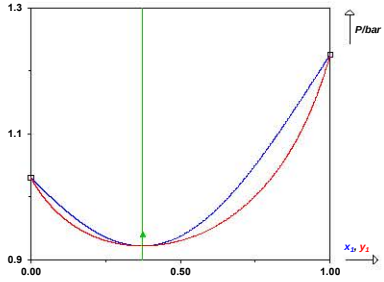

T/K = 323.15



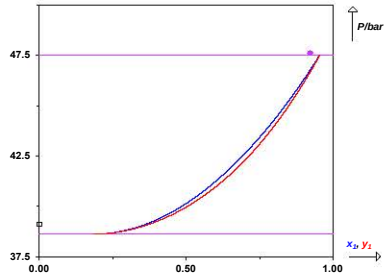

T/K = 328.25



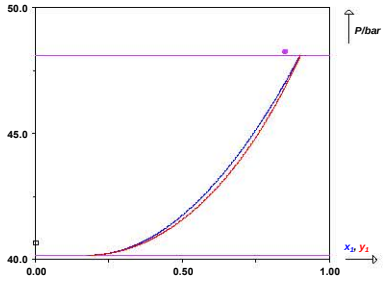

T/K = 335.16



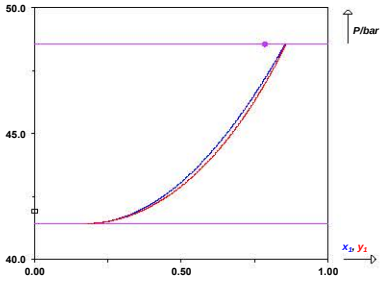

T/K = 510.68



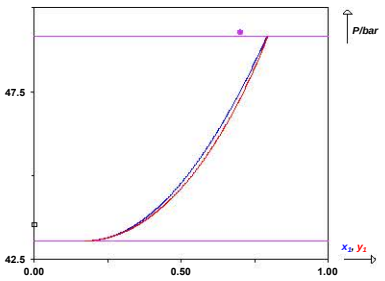
T/K = 513.52



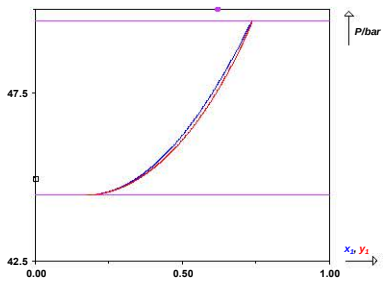

T/K = 515.78



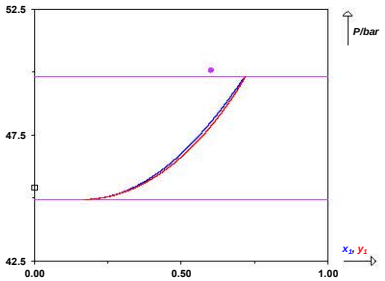

T/K = 518.63



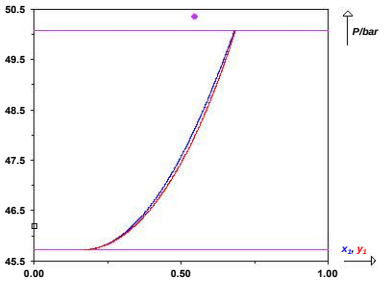

T/K = 521.04



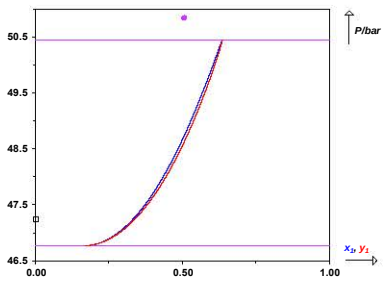

T/K = 521.86



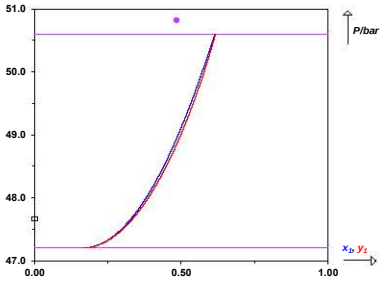

T/K = 523.15



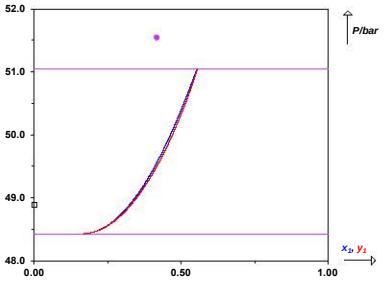

T/K = 524.86



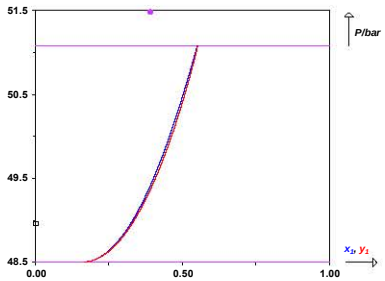

T/K = 525.56



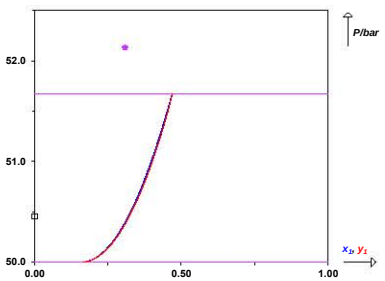

T/K = 527.52



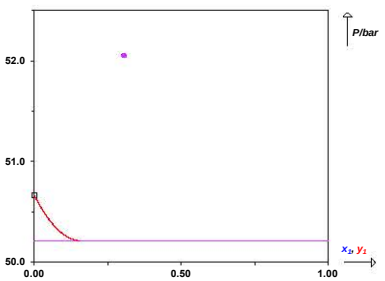

T/K = 527.64

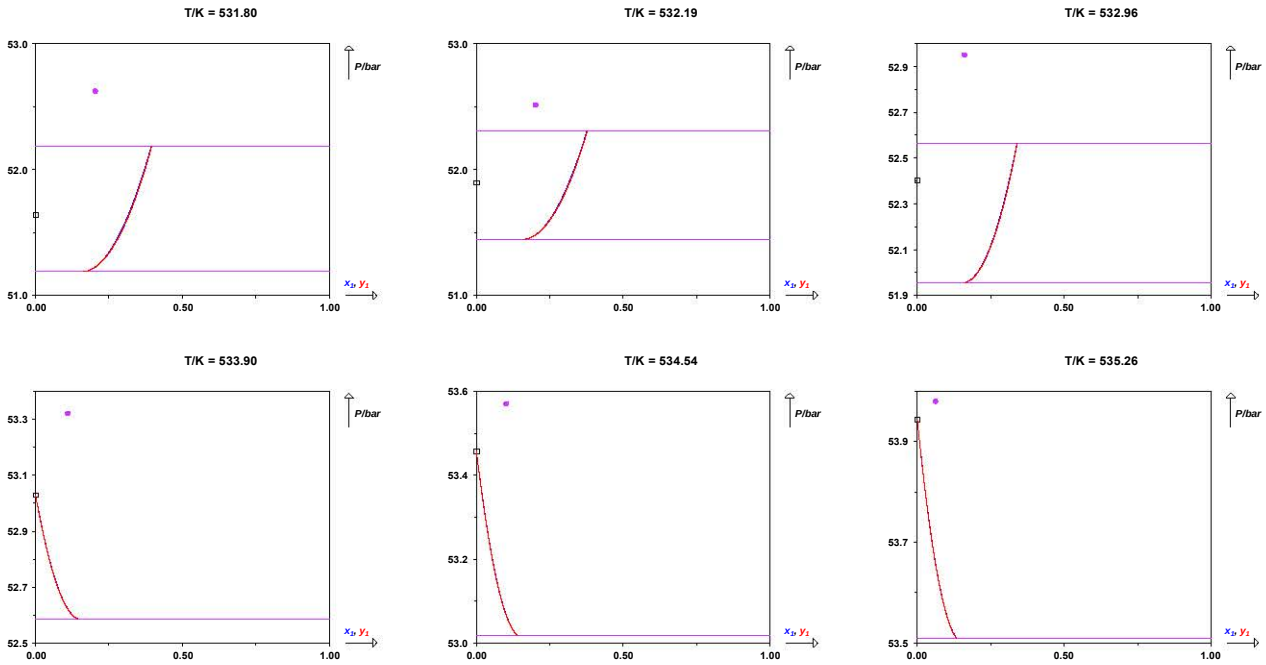



T/K = 529.98




T/K = 530.31




T/K = 531.80
T/K = 532.19
T/K = 532.96
T/K = 533.90
T/K = 534.54
T/K = 535.26
P/bar
x1, y1

## CHLOROFORM (1) + ETHYL ACETATE (2)

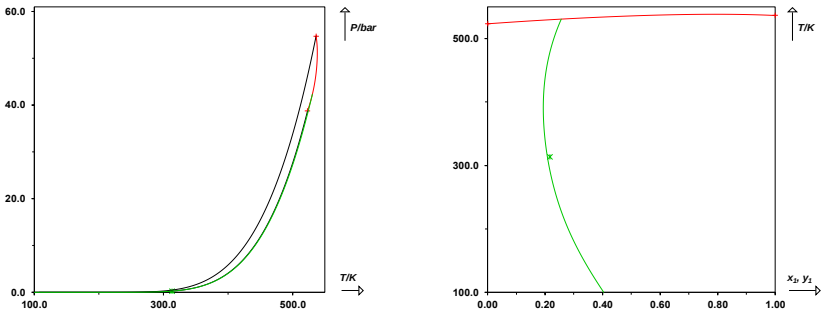
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 141-78-6 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | XEKOWRVHYACXOJ-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.40 | 523.30 |
| **$P_c$ / bar** | 54.72 | 38.80 |
| **ω** | 0.2220 | 0.3660 |

Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = -210
B/MPa = -530

*Deviations*
MAPE on x = 4.9 %
MAPE on y = 6.9 %
MAPE on $x_{az}$ = 2.0 %
MAPE on $P_{az}$ = 1.6 %
MAPE on $h^M$ = 10 %
MAPE on $c_P^M$ = 98 %



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**Isothermal phase equilibrium data**

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Ohta, Tatsuhiko - Asano, Hisashi - Nagata, Isamu, Thermodynamic study of complex formation in four binary liquid mixtures containing chloroform, Fluid Phase Equilibria 1-2 (1980) 105-114. doi:10.1016/0378-3812(80)80008-2

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2456 | 0.0680 | 0.0570 | |
| 0.2410 | 0.1680 | 0.1590 | |
| 0.2428 | 0.2160 | 0.2160 | AZEO |
| 0.2440 | 0.2360 | 0.2410 | |
| 0.2442 | 0.3050 | 0.3320 | |
| 0.2485 | 0.3740 | 0.4340 | |
| 0.2566 | 0.4260 | 0.5080 | |
| 0.2701 | 0.5160 | 0.6380 | |
| 0.2956 | 0.6150 | 0.7750 | |
| 0.3640 | 0.7900 | 0.9320 | |
| 0.3873 | 0.8390 | 0.9550 | |
| 0.4628 | 0.9660 | 0.9940 | |

Ohta, Tatsuhiko - Asano, Hisashi - Nagata, Isamu, Thermodynamic study of complex formation in four binary liquid mixtures containing chloroform, Fluid Phase Equilibria 1-2 (1980) 105-114. doi:10.1016/0378-3812(80)80008-2

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3774 | 0.0570 | 0.0490 |
| 0.3732 | 0.2480 | 0.2590 |
| 0.3752 | 0.2840 | 0.3050 |
| 0.3824 | 0.3860 | 0.4450 |
| 0.4025 | 0.4840 | 0.5860 |
| 0.4089 | 0.5140 | 0.6320 |
| 0.4494 | 0.6160 | 0.7580 |
| 0.5373 | 0.7870 | 0.9150 |
| 0.6430 | 0.9350 | 0.9880 |

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**Isobaric phase equilibrium data**

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Nagata, Isamu, Isobaric Vapor-Liquid Equilibria for the Ternary System Chloroform-Methanol-Ethyl Acetate., Journal of Chemical & Engineering Data 3 (1962) 367-373. doi:10.1021/je60014a013

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 350.65 | 0.0710 | 0.0640 |
| 350.75 | 0.1100 | 0.1020 |
| 350.85 | 0.1400 | 0.1340 |
| 350.65 | 0.2590 | 0.2700 |
| 350.45 | 0.3010 | 0.3230 |
| 349.95 | 0.3650 | 0.4080 |
| 349.15 | 0.4480 | 0.5220 |
| 348.25 | 0.5040 | 0.5960 |
| 347.85 | 0.5280 | 0.6280 |
| 346.65 | 0.5810 | 0.7000 |
| 344.95 | 0.6500 | 0.7800 |
| 343.55 | 0.7040 | 0.8390 |
| 342.05 | 0.7510 | 0.8790 |
| 340.85 | 0.7900 | 0.9100 |
| 338.75 | 0.8560 | 0.9500 |
| 336.85 | 0.9220 | 0.9780 |

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**Enthalpy of mixing**

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Ortega, J., Excess enthalpy. Trichloromethane-ethyl methanoate system, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1993)

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -253.80 | 0.0540 |
| -501.10 | 0.1129 |
| -800.50 | 0.1748 |
| -1110.1 | 0.2360 |
| -1361.5 | 0.2896 |
| -1575.1 | 0.3370 |
| -1777.9 | 0.3871 |
| -1912.8 | 0.4273 |
| -2029.2 | 0.4710 |
| -2098.6 | 0.5078 |
| -2145.3 | 0.5440 |
| -2159.2 | 0.5988 |
| -2123.3 | 0.6451 |
| -2047.9 | 0.6840 |
| -1923.1 | 0.7232 |
| -1772.3 | 0.7604 |
| -1609.5 | 0.7925 |
| -1403.6 | 0.8269 |
| -1165.0 | 0.8631 |
| -887.10 | 0.9010 |
| -596.40 | 0.9364 |
| -323.40 | 0.9656 |

Ohta, Tatsuhiko - Asano, Hisashi - Nagata, Isamu, Thermodynamic study of complex formation in four

binary liquid mixtures containing chloroform, Fluid Phase Equilibria 1-2 (1980) 105-114. doi:10.1016/0378-3812(80)80008-2

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -121.10 | 0.0240 |
| -391.40 | 0.0770 |
| -778.90 | 0.1560 |
| -1147.2 | 0.2380 |
| -1460.0 | 0.3170 |
| -1698.4 | 0.3910 |
| -1833.8 | 0.4460 |
| -1902.1 | 0.4860 |
| -1957.9 | 0.5500 |
| -1898.2 | 0.6240 |
| -1781.7 | 0.6820 |
| -1569.1 | 0.7480 |
| -1245.6 | 0.8180 |
| -1027.3 | 0.8580 |
| -633.10 | 0.9170 |
| -176.30 | 0.9770 |

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**Heat capacity of mixing**

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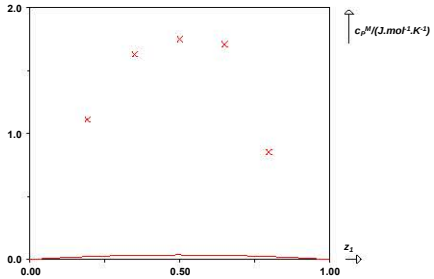
Fang, Wen-jun - Yu, Qing-sen - Lin, Rui-sen - Zong, Han-xing, Vapor heat capacities of some polar–polar binary systems, Thermochimica Acta (2000) 19-23. doi:10.1016/S0040-6031(99)00431-1

**T / K = 402.20**

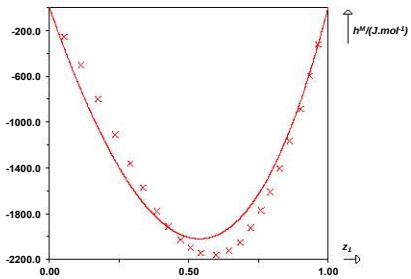
**P / bar = 1.013**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $z_1$ |
|---|---|
| 1.110 | 0.1929 |
| 1.630 | 0.3508 |
| 1.750 | 0.5020 |
| 1.710 | 0.6505 |
| 0.8500 | 0.7985 |

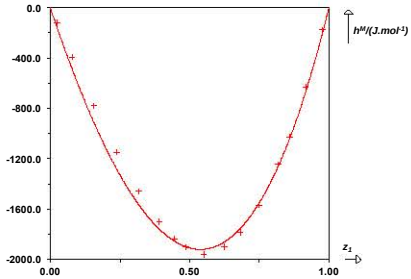
T/K = 402.20 - P/bar = 1.0130



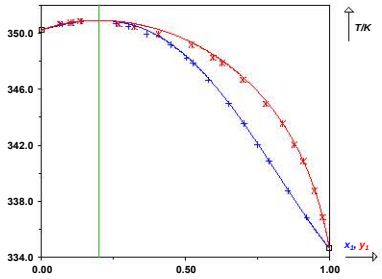

T/K = 298.15 - P/bar = 1.0100



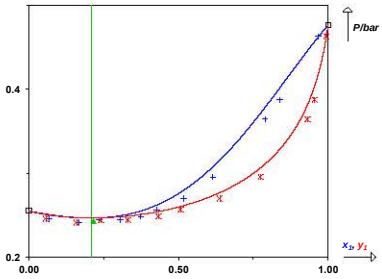

T/K = 308.15 - P/bar = 1.0132



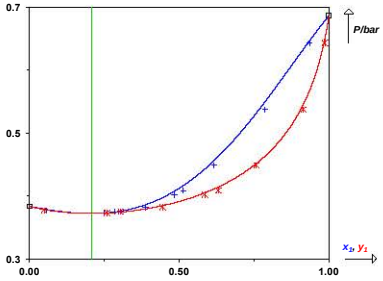

P/bar = 1.01330




T/K = 313.15




T/K = 323.15



## CHLOROFORM (1) + TETRAHYDROFURAN (2)

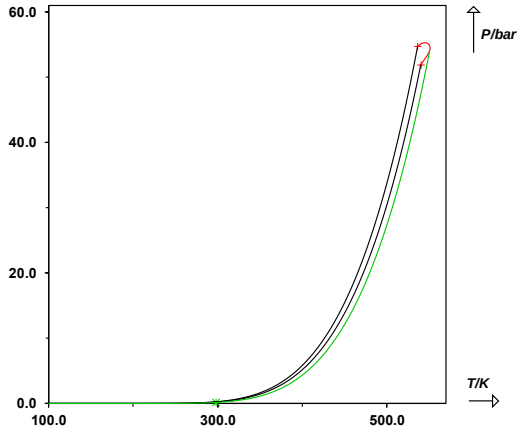
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 109-99-9 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | WYURNTSHIVDZCO-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.40 | 540.15 |
| **$P_c$ / bar** | 54.72 | 51.90 |
| **ω** | 0.2220 | 0.2250 |

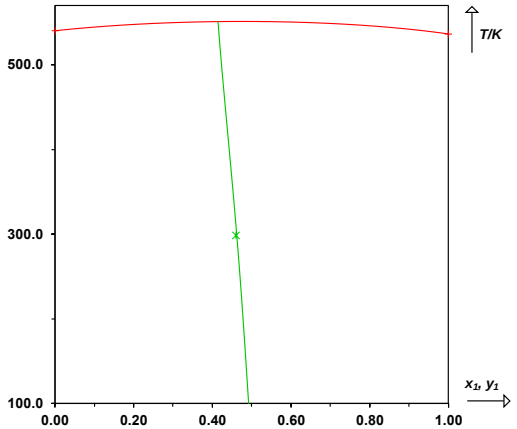
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = -349
B/MPa = -695

*Deviations*
MAPE on x = 5.1 %
MAPE on y = 4.1 %
MAPE on $x_{az}$ = 0.39 %
MAPE on $P_{az}$ = 0.10 %
MAPE on $h^M$ = 8.7 %
MAPE on $c_P^M$ = 29 %



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**Isothermal phase equilibrium data**

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Haase, R. - Tillmann, W., Negative values of the entropy of mixing, Z. Phys. Chem. Munich (1992) 209-216.

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2058 | 0.0716 | 0.0247 | |
| 0.1998 | 0.1050 | 0.0389 | |
| 0.1899 | 0.1648 | 0.0710 | |
| 0.1695 | 0.2910 | 0.1864 | |
| 0.1593 | 0.3808 | 0.3146 | |
| 0.1558 | 0.4600 | 0.4600 | AZEO |
| 0.1558 | 0.4612 | 0.4619 | |
| 0.1565 | 0.4887 | 0.5136 | |
| 0.1640 | 0.5791 | 0.6823 | |
| 0.1779 | 0.6573 | 0.8028 | |
| 0.2114 | 0.7901 | 0.9280 | |
| 0.2412 | 0.9006 | 0.9777 | |

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**Enthalpy of mixing**

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Suri, S.K. - Maheshwari, R.C., Molar excess enthalpies of arsenic tribromide + benzene, +cyclohexane, and +tetrachloromethane at 313.15 K, The Journal of Chemical Thermodynamics 12 (1980) 1191-1192. doi:10.1016/S0021-9614(80)80013-9

**T / K = 283.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -807.00 | 0.1005 |
| -1185.2 | 0.1507 |
| -1557.5 | 0.2008 |
| -1893.8 | 0.2510 |
| -2195.0 | 0.3011 |
| -2461.2 | 0.3512 |
| -2670.7 | 0.4012 |
| -2813.2 | 0.4513 |
| -2868.0 | 0.5013 |
| -2895.5 | 0.5513 |
| -2814.8 | 0.6012 |
| -2659.7 | 0.6512 |
| -2433.2 | 0.7011 |
| -2154.1 | 0.7510 |
| -1811.2 | 0.8008 |
| -1419.7 | 0.8507 |
| -981.30 | 0.9005 |

van Ness, H.C. - Abbott, M.M., Excess enthalpy. Trichloromethane (chloroform)-oxolane (tetrahydrofuran) system, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1974)

**T / K = 303.15**

**P / bar = 2.100**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -115.90 | 0.0138 |
| -213.30 | 0.0255 |
| -326.40 | 0.0393 |
| -573.40 | 0.0696 |
| -800.80 | 0.0987 |
| -990.90 | 0.1238 |
| -1294.7 | 0.1656 |
| -1618.4 | 0.2138 |
| -1887.5 | 0.2578 |
| -2099.7 | 0.2965 |
| -2256.5 | 0.3288 |
| -2419.0 | 0.3680 |
| -2548.6 | 0.4072 |
| -2639.7 | 0.4453 |
| -2697.6 | 0.4867 |
| -2708.8 | 0.5307 |
| -2678.5 | 0.5704 |
| -2617.5 | 0.6039 |
| -2513.1 | 0.6413 |
| -2355.9 | 0.6824 |
| -2145.0 | 0.7261 |
| -1989.5 | 0.7535 |
| -1779.1 | 0.7871 |
| -1624.8 | 0.8096 |
| -1428.6 | 0.8366 |
| -1261.4 | 0.8583 |
| -1031.1 | 0.8866 |
| -857.40 | 0.9072 |
| -619.70 | 0.9341 |
| -419.20 | 0.9560 |
| -234.00 | 0.9756 |
| -141.20 | 0.9853 |
| -69.50 | 0.9927 |

van Ness, H.C. - Abbott, M.M., Excess enthalpy. Trichloromethane (chloroform)-oxolane (tetrahydrofuran) system, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1974)

**T / K = 318.15**

**P / bar = 2.100**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -117.30 | 0.0144 |
| -316.80 | 0.0392 |

| | |
|---|---|
| -546.80 | 0.0684 |
| -777.50 | 0.0988 |
| -997.50 | 0.1286 |
| -1256.2 | 0.1658 |
| -1531.6 | 0.2081 |
| -1733.4 | 0.2417 |
| -1952.0 | 0.2819 |
| -2097.3 | 0.3118 |
| -2200.6 | 0.3355 |
| -2313.1 | 0.3644 |
| -2406.8 | 0.3934 |
| -2479.9 | 0.4207 |
| -2541.8 | 0.4523 |
| -2571.9 | 0.5633 |
| -2526.1 | 0.5934 |
| -2440.9 | 0.6293 |
| -2317.9 | 0.6669 |
| -2159.7 | 0.7048 |
| -1965.0 | 0.7435 |
| -1726.9 | 0.7842 |
| -1479.1 | 0.8217 |
| -1268.7 | 0.8510 |
| -1120.6 | 0.8704 |
| -898.50 | 0.8983 |
| -679.20 | 0.9246 |
| -474.10 | 0.9481 |
| -276.70 | 0.9702 |
| -109.60 | 0.9883 |

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**Heat capacity of mixing**

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Fenclova, D. - Dohnal, V. - Perez-Casas, S. - Frigolet, C. - Costas, M., Excess heat capacities, excess enthalpies, and excess volumes of trichloromethane + some oxygenated solvents or + the corresponding homomorphic hydrocarbons at 298.15 K, ELDATA Int. Electron. J. Phys. Chem. Data 3 (1995) 217-237.

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

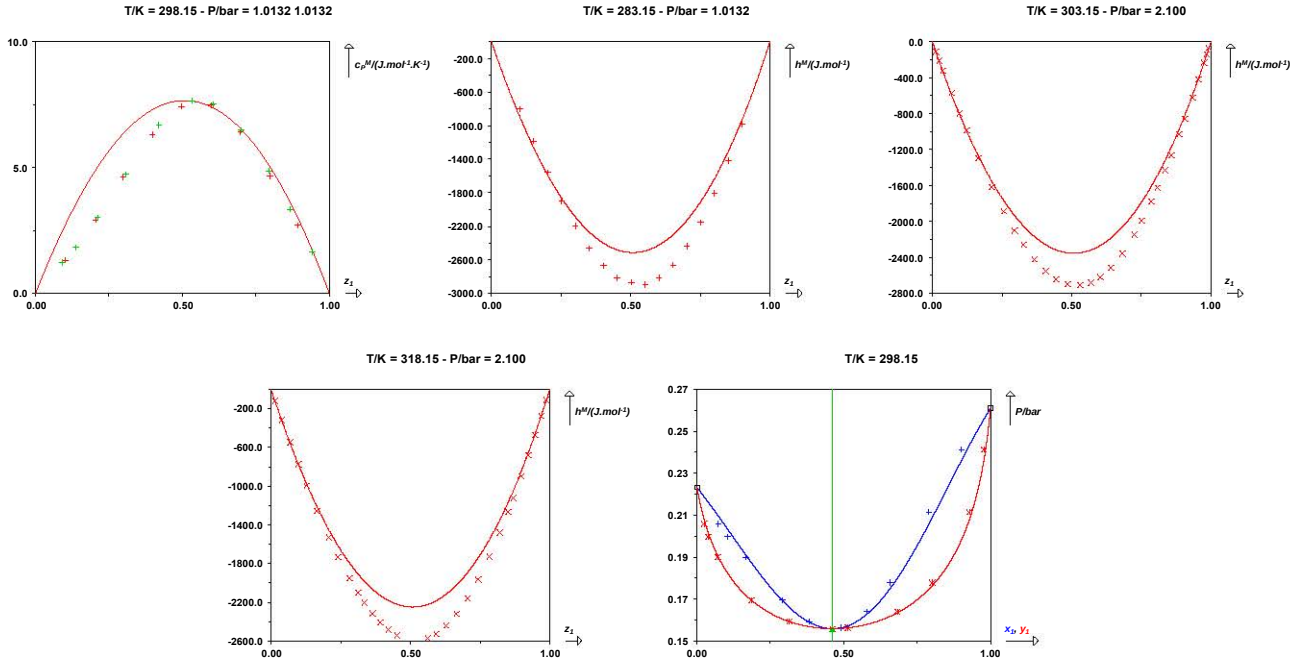
| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 1.330 | 0.1012 |
| 2.930 | 0.2036 |
| 4.610 | 0.2981 |
| 6.310 | 0.3969 |
| 7.430 | 0.4968 |
| 7.480 | 0.5992 |
| 6.400 | 0.6980 |
| 4.650 | 0.7981 |
| 2.710 | 0.8926 |

Inglese, Americo - Castagnolo, Maurizio - Dell'atti, Angelo - de Giglio, Angelo, Excess heat capacities and excess volumes of binary liquid mixtures of chloroform with cyclic ethers at 298.15 K, Thermochimica Acta 1 (1981) 77-87. doi:10.1016/0040-6031(81)80273-0

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 1.231 | 0.0904 |
| 1.814 | 0.1374 |
| 3.000 | 0.2112 |
| 4.722 | 0.3066 |
| 6.687 | 0.4195 |
| 7.655 | 0.5321 |
| 7.512 | 0.6052 |
| 6.480 | 0.6994 |
| 4.861 | 0.7934 |
| 3.341 | 0.8668 |
| 1.652 | 0.9413 |


T/K = 298.15 - P/bar = 1.0132 1.0132
$c_p^M$/(J.mol$^{-1}$.K$^{-1}$)
10.0
5.0
0.0
0.00
0.50
1.00
$z_1$
T/K = 283.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
-200.0
-600.0
-1000.0
-1400.0
-1800.0
-2200.0
-2600.0
-3000.0
T/K = 303.15 - P/bar = 2.100
$h^M$/(J.mol$^{-1}$)
0.0
-400.0
-800.0
-1200.0
-1600.0
-2000.0
-2400.0
-2800.0
T/K = 318.15 - P/bar = 2.100
$h^M$/(J.mol$^{-1}$)
T/K = 298.15
P/bar
0.27
0.25
0.23
0.21
0.19
0.17
0.15
$x_1$, $y_1$

## CHLOROFORM (1) + DI-n-PROPYL ETHER (2)

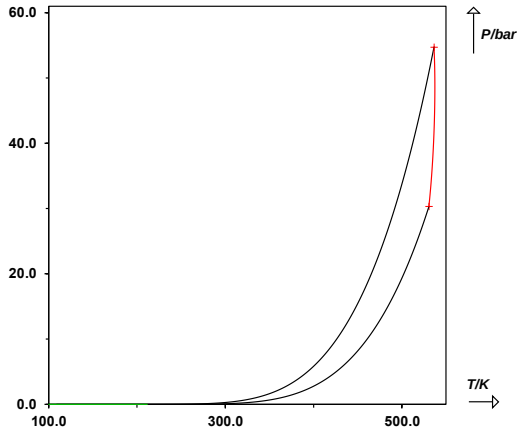
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 111-43-3 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | POLCUAVZOMRGSN-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.40 | 530.60 |
| **$P_c$ / bar** | 54.72 | 30.28 |
| **ω** | 0.2220 | 0.3690 |

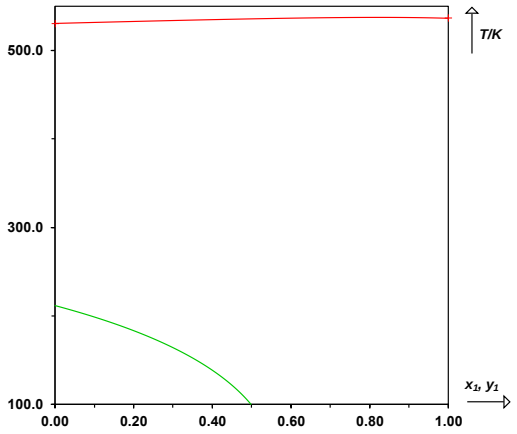
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = -101
B/MPa = -385

*Deviations*
MAPE on x = 9.9 %
MAPE on y = 11 %
MAPE on $h^M$ = 19 %
MAPE on $c_P^M$ = 85 %



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**Isobaric phase equilibrium data**

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Chevalier, J.L., Systèmes binaires chloroforme-éthers aliphatiques - III. — Équilibres liquide-vapeur, Journal de Chimie Physique et de Physico-Chimie Biologique (1969) 1457-1466.

**P / bar = 0.5333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 342.05 | 0.0510 | 0.0860 |
| 340.00 | 0.1580 | 0.2460 |
| 338.05 | 0.2400 | 0.3810 |
| 336.35 | 0.3050 | 0.4690 |
| 335.10 | 0.3460 | 0.5290 |
| 333.10 | 0.4240 | 0.6200 |
| 329.95 | 0.5210 | 0.7300 |
| 327.70 | 0.5900 | 0.7960 |
| 325.55 | 0.6580 | 0.8530 |
| 323.10 | 0.7300 | 0.9100 |
| 321.35 | 0.7810 | 0.9390 |
| 319.90 | 0.8350 | 0.9600 |

Chevalier, J.L., Systèmes binaires chloroforme-éthers aliphatiques - III. — Équilibres liquide-vapeur, Journal de Chimie Physique et de Physico-Chimie Biologique (1969) 1457-1466.

**P / bar = 0.8666**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 354.55 | 0.1330 | 0.2070 |
| 353.10 | 0.2020 | 0.3020 |
| 351.25 | 0.2730 | 0.4080 |
| 349.55 | 0.3450 | 0.5050 |
| 347.40 | 0.4240 | 0.6050 |
| 344.95 | 0.4970 | 0.6920 |
| 342.20 | 0.5770 | 0.7720 |
| 339.55 | 0.6460 | 0.8330 |
| 337.35 | 0.7150 | 0.8800 |
| 336.40 | 0.7390 | 0.8940 |
| 335.00 | 0.7800 | 0.9250 |
| 332.25 | 0.8800 | 0.9690 |
| 330.70 | 0.9350 | 0.9890 |

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**Enthalpy of mixing**

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Beath, L.A. - Williamson, A.G., Thermodynamics of ether solutions I. Enthalpies of mixing of ethers with carbon tetrachloride and with chloroform, The Journal of Chemical Thermodynamics 1 (1969) 51-57. doi:10.1016/0021-9614(69)90036-6

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -760.00 | 0.1197 |
| -1208.0 | 0.2145 |
| -1549.0 | 0.3040 |
| -1880.0 | 0.4120 |
| -1942.0 | 0.5070 |
| -1861.0 | 0.5939 |
| -1611.0 | 0.6909 |
| -1199.0 | 0.7942 |
| -669.00 | 0.8918 |

Becker, F. - Kiefer, M., Heat of mixing and formation of compounds in binary liquid systems. III. Ether-chloroform systems, Z. Naturforsch. Sec. A (1971) 1040-1046.

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -164.12 | 0.0250 |
| -323.22 | 0.0500 |
| -477.71 | 0.0750 |
| -625.51 | 0.1000 |
| -770.37 | 0.1250 |
| -907.28 | 0.1500 |
| -1037.5 | 0.1750 |
| -1162.3 | 0.2000 |
| -1278.2 | 0.2250 |
| -1387.9 | 0.2500 |
| -1488.4 | 0.2750 |
| -1580.1 | 0.3000 |
| -1663.4 | 0.3250 |
| -1737.1 | 0.3500 |
| -1800.7 | 0.3750 |
| -1853.9 | 0.4000 |
| -1895.8 | 0.4250 |
| -1926.8 | 0.4500 |
| -1945.6 | 0.4750 |
| -1953.1 | 0.5000 |
| -1949.4 | 0.5250 |
| -1933.0 | 0.5500 |
| -1905.0 | 0.5750 |
| -1865.2 | 0.6000 |
| -1812.0 | 0.6250 |
| -1742.5 | 0.6500 |
| -1668.0 | 0.6750 |
| -1585.5 | 0.7000 |
| -1493.0 | 0.7250 |
| -1392.1 | 0.7500 |

| | |
|---|---|
| -1282.0 | 0.7750 |
| -1164.3 | 0.8000 |
| -1039.2 | 0.8250 |
| -906.86 | 0.8500 |
| -768.28 | 0.8750 |
| -624.25 | 0.9000 |
| -475.62 | 0.9250 |
| -321.55 | 0.9500 |
| -162.87 | 0.9750 |

Becker, F. - Kiefer, M., Kontinuierliche Bestimmung von Mischungswärmen durch isotherme Enthalpietitration, Zeitschrift für Naturforschung A 1 (1969) doi:10.1515/zna-1969-0103

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -164.12 | 0.0250 |
| -323.22 | 0.0500 |
| -477.30 | 0.0749 |
| -769.12 | 0.1249 |
| -906.02 | 0.1498 |
| -1036.7 | 0.1748 |
| -1160.6 | 0.1997 |
| -1276.6 | 0.2246 |
| -1385.8 | 0.2495 |
| -1485.9 | 0.2744 |
| -1578.0 | 0.2994 |
| -1660.9 | 0.3243 |
| -1734.6 | 0.3492 |
| -1798.2 | 0.3740 |
| -1851.4 | 0.3989 |
| -1893.7 | 0.4238 |
| -1925.1 | 0.4487 |
| -1944.8 | 0.4736 |
| -1953.1 | 0.4986 |
| -1949.4 | 0.5236 |
| -1933.5 | 0.5486 |
| -1906.7 | 0.5736 |
| -1867.3 | 0.5968 |
| -1671.0 | 0.6759 |
| -1588.9 | 0.7009 |
| -1496.4 | 0.7258 |
| -1395.0 | 0.7507 |
| -1284.9 | 0.7756 |
| -1166.9 | 0.8005 |
| -1041.3 | 0.8254 |
| -769.95 | 0.8753 |
| -625.51 | 0.9002 |
| -476.04 | 0.9251 |
| -321.55 | 0.9500 |
| -162.87 | 0.9750 |

Chevalier, Jean-Louis - Bares, Daniel, Systèmes binaires chloroforme-éthers aliphatiques - I. — Chaleurs de mélange à 25 °C, Journal de Chimie Physique (1969) 1448-1452. doi:10.1051/jcp/196966s21448

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -1256.0 | 0.2340 |
| -1611.9 | 0.3250 |
| -1925.9 | 0.4770 |
| -1942.7 | 0.4970 |
| -1905.0 | 0.5150 |
| -1900.8 | 0.5340 |
| -1729.2 | 0.6470 |
| -1017.4 | 0.8260 |
| -695.01 | 0.8890 |
| -452.17 | 0.9260 |

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**Heat capacity of mixing**

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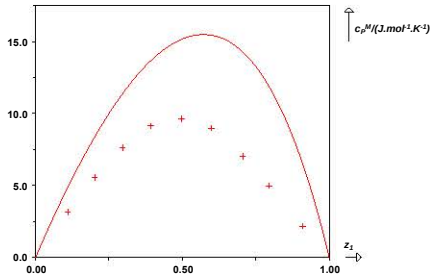
Fenclova, D. - Dohnal, V. - Perez-Casas, S. - Frigolet, C. - Costas, M., Excess heat capacities, excess enthalpies, and excess volumes of trichloromethane + some oxygenated solvents or + the corresponding homomorphic hydrocarbons at 298.15 K, ELDATA Int. Electron. J. Phys. Chem. Data 3 (1995) 217-237.

**T / K =** **298.15**

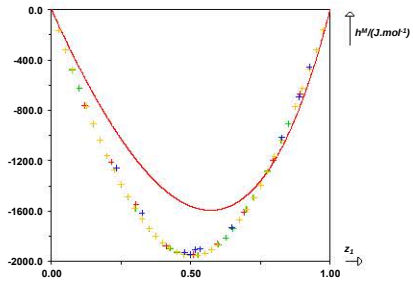
**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 3.160 | 0.1094 |
| 5.560 | 0.2014 |
| 7.620 | 0.2950 |
| 9.130 | 0.3931 |
| 9.630 | 0.4965 |
| 8.990 | 0.5968 |
| 7.030 | 0.7049 |
| 4.990 | 0.7945 |
| 2.190 | 0.9094 |

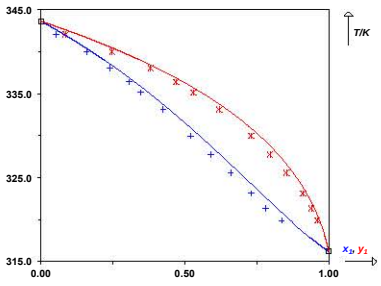
T/K = 298.15 - P/bar = 1.0132



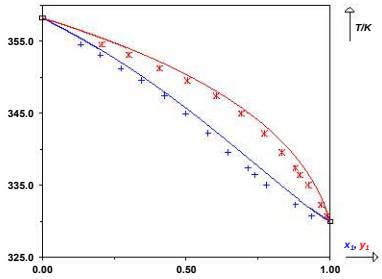

T/K = 298.15 - P/bar = 1.0132 1.0132 1.0132 1.0132




P/bar = 0.53329




P/bar = 0.86660



## METHYL ACETATE (1) + CHLOROFORM (2)

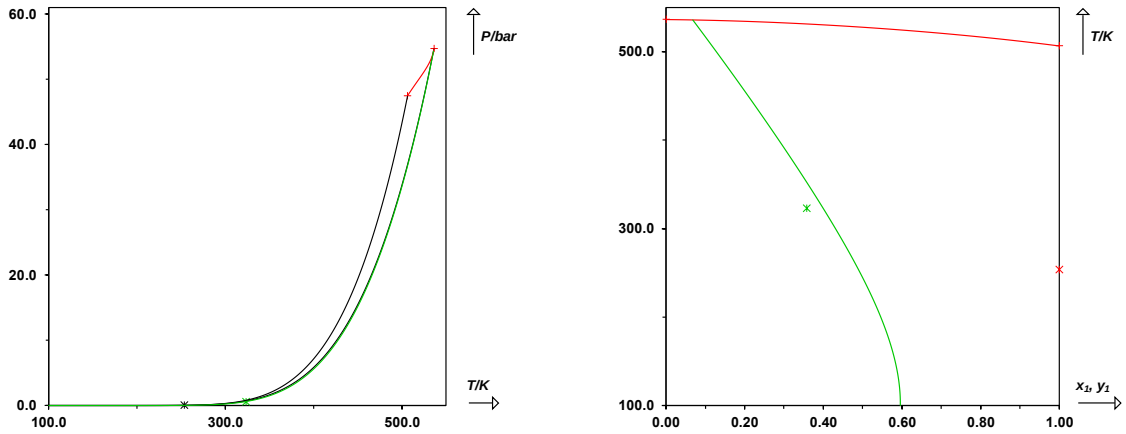
| | | |
|---|---|---|
| **CAS** | 79-20-9 | 67-66-3 |
| **InChiKey** | KXKVLQRXCPHEJC-UHFFFAOYSA-N | HEDRZPFGACZZDS-UHFFFAOYSA-N |
| **$T_c$ / K** | 506.55 | 536.40 |
| **$P_c$ / bar** | 47.50 | 54.72 |
| **ω** | 0.3310 | 0.2220 |

Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = -180
B/MPa = -365

*Deviations*
MAPE on x = 7.8 %
MAPE on y = 8.9 %
MAPE on $x_{az}$ = 9.2 %
MAPE on $P_{az}$ = 0.74 %
MAPE on $h^M$ = 22 %
MAPE on $c_P^M$ = 48 %



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**Isothermal phase equilibrium data**

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Ohta, Tatsuhiko - Asano, Hisashi - Nagata, Isamu, Thermodynamic study of complex formation in four binary liquid mixtures containing chloroform, Fluid Phase Equilibria 1-2 (1980) 105-114. doi:10.1016/0378-3812(80)80008-2

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4610 | 0.0590 | 0.0320 |
| 0.4398 | 0.1320 | 0.0830 |
| 0.4314 | 0.1640 | 0.1170 |
| 0.4190 | 0.2250 | 0.1890 |
| 0.4062 | 0.3560 | 0.3460 |
| 0.4080 | 0.3920 | 0.4040 |
| 0.4113 | 0.4470 | 0.4800 |
| 0.4132 | 0.4730 | 0.5170 |
| 0.4178 | 0.5050 | 0.5650 |
| 0.4276 | 0.5670 | 0.6480 |
| 0.4361 | 0.6040 | 0.6910 |
| 0.4624 | 0.7280 | 0.8220 |
| 0.4673 | 0.7410 | 0.8330 |
| 0.4800 | 0.7880 | 0.8720 |
| 0.4930 | 0.8410 | 0.9080 |
| 0.5277 | 0.9460 | 0.9730 |

Nagata, Isamu - Hayashida, Hiromichi, Vapor-Liquid Equilibrium Data For The Ternary Systems: Methyl Acetate-2-Propanol-Benzene And Methyl Acetate-Chloroform-Benzene, Journal of Chemical Engineering of Japan 2 (1970) 161-166. doi:10.1252/jcej.3.161

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.6670 | 0.0640 | 0.0400 | |
| 0.6426 | 0.1340 | 0.0890 | |
| 0.6294 | 0.1780 | 0.1310 | |
| 0.6074 | 0.2580 | 0.2200 | |
| 0.6001 | 0.3140 | 0.3080 | |
| 0.5988 | 0.3560 | 0.3540 | |
| 0.5988 | 0.3570 | 0.3570 | AZEO |
| 0.6008 | 0.3940 | 0.4050 | |
| 0.6050 | 0.4380 | 0.4700 | |
| 0.6108 | 0.4770 | 0.5260 | |
| 0.6204 | 0.5250 | 0.5840 | |
| 0.6448 | 0.6120 | 0.6980 | |
| 0.6773 | 0.7070 | 0.7960 | |
| 0.6837 | 0.7260 | 0.8140 | |
| 0.6906 | 0.7470 | 0.8350 | |
| 0.7135 | 0.8150 | 0.8860 | |
| 0.7625 | 0.9350 | 0.9660 | |

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**Enthalpy of mixing**

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Ortega, J. - Placido, J., Excess enthalpies of 14 binary liquid mixtures of trichloromethane + methyl n-alkanoates (C3-C16) at 298.15 K, ELDATA Int. Electron. J. Phys. Chem. Data 2 (1996) 85-96.

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -456.50 | 0.0613 |
| -802.90 | 0.1147 |
| -1119.6 | 0.1678 |
| -1368.4 | 0.2177 |
| -1560.3 | 0.2656 |
| -1705.9 | 0.3132 |
| -1804.8 | 0.3602 |
| -1859.2 | 0.4059 |
| -1876.9 | 0.4504 |
| -1860.2 | 0.4944 |
| -1781.0 | 0.5413 |
| -1660.9 | 0.5868 |
| -1504.4 | 0.6391 |
| -1303.1 | 0.6945 |
| -1089.7 | 0.7527 |
| -837.60 | 0.8126 |
| -588.10 | 0.8677 |
| -349.20 | 0.9194 |
| -185.30 | 0.9591 |

Ohta, Tatsuhiko - Asano, Hisashi - Nagata, Isamu, Thermodynamic study of complex formation in four binary liquid mixtures containing chloroform, Fluid Phase Equilibria 1-2 (1980) 105-114. doi:10.1016/0378-3812(80)80008-2

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -125.50 | 0.0170 |
| -330.80 | 0.0470 |
| -731.70 | 0.1130 |
| -1075.9 | 0.1810 |
| -1304.5 | 0.2400 |
| -1475.8 | 0.3010 |
| -1574.8 | 0.3620 |
| -1609.8 | 0.4130 |
| -1593.4 | 0.4750 |
| -1551.4 | 0.5200 |

| | |
|---|---|
| -1485.6 | 0.5610 |
| -1369.2 | 0.6160 |
| -1104.0 | 0.7100 |
| -873.00 | 0.7780 |
| -591.00 | 0.8530 |
| -374.80 | 0.9090 |
| -148.60 | 0.9650 |

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**Heat capacity of mixing**

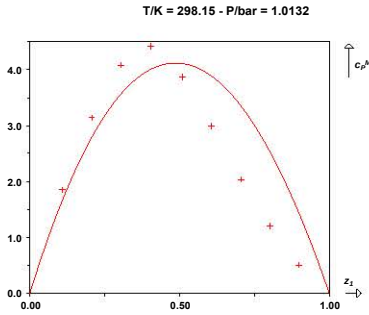
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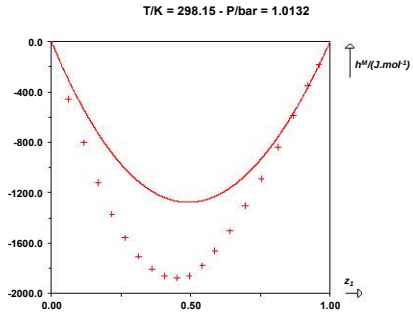
Fenclova, D. - Dohnal, V. - Perez-Casas, S. - Frigolet, C. - Costas, M., Excess heat capacities, excess enthalpies, and excess volumes of trichloromethane + some oxygenated solvents or + the corresponding homomorphic hydrocarbons at 298.15 K, ELDATA Int. Electron. J. Phys. Chem. Data 3 (1995) 217-237.

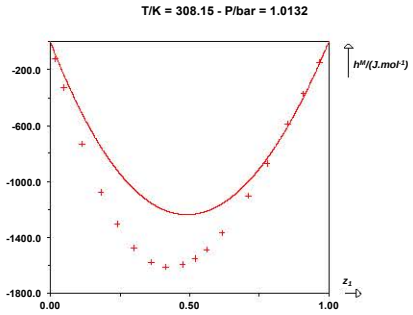
**T / K =** **298.15**

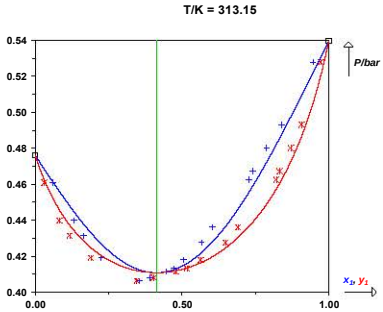
**P / bar =** **UNKNOWN (1.0132)**

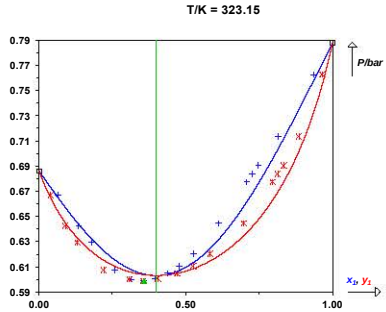
| $c_P^M$ / $J.mol^{-1}.K^{-1}$ | $x_1$ |
|---|---|
| 1.850 | 0.1081 |
| 3.140 | 0.2064 |
| 4.080 | 0.3043 |
| 4.420 | 0.4048 |
| 3.870 | 0.5093 |
| 2.990 | 0.6069 |
| 2.040 | 0.7046 |
| 1.210 | 0.8023 |
| 0.5100 | 0.8981 |


T/K = 298.15 - P/bar = 1.0132
$c_p^M/(J.mol^{-1}.K^{-1})$
$z_1$


T/K = 298.15 - P/bar = 1.0132
$h^M/(J.mol^{-1})$
$z_1$


T/K = 308.15 - P/bar = 1.0132
$h^M/(J.mol^{-1})$
$z_1$


T/K = 313.15
P/bar
$x_1, y_1$


T/K = 323.15
P/bar
$x_1, y_1$

## CYCLOPENTANONE (1) + 1,1,2,2-TETRACHLOROETHANE (2)

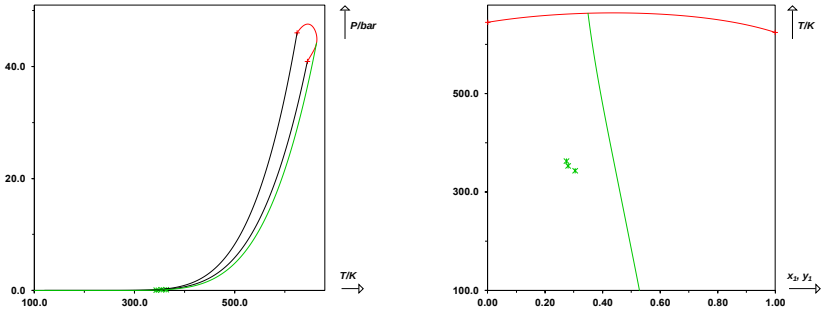
| | | |
|---|---|---|
| **CAS** | 120-92-3 | 79-34-5 |
| **InChiKey** | BGTOWKSIORTVQH-UHFFFAOYSA-N | QPFMBZIOSGYJDE-UHFFFAOYSA-N |
| **$T_c$ / K** | 624.50 | 645.00 |
| **$P_c$ / bar** | 46.00 | 40.90 |
| **ω** | 0.2880 | 0.2470 |

Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = -393
B/MPa = -518

*Deviations*
MAPE on x = 39 %
MAPE on y = 34 %
MAPE on $x_{az}$ = 38 %
MAPE on $P_{az}$ = 6.6 %
MAPE on $h^M$ = 8.6 %



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**Isothermal phase equilibrium data**

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Teodorescu, Mariana - Barhala, Alexandru - Dragoescu, Dana, Isothermal (vapour+liquid) equilibria for the binary (cyclopentanone or cyclohexanone with 1,1,2,2-tetrachloroethane) systems at temperatures of (343.15, 353.15, and 363.15)K, The Journal of Chemical Thermodynamics 11 (2006) 1432-1437. doi:10.1016/j.jct.2006.01.010

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.0717 | 0.0648 | 0.0497 | |
| 0.0697 | 0.1045 | 0.0748 | |
| 0.0675 | 0.1580 | 0.1266 | |
| 0.0663 | 0.2169 | 0.1889 | |
| 0.0656 | 0.2763 | 0.2718 | |
| 0.0654 | 0.3038 | 0.3038 | AZEO |
| 0.0664 | 0.3402 | 0.3892 | |
| 0.0679 | 0.4222 | 0.5284 | |
| 0.0708 | 0.4803 | 0.6260 | |
| 0.0752 | 0.5527 | 0.7244 | |
| 0.0816 | 0.6260 | 0.8093 | |
| 0.0880 | 0.6960 | 0.8796 | |
| 0.0972 | 0.7695 | 0.9312 | |
| 0.1073 | 0.8507 | 0.9648 | |
| 0.1185 | 0.9149 | 0.9851 | |
| 0.1256 | 0.9658 | 0.9960 | |
| 0.1283 | 0.9841 | 0.9969 | |

Teodorescu, Mariana - Barhala, Alexandru - Dragoescu, Dana, Isothermal (vapour+liquid) equilibria for the binary (cyclopentanone or cyclohexanone with 1,1,2,2-tetrachloroethane) systems at temperatures of (343.15, 353.15, and 363.15)K, The Journal of Chemical Thermodynamics 11 (2006) 1432-1437. doi:10.1016/j.jct.2006.01.010

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1067 | 0.0623 | 0.0497 | |
| 0.1040 | 0.1144 | 0.0848 | |
| 0.1032 | 0.1580 | 0.1266 | |
| 0.1017 | 0.2169 | 0.1959 | |
| 0.1018 | 0.2741 | 0.2786 | |
| 0.1007 | 0.2806 | 0.2806 | AZEO |
| 0.1023 | 0.3446 | 0.3892 | |
| 0.1049 | 0.4222 | 0.5284 | |
| 0.1092 | 0.4842 | 0.6225 | |
| 0.1169 | 0.5582 | 0.7244 | |
| 0.1253 | 0.6260 | 0.8107 | |
| 0.1344 | 0.6943 | 0.8709 | |
| 0.1478 | 0.7753 | 0.9238 | |
| 0.1626 | 0.8520 | 0.9568 | |
| 0.1772 | 0.9194 | 0.9832 | |
| 0.1888 | 0.9658 | 0.9951 | |

Teodorescu, Mariana - Barhala, Alexandru - Dragoescu, Dana, Isothermal (vapour+liquid) equilibria for the binary (cyclopentanone or cyclohexanone with 1,1,2,2-tetrachloroethane) systems at temperatures of (343.15, 353.15, and 363.15)K, The Journal of Chemical Thermodynamics 11 (2006) 1432-1437. doi:10.1016/j.jct.2006.01.010

**T / K = 363.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1613 | 0.0623 | 0.0522 | |
| 0.1574 | 0.1144 | 0.0897 | |
| 0.1560 | 0.1556 | 0.1314 | |
| 0.1538 | 0.2169 | 0.1959 | |
| 0.1536 | 0.2741 | 0.2853 | |
| 0.1527 | 0.2746 | 0.2746 | AZEO |
| 0.1553 | 0.3440 | 0.3912 | |
| 0.1597 | 0.4243 | 0.5208 | |
| 0.1658 | 0.4803 | 0.6225 | |
| 0.1762 | 0.5527 | 0.7244 | |
| 0.1880 | 0.6260 | 0.8079 | |
| 0.2016 | 0.6927 | 0.8659 | |
| 0.2221 | 0.7783 | 0.9249 | |
| 0.2409 | 0.8520 | 0.9588 | |
| 0.2609 | 0.9149 | 0.9832 | |
| 0.2781 | 0.9658 | 0.9951 | |
| 0.2840 | 0.9841 | 0.9969 | |

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**Enthalpy of mixing**

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Pathak, Gopal - Tripathi, A.D. - Phalgune, U.D. - Pradhan, S.D., Enthalpies of mixing of tetrachloroethane with furan, methylfuran, tetrahydrofuran, cyclopentanone and 1,4-dioxane, Thermochimica Acta (1995) 109-115. doi:10.1016/0040-6031(94)02236-H

**T / K = 303.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -657.00 | 0.0697 |
| -1668.0 | 0.2000 |
| -2188.0 | 0.2819 |
| -2784.0 | 0.4375 |
| -2767.0 | 0.5566 |
| -2681.0 | 0.6132 |
| -2360.0 | 0.6888 |

| | |
|---|---|
| -1659.0 | 0.7979 |
| -1084.0 | 0.8685 |
| -796.00 | 0.9086 |
| -420.00 | 0.9518 |

Chadha, Renu - Tripathi, Atri D., Excess Molar Enthalpies of 1,1,2,2-Tetrachloroethane + 2-Methylfuran, + Tetrahydrofuran, + 1,4-Dioxane, and + Cyclopentanone at 308.15 and 318.15 K, Journal of Chemical & Engineering Data 3 (1995) 645-646. doi:10.1021/je00019a024

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

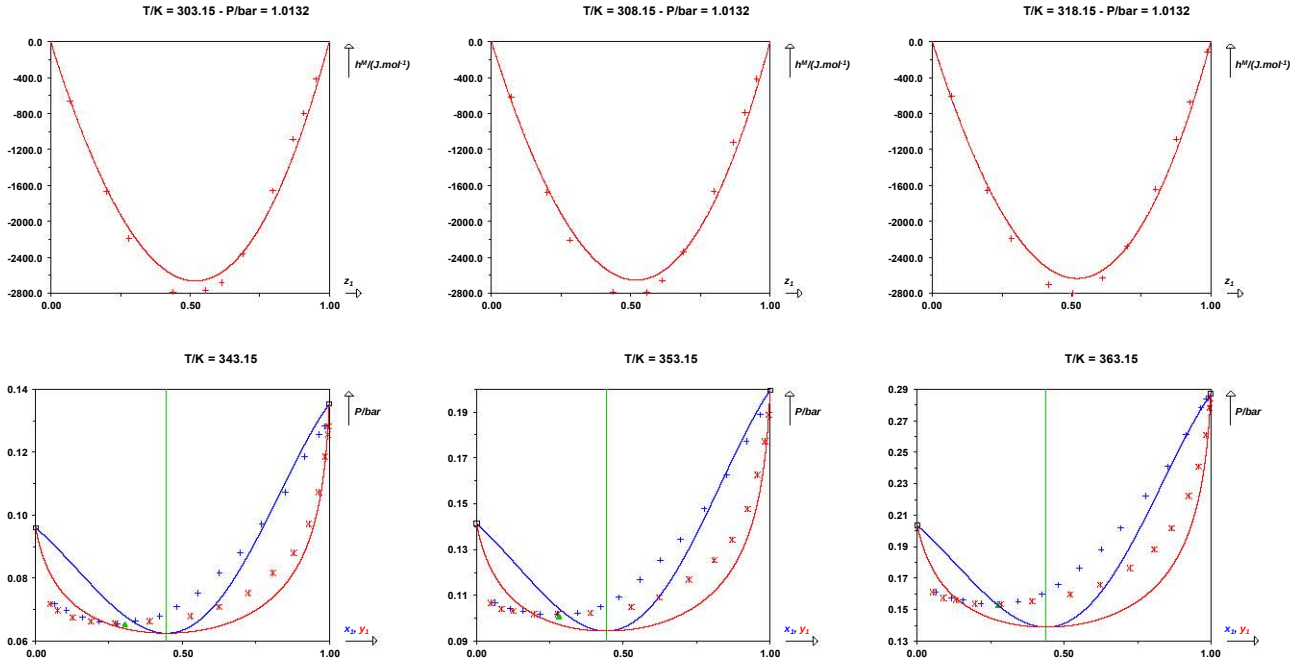
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -616.00 | 0.0697 |
| -1675.0 | 0.2000 |
| -2205.0 | 0.2819 |
| -2785.0 | 0.4375 |
| -2788.0 | 0.5566 |
| -2652.0 | 0.6132 |
| -2341.0 | 0.6888 |
| -1666.0 | 0.7979 |
| -1121.0 | 0.8685 |
| -787.00 | 0.9086 |
| -416.00 | 0.9518 |

Chadha, Renu - Tripathi, Atri D., Excess Molar Enthalpies of 1,1,2,2-Tetrachloroethane + 2-Methylfuran, + Tetrahydrofuran, + 1,4-Dioxane, and + Cyclopentanone at 308.15 and 318.15 K, Journal of Chemical & Engineering Data 3 (1995) 645-646. doi:10.1021/je00019a024

**T / K = 318.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -607.00 | 0.0682 |
| -1654.0 | 0.1986 |
| -2189.0 | 0.2835 |
| -2705.0 | 0.4167 |
| -2796.0 | 0.5045 |
| -2631.0 | 0.6112 |
| -2275.0 | 0.6995 |
| -1641.0 | 0.8025 |
| -1082.0 | 0.8752 |
| -675.00 | 0.9235 |
| -119.00 | 0.9867 |


T/K = 303.15 - P/bar = 1.0132
T/K = 308.15 - P/bar = 1.0132
T/K = 318.15 - P/bar = 1.0132
T/K = 343.15
T/K = 353.15
T/K = 363.15
P/bar
x1, y1
z1

## ETHYL ACETATE (1) + 1,1,2,2-TETRACHLOROETHANE (2)

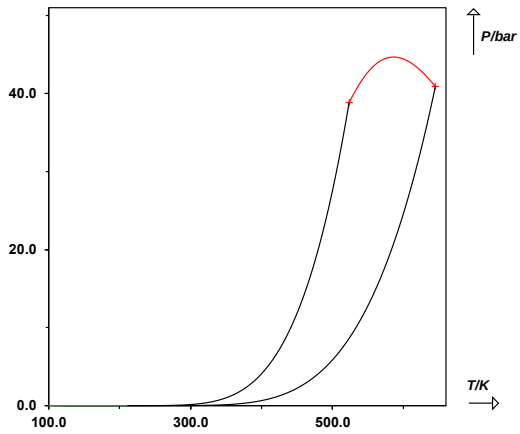
| | | |
|---|---|---|
| **CAS** | 141-78-6 | 79-34-5 |
| **InChiKey** | XEKOWRVHYACXOJ-UHFFFAOYSA-N | QPFMBZIOSGYJDE-UHFFFAOYSA-N |
| **$T_c$ / K** | 523.30 | 645.00 |
| **$P_c$ / bar** | 38.80 | 40.90 |
| **ω** | 0.3660 | 0.2470 |

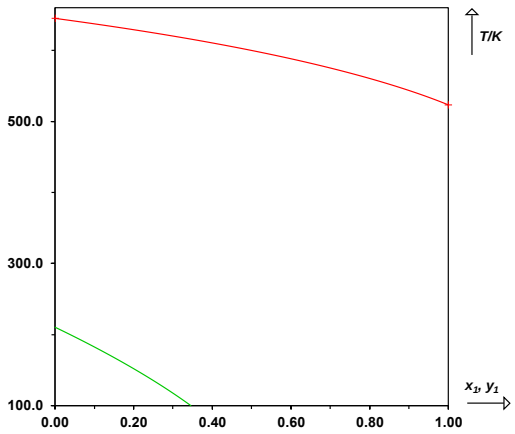
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = -223
B/MPa = -471

*Deviations*
MAPE on x = 2.1 %
MAPE on y = 9.6 %
MAPE on $h^M$ = 12 %



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**Isothermal phase equilibrium data**

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Narbutt, J. v., Die Schmelz-, Siede- und Dampfkurven (760 mm Druck) in den binären Systemen: Ortho- + Para-, Ortho- + Meta-, Para- + Metabromnitrobenzol, und die Schmelzkurven der Gemische von Diphenylamin und Phenanthren, Zeitschrift für Physikalische Chemie 1 (1905) doi:10.1515/zpch-1905-5337

**T / K = 330.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1738 | 0.4516 | 0.8954 |
| 0.1912 | 0.4826 | 0.9108 |
| 0.2255 | 0.5469 | 0.9385 |
| 0.3281 | 0.7060 | 0.9690 |
| 0.3592 | 0.7529 | 0.9827 |
| 0.4165 | 0.8510 | 0.9907 |
| 0.4633 | 0.9371 | 0.9978 |
| 0.4707 | 0.9458 | 0.9964 |

Narbutt, J. v., Die Schmelz-, Siede- und Dampfkurven (760 mm Druck) in den binären Systemen: Ortho- + Para-, Ortho- + Meta-, Para- + Metabromnitrobenzol, und die Schmelzkurven der Gemische von Diphenylamin und Phenanthren, Zeitschrift für Physikalische Chemie 1 (1905) doi:10.1515/zpch-1905-5337

**T / K = 350.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3379 | 0.4118 | 0.8361 |
| 0.3639 | 0.4389 | 0.8688 |
| 0.4588 | 0.5321 | 0.9130 |
| 0.7853 | 0.7978 | 0.9834 |
| 0.8015 | 0.8053 | 0.9856 |
| 0.8889 | 0.8836 | 0.9928 |

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**Enthalpy of mixing**

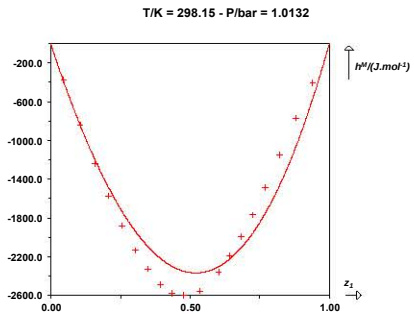
---

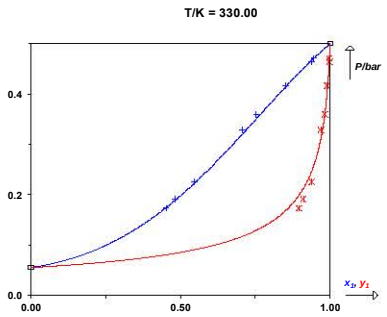
Fenby, D.V. - Scott, R.L., Excess enthalpy. Hexafluorobenzene-benzene system, Int. Data Ser. Sel. Data Mixtures Ser. A 2 (1975) 130-138.

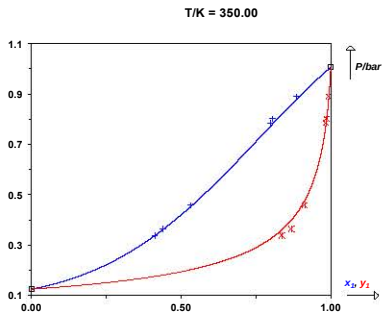
**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -377.10 | 0.0459 |
| -843.10 | 0.1063 |
| -1239.1 | 0.1586 |
| -1570.7 | 0.2066 |
| -1880.2 | 0.2558 |
| -2134.6 | 0.3032 |
| -2326.8 | 0.3480 |
| -2488.4 | 0.3929 |
| -2576.2 | 0.4364 |
| -2599.0 | 0.4776 |
| -2556.6 | 0.5341 |
| -2360.9 | 0.6029 |
| -2195.0 | 0.6427 |
| -1993.1 | 0.6835 |
| -1768.1 | 0.7245 |
| -1486.1 | 0.7699 |
| -1150.6 | 0.8213 |
| -768.60 | 0.8800 |
| -407.40 | 0.9406 |


T/K = 298.15 - P/bar = 1.0132
hᴱ/(J.mol⁻¹)
-200.0
-600.0
-1000.0
-1400.0
-1800.0
-2200.0
-2600.0
0.00
0.50
1.00
z₁


T/K = 330.00
P/bar
0.4
0.2
0.0
0.00
0.50
1.00
x₁, y₁


T/K = 350.00
P/bar
1.1
0.9
0.7
0.5
0.3
0.1
0.00
0.50
1.00
x₁, y₁

# H-SA systems (AC = 7)

## CHLOROFORM (1) + 1-BUTANOL (2)

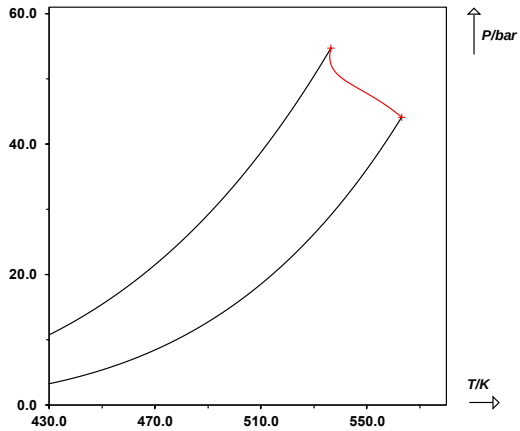
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 71-36-3 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | LRHPLDYGYMQRHN-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.40 | 563.10 |
| **$P_c$ / bar** | 54.72 | 44.14 |
| **ω** | 0.222 | 0.588 |

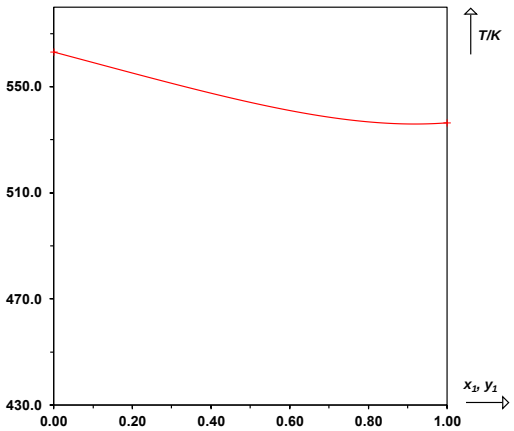
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 59.6
B/MPa = -25

*Deviations*
MAPE on x = 7.0 %
MAPE on y = 5.0 %
MAPE on $h^M$ = 98 %



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**Isobaric phase equilibrium data**

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Chen, Geng-Hua - Wang, Qi - Ma, Zhong-Min - Yan, Xin-Huan - Han, Shi-Jun, Phase equilibria at superatmospheric pressures for systems containing halohydrocarbon, aromatic hydrocarbon, and alcohol, Journal of Chemical & Engineering Data 2 (1995) 361-366. doi:10.1021/je00018a003

**P / bar = 1.050**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 390.62 | 0.0091 | 0.0449 |
| 388.96 | 0.0213 | 0.1255 |
| 387.43 | 0.0357 | 0.1801 |
| 383.69 | 0.0612 | 0.3066 |
| 380.17 | 0.0865 | 0.3937 |
| 376.14 | 0.1195 | 0.4974 |
| 370.37 | 0.1707 | 0.6171 |
| 365.64 | 0.2203 | 0.6899 |
| 361.90 | 0.2644 | 0.7575 |
| 357.72 | 0.3247 | 0.8065 |
| 354.43 | 0.3773 | 0.8499 |
| 351.34 | 0.4278 | 0.8767 |
| 349.62 | 0.4624 | 0.8909 |
| 347.67 | 0.5091 | 0.9166 |
| 343.31 | 0.6386 | 0.9405 |
| 341.13 | 0.6967 | 0.9461 |
| 340.09 | 0.7445 | 0.9497 |
| 339.67 | 0.7798 | 0.9608 |
| 339.36 | 0.7981 | 0.9633 |
| 339.09 | 0.8113 | 0.9635 |
| 337.54 | 0.8755 | 0.9762 |
| 335.56 | 0.9804 | 0.9921 |

Chen, Geng-Hua - Wang, Qi - Ma, Zhong-Min - Yan, Xin-Huan - Han, Shi-Jun, Phase equilibria at superatmospheric pressures for systems containing halohydrocarbon, aromatic hydrocarbon, and alcohol, Journal of Chemical & Engineering Data 2 (1995) 361-366. doi:10.1021/je00018a003

**P / bar = 2.050**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 405.03 | 0.0677 | 0.2509 |
| 402.09 | 0.0967 | 0.3336 |
| 401.06 | 0.1053 | 0.3525 |
| 398.92 | 0.1293 | 0.4149 |
| 395.84 | 0.1580 | 0.4940 |
| 392.70 | 0.1993 | 0.5650 |
| 384.13 | 0.3160 | 0.7129 |
| 379.79 | 0.3866 | 0.7805 |
| 375.54 | 0.4522 | 0.8342 |
| 375.70 | 0.4539 | 0.8343 |
| 373.25 | 0.4895 | 0.8650 |
| 370.13 | 0.5728 | 0.8967 |
| 367.67 | 0.6357 | 0.9151 |
| 365.94 | 0.7025 | 0.9329 |
| 363.50 | 0.7925 | 0.9580 |
| 362.03 | 0.8435 | 0.9653 |
| 360.93 | 0.8815 | 0.9763 |

Chen, Geng-Hua - Wang, Qi - Ma, Zhong-Min - Yan, Xin-Huan - Han, Shi-Jun, Phase equilibria at superatmospheric pressures for systems containing halohydrocarbon, aromatic hydrocarbon, and alcohol, Journal of Chemical & Engineering Data 2 (1995) 361-366. doi:10.1021/je00018a003

**P / bar = 3.030**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 421.35 | 0.0471 | 0.1560 |
| 421.05 | 0.0501 | 0.1709 |
| 420.29 | 0.0602 | 0.1970 |
| 418.27 | 0.0833 | 0.2583 |
| 415.33 | 0.1140 | 0.3422 |
| 412.51 | 0.1420 | 0.3981 |
| 409.16 | 0.1900 | 0.4901 |
| 408.39 | 0.2041 | 0.5163 |
| 407.12 | 0.2187 | 0.5462 |
| 406.10 | 0.2365 | 0.5756 |
| 404.14 | 0.2633 | 0.6087 |
| 399.76 | 0.3310 | 0.6834 |
| 397.69 | 0.3480 | 0.7111 |
| 396.56 | 0.3723 | 0.7249 |
| 394.10 | 0.4275 | 0.7630 |
| 389.90 | 0.5019 | 0.8226 |
| 385.93 | 0.5879 | 0.8676 |
| 382.06 | 0.6789 | 0.9096 |
| 379.32 | 0.7705 | 0.9419 |
| 376.85 | 0.8548 | 0.9617 |
| 373.91 | 0.9513 | 0.9871 |

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**Enthalpy of mixing**

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Ruiz, B. - Royo, F.M. - Otin, S., Excess molar enthalpies (HmE) of binary liquid mixtures, Rev. Acad. Cienc. Exact. Fis. Quim. Nat. Zaragoza (1989) 137-143.

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -111.80 | 0.0265 |

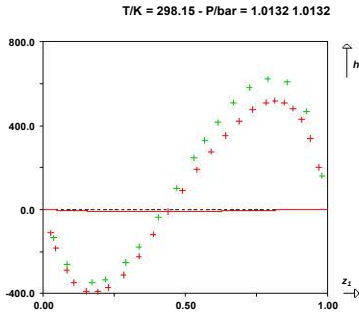
| | |
|---|---|
| -185.00 | 0.0453 |
| -289.20 | 0.0827 |
| -348.40 | 0.1098 |
| -388.80 | 0.1516 |
| -391.60 | 0.1931 |
| -372.70 | 0.2293 |
| -312.40 | 0.2829 |
| -223.10 | 0.3360 |
| -118.10 | 0.3883 |
| -10.50 | 0.4401 |
| 90.20 | 0.4912 |
| 189.20 | 0.5417 |
| 275.20 | 0.5915 |
| 350.80 | 0.6408 |
| 420.20 | 0.6895 |
| 475.80 | 0.7377 |
| 508.20 | 0.7852 |
| 518.60 | 0.8169 |
| 508.20 | 0.8478 |
| 482.60 | 0.8787 |
| 427.50 | 0.9099 |
| 337.90 | 0.9398 |
| 200.20 | 0.9700 |

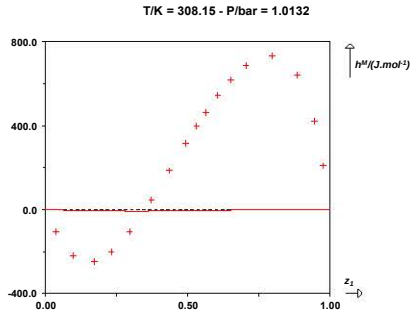
Nagata, I. - Kawamura, Y. - Asano, H. - Fujiwara, K. - Ogasawara, Y., Excess Enthalpies for Binary Mixtures of Chloroform with Alcohols, Z. Phys. Chem. Leipzig 6 (1978) 1109-1116.

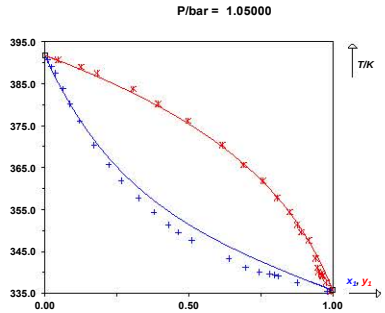
| **T / K =** | **298.15** |
|---|---|
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| -135.60 | 0.0371 |
| -260.60 | 0.0851 |
| -347.00 | 0.1718 |
| -333.30 | 0.2191 |
| -251.70 | 0.2918 |
| -176.80 | 0.3369 |
| -38.10 | 0.4062 |
| 101.80 | 0.4700 |
| 247.40 | 0.5320 |
| 327.20 | 0.5701 |
| 414.50 | 0.6150 |
| 507.90 | 0.6707 |
| 580.20 | 0.7264 |
| 620.40 | 0.7899 |
| 606.50 | 0.8579 |
| 467.60 | 0.9275 |
| 161.60 | 0.9822 |

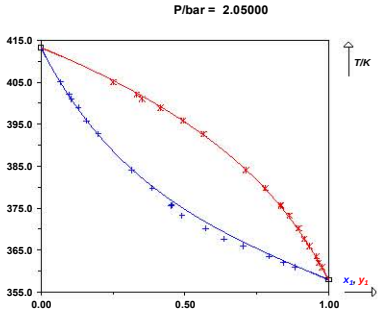
Nagata, I. - Kawamura, Y. - Asano, H. - Fujiwara, K. - Ogasawara, Y., Excess Enthalpies for Binary Mixtures of Chloroform with Alcohols, Z. Phys. Chem. Leipzig 6 (1978) 1109-1116.

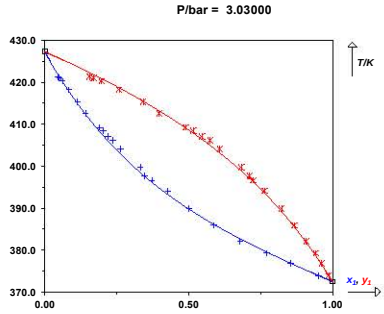
| **T / K =** | **308.15** |
|---|---|
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| -107.40 | 0.0352 |
| -220.10 | 0.0960 |
| -248.80 | 0.1699 |
| -202.60 | 0.2304 |
| -106.80 | 0.2947 |
| 45.50 | 0.3711 |
| 186.30 | 0.4344 |
| 315.00 | 0.4920 |
| 398.20 | 0.5308 |
| 461.90 | 0.5625 |
| 542.60 | 0.6055 |
| 615.60 | 0.6497 |
| 684.80 | 0.7042 |
| 732.40 | 0.7965 |
| 639.40 | 0.8852 |
| 420.60 | 0.9455 |
| 209.30 | 0.9772 |


T/K = 298.15 - P/bar = 1.0132 1.0132
800.0
400.0
0.0
-400.0
0.00
0.50
1.00
$h^M/(J.mol^{-1})$
$z_1$


T/K = 308.15 - P/bar = 1.0132
800.0
400.0
0.0
-400.0
0.00
0.50
1.00
$h^M/(J.mol^{-1})$
$z_1$


P/bar = 1.05000
395.0
385.0
375.0
365.0
355.0
345.0
335.0
0.00
0.50
1.00
T/K
$x_1, y_1$


P/bar = 2.05000
415.0
405.0
395.0
385.0
375.0
365.0
355.0
0.00
0.50
1.00
T/K
$x_1, y_1$


P/bar = 3.03000
430.0
420.0
410.0
400.0
390.0
380.0
370.0
0.00
0.50
1.00
T/K
$x_1, y_1$

## 1-PROPANOL (1) + TRICHLOROETHYLENE (2)

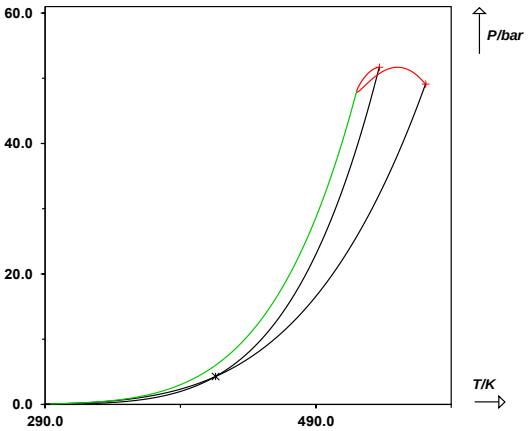
| | | |
|---|---|---|
| **CAS** | 71-23-8 | 79-01-6 |
| **InChiKey** | BDERNNFJNOPAEC-UHFFFAOYSA-N | XSTXAVWGXDQKEL-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.80 | 571.00 |
| **$P_c$ / bar** | 51.69 | 49.10 |
| **ω** | 0.621 | 0.217 |

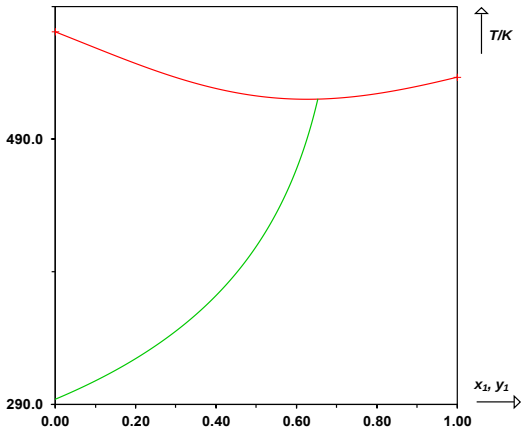
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 242
B/MPa = -53.5

*Deviations*
MAPE on x = 17 %
MAPE on y = 11 %
MAPE on $h^M$ = 100 %



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**Isobaric phase equilibrium data**

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Aucejo, Antonio - Gonzalez-Alfaro, Vicenta - Monton, Juan B. - Vazquez, M. Isabel, Isobaric Vapor-Liquid Equilibria of Trichloroethylene with 1-Propanol and 2-Propanol at 20 and 100 kPa, Journal of Chemical & Engineering Data 1 (1995) 332-335. doi:10.1021/je00017a073

**P / bar = 0.2000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 331.45 | 0.9890 | 0.9330 |
| 330.55 | 0.9810 | 0.8890 |
| 329.75 | 0.9730 | 0.8500 |
| 329.05 | 0.9640 | 0.8100 |
| 328.15 | 0.9510 | 0.7600 |
| 326.55 | 0.9330 | 0.6910 |
| 324.75 | 0.9100 | 0.6200 |
| 323.05 | 0.8810 | 0.5500 |
| 321.55 | 0.8490 | 0.4930 |
| 319.45 | 0.8130 | 0.4250 |
| 317.65 | 0.7590 | 0.3710 |
| 316.55 | 0.7110 | 0.3440 |
| 315.15 | 0.6560 | 0.2970 |
| 313.95 | 0.5650 | 0.2580 |
| 313.15 | 0.4850 | 0.2340 |
| 312.75 | 0.4200 | 0.2180 |
| 312.35 | 0.3310 | 0.1990 |
| 312.15 | 0.2490 | 0.1810 |
| 312.35 | 0.0650 | 0.1190 |
| 313.35 | 0.0180 | 0.0540 |

Aucejo, Antonio - Gonzalez-Alfaro, Vicenta - Monton, Juan B. - Vazquez, M. Isabel, Isobaric Vapor-Liquid Equilibria of Trichloroethylene with 1-Propanol and 2-Propanol at 20 and 100 kPa, Journal of Chemical & Engineering Data 1 (1995) 332-335. doi:10.1021/je00017a073

**P / bar = 1.0000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 369.05 | 0.9910 | 0.9680 |
| 367.25 | 0.9670 | 0.8870 |
| 365.55 | 0.9400 | 0.8110 |
| 364.45 | 0.9200 | 0.7600 |
| 362.75 | 0.8860 | 0.6910 |
| 359.75 | 0.8040 | 0.5780 |
| 358.15 | 0.7490 | 0.5100 |
| 356.85 | 0.6860 | 0.4640 |
| 355.85 | 0.6170 | 0.4230 |
| 355.05 | 0.5320 | 0.3810 |
| 354.55 | 0.4590 | 0.3520 |
| 354.35 | 0.3850 | 0.3320 |
| 354.45 | 0.1890 | 0.2480 |
| 354.95 | 0.1260 | 0.2160 |
| 355.35 | 0.1000 | 0.1890 |
| 355.75 | 0.0810 | 0.1630 |
| 356.55 | 0.0530 | 0.1280 |
| 356.85 | 0.0440 | 0.1100 |
| 357.75 | 0.0260 | 0.0710 |
| 358.45 | 0.0140 | 0.0420 |

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**Enthalpy of mixing**

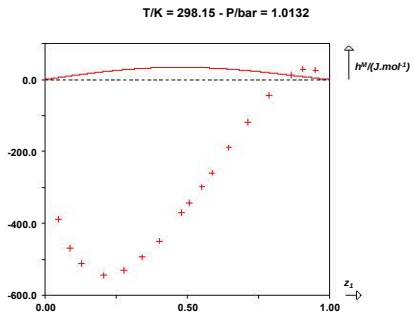
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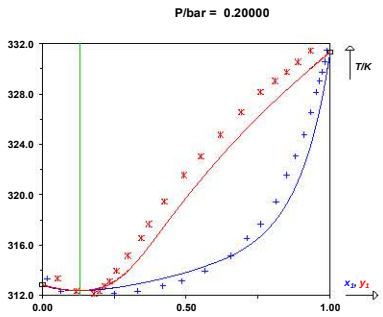
Marcus, Y. - Kolarik, Z., The enthalpies of mixing of organophosphate esters with hydrocarbons, Journal of Solution Chemistry 1 (1977) 39-56. doi:10.1007/BF00650791

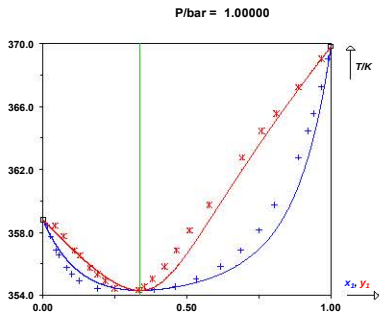
**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 26.10 | 0.9514 |
| 28.60 | 0.9074 |
| 11.90 | 0.8672 |
| -43.60 | 0.7870 |
| -117.90 | 0.7139 |
| -189.20 | 0.6474 |
| -259.10 | 0.5872 |
| -298.30 | 0.5529 |
| -342.50 | 0.5073 |
| -369.50 | 0.4816 |
| -449.10 | 0.4028 |
| -493.30 | 0.3427 |
| -530.10 | 0.2776 |
| -544.40 | 0.2062 |
| -510.70 | 0.1281 |
| -468.10 | 0.0892 |
| -388.90 | 0.0467 |


T/K = 298.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
0.0
-200.0
-400.0
-600.0
0.00
0.50
1.00
$z_1$


P/bar = 0.20000
T/K
332.0
328.0
324.0
320.0
316.0
312.0
0.00
0.50
1.00
$x_1$, $y_1$


P/bar = 1.00000
T/K
370.0
366.0
362.0
358.0
354.0
0.00
0.50
1.00
$x_1$, $y_1$

## TRICHLOROETHYLENE (1) + 1-BUTANOL (2)

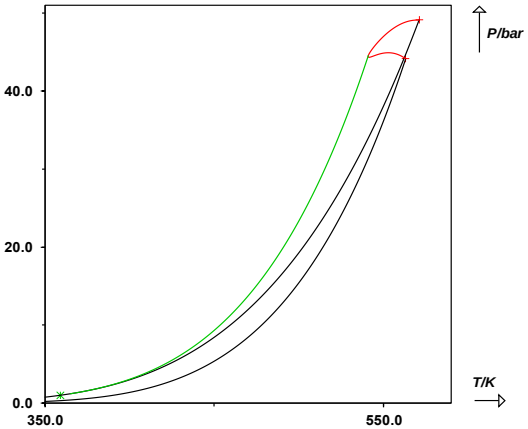
| | | |
|---|---|---|
| **CAS** | 79-01-6 | 71-36-3 |
| **InChiKey** | XSTXAVWGXDQKEL-UHFFFAOYSA-N | LRHPLDYGYMQRHN-UHFFFAOYSA-N |
| **$T_c$ / K** | 571 | 563.1 |
| **$P_c$ / bar** | 49.1 | 44.14 |
| **ω** | 0.217 | 0.588 |

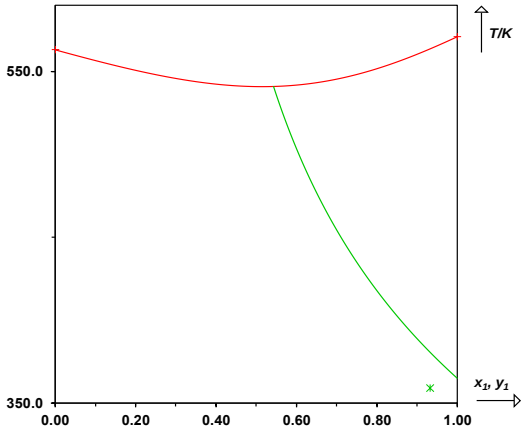
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 168
B/MPa = -51.4

*Deviations*
MAPE on x = 14 %
MAPE on y = 12 %
MAPE on $h^M$ = 96 %



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**Isobaric phase equilibrium data**

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Dejoz, Ana - González-Alfaro, Vicenta - Miguel, Pablo J. - Vázquez, M. Isabel, Isobaric Vapor−Liquid Equilibria of Trichloroethylene with 1-Butanol and 2-Butanol at 20 and 100 kPa, Journal of Chemical & Engineering Data 1 (1996) 89-92. doi:10.1021/je950163g

**P / bar = 0.2000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 348.15 | 0.0160 | 0.1370 |
| 345.75 | 0.0310 | 0.2430 |
| 343.15 | 0.0510 | 0.3450 |
| 339.85 | 0.0770 | 0.4490 |
| 336.05 | 0.1160 | 0.5860 |
| 332.45 | 0.1530 | 0.6590 |
| 329.05 | 0.1990 | 0.7330 |
| 325.75 | 0.2530 | 0.7900 |
| 323.25 | 0.3060 | 0.8290 |
| 321.25 | 0.3640 | 0.8580 |
| 319.65 | 0.4230 | 0.8740 |
| 318.25 | 0.4740 | 0.8900 |
| 317.25 | 0.5420 | 0.9020 |
| 316.45 | 0.6040 | 0.9120 |
| 315.85 | 0.6580 | 0.9190 |
| 315.45 | 0.7040 | 0.9250 |
| 315.05 | 0.7520 | 0.9310 |
| 314.75 | 0.8070 | 0.9390 |
| 314.55 | 0.8430 | 0.9440 |

Dejoz, Ana - González-Alfaro, Vicenta - Miguel, Pablo J. - Vázquez, M. Isabel, Isobaric Vapor−Liquid Equilibria of Trichloroethylene with 1-Butanol and 2-Butanol at 20 and 100 kPa, Journal of Chemical & Engineering Data 1 (1996) 89-92. doi:10.1021/je950163g

**P / bar = 1.0000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 389.15 | 0.0110 | 0.0520 |
| 388.05 | 0.0230 | 0.1000 |
| 385.55 | 0.0440 | 0.1940 |
| 383.15 | 0.0760 | 0.2880 |
| 379.65 | 0.1170 | 0.4030 |
| 376.15 | 0.1720 | 0.4990 |
| 372.75 | 0.2270 | 0.5760 |
| 369.85 | 0.2950 | 0.6480 |
| 367.55 | 0.3510 | 0.6920 |
| 365.55 | 0.4120 | 0.7400 |
| 363.95 | 0.4780 | 0.7720 |
| 362.65 | 0.5460 | 0.8020 |
| 361.65 | 0.6080 | 0.8210 |
| 360.85 | 0.6680 | 0.8400 |
| 360.35 | 0.7270 | 0.8580 |
| 359.85 | 0.7810 | 0.8710 |
| 359.55 | 0.8310 | 0.8850 |
| 359.25 | 0.8710 | 0.9020 |
| 359.15 | 0.9800 | 0.9760 |

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**Enthalpy of mixing**

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Marcus, Y. - Kolarik, Z., The enthalpies of mixing of organophosphate esters with hydrocarbons, Journal of Solution Chemistry 1 (1977) 39-56. doi:10.1007/BF00650791

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 21.50 | 0.0400 |
| 27.30 | 0.0764 |
| 18.50 | 0.1111 |
| -22.30 | 0.1809 |
| -81.70 | 0.2461 |
| -150.30 | 0.3071 |
| -223.90 | 0.3639 |
| -266.10 | 0.4004 |
| -288.80 | 0.4168 |
| -347.10 | 0.4658 |
| -376.90 | 0.4933 |
| -399.30 | 0.5113 |
| -435.70 | 0.5484 |
| -495.10 | 0.6102 |
| -540.20 | 0.6797 |
| -557.80 | 0.7583 |
| -531.10 | 0.8474 |
| -488.90 | 0.8928 |
| -418.50 | 0.9434 |

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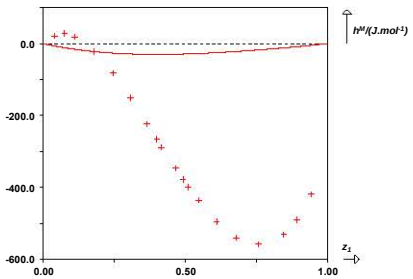
**Azeotropic point**

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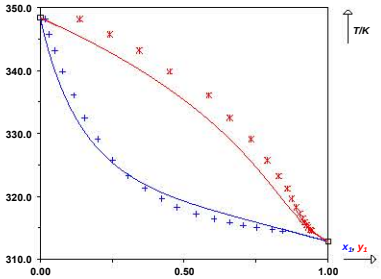
Dejoz, Ana - González-Alfaro, Vicenta - Miguel, Pablo J. - Vázquez, M. Isabel, Isobaric Vapor−Liquid Equilibria of Trichloroethylene with 1-Butanol and 2-Butanol at 20 and 100 kPa, Journal of Chemical & Engineering Data 1 (1996) 89-92. doi:10.1021/je950163g

| T / K | P / bar | $x_1$ |
|---|---|---|
| 359.05 | 1.0000 | 0.9320 |

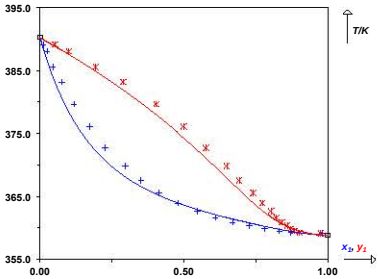
T/K = 298.15 - P/bar = 1.0132



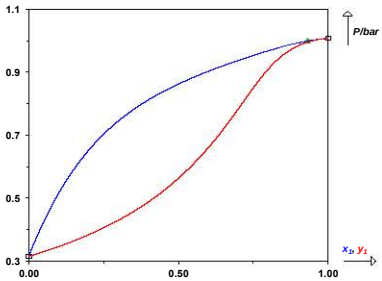

P/bar = 0.20000




P/bar = 1.00000




T/K = 359.05



## ISOPROPANOL (1) + TRICHLOROETHYLENE (2)

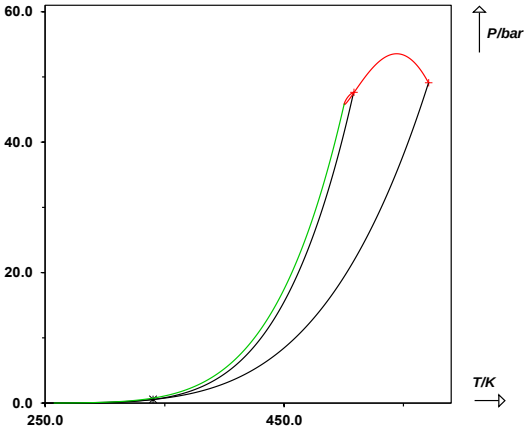
| | | |
|---|---|---|
| **CAS** | 67-63-0 | 79-01-6 |
| **InChiKey** | KFZMGEQAYNKOFK-UHFFFAOYSA-N | XSTXAVWGXDQKEL-UHFFFAOYSA-N |
| **$T_c$ / K** | 508.30 | 571.00 |
| **$P_c$ / bar** | 47.65 | 49.10 |
| **ω** | 0.663 | 0.217 |

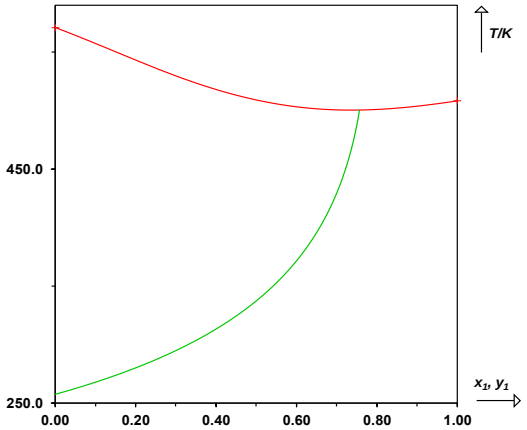
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 228
B/MPa = -78

*Deviations*
MAPE on x = 18 %
MAPE on y = 14 %
MAPE on $h^M$ = 72 %



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**Isobaric phase equilibrium data**

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Aucejo, Antonio - Gonzalez-Alfaro, Vicenta - Monton, Juan B. - Vazquez, M. Isabel, Isobaric Vapor-Liquid Equilibria of Trichloroethylene with 1-Propanol and 2-Propanol at 20 and 100 kPa, Journal of Chemical & Engineering Data 1 (1995) 332-335. doi:10.1021/je00017a073

**P / bar = 0.2000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 313.05 | 0.0130 | 0.0590 |
| 311.95 | 0.0260 | 0.1020 |
| 309.95 | 0.0680 | 0.1940 |
| 309.35 | 0.1090 | 0.2310 |
| 308.95 | 0.1640 | 0.2620 |
| 308.65 | 0.2300 | 0.2870 |
| 308.55 | 0.3040 | 0.3100 |
| 308.65 | 0.3860 | 0.3340 |
| 308.85 | 0.4580 | 0.3560 |
| 309.15 | 0.5390 | 0.3830 |
| 309.75 | 0.6190 | 0.4210 |
| 310.25 | 0.6810 | 0.4570 |
| 310.85 | 0.7440 | 0.4900 |
| 311.75 | 0.7870 | 0.5360 |
| 312.75 | 0.8300 | 0.5880 |
| 313.75 | 0.8650 | 0.6410 |
| 314.75 | 0.8970 | 0.6960 |
| 315.75 | 0.9230 | 0.7540 |
| 316.75 | 0.9450 | 0.8120 |
| 317.35 | 0.9580 | 0.8440 |
| 317.85 | 0.9680 | 0.8820 |
| 318.25 | 0.9770 | 0.9070 |
| 318.95 | 0.9870 | 0.9490 |
| 319.25 | 0.9930 | 0.9700 |

Aucejo, Antonio - Gonzalez-Alfaro, Vicenta - Monton, Juan B. - Vazquez, M. Isabel, Isobaric Vapor-Liquid Equilibria of Trichloroethylene with 1-Propanol and 2-Propanol at 20 and 100 kPa, Journal of Chemical & Engineering Data 1 (1995) 332-335. doi:10.1021/je00017a073

**P / bar = 1.0000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 358.15 | 0.0090 | 0.0490 |
| 357.35 | 0.0150 | 0.0710 |
| 356.65 | 0.0210 | 0.0930 |
| 355.65 | 0.0330 | 0.1290 |
| 354.45 | 0.0510 | 0.1700 |
| 353.65 | 0.0590 | 0.1990 |
| 352.05 | 0.0920 | 0.2550 |
| 350.55 | 0.1380 | 0.3120 |
| 349.35 | 0.2020 | 0.3590 |
| 348.85 | 0.2480 | 0.3890 |
| 348.45 | 0.3050 | 0.4130 |
| 348.15 | 0.3680 | 0.4380 |
| 348.05 | 0.5670 | 0.5230 |
| 348.35 | 0.6430 | 0.5630 |
| 348.75 | 0.7100 | 0.6060 |
| 349.45 | 0.7820 | 0.6630 |
| 350.35 | 0.8440 | 0.7270 |
| 351.45 | 0.8940 | 0.7910 |
| 352.45 | 0.9320 | 0.8530 |
| 353.55 | 0.9680 | 0.9200 |
| 354.55 | 0.9920 | 0.9790 |

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**Enthalpy of mixing**

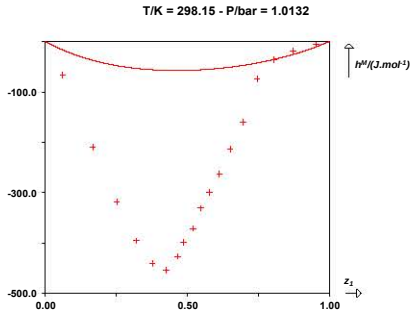
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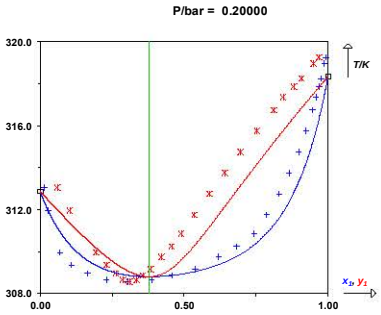
Iloukhani, H. - Parsa, J.B., Excess Molar Enthalpies of Binary Mixtures of Trichloroethylene with Six 2-Alkanols at 25°C, J. Solution Chem. 5 (2001) 425-433. doi:10.1023/A:1010396430848

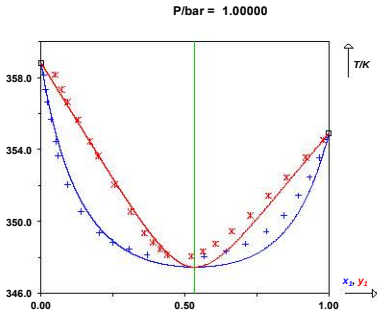
**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -66.80 | 0.0631 |
| -209.40 | 0.1680 |
| -318.60 | 0.2518 |
| -395.70 | 0.3203 |
| -440.20 | 0.3773 |
| -453.50 | 0.4254 |
| -426.20 | 0.4667 |
| -398.40 | 0.4872 |
| -371.50 | 0.5204 |
| -330.80 | 0.5480 |
| -299.50 | 0.5788 |
| -263.00 | 0.6133 |
| -213.30 | 0.6521 |
| -159.80 | 0.6961 |
| -73.80 | 0.7465 |
| -35.60 | 0.8048 |
| -18.60 | 0.8730 |
| -6.300 | 0.9537 |


T/K = 298.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
-100.0
-300.0
-500.0
0.00
0.50
1.00
$z_1$


P/bar = 0.20000
T/K
320.0
316.0
312.0
308.0
0.00
0.50
1.00
$x_1$, $y_1$


P/bar = 1.00000
T/K
358.0
354.0
350.0
346.0
0.00
0.50
1.00
$x_1$, $y_1$

## 2-BUTANOL (1) + TRICHLOROETHYLENE (2)

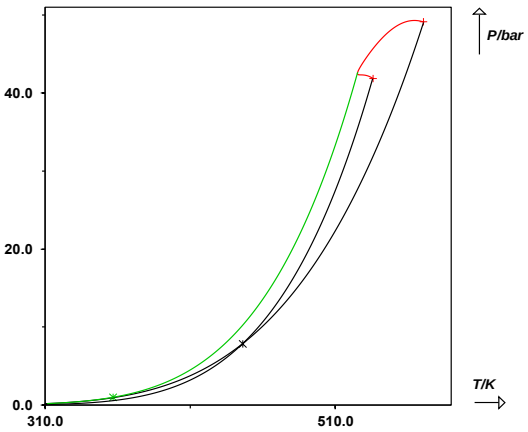
| | | |
|---|---|---|
| **CAS** | 78-92-2 | 79-01-6 |
| **InChiKey** | BTANRVKWQNVYAZ-UHFFFAOYSA-N | XSTXAVWGXDQKEL-UHFFFAOYSA-N |
| **$T_c$ / K** | 535.9 | 571 |
| **$P_c$ / bar** | 41.885 | 49.1 |
| **ω** | 0.581 | 0.217 |

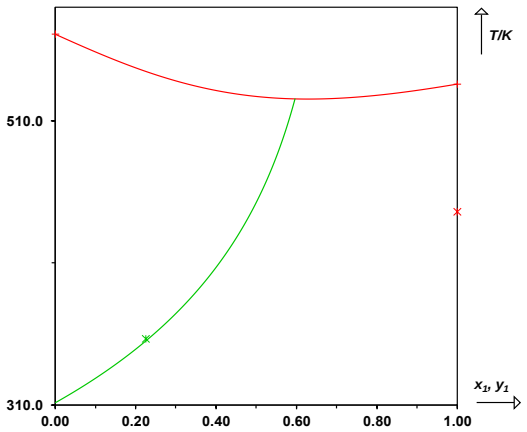
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 151
B/MPa = -67.9

*Deviations*
MAPE on x = 11 %
MAPE on y = 13 %
MAPE on $x_{az}$ = 2.1 %
MAPE on $P_{az}$ = 0.51 %
MAPE on $h^M$ = 70 %



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**Isobaric phase equilibrium data**

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Dejoz, Ana - González-Alfaro, Vicenta - Miguel, Pablo J. - Vázquez, M. Isabel, Isobaric Vapor−Liquid Equilibria of Trichloroethylene with 1-Butanol and 2-Butanol at 20 and 100 kPa, Journal of Chemical & Engineering Data 1 (1996) 89-92. doi:10.1021/je950163g

**P / bar = 0.2000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 333.85 | 0.9910 | 0.9530 |
| 332.85 | 0.9750 | 0.8980 |
| 331.15 | 0.9540 | 0.8080 |
| 329.55 | 0.9280 | 0.7140 |
| 327.55 | 0.8990 | 0.6250 |
| 325.55 | 0.8690 | 0.5520 |
| 323.55 | 0.8290 | 0.4720 |
| 321.55 | 0.7850 | 0.4030 |
| 319.85 | 0.7300 | 0.3490 |
| 318.45 | 0.6780 | 0.3130 |
| 317.05 | 0.6010 | 0.2680 |
| 315.95 | 0.5300 | 0.2370 |
| 315.25 | 0.4890 | 0.2230 |
| 314.55 | 0.4330 | 0.2020 |
| 314.15 | 0.3630 | 0.1830 |
| 313.85 | 0.3110 | 0.1670 |
| 313.55 | 0.2560 | 0.1600 |
| 313.35 | 0.2220 | 0.1470 |
| 313.25 | 0.0610 | 0.0780 |
| 313.35 | 0.0490 | 0.0710 |
| 313.45 | 0.0430 | 0.0570 |
| 313.55 | 0.0300 | 0.0460 |
| 313.75 | 0.0180 | 0.0330 |
| 313.85 | 0.0080 | 0.0150 |
| 314.05 | 0.0010 | 0.0020 |

Dejoz, Ana - González-Alfaro, Vicenta - Miguel, Pablo J. - Vázquez, M. Isabel, Isobaric Vapor−Liquid Equilibria of Trichloroethylene with 1-Butanol and 2-Butanol at 20 and 100 kPa, Journal of Chemical & Engineering Data 1 (1996) 89-92. doi:10.1021/je950163g

**P / bar = 1.0000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 371.25 | 0.9880 | 0.9620 |
| 370.75 | 0.9790 | 0.9400 |
| 369.75 | 0.9570 | 0.8800 |
| 368.25 | 0.9140 | 0.8070 |
| 366.45 | 0.8640 | 0.7120 |
| 364.55 | 0.7950 | 0.6090 |
| 362.95 | 0.7390 | 0.5390 |
| 361.55 | 0.6970 | 0.4850 |
| 360.25 | 0.6370 | 0.4360 |
| 359.25 | 0.5850 | 0.3920 |
| 358.45 | 0.5330 | 0.3410 |
| 357.95 | 0.4750 | 0.3120 |
| 357.55 | 0.4300 | 0.2970 |
| 357.15 | 0.3580 | 0.2740 |
| 356.95 | 0.3070 | 0.2550 |
| 356.85 | 0.2660 | 0.2430 |
| 356.85 | 0.1620 | 0.1790 |
| 357.05 | 0.1350 | 0.1610 |
| 357.25 | 0.1080 | 0.1400 |
| 357.45 | 0.0900 | 0.1230 |
| 357.65 | 0.0680 | 0.1050 |
| 357.95 | 0.0520 | 0.0840 |
| 358.25 | 0.0370 | 0.0640 |
| 358.75 | 0.0200 | 0.0390 |
| 358.95 | 0.0120 | 0.0220 |
| 359.15 | 0.0060 | 0.0120 |
| 359.35 | 0.0020 | 0.0050 |

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**Enthalpy of mixing**

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Iloukhani, H. - Parsa, J.B., Excess Molar Enthalpies of Binary Mixtures of Trichloroethylene with Six 2-Alkanols at 25°C, J. Solution Chem. 5 (2001) 425-433. doi:10.1023/A:1010396430848

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -11.10 | 0.9450 |
| -29.50 | 0.8513 |
| -72.50 | 0.7745 |
| -169.30 | 0.7104 |
| -251.70 | 0.6561 |
| -311.50 | 0.6095 |
| -352.10 | 0.5691 |
| -384.30 | 0.5337 |
| -413.60 | 0.5025 |
| -437.80 | 0.4747 |
| -457.40 | 0.4609 |
| -469.80 | 0.4216 |
| -457.20 | 0.3815 |
| -425.40 | 0.3354 |
| -372.90 | 0.2819 |
| -290.30 | 0.2190 |
| -208.70 | 0.1440 |
| -63.00 | 0.0531 |

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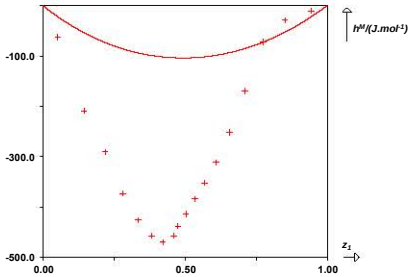
**Azeotropic point**

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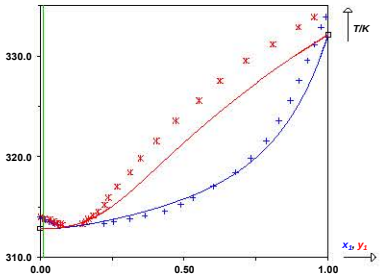
Dejoz, Ana - González-Alfaro, Vicenta - Miguel, Pablo J. - Vázquez, M. Isabel, Isobaric Vapor−Liquid Equilibria of Trichloroethylene with 1-Butanol and 2-Butanol at 20 and 100 kPa, Journal of Chemical & Engineering Data 1 (1996) 89-92. doi:10.1021/je950163g

| T / K | P / bar | $x_1$ |
|---|---|---|
| 356.75 | 1.0000 | 0.2250 |

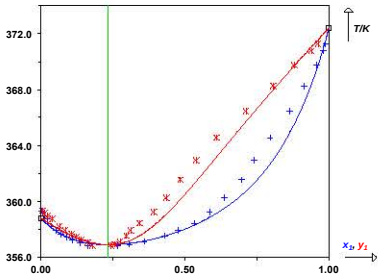
T/K = 298.15 - P/bar = 1.0132



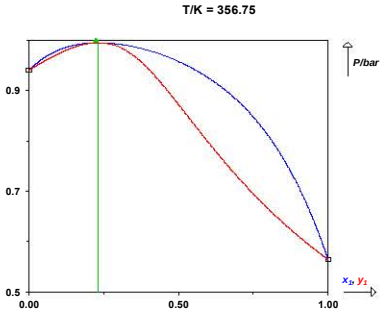

P/bar = 0.20000




P/bar = 1.00000




T/K = 356.75



## 1-HEXYNE (1) + ACETONITRILE (2)

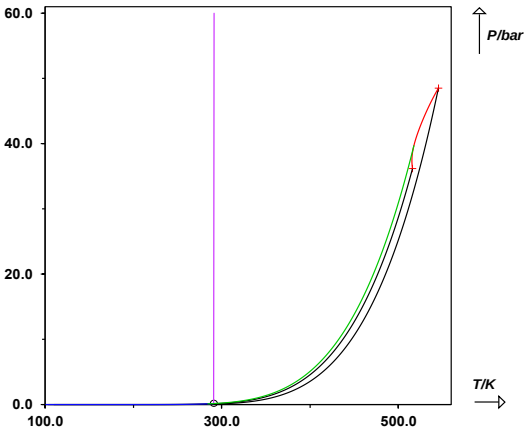
| | | |
|---|---|---|
| **CAS** | 693-02-7 | 75-05-8 |
| **InChiKey** | CGHIBGNXEGJPQZ-UHFFFAOYSA-N | WEVYAHXRMPXWCK-UHFFFAOYSA-N |
| **$T_c$ / K** | 516.20 | 545.50 |
| **$P_c$ / bar** | 36.20 | 48.50 |
| **ω** | 0.333 | 0.342 |

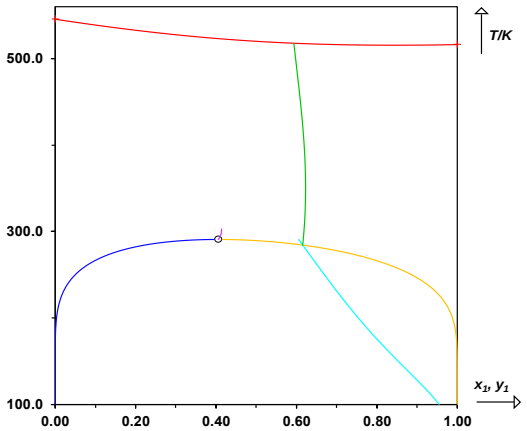
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 304
B/MPa = 711

*Deviations*
MAPE on x = 14 %
MAPE on y = 31 %



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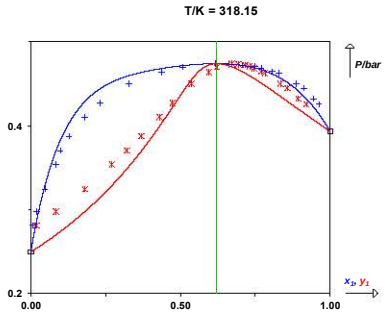
**Isothermal phase equilibrium data**

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Desplanches, Hervé - Chevalier, Jean-Louis - Llinas, Richard, Étude thermodynamique de solutions d'acétonitrile et d'hydrocarbures acétyléniques, Journal de Chimie Physique (1977) 259-265. doi:10.1051/jcp/1977740259

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2813 | 0.0050 | 0.0190 |
| 0.2976 | 0.0200 | 0.0840 |
| 0.3245 | 0.0470 | 0.1820 |
| 0.3537 | 0.0830 | 0.2720 |
| 0.3701 | 0.0980 | 0.3220 |
| 0.3872 | 0.1280 | 0.3700 |
| 0.4098 | 0.1800 | 0.4310 |
| 0.4265 | 0.2310 | 0.4740 |
| 0.4496 | 0.3270 | 0.5370 |
| 0.4634 | 0.4380 | 0.5950 |
| 0.4697 | 0.5070 | 0.6220 |
| 0.4737 | 0.6170 | 0.6720 |
| 0.4726 | 0.6640 | 0.6940 |
| 0.4718 | 0.7070 | 0.7170 |
| 0.4702 | 0.7480 | 0.7310 |
| 0.4680 | 0.7700 | 0.7460 |
| 0.4641 | 0.8060 | 0.7700 |
| 0.4625 | 0.8300 | 0.7820 |
| 0.4498 | 0.8880 | 0.8350 |
| 0.4445 | 0.9130 | 0.8570 |
| 0.4320 | 0.9450 | 0.8950 |
| 0.4254 | 0.9620 | 0.9210 |


T/K = 318.15
P/bar
0.4
0.2
0.00
0.50
1.00
x1, y1

## ISOPROPANOL (1) + CHLOROFORM (2)

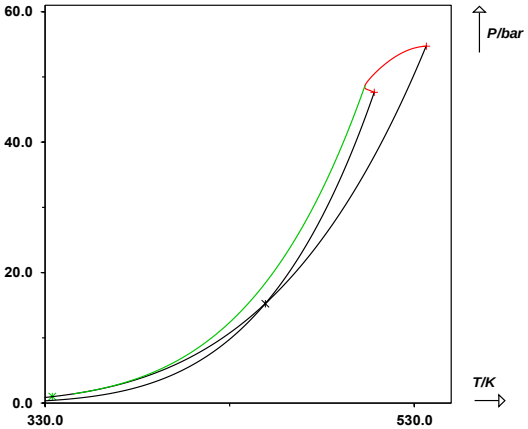
| | | |
|---|---|---|
| **CAS** | 67-63-0 | 67-66-3 |
| **InChiKey** | KFZMGEQAYNKOFK-UHFFFAOYSA-N | HEDRZPFGACZZDS-UHFFFAOYSA-N |
| **$T_c$ / K** | 508.30 | 536.40 |
| **$P_c$ / bar** | 47.65 | 54.72 |
| **ω** | 0.663 | 0.222 |

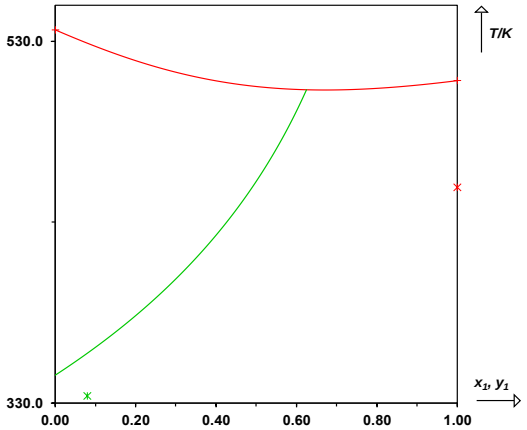
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 137
B/MPa = -36.8

*Deviations*
MAPE on x = 15 %
MAPE on y = 13 %
MAPE on $h^M$ = 97 %



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**Isothermal phase equilibrium data**

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Nagata, Isamu, Vapor-liquid equilibria for the ternary system 2-propanol-chloroform-benzene at 50°C, Journal of Chemical & Engineering Data 1 (1985) 80-82. doi:10.1021/je00039a027

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3308 | 0.9010 | 0.6580 |
| 0.3976 | 0.8240 | 0.5080 |
| 0.4726 | 0.7130 | 0.3830 |
| 0.5276 | 0.6200 | 0.3060 |
| 0.5789 | 0.5110 | 0.2430 |
| 0.6125 | 0.4110 | 0.1990 |
| 0.6240 | 0.3770 | 0.1880 |
| 0.6629 | 0.2300 | 0.1350 |
| 0.6786 | 0.1640 | 0.1050 |
| 0.6887 | 0.0610 | 0.0530 |
| 0.6909 | 0.0470 | 0.0430 |

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**Isobaric phase equilibrium data**

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Komarov, V.M. - Boldyrev, A.V. - Pelevina, R.S., Liquid-vapor equilibrium in the methyl cyclopropyl ketone-water system, J. Appl. Chem. USSR 6 (1973) 1371-1372.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 354.15 | 0.9700 | 0.9090 |
| 353.15 | 0.9480 | 0.8700 |
| 351.65 | 0.9090 | 0.7830 |
| 348.85 | 0.8650 | 0.6660 |
| 347.15 | 0.8080 | 0.5800 |
| 345.75 | 0.7680 | 0.5150 |
| 343.95 | 0.6900 | 0.4290 |
| 341.65 | 0.6100 | 0.3500 |
| 340.35 | 0.5450 | 0.2900 |
| 339.25 | 0.4950 | 0.2550 |
| 338.65 | 0.4500 | 0.2450 |
| 337.75 | 0.3900 | 0.2200 |
| 336.65 | 0.3150 | 0.1890 |
| 335.95 | 0.2700 | 0.1700 |
| 335.15 | 0.2100 | 0.1500 |
| 334.85 | 0.1850 | 0.1350 |
| 334.35 | 0.1300 | 0.1100 |
| 334.05 | 0.0200 | 0.0400 |

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**Enthalpy of mixing**

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Nagata, I. - Kawamura, Y. - Asano, H. - Fujiwara, K. - Ogasawara, Y., Excess Enthalpies for Binary Mixtures of Chloroform with Alcohols, Z. Phys. Chem. Leipzig 6 (1978) 1109-1116.

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -49.40 | 0.9844 |
| -130.80 | 0.9479 |
| -171.40 | 0.9100 |
| -177.10 | 0.8843 |
| -172.60 | 0.8577 |
| -129.30 | 0.8121 |
| -63.60 | 0.7682 |
| 22.50 | 0.7222 |
| 201.60 | 0.6375 |
| 392.50 | 0.5472 |
| 456.10 | 0.5171 |
| 556.40 | 0.4644 |
| 678.30 | 0.3852 |
| 739.70 | 0.3291 |
| 763.70 | 0.2953 |
| 777.20 | 0.2604 |
| 778.90 | 0.2320 |
| 772.00 | 0.2082 |
| 746.30 | 0.1736 |
| 675.60 | 0.1285 |
| 550.90 | 0.0853 |
| 258.80 | 0.0304 |

Nagata, I. - Kawamura, Y. - Asano, H. - Fujiwara, K. - Ogasawara, Y., Excess Enthalpies for Binary Mixtures of Chloroform with Alcohols, Z. Phys. Chem. Leipzig 6 (1978) 1109-1116.

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -48.60 | 0.9777 |
| -95.60 | 0.9379 |
| -104.60 | 0.8980 |
| -100.40 | 0.8806 |
| -46.90 | 0.8322 |
| 38.00 | 0.7826 |
| 252.30 | 0.6833 |
| 674.50 | 0.4875 |
| 796.90 | 0.4101 |
| 879.60 | 0.3258 |
| 895.90 | 0.2832 |

| | |
|---|---|
| 893.60 | 0.2495 |
| 881.50 | 0.2227 |
| 851.30 | 0.1908 |
| 851.00 | 0.1884 |
| 780.60 | 0.1474 |
| 658.10 | 0.1043 |
| 541.40 | 0.0757 |
| 418.50 | 0.0532 |
| 251.90 | 0.0299 |

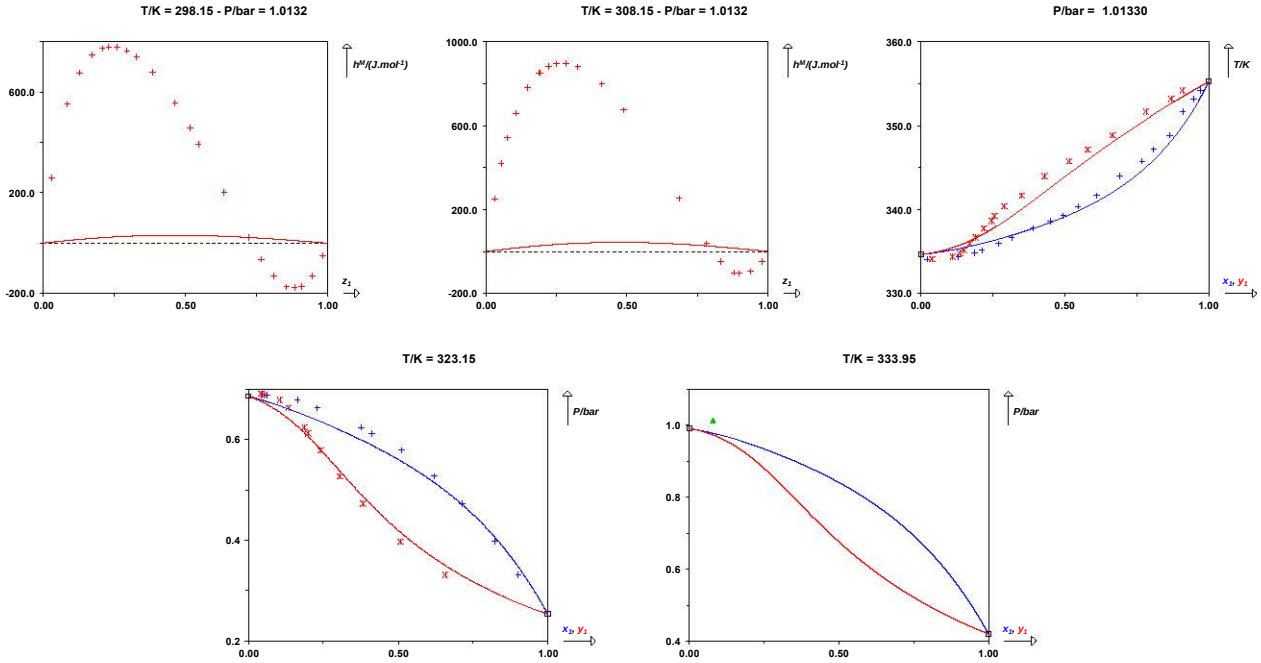
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**Azeotropic point**

---

Komarov, V.M. - Boldyrev, A.V. - Pelevina, R.S., Liquid-vapor equilibrium in the methyl cyclopropyl ketone-water system, J. Appl. Chem. USSR 6 (1973) 1371-1372.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 333.95 | 1.013 | 0.0790 |


T/K = 298.15 - P/bar = 1.0132
T/K = 308.15 - P/bar = 1.0132
P/bar = 1.01330
T/K = 323.15
T/K = 333.95
P/bar
T/K
x1, y1
z1

## ETHANOL (1) + 1-HEPTYNE (2)

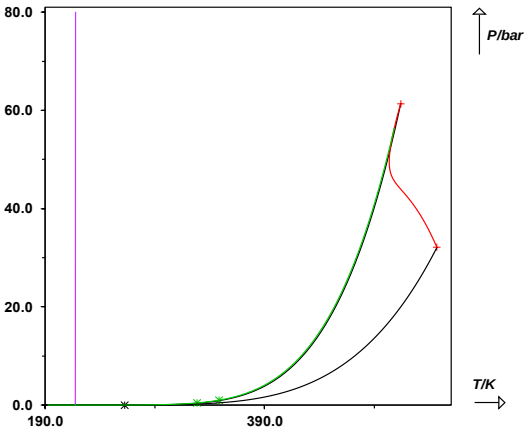
| | | |
|---|---|---|
| **CAS** | 64-17-5 | 628-71-7 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | YVXHZKKCZYLQOP-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 547.00 |
| **$P_c$ / bar** | 61.37 | 32.10 |
| **ω** | 0.644 | 0.378 |

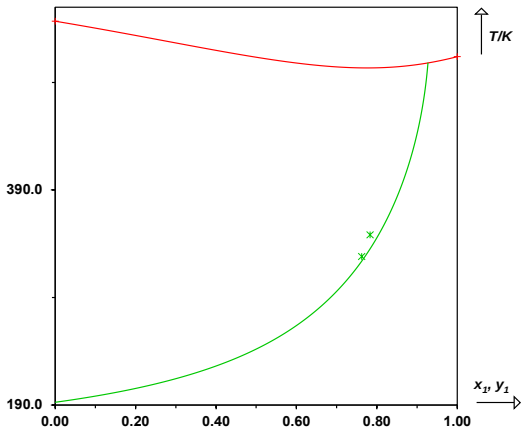
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 281
B/MPa = 141

*Deviations*
MAPE on x = 18 %
MAPE on y = 6.6 %
MAPE on $x_{az}$ = 4.3 %
MAPE on $P_{az}$ = 0.94 %
MAPE on $h^M$ = 43 %



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**Isothermal phase equilibrium data**

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Zudkevitch, David - Lindrud, Mark - Chu, Yi-Zhi, Vapor−Liquid Equilibria for Ethanol + Hept-1-yne and Butyric Acid + Butyric Anhydride, Journal of Chemical & Engineering Data 3 (1999) 393-397. doi:10.1021/je980210f

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2573 | 0.0653 | 0.2792 | |
| 0.3033 | 0.1299 | 0.4249 | |
| 0.3429 | 0.2028 | 0.5073 | |
| 0.3778 | 0.2767 | 0.5703 | |
| 0.4034 | 0.4248 | 0.6514 | |
| 0.4125 | 0.4768 | 0.6698 | |
| 0.4196 | 0.5803 | 0.7050 | |
| 0.4226 | 0.7334 | 0.7455 | |
| 0.4258 | 0.7619 | 0.7619 | AZEO |
| 0.4253 | 0.7876 | 0.7575 | |
| 0.4166 | 0.8370 | 0.7916 | |
| 0.3832 | 0.9814 | 0.9526 | |

Zudkevitch, David - Lindrud, Mark - Chu, Yi-Zhi, Vapor−Liquid Equilibria for Ethanol + Hept-1-yne and Butyric Acid + Butyric Anhydride, Journal of Chemical & Engineering Data 3 (1999) 393-397. doi:10.1021/je980210f

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.5811 | 0.0670 | 0.2915 | |
| 0.6783 | 0.1319 | 0.4357 | |
| 0.8126 | 0.2506 | 0.5603 | |
| 0.9069 | 0.4248 | 0.6527 | |
| 0.9392 | 0.5576 | 0.7038 | |
| 0.9506 | 0.6998 | 0.7469 | |
| 0.9546 | 0.7201 | 0.7542 | |
| 0.9594 | 0.7617 | 0.7631 | |
| 0.9626 | 0.7830 | 0.7830 | AZEO |
| 0.9614 | 0.8439 | 0.8069 | |
| 0.9107 | 0.9658 | 0.9398 | |

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**Enthalpy of mixing**

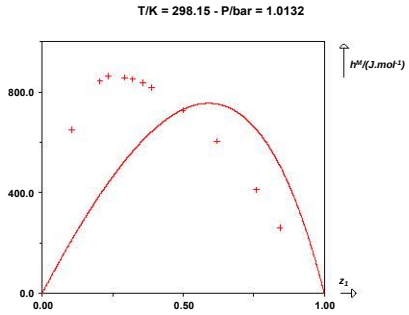
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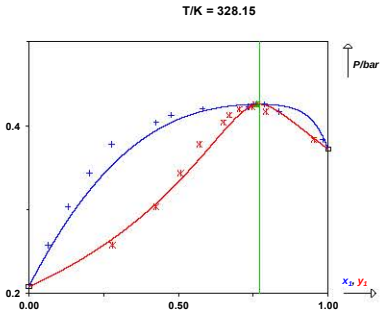
Letcher, Trevor M. - Schoonbaert, Fabienne E.Z. - Bean, Bruce, The molar excess enthalpies and volumes of 1-alkyne + methanol and + ethanol mixtures at 298.15 K, Fluid Phase Equilibria 1-2 (1990) 111-119. doi:10.1016/0378-3812(90)90008-B

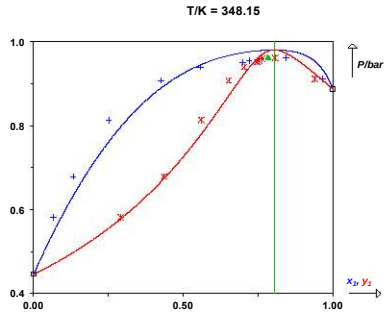
**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 650.00 | 0.1039 |
| 842.60 | 0.2045 |
| 863.00 | 0.2340 |
| 857.20 | 0.2917 |
| 850.20 | 0.3211 |
| 836.60 | 0.3566 |
| 816.60 | 0.3877 |
| 727.20 | 0.4988 |
| 605.80 | 0.6186 |
| 412.00 | 0.7585 |
| 261.20 | 0.8422 |


T/K = 298.15 - P/bar = 1.0132
$h^{M}$/(J.mol$^{-1}$)
800.0
400.0
0.0
0.00
0.50
1.00
$z_1$


T/K = 328.15
P/bar
0.4
0.2
0.00
0.50
1.00
$x_1$, $y_1$


T/K = 348.15
P/bar
1.0
0.8
0.6
0.4
0.00
0.50
1.00
$x_1$, $y_1$

## CHLOROFORM (1) + ACETONITRILE (2)

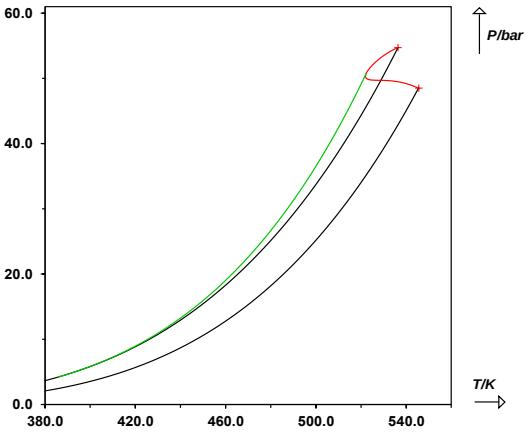
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 75-05-8 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | WEVYAHXRMPXWCK-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.40 | 545.50 |
| **$P_c$ / bar** | 54.72 | 48.50 |
| **ω** | 0.222 | 0.342 |

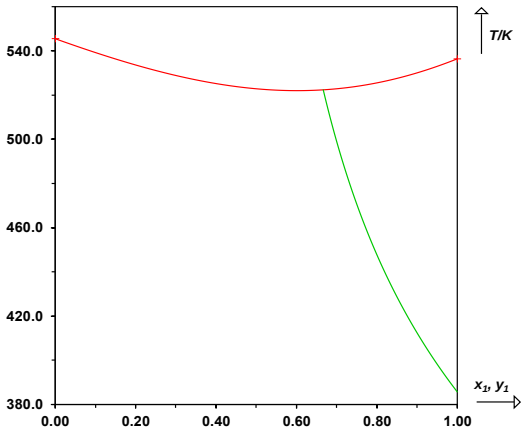
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 70.3
B/MPa = -104

*Deviations*
MAPE on x = 12 %
MAPE on y = 14 %
MAPE on $h^M$ = 60 %
MAPE on $c_P^M$ = 140 %



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**Isothermal phase equilibrium data**

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Lazarte, Manuel - Gómez Marigliano, Ana C. - Sólimo, Horacio N., Excess Molar Volume, Viscosity, and Molar Refraction Deviations, and Liquid?Vapor Equilibrium at 303.15 K for Chloroform + Acetonitrile Binary Mixture. An Infrared Study, Journal of Solution Chemistry 12 (2004) 1549-1563. doi:10.1007/s10953-004-1393-9

**T / K =** **303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1727 | 0.0750 | 0.1830 |
| 0.1840 | 0.1200 | 0.2570 |
| 0.2019 | 0.2120 | 0.3920 |
| 0.2160 | 0.2990 | 0.4990 |
| 0.2287 | 0.3680 | 0.5520 |
| 0.2446 | 0.4690 | 0.6460 |
| 0.2600 | 0.5550 | 0.7190 |
| 0.2800 | 0.6600 | 0.7950 |
| 0.2993 | 0.8040 | 0.8930 |
| 0.3079 | 0.8520 | 0.9160 |

Nagata, Isamu - Kawamura, Yuji, Excess thermodynamic functions and complex formation in binary liquid mixtures containing acetonitrile, Fluid Phase Equilibria 1 (1979) 1-11. doi:10.1016/0378-3812(79)80023-0

**T / K =** **328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4440 | 0.0400 | 0.0950 |
| 0.4897 | 0.1090 | 0.2320 |
| 0.5445 | 0.2300 | 0.3950 |
| 0.5929 | 0.3380 | 0.5090 |
| 0.6279 | 0.4240 | 0.5860 |
| 0.6767 | 0.5490 | 0.6930 |
| 0.7045 | 0.6380 | 0.7560 |
| 0.7546 | 0.7850 | 0.8620 |
| 0.7735 | 0.8590 | 0.9100 |
| 0.7983 | 0.9340 | 0.9550 |
| 0.7999 | 0.9380 | 0.9580 |

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**Isobaric phase equilibrium data**

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Mato, F. - Sanchez, M., Liquid-vapor equilibriums of binary mixtures of acetonitrile, Anales de la Real Sociedad Espanola de Fisica y Quimica, Serie B: Quimica (1967) 1-11.

**P / bar =** **1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 354.15 | 0.0150 | 0.0420 |
| 353.25 | 0.0350 | 0.0880 |
| 352.15 | 0.0570 | 0.1380 |
| 351.25 | 0.0790 | 0.1790 |
| 350.15 | 0.1070 | 0.2320 |
| 348.75 | 0.1470 | 0.2930 |
| 347.75 | 0.1780 | 0.3410 |
| 346.85 | 0.2130 | 0.3850 |
| 345.75 | 0.2520 | 0.4350 |
| 344.85 | 0.2930 | 0.4760 |
| 343.95 | 0.3340 | 0.5190 |
| 343.15 | 0.3790 | 0.5600 |
| 342.35 | 0.4240 | 0.6010 |
| 341.75 | 0.4620 | 0.6310 |
| 341.05 | 0.5020 | 0.6630 |
| 340.45 | 0.5430 | 0.6950 |
| 339.85 | 0.5790 | 0.7230 |
| 339.25 | 0.6160 | 0.7500 |
| 338.75 | 0.6440 | 0.7710 |
| 338.55 | 0.6630 | 0.7840 |
| 338.25 | 0.6860 | 0.8030 |
| 337.75 | 0.7110 | 0.8220 |
| 337.45 | 0.7420 | 0.8400 |
| 337.05 | 0.7690 | 0.8570 |
| 336.65 | 0.8060 | 0.8800 |
| 336.15 | 0.8620 | 0.9130 |
| 335.85 | 0.8840 | 0.9280 |
| 335.05 | 0.9660 | 0.9760 |

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**Enthalpy of mixing**

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Handa, Yash Paul - Jones, David Edward, Molar excess enthalpies of acetonitrile + chloroform and of acetonitrile + chloroform-d1 at 298 K, Canadian Journal of Chemistry 16 (1977) 2977-2979. doi:10.1139/v77-414

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -24.80 | 0.0140 |
| -79.30 | 0.0480 |
| -197.60 | 0.1160 |
| -325.10 | 0.1860 |
| -438.70 | 0.2490 |
| -534.70 | 0.3050 |
| -612.80 | 0.3530 |
| -683.10 | 0.4010 |
| -759.10 | 0.4770 |
| -810.30 | 0.5520 |

| | |
|---|---|
| -821.10 | 0.6250 |
| -751.40 | 0.7230 |
| -607.30 | 0.8100 |
| -365.60 | 0.9000 |
| -115.70 | 0.9720 |

Nagata, Isamura - Tamura, Kazuhiro, Excess enthalpies of acetonitrile + trichloromethane, + ethyl acetate, and + methyl acetate, and of (acetonitrile + trichloromethane) + ethyl acetate and + methyl acetate at 308.15 K, The Journal of Chemical Thermodynamics 8 (1983) 721-724. doi:10.1016/0021-9614(83)90138-6

**T / K =** **308.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -70.60 | 0.0442 |
| -205.80 | 0.1234 |
| -400.60 | 0.2355 |
| -527.80 | 0.3100 |
| -615.00 | 0.3645 |
| -678.40 | 0.4139 |
| -711.00 | 0.4423 |
| -760.40 | 0.5244 |
| -785.90 | 0.5932 |
| -778.70 | 0.6437 |
| -734.60 | 0.7137 |
| -601.40 | 0.8011 |
| -405.60 | 0.8819 |
| -203.40 | 0.9450 |
| -63.70 | 0.9825 |

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**Heat capacity of mixing**

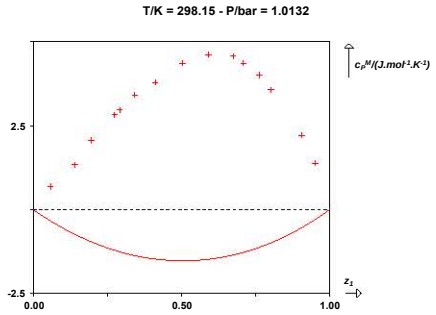
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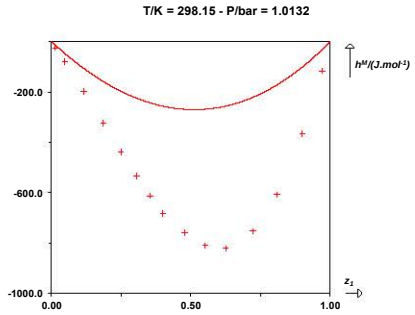
Zegers, H.C. - Somsen, G., Volumes and heat capacities of mixtures of dimethylformamide with several dialkylacetamides, Fluid Phase Equilibria 3 (1984) 299-311. doi:10.1016/0378-3812(84)85013-X

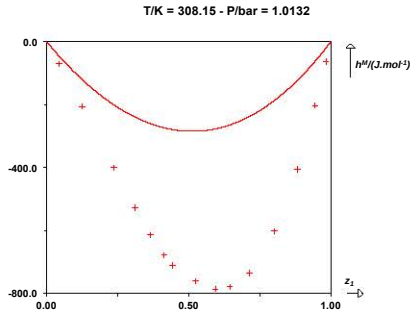
**T / K =** **298.15**

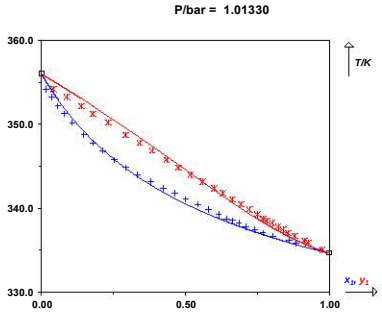
**P / bar =** **UNKNOWN (1.0132)**

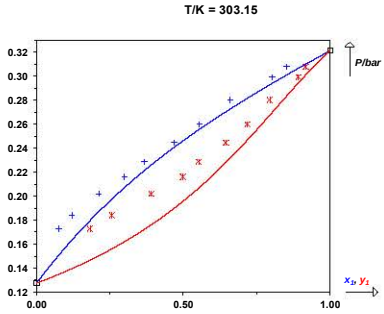
| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.6760 | 0.0577 |
| 1.334 | 0.1399 |
| 2.064 | 0.1950 |
| 2.822 | 0.2739 |
| 2.968 | 0.2914 |
| 3.407 | 0.3433 |
| 3.781 | 0.4111 |
| 4.357 | 0.5034 |
| 4.611 | 0.5907 |
| 4.566 | 0.6745 |
| 4.352 | 0.7100 |
| 3.993 | 0.7631 |
| 3.566 | 0.8034 |
| 2.207 | 0.9063 |
| 1.373 | 0.9517 |

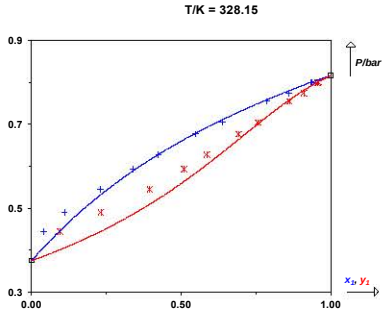

T/K = 298.15 - P/bar = 1.0132
$c_p^M/(J.mol^{-1}.K^{-1})$
2.5
-2.5
0.00
0.50
1.00
$z_1$


T/K = 298.15 - P/bar = 1.0132
$h^M/(J.mol^{-1})$
-200.0
-600.0
-1000.0
0.00
0.50
1.00
$z_1$


T/K = 308.15 - P/bar = 1.0132
$h^M/(J.mol^{-1})$
0.0
-400.0
-800.0
0.00
0.50
1.00
$z_1$


P/bar = 1.01330
T/K
360.0
350.0
340.0
330.0
0.00
0.50
1.00
$x_1, y_1$


T/K = 303.15
P/bar
0.32
0.30
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.00
0.50
1.00
$x_1, y_1$


T/K = 328.15
P/bar
0.9
0.7
0.5
0.3
0.00
0.50
1.00
$x_1, y_1$

## ETHYL FORMATE (1) + CHLOROFORM (2)

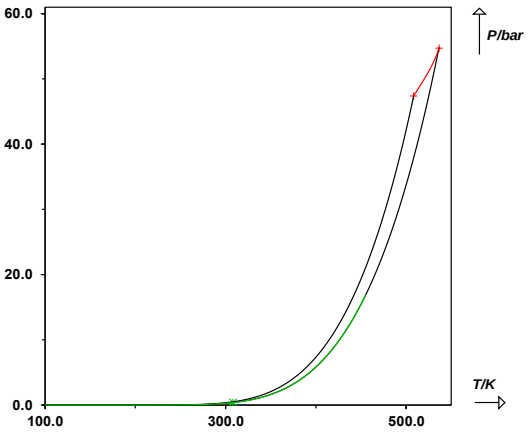
| | | |
|---|---|---|
| **CAS** | 109-94-4 | 67-66-3 |
| **InChiKey** | WBJINCZRORDGAQ-UHFFFAOYSA-N | HEDRZPFGACZZDS-UHFFFAOYSA-N |
| **$T_c$ / K** | 508.40 | 536.40 |
| **$P_c$ / bar** | 47.40 | 54.72 |
| **ω** | 0.285 | 0.222 |

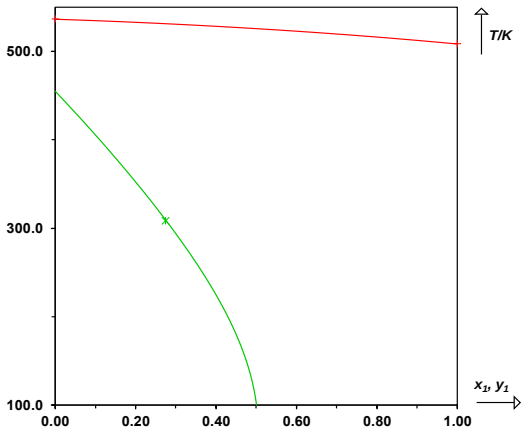
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = -121
B/MPa = -302

*Deviations*
MAPE on x = 7.2 %
MAPE on y = 7.0 %
MAPE on $x_{az}$ = 0.95 %
MAPE on $P_{az}$ = 0.31 %
MAPE on $h^M$ = 14 %



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**Isothermal phase equilibrium data**

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Ohta, Tatsuhiko - Asano, Hisashi - Nagata, Isamu, Thermodynamic study of complex formation in four binary liquid mixtures containing chloroform, Fluid Phase Equilibria 1-2 (1980) 105-114. doi:10.1016/0378-3812(80)80008-2

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.3894 | 0.0410 | 0.0290 | |
| 0.3817 | 0.1280 | 0.1100 | |
| 0.3765 | 0.1890 | 0.1720 | |
| 0.3750 | 0.2360 | 0.2240 | |
| 0.3733 | 0.2730 | 0.2710 | |
| 0.3733 | 0.2740 | 0.2740 | AZEO |
| 0.3760 | 0.3570 | 0.3820 | |
| 0.3848 | 0.4540 | 0.5080 | |
| 0.3898 | 0.5050 | 0.5670 | |
| 0.4001 | 0.5800 | 0.6590 | |
| 0.4228 | 0.7210 | 0.7980 | |
| 0.4418 | 0.8000 | 0.8640 | |
| 0.4672 | 0.8970 | 0.9380 | |
| 0.4773 | 0.9440 | 0.9680 | |

Ohta, Tatsuhiko - Asano, Hisashi - Nagata, Isamu, Thermodynamic study of complex formation in four binary liquid mixtures containing chloroform, Fluid Phase Equilibria 1-2 (1980) 105-114. doi:10.1016/0378-3812(80)80008-2

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5642 | 0.0580 | 0.0440 |
| 0.5526 | 0.1900 | 0.1790 |
| 0.5541 | 0.2160 | 0.2120 |
| 0.5646 | 0.3960 | 0.4350 |
| 0.5748 | 0.4660 | 0.5250 |
| 0.5788 | 0.4900 | 0.5560 |
| 0.6102 | 0.6220 | 0.7050 |
| 0.6227 | 0.6740 | 0.7580 |
| 0.6698 | 0.8460 | 0.8980 |
| 0.6930 | 0.9050 | 0.9410 |

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**Enthalpy of mixing**

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Ortega, J., Excess enthalpy. Trichloromethane-ethyl methanoate system, Int. Data Ser. Sel. Data Mixtures Ser. A 1 (1993)

**T / K = 298.15**

**P / bar = 1.010**

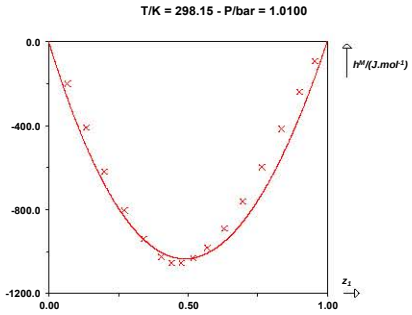
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -200.70 | 0.0689 |
| -411.20 | 0.1356 |
| -620.70 | 0.2004 |
| -804.40 | 0.2722 |
| -940.80 | 0.3419 |
| -1025.7 | 0.4045 |
| -1054.7 | 0.4415 |
| -1054.3 | 0.4769 |
| -1031.4 | 0.5198 |
| -982.80 | 0.5694 |
| -891.70 | 0.6309 |
| -762.80 | 0.6968 |
| -599.50 | 0.7665 |
| -416.30 | 0.8367 |
| -239.00 | 0.8999 |
| -93.20 | 0.9568 |

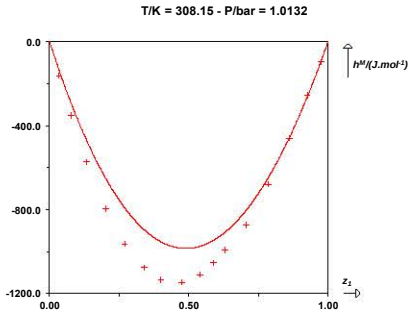
Ohta, Tatsuhiko - Asano, Hisashi - Nagata, Isamu, Thermodynamic study of complex formation in four binary liquid mixtures containing chloroform, Fluid Phase Equilibria 1-2 (1980) 105-114. doi:10.1016/0378-3812(80)80008-2

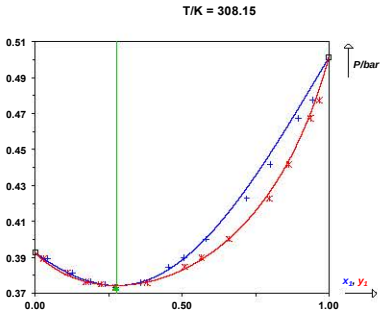
**T / K = 308.15**

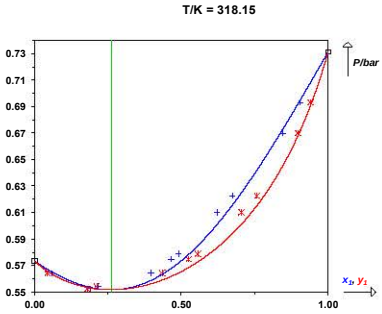
**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -162.00 | 0.0340 |
| -351.80 | 0.0770 |
| -573.80 | 0.1330 |
| -797.00 | 0.2010 |
| -963.90 | 0.2700 |
| -1077.8 | 0.3400 |
| -1136.1 | 0.4010 |
| -1147.4 | 0.4750 |
| -1109.7 | 0.5400 |
| -1054.4 | 0.5890 |
| -992.80 | 0.6300 |
| -873.30 | 0.7060 |
| -678.70 | 0.7850 |
| -460.20 | 0.8610 |
| -255.70 | 0.9260 |
| -97.10 | 0.9740 |


T/K = 298.15 - P/bar = 1.0100
0.0
-400.0
-800.0
-1200.0
0.00
0.50
1.00
$h^M$/(J.mol$^{-1}$)
$z_1$


T/K = 308.15 - P/bar = 1.0132
0.0
-400.0
-800.0
-1200.0
0.00
0.50
1.00
$h^M$/(J.mol$^{-1}$)
$z_1$


T/K = 308.15
0.51
0.49
0.47
0.45
0.43
0.41
0.39
0.37
0.00
0.50
1.00
P/bar
$x_1$, $y_1$


T/K = 318.15
0.73
0.71
0.69
0.67
0.65
0.63
0.61
0.59
0.57
0.55
0.00
0.50
1.00
P/bar
$x_1$, $y_1$

## CHLOROFORM (1) + 1-PROPANOL (2)

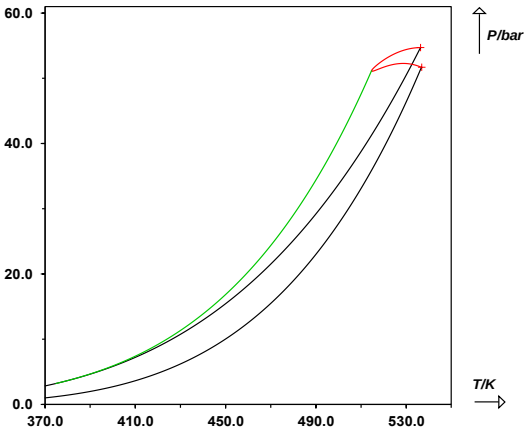
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 71-23-8 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | BDERNNFJNOPAEC-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.40 | 536.80 |
| **$P_c$ / bar** | 54.72 | 51.69 |
| **ω** | 0.222 | 0.621 |

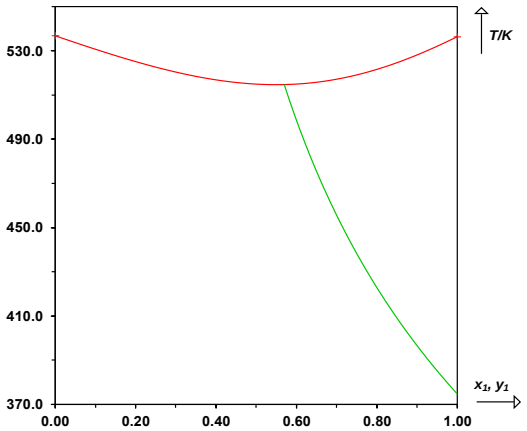
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 186
B/MPa = -56.8

*Deviations*
MAPE on x = 14 %
MAPE on y = 13 %
MAPE on $h^M$ = 97 %



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**Isothermal phase equilibrium data**

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Nagata, Isamu, Isothermal (vapour + liquid) equilibria of propan-1-ol + acetonitrile and + trichloromethane and of (propan-1-ol + acetonitrile + trichloromethane), The Journal of Chemical Thermodynamics 11 (1985) 1017-1022. doi:10.1016/0021-9614(85)90086-2

**T / K =** **328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3396 | 0.1670 | 0.6110 |
| 0.4380 | 0.2660 | 0.7310 |
| 0.4698 | 0.3000 | 0.7490 |
| 0.5766 | 0.4230 | 0.8220 |
| 0.6645 | 0.5580 | 0.8740 |
| 0.7507 | 0.7690 | 0.9150 |
| 0.7719 | 0.8270 | 0.9300 |
| 0.7845 | 0.8660 | 0.9400 |
| 0.8059 | 0.9320 | 0.9640 |

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**Isobaric phase equilibrium data**

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Wang Shouyu - Cai Shuxing, VLE Data for Chloroform - n-Propanol and its System Containing Salt, Huaxue Gongcheng 5 (1994) 36-40.

**P / bar =** **1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 365.65 | 0.0480 | 0.2040 |
| 362.25 | 0.0930 | 0.3460 |
| 357.45 | 0.1570 | 0.4990 |
| 355.05 | 0.1940 | 0.5650 |
| 351.35 | 0.2530 | 0.6560 |
| 347.85 | 0.3270 | 0.7360 |
| 344.35 | 0.4030 | 0.7920 |
| 342.05 | 0.4960 | 0.8400 |
| 340.35 | 0.5610 | 0.8680 |
| 338.45 | 0.6640 | 0.8940 |
| 337.35 | 0.7530 | 0.9120 |
| 336.05 | 0.8600 | 0.9390 |
| 335.25 | 0.9400 | 0.9690 |
| 334.85 | 0.9840 | 0.9870 |

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**Enthalpy of mixing**

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Nagata, I. - Kawamura, Y. - Asano, H. - Fujiwara, K. - Ogasawara, Y., Excess Enthalpies for Binary Mixtures of Chloroform with Alcohols, Z. Phys. Chem. Leipzig 6 (1978) 1109-1116.

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -76.90 | 0.0171 |
| -214.60 | 0.0556 |
| -364.30 | 0.1184 |
| -411.50 | 0.1701 |
| -394.30 | 0.2351 |
| -334.50 | 0.2868 |
| -232.60 | 0.3453 |
| -141.80 | 0.3887 |
| -47.80 | 0.4306 |
| 36.20 | 0.4668 |
| 263.10 | 0.5667 |
| 403.00 | 0.6369 |
| 510.80 | 0.7037 |
| 573.80 | 0.7601 |
| 601.50 | 0.8190 |
| 589.50 | 0.8569 |
| 445.00 | 0.9326 |
| 227.50 | 0.9739 |

Hirobe, H., Thermochemical studies, J. Fac. Sci. Univ. Tokyo Sect. 1 4 (1926) 155-222.

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -211.85 | 0.0486 |
| -415.33 | 0.1640 |
| -342.06 | 0.2794 |
| -244.51 | 0.3399 |
| 131.47 | 0.5011 |
| 151.56 | 0.5123 |
| 515.81 | 0.6823 |
| 586.99 | 0.7411 |
| 636.81 | 0.8347 |
| 449.66 | 0.9359 |

Nagata, I. - Kawamura, Y. - Asano, H. - Fujiwara, K. - Ogasawara, Y., Excess Enthalpies for Binary Mixtures of Chloroform with Alcohols, Z. Phys. Chem. Leipzig 6 (1978) 1109-1116.

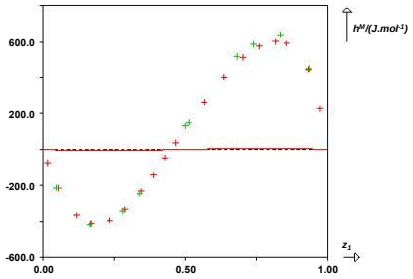
**T / K =** **308.15**

**P / bar =** **UNKNOWN (1.0132)**

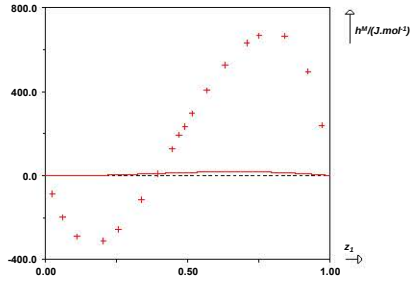
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -88.00 | 0.0226 |
| -197.90 | 0.0586 |
| -291.90 | 0.1103 |
| -311.30 | 0.2020 |

| | |
|---|---|
| -256.60 | 0.2552 |
| -113.80 | 0.3363 |
| 9.800 | 0.3935 |
| 126.40 | 0.4438 |
| 193.10 | 0.4698 |
| 233.50 | 0.4903 |
| 295.20 | 0.5147 |
| 404.20 | 0.5659 |
| 526.40 | 0.6314 |
| 631.50 | 0.7069 |
| 667.40 | 0.7507 |
| 664.00 | 0.8388 |
| 494.40 | 0.9223 |
| 239.60 | 0.9709 |

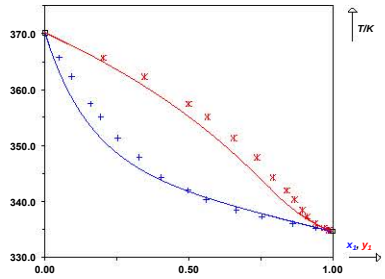
T/K = 298.15 - P/bar = 1.0132 1.0132



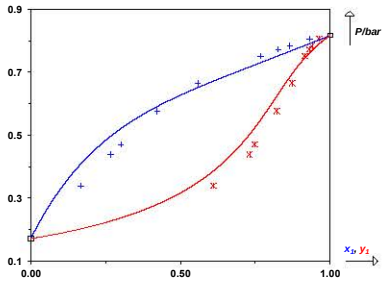

T/K = 308.15 - P/bar = 1.0132




P/bar = 1.01300




T/K = 328.15



## n-PROPYL FORMATE (1) + 1,1,2,2-TETRACHLOROETHANE (2)

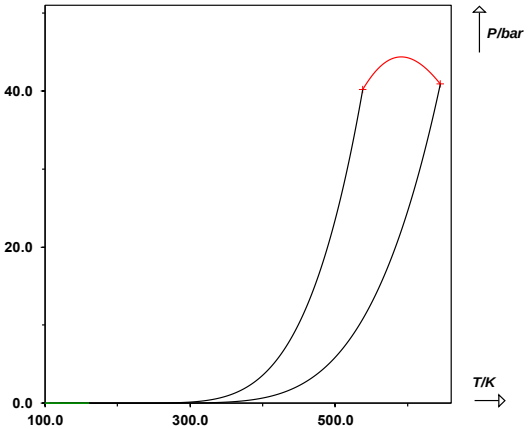
| | | |
|---|---|---|
| **CAS** | 110-74-7 | 79-34-5 |
| **InChiKey** | KFNNIILCVOLYIR-UHFFFAOYSA-N | QPFMBZIOSGYJDE-UHFFFAOYSA-N |
| **$T_c$ / K** | 538.00 | 645.00 |
| **$P_c$ / bar** | 40.20 | 40.90 |
| **ω** | 0.309 | 0.247 |

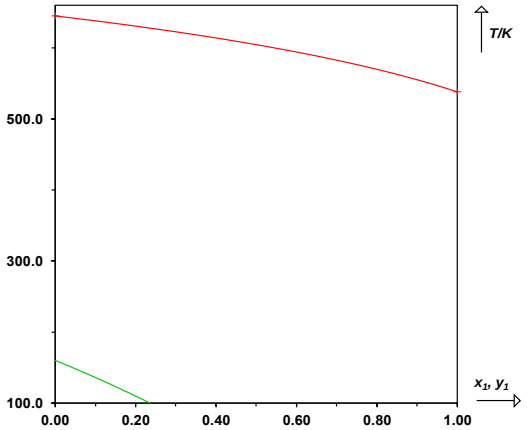
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = -168
B/MPa = -352

*Deviations*
MAPE on x = 6.2 %
MAPE on y = 11 %
MAPE on $h^M$ = 11 %



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**Isothermal phase equilibrium data**

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Narbutt, J. v., Die Schmelz-, Siede- und Dampfkurven (760 mm Druck) in den binären Systemen: Ortho- + Para-, Ortho- + Meta-, Para- + Metabromnitrobenzol, und die Schmelzkurven der Gemische von Diphenylamin und Phenanthren, Zeitschrift für Physikalische Chemie 1 (1905) doi:10.1515/zpch-1905-5337

**T / K = 330.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1178 | 0.2965 | 0.7416 |
| 0.1329 | 0.3406 | 0.7851 |
| 0.1464 | 0.3780 | 0.8178 |
| 0.1656 | 0.4213 | 0.8572 |
| 0.2093 | 0.5196 | 0.9155 |
| 0.2277 | 0.5606 | 0.9317 |
| 0.2505 | 0.6088 | 0.9470 |
| 0.2709 | 0.6514 | 0.9561 |
| 0.2912 | 0.6877 | 0.9645 |
| 0.3106 | 0.7270 | 0.9706 |
| 0.3290 | 0.7666 | 0.9728 |
| 0.3499 | 0.8090 | 0.9766 |
| 0.3935 | 0.8977 | 0.9917 |
| 0.4098 | 0.9324 | 0.9932 |
| 0.4278 | 0.9713 | 0.9970 |

Narbutt, J. v., Die Schmelz-, Siede- und Dampfkurven (760 mm Druck) in den binären Systemen: Ortho- + Para-, Ortho- + Meta-, Para- + Metabromnitrobenzol, und die Schmelzkurven der Gemische von Diphenylamin und Phenanthren, Zeitschrift für Physikalische Chemie 1 (1905) doi:10.1515/zpch-1905-5337

**T / K = 350.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1234 | 0.0651 | 0.2539 |
| 0.1339 | 0.0857 | 0.3172 |
| 0.1460 | 0.0997 | 0.3886 |
| 0.1679 | 0.1481 | 0.4911 |
| 0.2225 | 0.2411 | 0.6555 |
| 0.2668 | 0.3046 | 0.7392 |
| 0.2915 | 0.3334 | 0.7739 |
| 0.3286 | 0.3780 | 0.8170 |
| 0.3583 | 0.4178 | 0.8454 |
| 0.4085 | 0.4755 | 0.8799 |
| 0.4454 | 0.5161 | 0.9008 |
| 0.5257 | 0.6037 | 0.9332 |
| 0.5717 | 0.6505 | 0.9462 |
| 0.6059 | 0.6861 | 0.9569 |
| 0.6828 | 0.7674 | 0.9713 |
| 0.7212 | 0.8074 | 0.9789 |
| 0.8075 | 0.8954 | 0.9895 |
| 0.8407 | 0.9324 | 0.9932 |
| 0.8750 | 0.9706 | 0.9970 |

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**Enthalpy of mixing**

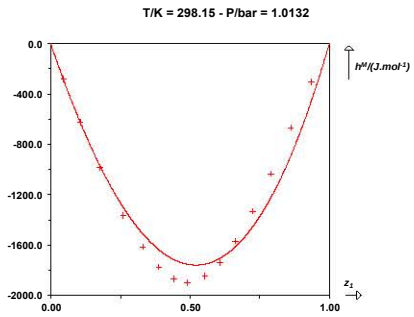
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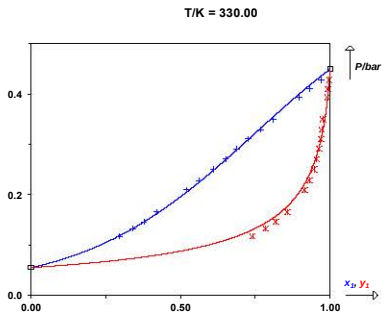
Fenby, D.V. - Scott, R.L., Excess enthalpy. Hexafluorobenzene-benzene system, Int. Data Ser. Sel. Data Mixtures Ser. A 2 (1975) 130-138.

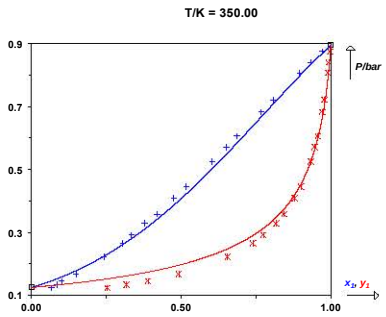
**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -279.60 | 0.0455 |
| -622.30 | 0.1058 |
| -984.30 | 0.1754 |
| -1365.2 | 0.2602 |
| -1614.7 | 0.3298 |
| -1773.9 | 0.3889 |
| -1868.8 | 0.4414 |
| -1897.4 | 0.4899 |
| -1844.1 | 0.5535 |
| -1737.2 | 0.6072 |
| -1566.9 | 0.6635 |
| -1330.9 | 0.7248 |
| -1034.3 | 0.7906 |
| -668.00 | 0.8615 |
| -303.90 | 0.9358 |


T/K = 298.15 - P/bar = 1.0132
0.0
-400.0
-800.0
-1200.0
-1600.0
-2000.0
0.00
0.50
1.00
hᴱ/(J.mol⁻¹)
z₁


T/K = 330.00
0.4
0.2
0.0
0.00
0.50
1.00
P/bar
x₁, y₁


T/K = 350.00
0.9
0.7
0.5
0.3
0.1
0.00
0.50
1.00
P/bar
x₁, y₁

## ETHANOL (1) + CHLOROFORM (2)

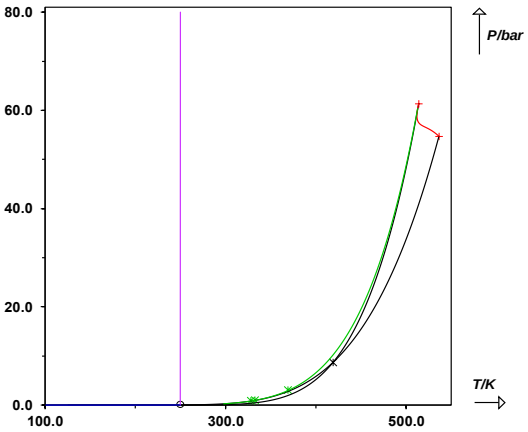
| | | |
|---|---|---|
| **CAS** | 64-17-5 | 67-66-3 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | HEDRZPFGACZZDS-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 536.40 |
| **$P_c$ / bar** | 61.37 | 54.72 |
| **ω** | 0.644 | 0.222 |

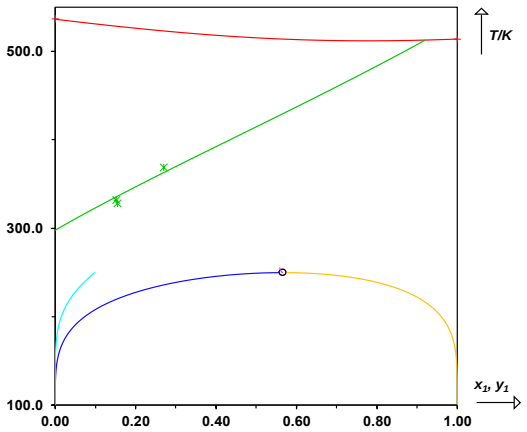
Non ideal with entropic causes

**PPR78 results**

*Parameters*
A/MPa = 300
B/MPa = 600

*Deviations*
MAPE on x = 19 %
MAPE on y = 9.1 %
MAPE on $x_{az}$ = 8.3 %
MAPE on $P_{az}$ = 4.4 %
MAPE on $h^M$ = 2200 %



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**Isothermal phase equilibrium data**

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Scatchard, George - Raymond, C. L., Vapor—Liquid Equilibrium. II. Chloroform—Ethanol Mixtures at 35, 45 and 55°, Journal of the American Chemical Society 6 (1938) 1278-1287. doi:10.1021/ja01273a002

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1398 | 0.9938 | 0.9746 |
| 0.1484 | 0.9759 | 0.9009 |
| 0.1515 | 0.9703 | 0.8790 |
| 0.1647 | 0.9458 | 0.7846 |
| 0.1678 | 0.9406 | 0.7657 |
| 0.1977 | 0.8891 | 0.6115 |
| 0.2368 | 0.8270 | 0.4696 |
| 0.2742 | 0.7639 | 0.3793 |
| 0.3001 | 0.7127 | 0.3253 |
| 0.3056 | 0.6986 | 0.3130 |
| 0.3153 | 0.6773 | 0.2991 |
| 0.3378 | 0.6155 | 0.2630 |
| 0.3404 | 0.6078 | 0.2588 |
| 0.3568 | 0.5616 | 0.2354 |
| 0.3654 | 0.5173 | 0.2203 |
| 0.3892 | 0.3815 | 0.1819 |
| 0.3959 | 0.3217 | 0.1673 |
| 0.4040 | 0.2254 | 0.1446 |
| 0.4072 | 0.1735 | 0.1302 |
| 0.4068 | 0.1577 | 0.1248 |
| 0.4083 | 0.1517 | 0.1217 |
| 0.4080 | 0.0685 | 0.0839 |
| 0.4065 | 0.0440 | 0.0637 |
| 0.4055 | 0.0414 | 0.0615 |
| 0.4049 | 0.0400 | 0.0597 |
| 0.4052 | 0.0384 | 0.0586 |

Scatchard, George - Raymond, C. L., Vapor—Liquid Equilibrium. II. Chloroform—Ethanol Mixtures at 35, 45 and 55°, Journal of the American Chemical Society 6 (1938) 1278-1287. doi:10.1021/ja01273a002

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2413 | 0.9843 | 0.9400 |
| 0.2435 | 0.9811 | 0.9284 |
| 0.2661 | 0.9524 | 0.8283 |
| 0.2859 | 0.9288 | 0.7533 |
| 0.3332 | 0.8740 | 0.6026 |
| 0.3974 | 0.8003 | 0.4634 |
| 0.3995 | 0.7989 | 0.4605 |
| 0.4395 | 0.7431 | 0.3940 |
| 0.4742 | 0.6884 | 0.3443 |
| 0.4867 | 0.6702 | 0.3286 |
| 0.5220 | 0.5985 | 0.2857 |
| 0.5385 | 0.5561 | 0.2660 |
| 0.5608 | 0.4860 | 0.2397 |
| 0.5670 | 0.4595 | 0.2297 |
| 0.5851 | 0.3717 | 0.2046 |
| 0.5975 | 0.2852 | 0.1809 |
| 0.6074 | 0.1794 | 0.1484 |
| 0.6077 | 0.1148 | 0.1217 |
| 0.6060 | 0.0900 | 0.1067 |
| 0.6053 | 0.0875 | 0.1054 |
| 0.6050 | 0.0837 | 0.1026 |
| 0.5979 | 0.0443 | 0.0681 |
| 0.5938 | 0.0323 | 0.0546 |
| 0.5907 | 0.0242 | 0.0421 |
| 0.5865 | 0.0134 | 0.0273 |

Roeck, H. - Schroeder, W., Beitrag zur Kenntnis des Konzentrationsverlaufs thermodynamischer Mischungsfunktionen, Z. Phys. Chem. NF (1956) 277-284.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3946 | 0.9790 | 0.9250 |
| 0.4913 | 0.8940 | 0.6790 |
| 0.5502 | 0.8400 | 0.5720 |
| 0.6062 | 0.7890 | 0.4870 |
| 0.6533 | 0.7410 | 0.4280 |
| 0.6931 | 0.6970 | 0.3840 |
| 0.7215 | 0.6570 | 0.3530 |
| 0.7495 | 0.6150 | 0.3300 |

Bourrelly, Viviane - Chevalier, Jean-Louis, Appareil pour la détermination rapide des équilibres isothermes liquide-vapeur, Journal de Chimie Physique (1968) 1561-1564. doi:10.1051/jcp/1968651561

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3986 | 0.9750 | 0.9090 |
| 0.4380 | 0.9410 | 0.8040 |
| 0.4806 | 0.9080 | 0.7040 |
| 0.5633 | 0.8400 | 0.5640 |
| 0.6046 | 0.8080 | 0.5000 |
| 0.6173 | 0.7870 | 0.4790 |
| 0.7033 | 0.6920 | 0.3760 |
| 0.7466 | 0.6300 | 0.3380 |
| 0.7559 | 0.6030 | 0.3200 |
| 0.7753 | 0.5750 | 0.3070 |
| 0.7919 | 0.5380 | 0.2890 |

| | | | |
|---|---|---|---|
| 0.8006 | 0.5170 | 0.2800 | |
| 0.8113 | 0.4900 | 0.2700 | |
| 0.8173 | 0.4830 | 0.2640 | |
| 0.8499 | 0.3400 | 0.2160 | |
| 0.8599 | 0.3050 | 0.2070 | |
| 0.8673 | 0.2340 | 0.1810 | |
| 0.8706 | 0.1850 | 0.1650 | |
| 0.8713 | 0.1740 | 0.1590 | |
| 0.8719 | 0.1560 | 0.1520 | |
| 0.8719 | 0.1540 | 0.1540 | AZEO |
| 0.8686 | 0.1010 | 0.1240 | |
| 0.8626 | 0.0720 | 0.1000 | |
| 0.8506 | 0.0600 | 0.0900 | |
| 0.8359 | 0.0330 | 0.0620 | |

Scatchard, George - Raymond, C. L., Vapor—Liquid Equilibrium. II. Chloroform—Ethanol Mixtures at 35, 45 and 55°, Journal of the American Chemical Society 6 (1938) 1278-1287. doi:10.1021/ja01273a002

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4085 | 0.9669 | 0.8838 |
| 0.4532 | 0.9288 | 0.7698 |
| 0.4625 | 0.9198 | 0.7467 |
| 0.4893 | 0.8971 | 0.6877 |
| 0.5438 | 0.8521 | 0.5965 |
| 0.5880 | 0.8131 | 0.5205 |
| 0.6258 | 0.7799 | 0.4729 |
| 0.6783 | 0.7194 | 0.4058 |
| 0.7247 | 0.6588 | 0.3593 |
| 0.7276 | 0.6555 | 0.3581 |
| 0.7469 | 0.6233 | 0.3359 |
| 0.7556 | 0.6096 | 0.3280 |
| 0.7586 | 0.6035 | 0.3240 |
| 0.7986 | 0.5206 | 0.2839 |
| 0.8315 | 0.4270 | 0.2473 |
| 0.8428 | 0.3789 | 0.2361 |
| 0.8553 | 0.3149 | 0.2143 |
| 0.8623 | 0.2731 | 0.1990 |
| 0.8679 | 0.2236 | 0.1819 |
| 0.8707 | 0.1610 | 0.1583 |
| 0.8671 | 0.0963 | 0.1202 |
| 0.8589 | 0.0570 | 0.0850 |
| 0.8357 | 0.0348 | 0.0592 |

Hala, E. - Fried, V. - Pick, J. - Vilim, O., Liquid-vapor equilibria. VII. Calculation of liquid-vapor equilibria in two-component systems from isothermal p-x curves, Chem. Listy (1953) 1423-1427.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3836 | 0.9900 | 0.9615 |
| 0.3866 | 0.9872 | 0.9532 |
| 0.4000 | 0.9760 | 0.9095 |
| 0.4266 | 0.9510 | 0.8350 |
| 0.4533 | 0.9275 | 0.7610 |
| 0.5066 | 0.8825 | 0.6520 |
| 0.5600 | 0.8375 | 0.5540 |
| 0.6133 | 0.7900 | 0.4870 |
| 0.6666 | 0.7340 | 0.4110 |
| 0.7199 | 0.6660 | 0.3670 |
| 0.7733 | 0.5760 | 0.3110 |
| 0.8266 | 0.4195 | 0.2550 |
| 0.8650 | 0.0830 | 0.1110 |
| 0.8567 | 0.0510 | 0.0780 |
| 0.8485 | 0.0325 | 0.0600 |
| 0.8319 | 0.0100 | 0.0200 |

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**Isobaric phase equilibrium data**

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Orchillés, A. Vicent - Miguel, Pablo J. - Vercher, Ernesto - Martínez-Andreu, Antoni, Isobaric Vapor−Liquid and Liquid−Liquid Equilibria for Chloroform + Ethanol + 1-Ethyl-3-methylimidazolium Trifluoromethanesulfonate at 100 kPa, Journal of Chemical & Engineering Data 11 (2008) 2642-2648. doi:10.1021/je800548t

**P / bar = 1.0000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 350.29 | 0.9840 | 0.9510 |
| 349.54 | 0.9710 | 0.9110 |
| 348.30 | 0.9470 | 0.8490 |
| 347.13 | 0.9260 | 0.7920 |
| 345.70 | 0.8980 | 0.7320 |
| 344.13 | 0.8620 | 0.6540 |
| 342.39 | 0.8220 | 0.5850 |
| 340.48 | 0.7740 | 0.5120 |
| 338.66 | 0.7160 | 0.4470 |
| 337.04 | 0.6530 | 0.3910 |
| 335.84 | 0.6020 | 0.3540 |
| 334.92 | 0.5430 | 0.3160 |
| 334.29 | 0.4950 | 0.2890 |
| 333.75 | 0.4500 | 0.2680 |
| 333.35 | 0.4090 | 0.2510 |
| 333.03 | 0.3680 | 0.2350 |
| 332.78 | 0.3260 | 0.2180 |
| 332.59 | 0.2910 | 0.2060 |
| 332.49 | 0.2650 | 0.1970 |
| 332.34 | 0.2310 | 0.1850 |

| | | |
|---|---|---|
| 332.20 | 0.1400 | 0.1460 |
| 332.27 | 0.1110 | 0.1310 |
| 332.37 | 0.0890 | 0.1150 |
| 332.53 | 0.0680 | 0.0980 |
| 332.77 | 0.0490 | 0.0740 |
| 333.07 | 0.0300 | 0.0520 |
| 333.44 | 0.0150 | 0.0290 |

Chen, Geng-Hua - Wang, Qi - Ma, Zhong-Min - Yan, Xin-Huan - Han, Shi-Jun, Phase equilibria at superatmospheric pressures for systems containing halohydrocarbon, aromatic hydrocarbon, and alcohol, Journal of Chemical & Engineering Data 2 (1995) 361-366. doi:10.1021/je00018a003

**P / bar = 3.025**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 381.62 | 0.9936 | 0.9864 |
| 380.48 | 0.9617 | 0.9134 |
| 380.11 | 0.9525 | 0.8945 |
| 379.45 | 0.9391 | 0.8676 |
| 379.03 | 0.9275 | 0.8458 |
| 378.16 | 0.9090 | 0.8126 |
| 377.39 | 0.8892 | 0.7712 |
| 376.58 | 0.8654 | 0.7321 |
| 375.72 | 0.8412 | 0.6988 |
| 374.70 | 0.8078 | 0.6528 |
| 373.68 | 0.7690 | 0.6086 |
| 372.97 | 0.7369 | 0.5753 |
| 372.66 | 0.7103 | 0.5553 |
| 372.10 | 0.6828 | 0.5319 |
| 371.66 | 0.6587 | 0.5088 |
| 371.16 | 0.6371 | 0.4887 |
| 370.71 | 0.6000 | 0.4595 |
| 370.69 | 0.5760 | 0.4500 |
| 370.27 | 0.5555 | 0.4264 |
| 370.05 | 0.5280 | 0.4187 |
| 369.93 | 0.5126 | 0.3999 |
| 369.72 | 0.4818 | 0.3840 |
| 368.91 | 0.3705 | 0.3215 |
| 368.88 | 0.3378 | 0.3073 |
| 368.70 | 0.3110 | 0.2914 |
| 368.67 | 0.2887 | 0.2811 |
| 368.80 | 0.2701 | 0.2700 |
| 368.76 | 0.2319 | 0.2466 |
| 368.78 | 0.2059 | 0.2277 |
| 368.86 | 0.1961 | 0.2209 |
| 368.88 | 0.1911 | 0.2200 |
| 369.20 | 0.1508 | 0.1887 |
| 369.23 | 0.1348 | 0.1731 |
| 369.49 | 0.1119 | 0.1545 |
| 369.66 | 0.0858 | 0.1266 |
| 370.43 | 0.0537 | 0.0879 |
| 370.78 | 0.0372 | 0.0645 |
| 371.74 | 0.0077 | 0.0136 |

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**Enthalpy of mixing**

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Nagata, I. - Kawamura, Y. - Asano, H. - Fujiwara, K. - Ogasawara, Y., Excess Enthalpies for Binary Mixtures of Chloroform with Alcohols, Z. Phys. Chem. Leipzig 6 (1978) 1109-1116.

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -45.10 | 0.9919 |
| -106.70 | 0.9802 |
| -257.40 | 0.9485 |
| -369.20 | 0.9198 |
| -532.10 | 0.8614 |
| -605.70 | 0.8101 |
| -622.60 | 0.7707 |
| -613.50 | 0.7362 |
| -595.20 | 0.7099 |
| -526.70 | 0.6541 |
| -420.30 | 0.5960 |
| -276.90 | 0.5307 |
| -185.30 | 0.4902 |
| -70.90 | 0.4406 |
| -13.40 | 0.4146 |
| 29.60 | 0.3946 |
| 115.90 | 0.3530 |
| 232.10 | 0.2897 |
| 302.20 | 0.2442 |
| 353.40 | 0.1963 |
| 371.40 | 0.1683 |
| 377.80 | 0.1425 |
| 377.60 | 0.1233 |
| 360.30 | 0.0930 |
| 342.10 | 0.0786 |
| 317.90 | 0.0626 |
| 247.00 | 0.0410 |
| 161.70 | 0.0234 |
| 80.70 | 0.0105 |

Shatas, Joseph P. - Abbott, Michael M. - Van Ness, Hendrick C., Excess thermodynamic functions for ternary systems. II. Chloroform-ethanol-n-heptane at

50°C, Journal of Chemical & Engineering Data 4 (1975) 406-409. doi:10.1021/je60067a020

**T / K = 303.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -68.80 | 0.9880 |
| -101.30 | 0.9817 |
| -179.10 | 0.9660 |
| -244.40 | 0.9518 |
| -344.60 | 0.9264 |
| -451.10 | 0.8925 |
| -565.30 | 0.8291 |
| -581.00 | 0.8081 |
| -585.00 | 0.7699 |
| -566.10 | 0.7364 |
| -561.90 | 0.7319 |
| -557.80 | 0.7279 |
| -519.60 | 0.6927 |
| -508.00 | 0.6779 |
| -468.50 | 0.6514 |
| -424.40 | 0.6280 |
| -369.10 | 0.6017 |
| -197.10 | 0.5396 |
| -135.40 | 0.5146 |
| -66.10 | 0.4863 |
| -1.900 | 0.4609 |
| 117.10 | 0.4142 |
| 186.50 | 0.3828 |
| 266.90 | 0.3453 |
| 360.30 | 0.2959 |
| 436.60 | 0.2481 |
| 470.50 | 0.2228 |
| 495.90 | 0.2005 |
| 510.00 | 0.1761 |
| 515.80 | 0.1480 |
| 505.30 | 0.1216 |
| 486.00 | 0.1037 |
| 420.50 | 0.0721 |
| 329.20 | 0.0468 |
| 184.70 | 0.0222 |
| 123.30 | 0.0140 |
| 25.10 | 0.0029 |

Roach, Mark - Van Ness, Hendrick C., Excess thermodynamic functions for ternary systems. 10. HE and SE for ethanol/chloroform/1,4-dioxane at 50°C, Journal of Chemical & Engineering Data 2 (1984) 181-183. doi:10.1021/je00036a026

**T / K = 323.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -47.80 | 0.9893 |
| -130.30 | 0.9681 |
| -196.10 | 0.9483 |
| -262.40 | 0.9238 |
| -309.70 | 0.9006 |
| -361.90 | 0.8558 |
| -369.40 | 0.8173 |
| -330.90 | 0.7625 |
| -262.20 | 0.7156 |
| -159.00 | 0.6644 |
| -85.10 | 0.6316 |
| -46.20 | 0.6165 |
| -3.700 | 0.5985 |
| 73.80 | 0.5690 |
| 126.00 | 0.5481 |
| 195.70 | 0.5216 |
| 259.00 | 0.4960 |
| 386.60 | 0.4437 |
| 481.10 | 0.4017 |
| 567.20 | 0.3586 |
| 641.70 | 0.3144 |
| 719.70 | 0.2457 |
| 734.10 | 0.2191 |
| 719.90 | 0.1587 |
| 645.70 | 0.1125 |
| 430.40 | 0.0560 |
| 254.10 | 0.0288 |

Shatas, Joseph P. - Abbott, Michael M. - Van Ness, Hendrick C., Excess thermodynamic functions for ternary systems. II. Chloroform-ethanol-n-heptane at 50°C, Journal of Chemical & Engineering Data 4 (1975) 406-409. doi:10.1021/je60067a020

**T / K = 323.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -149.40 | 0.9628 |
| -253.40 | 0.9297 |
| -355.90 | 0.8679 |
| -366.00 | 0.8521 |
| -370.10 | 0.8134 |
| -362.30 | 0.7969 |
| -351.10 | 0.7818 |
| -318.30 | 0.7529 |
| -269.40 | 0.7205 |
| -206.70 | 0.6871 |
| -138.50 | 0.6551 |

| | |
|---|---|
| -68.70 | 0.6256 |
| -2.700 | 0.5990 |
| 102.10 | 0.5661 |
| 180.20 | 0.5363 |
| 264.60 | 0.5040 |
| 335.50 | 0.4766 |
| 432.20 | 0.4368 |
| 484.40 | 0.4117 |
| 542.60 | 0.3830 |
| 623.50 | 0.3395 |
| 688.80 | 0.2959 |
| 720.10 | 0.2677 |
| 727.90 | 0.2560 |
| 749.20 | 0.2049 |
| 721.80 | 0.1535 |
| 610.90 | 0.0982 |
| 512.00 | 0.0719 |
| 426.10 | 0.0547 |
| 328.30 | 0.0391 |
| 268.90 | 0.0308 |
| 203.30 | 0.0225 |
| 163.50 | 0.0178 |
| 100.80 | 0.0107 |

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**Azeotropic point**

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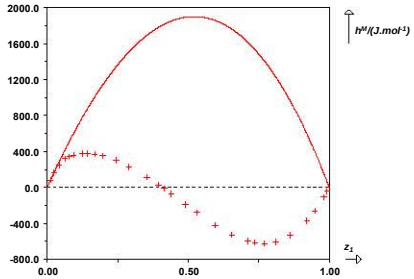
Chen, Geng-Hua - Wang, Qi - Ma, Zhong-Min - Yan, Xin-Huan - Han, Shi-Jun, Phase equilibria at superatmospheric pressures for systems containing halohydrocarbon, aromatic hydrocarbon, and alcohol, Journal of Chemical & Engineering Data 2 (1995) 361-366. doi:10.1021/je00018a003

| T / K | P / bar | $x_1$ |
|---|---|---|
| 368.80 | 3.025 | 0.2700 |

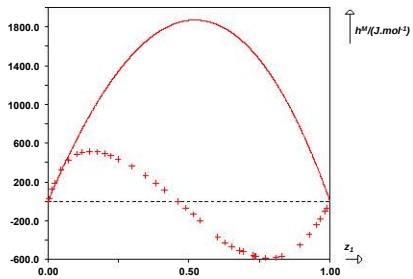
Orchillés, A. Vicent - Miguel, Pablo J. - Vercher, Ernesto - Martínez-Andreu, Antoni, Isobaric Vapor−Liquid and Liquid−Liquid Equilibria for Chloroform + Ethanol + 1-Ethyl-3-methylimidazolium Trifluoromethanesulfonate at 100 kPa, Journal of Chemical & Engineering Data 11 (2008) 2642-2648. doi:10.1021/je800548t

| T / K | P / bar | $x_1$ |
|---|---|---|
| 332.20 | 1.0000 | 0.1520 |

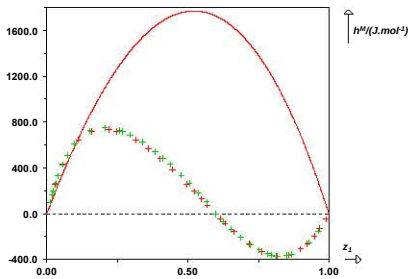
T/K = 298.15 - P/bar = 1.0132



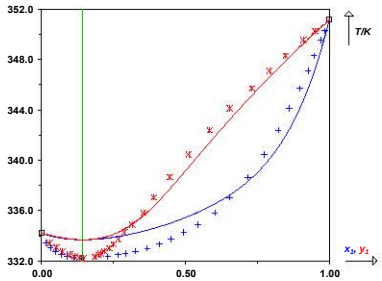

T/K = 303.15 - P/bar = 1.0132



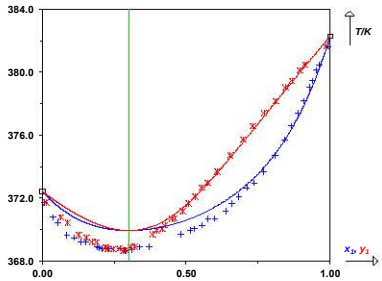

T/K = 323.15 - P/bar = 1.0132 1.0132



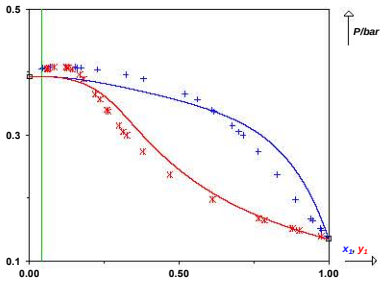

P/bar = 1.00000



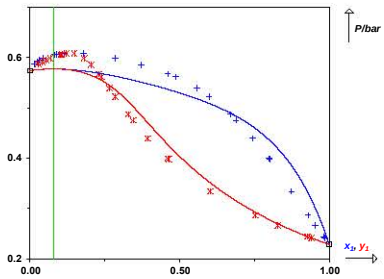

P/bar = 3.02500



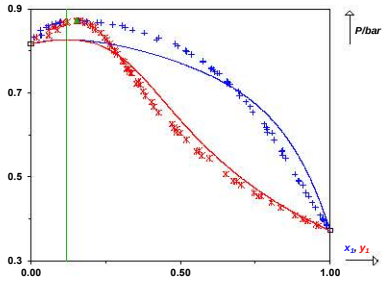

T/K = 308.15



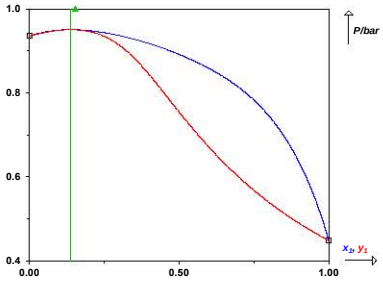

T/K = 318.15



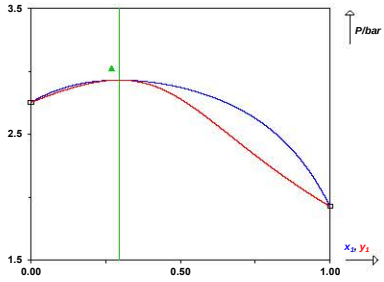

T/K = 328.15




T/K = 332.20




T/K = 368.80



## CHLOROFORM (1) + ACETIC ACID (2)

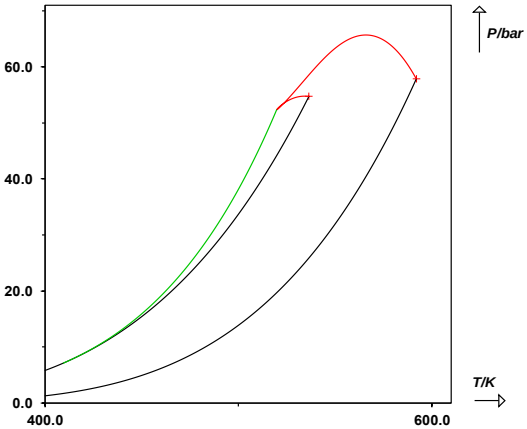
| | | |
|---|---|---|
| **CAS** | 67-66-3 | 64-19-7 |
| **InChiKey** | HEDRZPFGACZZDS-UHFFFAOYSA-N | QTBSBXVTEAMEQO-UHFFFAOYSA-N |
| **$T_c$ / K** | 536.4 | 591.95 |
| **$P_c$ / bar** | 54.72 | 57.86 |
| **ω** | 0.222 | 0.467 |

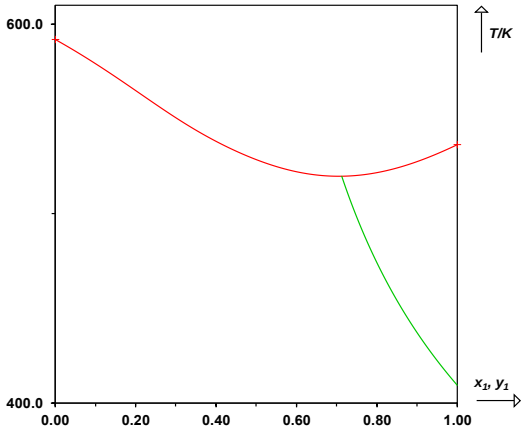
Non ideal with entropic causes

**PPR78 results**

*Parameters*
A/MPa = 198
B/MPa = -242

*Deviations*
MAPE on x = 16 %
MAPE on y = 24 %
MAPE on $h^M$ = 4.9 %



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**Isothermal phase equilibrium data**

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Campbell, A. N. - Kartzmark, E. M. - Gieskes, J. M. T. M., Vapor–Liquid Equilibria, Densities, And Refractivities In The System Acetic Acid – Chloroform – Water At 25 °C, Canadian Journal of Chemistry 2 (1963) 407-429. doi:10.1139/v63-059

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0619 | 0.0851 | 0.5236 |
| 0.0684 | 0.1068 | 0.5875 |
| 0.0781 | 0.1338 | 0.6543 |
| 0.1032 | 0.2087 | 0.7725 |
| 0.1247 | 0.2816 | 0.8274 |
| 0.1356 | 0.3136 | 0.8458 |
| 0.1881 | 0.5259 | 0.9272 |
| 0.2313 | 0.7463 | 0.9648 |

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**Isobaric phase equilibrium data**

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Conti, J. J. - Othmer, D. F. - Gilmont, Roger, Composition of Vapors from Boiling Binary Solutions. Systems Containing Formic Acid, Acetic Acid, Water, and Chloroform., Journal of Chemical & Engineering Data 3 (1960) 301-307. doi:10.1021/je60007a019

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 374.45 | 0.0810 | 0.3380 |
| 368.85 | 0.1172 | 0.4515 |
| 368.55 | 0.1222 | 0.4568 |
| 361.95 | 0.1863 | 0.5785 |
| 354.55 | 0.2814 | 0.7061 |
| 347.55 | 0.4008 | 0.8058 |
| 343.65 | 0.5062 | 0.8572 |
| 343.05 | 0.5256 | 0.8802 |
| 340.95 | 0.6127 | 0.9088 |
| 338.05 | 0.7507 | 0.9428 |

Campbell, A. N. - Gieskes, J. M. T. M., The Isobaric Boiling Points Of The System: Acetic Acid – Chloroform – Water At A Pressure Of 760 Mm Hg, Canadian Journal of Chemistry 1 (1964) 186-189. doi:10.1139/v64-032

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 386.85 | 0.0071 | 0.0699 |
| 379.15 | 0.0474 | 0.2213 |
| 369.95 | 0.0994 | 0.4383 |
| 366.65 | 0.1205 | 0.5064 |
| 354.95 | 0.2630 | 0.7019 |
| 354.65 | 0.2751 | 0.6962 |
| 344.15 | 0.4808 | 0.8595 |
| 342.95 | 0.5109 | 0.8716 |
| 336.45 | 0.8340 | 0.9687 |
| 334.65 | 0.9764 | 0.9960 |

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**Enthalpy of mixing**

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Abramov, E.V. - Mirzayan, A.S. - Fedorova, V.I., Heats of formation of ternary systems. 1. Acetic acid-pyridine-chloroform system, Izv. Akad. Nauk Kaz. SSR Ser. Khim. 4 (1972) 26-32.

**T / K = 293.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -212.00 | 0.0930 |
| -222.00 | 0.1000 |
| -402.00 | 0.2040 |
| -531.00 | 0.2990 |
| -541.00 | 0.3000 |
| -605.00 | 0.3930 |
| -611.00 | 0.3970 |
| -632.00 | 0.4900 |
| -630.00 | 0.4950 |
| -626.00 | 0.5000 |
| -619.00 | 0.5310 |
| -582.00 | 0.6030 |
| -531.00 | 0.6670 |
| -441.00 | 0.7560 |
| -354.00 | 0.8110 |
| -213.00 | 0.8900 |

Abramov, E.V. - Mirzayan, A.S. - Fedorova, V.I., Heats of formation of ternary systems. 1. Acetic acid-pyridine-chloroform system, Izv. Akad. Nauk Kaz. SSR Ser. Khim. 4 (1972) 26-32.

**T / K = 298.15**

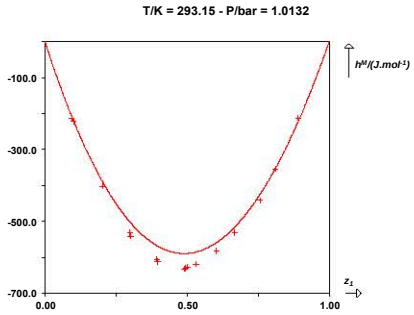
**P / bar = UNKNOWN (1.0132)**

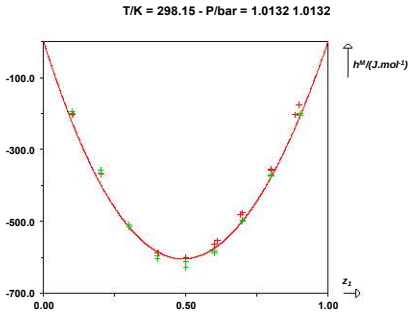
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -204.00 | 0.1020 |
| -370.00 | 0.2020 |
| -516.00 | 0.3000 |
| -586.00 | 0.4000 |
| -588.00 | 0.4030 |
| -599.00 | 0.5000 |
| -563.00 | 0.6000 |
| -554.00 | 0.6110 |
| -480.00 | 0.6920 |

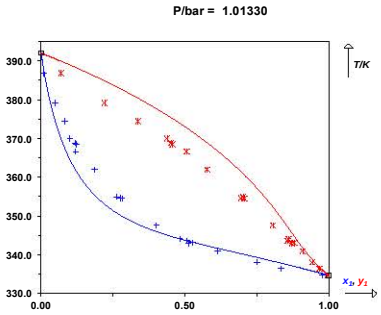
| | |
|---|---|
| -476.00 | 0.7000 |
| -358.00 | 0.7980 |
| -355.00 | 0.8000 |
| -203.00 | 0.8830 |
| -175.00 | 0.8980 |

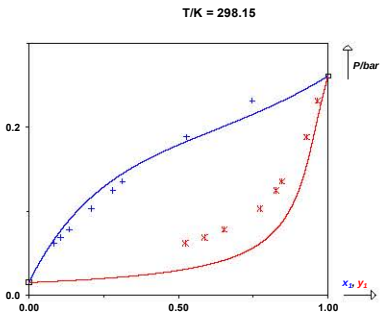
Ratkovics, F., Adiabatic calorimeter for determining heats of mixing, Magy. Kem. Foly. 10 (1971) 499-502.

| **T / K =** | **298.15** |
|---|---|
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| -200.13 | 0.1000 |
| -193.43 | 0.1000 |
| -357.13 | 0.2000 |
| -366.35 | 0.2000 |
| -515.81 | 0.3000 |
| -508.28 | 0.3000 |
| -594.53 | 0.4000 |
| -603.74 | 0.4000 |
| -628.86 | 0.5000 |
| -612.11 | 0.5000 |
| -586.99 | 0.6000 |
| -581.97 | 0.6000 |
| -494.88 | 0.7000 |
| -499.49 | 0.7000 |
| -373.04 | 0.8000 |
| -371.37 | 0.8000 |
| -200.97 | 0.9000 |
| -205.99 | 0.9000 |


T/K = 293.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
-100.0
-300.0
-500.0
-700.0
0.00
0.50
1.00
$z_1$


T/K = 298.15 - P/bar = 1.0132 1.0132
$h^M$/(J.mol$^{-1}$)
-100.0
-300.0
-500.0
-700.0
0.00
0.50
1.00
$z_1$


P/bar = 1.01330
T/K
390.0
380.0
370.0
360.0
350.0
340.0
330.0
0.00
0.50
1.00
$x_1, y_1$


T/K = 298.15
P/bar
0.2
0.0
0.00
0.50
1.00
$x_1, y_1$

## METHANOL (1) + HALOTHANE (2)

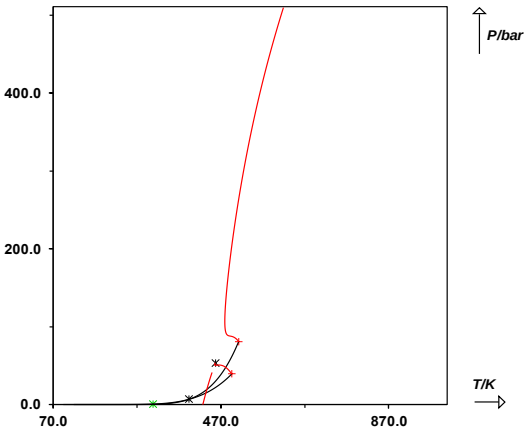
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 151-67-7 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | BCQZXOMGPXTTIC-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.5 | 496 |
| **$P_c$ / bar** | 80.84 | 39.2 |
| **ω** | 0.566 | 0.275 |

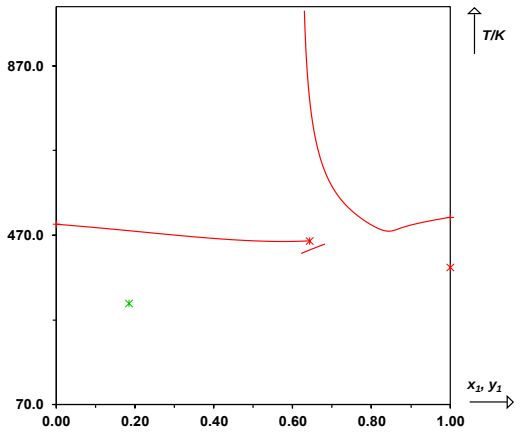
Non ideal with entropic causes

**PPR78 results**

*Parameters*
A/MPa = 643
B/MPa = -149

*Deviations*
MAPE on x = 76 %
MAPE on y = 30 %
MAPE on $h^M$ = 96 %
MAPE on $c_P^M$ = 79 %



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**Isothermal phase equilibrium data**

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Gmehling, Juergen - Onken, Ulfert - Schulte, Hans Werner, Vapor-liquid equilibriums for the binary systems diethyl ether-halothane (1,1,1-trifluoro-2-bromo-2-chloroethane), halothane-methanol, and diethyl ether-methanol, Journal of Chemical & Engineering Data 1 (1980) 29-32. doi:10.1021/je60084a016

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2623 | 0.9247 | 0.8054 |
| 0.3621 | 0.7946 | 0.4737 |
| 0.4134 | 0.7216 | 0.3794 |
| 0.4557 | 0.6398 | 0.3164 |
| 0.4826 | 0.5675 | 0.2806 |
| 0.4920 | 0.5348 | 0.2674 |
| 0.5006 | 0.4991 | 0.2566 |
| 0.5324 | 0.2328 | 0.1902 |
| 0.5333 | 0.1685 | 0.1721 |
| 0.5339 | 0.1535 | 0.1678 |

Fenclova, D. - Dohnal, V., Excess Gibbs energy. Bromochloro-1,1,1-trifluoroethane - methanol system, Int. Data Ser. Sel. Data Mixtures Ser. A 2 (1993)

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.2842 | 0.9936 | 0.9787 | |
| 0.2906 | 0.9845 | 0.9484 | |
| 0.3139 | 0.9540 | 0.8520 | |
| 0.3388 | 0.9236 | 0.7639 | |
| 0.3530 | 0.9069 | 0.7203 | |
| 0.3664 | 0.8923 | 0.6812 | |
| 0.3911 | 0.8652 | 0.6179 | |
| 0.4252 | 0.8281 | 0.5434 | |
| 0.4507 | 0.7994 | 0.4950 | |
| 0.4959 | 0.7453 | 0.4217 | |
| 0.5257 | 0.7048 | 0.3790 | |
| 0.5688 | 0.6312 | 0.3242 | |
| 0.6093 | 0.5257 | 0.2740 | |
| 0.6349 | 0.4057 | 0.2385 | |
| 0.6454 | 0.3164 | 0.2175 | |
| 0.6500 | 0.2449 | 0.2003 | |
| 0.6515 | 0.1896 | 0.1854 | |
| 0.6518 | 0.1838 | 0.1838 | AZEO |
| 0.6510 | 0.1486 | 0.1722 | |
| 0.6506 | 0.1403 | 0.1691 | |
| 0.6482 | 0.1113 | 0.1556 | |
| 0.6350 | 0.0551 | 0.1133 | |
| 0.6121 | 0.0204 | 0.0577 | |

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**Isobaric phase equilibrium data**

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Gmehling, Juergen - Onken, Ulfert - Schulte, Hans Werner, Vapor-liquid equilibriums for the binary systems diethyl ether-halothane (1,1,1-trifluoro-2-bromo-2-chloroethane), halothane-methanol, and diethyl ether-methanol, Journal of Chemical & Engineering Data 1 (1980) 29-32. doi:10.1021/je60084a016

**P / bar = 0.9333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 331.09 | 0.9178 | 0.7716 |
| 325.40 | 0.7964 | 0.5255 |
| 322.78 | 0.7227 | 0.4302 |
| 320.83 | 0.6412 | 0.3641 |
| 319.52 | 0.5643 | 0.3219 |
| 318.79 | 0.5008 | 0.2965 |
| 317.50 | 0.2316 | 0.2194 |
| 317.60 | 0.1525 | 0.1904 |

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**Heat capacity of mixing**

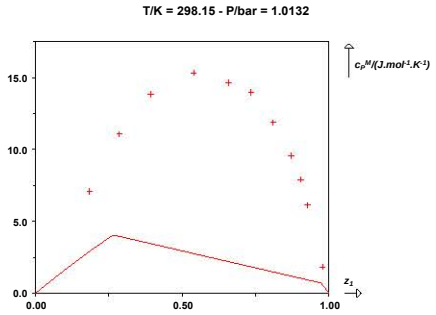
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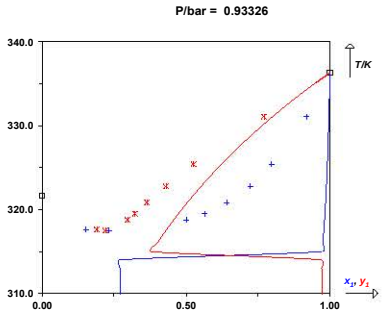
Costas, M., Excess heat capacity. Bromochloro-1,1,1-trifluoroethane - methanol system, Int. Data Ser. Sel. Data Mixtures Ser. A 2 (1993)

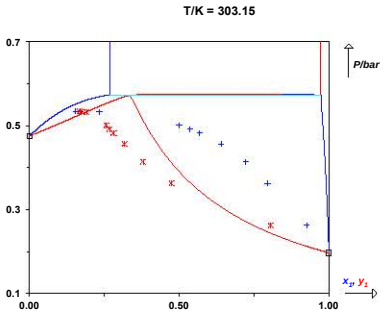
**T / K = 298.15**

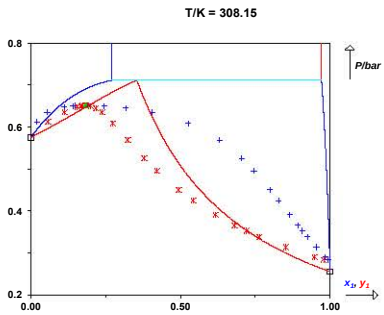
**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / $J.mol^{-1}.K^{-1}$ | $x_1$ |
|---|---|
| 1.830 | 0.9779 |
| 6.130 | 0.9265 |
| 7.930 | 0.9026 |
| 9.550 | 0.8703 |
| 11.89 | 0.8086 |
| 13.97 | 0.7347 |
| 14.62 | 0.6566 |
| 15.34 | 0.5388 |
| 13.85 | 0.3910 |
| 11.07 | 0.2850 |
| 7.090 | 0.1844 |


T/K = 298.15 - P/bar = 1.0132
$c_p^M$/(J.mol$^{-1}$.K$^{-1}$)
15.0
10.0
5.0
0.0
0.00
0.50
1.00
$z_1$


P/bar = 0.93326
T/K
340.0
330.0
320.0
310.0
0.00
0.50
1.00
$x_1$, $y_1$


T/K = 303.15
P/bar
0.7
0.5
0.3
0.1
0.00
0.50
1.00
$x_1$, $y_1$


T/K = 308.15
P/bar
0.8
0.6
0.4
0.2
0.00
0.50
1.00
$x_1$, $y_1$

## TRICHLOROETHYLENE (1) + 2-METHOXYETHANOL (2)

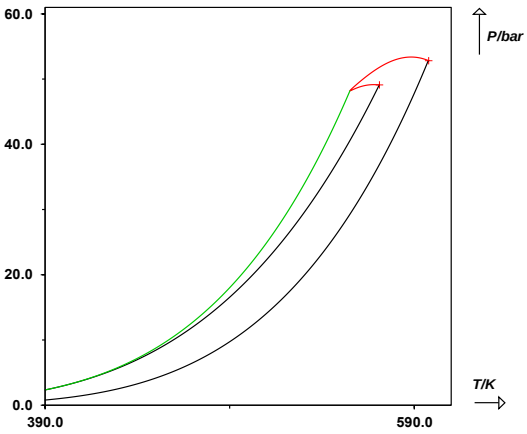
| | | |
|---|---|---|
| **CAS** | 79-01-6 | 109-86-4 |
| **InChiKey** | XSTXAVWGXDQKEL-UHFFFAOYSA-N | XNWFRZJHXBZDAG-UHFFFAOYSA-N |
| **$T_c$ / K** | 571.00 | 597.60 |
| **$P_c$ / bar** | 49.10 | 52.85 |
| **ω** | 0.217 | 0.454 |

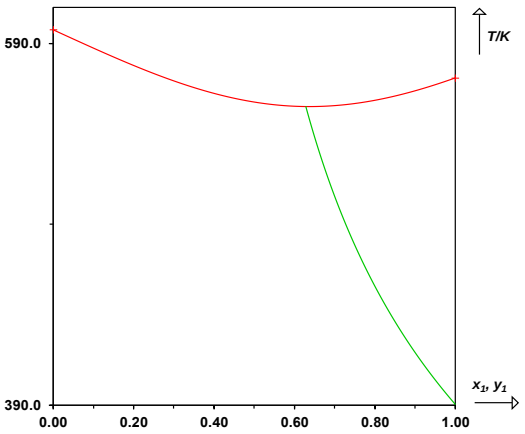
Non ideal with entropic causes

**PPR78 results**

*Parameters*
A/MPa = 184
B/MPa = -51.4

*Deviations*
MAPE on x = 8.8 %
MAPE on y = 3.5 %
MAPE on $h^M$ = 91 %



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**Isothermal phase equilibrium data**

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Jonasson, Ari - Savoia, Marco - Persson, Ole - Fredenslund, Aage, Isothermal vapor-liquid equilibrium data for ether + glycol, chloroalkene + glycol, epoxy ether + alkane, epoxy ether + alkene, and epoxy ether + chloroalkane systems, Journal of Chemical & Engineering Data 1 (1994) 134-139. doi:10.1021/je00013a038

**T / K = 341.01**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1436 | 0.0220 | 0.1796 |
| 0.1735 | 0.0474 | 0.3311 |
| 0.2594 | 0.1370 | 0.5867 |
| 0.3217 | 0.2201 | 0.6942 |
| 0.3778 | 0.3139 | 0.7604 |
| 0.4317 | 0.4319 | 0.8139 |
| 0.4705 | 0.5446 | 0.8483 |
| 0.5046 | 0.6782 | 0.8809 |
| 0.5288 | 0.7991 | 0.9083 |
| 0.5427 | 0.8928 | 0.9347 |

Jonasson, Ari - Savoia, Marco - Persson, Ole - Fredenslund, Aage, Isothermal vapor-liquid equilibrium data for ether + glycol, chloroalkene + glycol, epoxy ether + alkane, epoxy ether + alkene, and epoxy ether + chloroalkane systems, Journal of Chemical & Engineering Data 1 (1994) 134-139. doi:10.1021/je00013a038

**T / K = 357.98**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2931 | 0.0227 | 0.1608 |
| 0.3642 | 0.0608 | 0.3470 |
| 0.4835 | 0.1373 | 0.5416 |
| 0.5853 | 0.2181 | 0.6523 |
| 0.6907 | 0.3265 | 0.7345 |
| 0.7672 | 0.4319 | 0.7841 |
| 0.8381 | 0.5578 | 0.8281 |
| 0.8868 | 0.6779 | 0.8609 |
| 0.9260 | 0.8000 | 0.8922 |
| 0.9482 | 0.8939 | 0.9245 |

---

**Enthalpy of mixing**

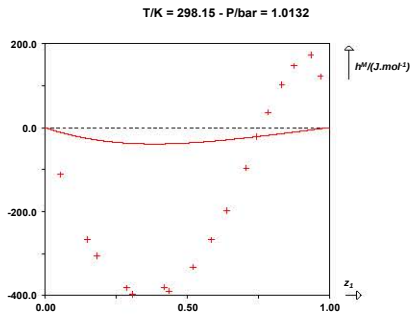
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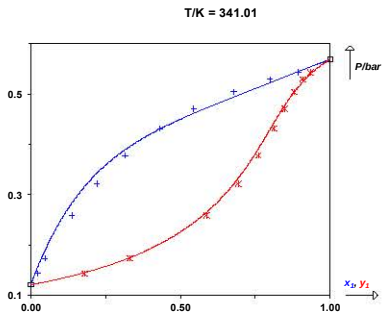
Venkatesulu, D. - Rao, M.V.Prabhakara - Veeranna, D., Excess enthalpies of 2-alkoxyethanols with trichloroethylene and tetrachloroethylene at 298.15 K, Thermochimica Acta (1994) 33-39. doi:10.1016/0040-6031(94)85006-2

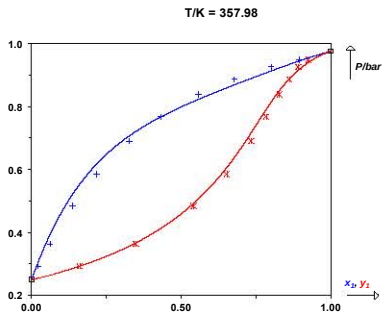
**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -111.70 | 0.0535 |
| -266.80 | 0.1487 |
| -306.20 | 0.1827 |
| -381.80 | 0.2865 |
| -397.90 | 0.3077 |
| -380.10 | 0.4202 |
| -390.00 | 0.4365 |
| -332.30 | 0.5223 |
| -267.50 | 0.5854 |
| -198.30 | 0.6388 |
| -96.10 | 0.7086 |
| -21.70 | 0.7442 |
| 36.20 | 0.7847 |
| 101.10 | 0.8335 |
| 147.10 | 0.8760 |
| 172.80 | 0.9350 |
| 121.90 | 0.9695 |


T/K = 298.15 - P/bar = 1.0132
200.0
0.0
-200.0
-400.0
0.00
0.50
1.00
$h^{M}$/(J.mol$^{-1}$)
$z_1$


T/K = 341.01
0.5
0.3
0.1
0.00
0.50
1.00
P/bar
$x_1$, $y_1$


T/K = 357.98
1.0
0.8
0.6
0.4
0.2
0.00
0.50
1.00
P/bar
$x_1$, $y_1$

# E-SA systems (AC = 8)

## CARBON DIOXIDE (1) + WATER (2)

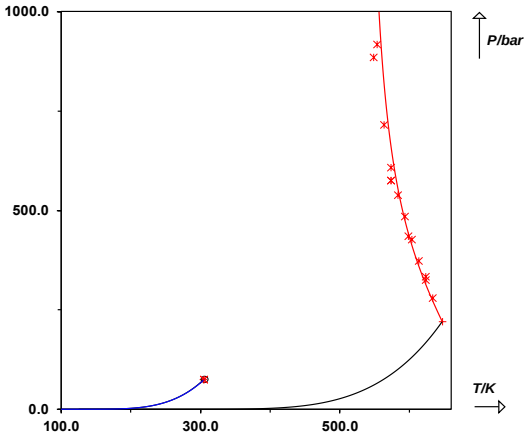
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 7732-18-5 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | XLYOFNOQVPJJNP-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 647.10 |
| **$P_c$ / bar** | 73.83 | 220.64 |
| **ω** | 0.2240 | 0.3450 |

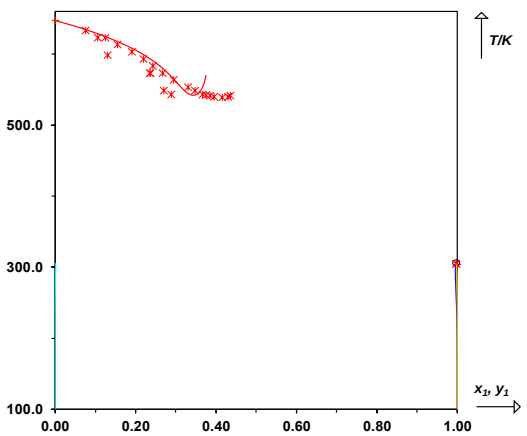
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 2830
B/MPa = 4000

*Deviations*
MAPE on x = 24 %
MAPE on y = 11 %
MAPE on $x_c$ = 7.5 %
MAPE on $P_c$ = 3.2 %
MAPE on $h^M$ = 39 %



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**Isothermal phase equilibrium data**

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Hou, Shu-Xin - Maitland, Geoffrey C. - Trusler, J.P. Martin, Measurement and modeling of the phase behavior of the (carbon dioxide+water) mixture at temperatures from 298.15K to 448.15K, The Journal of Supercritical Fluids (2013) 87-96. doi:10.1016/j.supflu.2012.11.011

| **T / K =** | **298.15** | |
|---|---|---|
| P / bar | $x_1$ | $y_1$ |
| 16.66 | 0.0089 | 0.9973 |
| 32.58 | 0.0154 | 0.9984 |

Zel'venskii, Ya.D., The solubility of carbon dioxide in water under pressure, Zh. Khim. Prom. (1937) 1250-1257.

| **T / K =** | **298.15** |
|---|---|
| P / bar | $x_1$ |
| 10.74 | 0.0064 |
| 10.82 | 0.0062 |
| 21.33 | 0.0118 |
| 22.48 | 0.0124 |
| 24.29 | 0.0129 |
| 25.50 | 0.0134 |
| 30.79 | 0.0156 |
| 33.70 | 0.0166 |
| 33.79 | 0.0166 |
| 38.08 | 0.0185 |
| 38.42 | 0.0186 |
| 43.25 | 0.0203 |
| 44.18 | 0.0204 |
| 54.98 | 0.0229 |
| 55.06 | 0.0230 |
| 61.68 | 0.0240 |

Gillespie, P.C. - Wilson, G.M., Vapor-Liquid and Liquid-Liquid Equilibria: Water - Methane, Water - Carbon Dioxide, Water - Hydrogen Sulfide, Water - n-Pentane, Water - Methane - n-Pentane, GPA Research Report (1982) 1-73.

| **T / K =** | **304.21** | |
|---|---|---|
| P / bar | $x_1$ | $y_1$ |
| 6.895 | 0.0033 | 0.9931 |
| 25.34 | 0.0106 | 0.9976 |
| 50.68 | 0.0182 | 0.9984 |

Liu, Yuanhui - Hou, Minqiang - Ning, Hui - Yang, Dezhong - Yang, Guanying - Han, Buxing, Phase Equilibria of CO2 + N2 + H2O and N2 + CO2 + H2O + NaCl + KCl + CaCl2 Systems at Different Temperatures and Pressures, Journal of Chemical & Engineering Data 7 (2012) 1928-1932. doi:10.1021/je3000958

| **T / K =** | **308.15** |
|---|---|
| P / bar | $x_1$ |
| 80.00 | 0.0224 |
| 120.00 | 0.0238 |
| 160.00 | 0.0250 |

Ferrentino, Giovanna - Barletta, Diego - Balaban, Murat Omer - Ferrari, Giovanna - Poletto, Massimo, Measurement and prediction of CO2 solubility in sodium phosphate monobasic solutions for food treatment with high pressure carbon dioxide, The Journal of Supercritical Fluids 1 (2010) 142-150. doi:10.1016/j.supflu.2009.10.005

| **T / K =** | **308.15** |
|---|---|
| P / bar | $x_1$ |
| 75.80 | 0.0229 |
| 103.40 | 0.0239 |
| 131.00 | 0.0246 |
| 54.50 | 0.0229 |
| 57.20 | 0.0239 |
| 58.50 | 0.0246 |

Liu, Yuanhui - Hou, Minqiang - Yang, Guanying - Han, Buxing, Solubility of CO2 in aqueous solutions of NaCl, KCl, CaCl2 and their mixed salts at different temperatures and pressures, The Journal of Supercritical Fluids 2 (2011) 125-129. doi:10.1016/j.supflu.2010.12.003

| **T / K =** | **308.15** |
|---|---|
| P / bar | $x_1$ |
| 21.00 | 0.0093 |
| 40.90 | 0.0157 |
| 60.80 | 0.0204 |
| 80.90 | 0.0224 |
| 100.80 | 0.0231 |
| 120.50 | 0.0238 |
| 140.10 | 0.0245 |
| 158.30 | 0.0249 |

King, M.B. - Mubarak, A. - Kim, J.D. - Bott, T.R., The mutual solubilities of water with supercritical and liquid carbon dioxides, The Journal of Supercritical Fluids 4 (1992) 296-302. doi:10.1016/0896-8446(92)90021-B

| **T / K =** | **308.15** |
|---|---|
| P / bar | $x_1$ |
| 91.20 | 0.9962 |
| 101.30 | 0.9959 |
| 111.50 | 0.9959 |
| 126.70 | 0.9957 |
| 136.80 | 0.9956 |

| | |
|---|---|
| 152.00 | 0.9954 |
| 202.70 | 0.9950 |

Zaalishvili, S.D., Solubility of carbon dioxide from its mixtures with hydrogen and nitrogen in water under pressure, Zh. Fiz. Khim. 3 (1940) 413-417.

**T / K = 308.15**

| P / bar | $x_1$ |
|---|---|
| 3.242 | 0.0019 |
| 6.080 | 0.0035 |
| 10.23 | 0.0059 |
| 13.68 | 0.0079 |
| 3.546 | 0.0021 |
| 3.040 | 0.0018 |
| 6.688 | 0.0039 |
| 9.018 | 0.0053 |

Hou, Shu-Xin - Maitland, Geoffrey C. - Trusler, J.P. Martin, Measurement and modeling of the phase behavior of the (carbon dioxide+water) mixture at temperatures from 298.15K to 448.15K, The Journal of Supercritical Fluids (2013) 87-96. doi:10.1016/j.supflu.2012.11.011

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.89 | 0.0033 | 0.9719 |
| 29.80 | 0.0090 | 0.9949 |
| 74.06 | 0.0183 | 0.9965 |
| 100.21 | 0.0205 | 0.9960 |
| 129.73 | 0.0214 | 0.9947 |
| 175.33 | 0.0226 | 0.9939 |

Dohrn, R. - Bünz, A.P. - Devlieghere, F. - Thelen, D., Experimental measurements of phase equilibria for ternary and quaternary systems of glucose, water, CO2 and ethanol with a novel apparatus, Fluid Phase Equilibria (1993) 149-158. doi:10.1016/0378-3812(93)87017-U

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 101.00 | 0.0208 | 0.9945 |
| 201.00 | 0.0235 | 0.9932 |
| 301.00 | 0.0251 | 0.9922 |

D'souza, Rupert - Patrick, Jennie R. - Teja, Amyn S., High Pressure Phase Equilibria in the Carbon Dioxide - n-Hexadecane and Carbon Dioxide - Water Systems, The Canadian Journal of Chemical Engineering 2 (1988) 319-323. doi:10.1002/cjce.5450660221

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 101.33 | 0.0198 | 0.9945 |
| 152.00 | 0.0210 | 0.9921 |

Briones, J.A. - Mullins, J.C. - Thies, M.C. - Kim, B.-U., Ternary phase equilibria for acetic acid-water mixtures with supercritical carbon dioxide, Fluid Phase Equilibria (1987) 235-246. doi:10.1016/0378-3812(87)85026-4

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 68.20 | 0.0165 | 0.9966 |
| 75.30 | 0.0175 | 0.9966 |
| 87.20 | 0.0177 | 0.9964 |
| 101.30 | 0.0208 | 0.9956 |
| 122.10 | 0.0210 | 0.9946 |
| 147.50 | 0.0221 | 0.9939 |
| 176.80 | 0.0226 | 0.9936 |

Bamberger, A. - Sieder, G. - Maurer, G., High-pressure (vapor+liquid) equilibrium in binary mixtures of (carbon dioxide+water or acetic acid) at temperatures from 313 to 353 K, The Journal of Supercritical Fluids 2 (2000) 97-110. doi:10.1016/S0896-8446(99)00054-6

**T / K = 333.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 40.50 | 0.0096 | 0.9934 |
| 70.80 | 0.0157 | 0.9949 |
| 80.80 | 0.0166 | 0.9950 |
| 90.90 | 0.0179 | 0.9953 |
| 100.90 | 0.0186 | 0.9951 |
| 111.00 | 0.0195 | 0.9947 |
| 121.00 | 0.0201 | 0.9942 |
| 141.10 | 0.0208 | 0.9922 |

Hou, Shu-Xin - Maitland, Geoffrey C. - Trusler, J.P. Martin, Measurement and modeling of the phase behavior of the (carbon dioxide+water) mixture at temperatures from 298.15K to 448.15K, The Journal of Supercritical Fluids (2013) 87-96. doi:10.1016/j.supflu.2012.11.011

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.01 | 0.0022 | 0.9687 |
| 29.21 | 0.0061 | 0.9858 |
| 71.23 | 0.0127 | 0.9916 |
| 101.67 | 0.0159 | 0.9919 |
| 132.82 | 0.0186 | 0.9916 |
| 169.18 | 0.0199 | 0.9900 |

D'souza, Rupert - Patrick, Jennie R. - Teja, Amyn S., High Pressure Phase Equilibria in the Carbon Dioxide - n-Hexadecane and Carbon Dioxide - Water Systems, The Canadian Journal of Chemical Engineering 2 (1988) 319-323. doi:10.1002/cjce.5450660221

**T / K =** **348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 101.33 | 0.0156 | 0.9926 |
| 152.00 | 0.0188 | 0.9910 |

Gillespie, P.C. - Wilson, G.M., Vapor-Liquid and Liquid-Liquid Equilibria: Water - Methane, Water - Carbon Dioxide, Water - Hydrogen Sulfide, Water - n-Pentane, Water - Methane - n-Pentane, GPA Research Report (1982) 1-73.

**T / K =** **348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0015 | 0.9399 |
| 25.34 | 0.0054 | 0.9818 |
| 50.68 | 0.0101 | 0.9891 |
| 101.35 | 0.0162 | 0.9927 |
| 202.71 | 0.0209 | 0.9906 |

Bamberger, A. - Sieder, G. - Maurer, G., High-pressure (vapor+liquid) equilibrium in binary mixtures of (carbon dioxide+water or acetic acid) at temperatures from 313 to 353 K, The Journal of Supercritical Fluids 2 (2000) 97-110. doi:10.1016/S0896-8446(99)00054-6

**T / K =** **353.10**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 40.50 | 0.0080 | 0.9857 |
| 60.60 | 0.0114 | 0.9891 |
| 70.80 | 0.0128 | 0.9896 |
| 80.80 | 0.0140 | 0.9903 |
| 90.90 | 0.0151 | 0.9908 |
| 100.90 | 0.0160 | 0.9907 |
| 111.00 | 0.0172 | 0.9910 |
| 121.00 | 0.0176 | 0.9904 |
| 131.00 | 0.0184 | 0.9900 |

Gillespie, P.C. - Wilson, G.M., Vapor-Liquid and Liquid-Liquid Equilibria: Water - Methane, Water - Carbon Dioxide, Water - Hydrogen Sulfide, Water - n-Pentane, Water - Methane - n-Pentane, GPA Research Report (1982) 1-73.

**T / K =** **366.48**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0010 | 0.8797 |
| 25.34 | 0.0043 | 0.9653 |
| 50.68 | 0.0085 | 0.9803 |
| 101.35 | 0.0145 | 0.9863 |
| 202.71 | 0.0206 | 0.9857 |

Hou, Shu-Xin - Maitland, Geoffrey C. - Trusler, J.P. Martin, Measurement and modeling of the phase behavior of the (carbon dioxide+water) mixture at temperatures from 298.15K to 448.15K, The Journal of Supercritical Fluids (2013) 87-96. doi:10.1016/j.supflu.2012.11.011

**T / K =** **373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.07 | 0.0017 | 0.9120 |
| 24.26 | 0.0039 | 0.9531 |
| 70.88 | 0.0109 | 0.9790 |
| 102.35 | 0.0137 | 0.9825 |
| 133.52 | 0.0163 | 0.9832 |
| 170.70 | 0.0187 | 0.9829 |

Pfohl, O. - Avramova, Pavlina - Brunner, Gerd, Two- and three-phase equilibria in systems containing benzene derivatives, carbon dioxide, and water at 373.15 K and 10-30 MPa, Fluid Phase Equilibria (1998) 179-206. doi:10.1016/S0378-3812(97)00210-0

**T / K =** **373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 100.00 | 0.0110 | 0.9799 |
| 200.00 | 0.0179 | 0.9810 |
| 300.00 | 0.0204 | 0.9767 |

Takenouchi, S. - Kennedy, G. C., The binary system H2O-CO2 at high temperatures and pressures, American Journal of Science 9 (1964) 1055-1074. doi:10.2475/ajs.262.9.1055

**T / K =** **383.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 100.00 | 0.0140 | 0.9560 |
| 200.00 | 0.0210 | 0.9580 |
| 300.00 | 0.0240 | 0.9480 |
| 399.99 | 0.0260 | 0.9320 |
| 500.00 | 0.0280 | 0.9140 |
| 600.00 | 0.0300 | 0.8930 |
| 700.00 | 0.0315 | 0.8720 |
| 800.00 | 0.0330 | 0.8540 |
| 900.01 | 0.0345 | 0.8400 |
| 1000.0 | 0.0360 | 0.8300 |
| 1100.0 | 0.0370 | 0.8220 |
| 1200.0 | 0.0375 | 0.8160 |
| 1300.0 | 0.0385 | 0.8100 |
| 1400.0 | 0.0390 | 0.8040 |
| 1500.0 | 0.0400 | 0.8000 |

Gillespie, P.C. - Wilson, G.M., Vapor-Liquid and Liquid-Liquid Equilibria: Water - Methane, Water - Carbon Dioxide, Water - Hydrogen Sulfide, Water - n-Pentane, Water - Methane - n-Pentane, GPA Research Report (1982) 1-73.

**T / K =** **394.26**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|

| | | |
|---|---|---|
| 6.895 | 0.0009 | 0.6889 |
| 25.34 | 0.0036 | 0.9078 |
| 50.68 | 0.0073 | 0.9483 |
| 101.35 | 0.0132 | 0.9677 |
| 202.71 | 0.0205 | 0.9728 |

Hou, Shu-Xin - Maitland, Geoffrey C. - Trusler, J.P. Martin, Measurement and modeling of the phase behavior of the (carbon dioxide+water) mixture at temperatures from 298.15K to 448.15K, The Journal of Supercritical Fluids (2013) 87-96. doi:10.1016/j.supflu.2012.11.011

**T / K = 398.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.58 | 0.0014 | 0.7869 |
| 31.76 | 0.0044 | 0.9147 |
| 73.21 | 0.0100 | 0.9554 |
| 99.84 | 0.0131 | 0.9644 |
| 134.56 | 0.0157 | 0.9664 |
| 174.35 | 0.0186 | 0.9691 |

Hou, Shu-Xin - Maitland, Geoffrey C. - Trusler, J.P. Martin, Measurement and modeling of the phase behavior of the (carbon dioxide+water) mixture at temperatures from 298.15K to 448.15K, The Journal of Supercritical Fluids (2013) 87-96. doi:10.1016/j.supflu.2012.11.011

**T / K = 423.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 14.28 | 0.0013 | 0.6536 |
| 29.87 | 0.0035 | 0.8107 |
| 71.97 | 0.0087 | 0.9055 |
| 100.14 | 0.0123 | 0.9250 |
| 134.18 | 0.0156 | 0.9363 |
| 173.55 | 0.0191 | 0.9434 |

Takenouchi, S. - Kennedy, G. C., The binary system H2O-CO2 at high temperatures and pressures, American Journal of Science 9 (1964) 1055-1074. doi:10.2475/ajs.262.9.1055

**T / K = 423.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 100.00 | 0.0135 | 0.8800 |
| 200.00 | 0.0215 | 0.9100 |
| 300.00 | 0.0260 | 0.9000 |
| 399.99 | 0.0290 | 0.8820 |
| 500.00 | 0.0320 | 0.8620 |
| 600.00 | 0.0345 | 0.8400 |
| 700.00 | 0.0370 | 0.8240 |
| 800.00 | 0.0390 | 0.8080 |
| 900.01 | 0.0405 | 0.7940 |
| 1000.0 | 0.0420 | 0.7800 |
| 1100.0 | 0.0440 | 0.7700 |
| 1200.0 | 0.0450 | 0.7640 |
| 1300.0 | 0.0460 | 0.7580 |
| 1400.0 | 0.0470 | 0.7540 |
| 1500.0 | 0.0480 | 0.7520 |

Hou, Shu-Xin - Maitland, Geoffrey C. - Trusler, J.P. Martin, Measurement and modeling of the phase behavior of the (carbon dioxide+water) mixture at temperatures from 298.15K to 448.15K, The Journal of Supercritical Fluids (2013) 87-96. doi:10.1016/j.supflu.2012.11.011

**T / K = 448.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.27 | 0.0006 | 0.2957 |
| 36.57 | 0.0037 | 0.7100 |
| 75.65 | 0.0086 | 0.8427 |
| 104.97 | 0.0114 | 0.8808 |
| 134.42 | 0.0141 | 0.8933 |
| 174.59 | 0.0176 | 0.8982 |

Zawisza, Andrzej - Malesinska, Boguslawa, Solubility of carbon dioxide in liquid water and of water in gaseous carbon dioxide in the range 0.2-5 MPa and at temperatures up to 473 K, Journal of Chemical & Engineering Data 4 (1981) 388-391. doi:10.1021/je00026a012

**T / K = 448.15**

| P / bar | $x_1$ |
|---|---|
| 11.97 | 0.0005 |
| 19.77 | 0.0016 |
| 25.96 | 0.0025 |
| 30.37 | 0.0030 |
| 40.80 | 0.0046 |

Takenouchi, S. - Kennedy, G. C., The binary system H2O-CO2 at high temperatures and pressures, American Journal of Science 9 (1964) 1055-1074. doi:10.2475/ajs.262.9.1055

**T / K = 473.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 100.00 | 0.0130 | 0.7150 |
| 200.00 | 0.0260 | 0.8200 |
| 300.00 | 0.0340 | 0.8250 |
| 399.99 | 0.0410 | 0.8160 |
| 500.00 | 0.0470 | 0.8000 |
| 600.00 | 0.0520 | 0.7800 |
| 700.00 | 0.0560 | 0.7600 |
| 800.00 | 0.0580 | 0.7450 |
| 900.01 | 0.0610 | 0.7320 |

| | | |
|---|---|---|
| 1000.0 | 0.0630 | 0.7200 |
| 1100.0 | 0.0650 | 0.7160 |
| 1200.0 | 0.0670 | 0.7060 |
| 1300.0 | 0.0690 | 0.7000 |
| 1400.0 | 0.0700 | 0.6940 |
| 1500.0 | 0.0720 | 0.6900 |

Takenouchi, S. - Kennedy, G. C., The binary system H2O-CO2 at high temperatures and pressures, American Journal of Science 9 (1964) 1055-1074. doi:10.2475/ajs.262.9.1055

**T / K = 473.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 100.00 | 0.0130 | 0.7150 |
| 200.00 | 0.0260 | 0.8200 |
| 300.00 | 0.0340 | 0.8250 |
| 400.00 | 0.0410 | 0.8160 |
| 500.00 | 0.0470 | 0.8000 |
| 600.00 | 0.0520 | 0.7800 |
| 700.00 | 0.0560 | 0.7600 |
| 799.99 | 0.0580 | 0.7450 |
| 899.99 | 0.0610 | 0.7320 |
| 1000.0 | 0.0630 | 0.7200 |
| 1100.0 | 0.0650 | 0.7160 |
| 1200.0 | 0.0670 | 0.7060 |
| 1300.0 | 0.0690 | 0.7000 |
| 1400.0 | 0.0700 | 0.6940 |
| 1500.0 | 0.0720 | 0.6900 |

Takenouchi, S. - Kennedy, G. C., The binary system H2O-CO2 at high temperatures and pressures, American Journal of Science 9 (1964) 1055-1074. doi:10.2475/ajs.262.9.1055

**T / K = 523.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 100.00 | 0.0120 | 0.4100 |
| 200.00 | 0.0270 | 0.6360 |
| 300.00 | 0.0420 | 0.6800 |
| 399.99 | 0.0550 | 0.6760 |
| 500.00 | 0.0640 | 0.6600 |
| 600.00 | 0.0740 | 0.6360 |
| 700.00 | 0.0840 | 0.6130 |
| 800.00 | 0.0940 | 0.5930 |
| 900.01 | 0.1040 | 0.5800 |
| 1000.0 | 0.1150 | 0.5670 |
| 1100.0 | 0.1250 | 0.5550 |
| 1200.0 | 0.1320 | 0.5480 |
| 1300.0 | 0.1360 | 0.5420 |

Takenouchi, S. - Kennedy, G. C., The binary system H2O-CO2 at high temperatures and pressures, American Journal of Science 9 (1964) 1055-1074. doi:10.2475/ajs.262.9.1055

**T / K = 533.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 200.00 | 0.0270 | 0.5720 |
| 250.01 | 0.0350 | 0.6200 |
| 300.00 | 0.0440 | 0.6400 |
| 399.99 | 0.0590 | 0.6420 |
| 500.00 | 0.0730 | 0.6240 |
| 600.00 | 0.0870 | 0.6040 |
| 700.00 | 0.1000 | 0.5800 |
| 800.00 | 0.1130 | 0.5600 |
| 900.01 | 0.1250 | 0.5480 |
| 1000.0 | 0.1350 | 0.5360 |
| 1100.0 | 0.1450 | 0.5240 |
| 1200.0 | 0.1550 | 0.5100 |
| 1300.0 | 0.1600 | 0.5040 |
| 1400.0 | 0.1650 | 0.5020 |
| 1500.0 | 0.1750 | 0.5000 |

Tödheide, K. - Franck, E. U., Das Zweiphasengebiet und die kritische Kurve im System Kohlendioxid–Wasser bis zu Drucken von 3500 bar, Zeitschrift für Physikalische Chemie 5_6 (1963) 387-401. doi:10.1524/zpch.1963.37.5_6.387

**T / K = 538.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 200.00 | 0.0260 | 0.5770 |
| 500.00 | 0.0800 | 0.6570 |
| 1000.0 | 0.1550 | 0.6000 |
| 1500.0 | 0.2150 | 0.5460 |
| 2000.0 | 0.2720 | 0.5080 |
| 2500.0 | 0.2980 | 0.4930 |
| 3000.0 | 0.2920 | 0.5500 |
| 3500.0 | 0.2800 | 0.5700 |

Tödheide, K. - Franck, E. U., Das Zweiphasengebiet und die kritische Kurve im System Kohlendioxid–Wasser bis zu Drucken von 3500 bar, Zeitschrift für Physikalische Chemie 5_6 (1963) 387-401. doi:10.1524/zpch.1963.37.5_6.387

**T / K = 540.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 200.00 | 0.0260 | 0.5670 | |
| 500.00 | 0.0820 | 0.6500 | |
| 1000.0 | 0.1700 | 0.5750 | |
| 1500.0 | 0.2400 | 0.5260 | |
| 3500.0 | 0.3550 | 0.5100 | |
| 1890.0 | 0.3950 | 0.3950 | CRIT |

Tödheide, K. - Franck, E. U., Das Zweiphasengebiet und die kritische Kurve im System Kohlendioxid–Wasser bis zu Drucken von 3500 bar, Zeitschrift für Physikalische Chemie 5_6 (1963) 387-401. doi:10.1524/zpch.1963.37.5_6.387

**T / K = 541.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 200.00 | 0.0260 | 0.5590 | |
| 300.00 | 0.0480 | 0.6200 | |
| 400.00 | 0.0640 | 0.6440 | |
| 500.00 | 0.0830 | 0.6420 | |
| 600.00 | 0.0950 | 0.6380 | |
| 700.00 | 0.1180 | 0.6220 | |
| 799.99 | 0.1380 | 0.6030 | |
| 899.99 | 0.1600 | 0.5860 | |
| 1000.0 | 0.1790 | 0.5690 | |
| 1100.0 | 0.1970 | 0.5560 | |
| 1200.0 | 0.2110 | 0.5470 | |
| 1300.0 | 0.2280 | 0.5300 | |
| 1400.0 | 0.2480 | 0.5180 | |
| 1500.0 | 0.2780 | 0.4970 | |
| 1620.0 | 0.3850 | 0.3850 | CRIT |

Takenouchi, S. - Kennedy, G. C., The binary system H2O-CO2 at high temperatures and pressures, American Journal of Science 9 (1964) 1055-1074. doi:10.2475/ajs.262.9.1055

**T / K = 543.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 200.00 | 0.0270 | 0.5300 | |
| 250.01 | 0.0360 | 0.5700 | |
| 500.00 | 0.0870 | 0.5700 | |
| 600.00 | 0.1060 | 0.5460 | |
| 700.00 | 0.1250 | 0.5200 | |
| 800.00 | 0.1450 | 0.4960 | |
| 900.01 | 0.1660 | 0.4620 | |
| 1000.0 | 0.1900 | 0.4240 | |
| 1100.0 | 0.2150 | 0.3820 | |
| 1200.0 | 0.2500 | 0.3400 | |
| 1230.0 | 0.2880 | 0.2880 | CRIT |

Takenouchi, S. - Kennedy, G. C., The binary system H2O-CO2 at high temperatures and pressures, American Journal of Science 9 (1964) 1055-1074. doi:10.2475/ajs.262.9.1055

**T / K = 548.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 100.00 | 0.0100 | 0.2560 | |
| 150.00 | 0.0190 | 0.4260 | |
| 200.00 | 0.0280 | 0.5000 | |
| 250.01 | 0.0380 | 0.5400 | |
| 500.00 | 0.0960 | 0.5300 | |
| 600.00 | 0.1200 | 0.4960 | |
| 700.00 | 0.1440 | 0.4600 | |
| 800.00 | 0.1750 | 0.4200 | |
| 885.00 | 0.2700 | 0.2700 | CRIT |

Takenouchi, S. - Kennedy, G. C., The binary system H2O-CO2 at high temperatures and pressures, American Journal of Science 9 (1964) 1055-1074. doi:10.2475/ajs.262.9.1055

**T / K = 573.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 100.00 | 0.0040 | 0.0800 | |
| 150.00 | 0.0160 | 0.2900 | |
| 200.00 | 0.0290 | 0.3900 | |
| 250.01 | 0.0410 | 0.4340 | |
| 300.00 | 0.0540 | 0.4540 | |
| 350.00 | 0.0680 | 0.4560 | |
| 399.99 | 0.0840 | 0.4480 | |
| 450.00 | 0.1040 | 0.4220 | |
| 500.00 | 0.1270 | 0.3800 | |
| 549.99 | 0.1700 | 0.3200 | |
| 575.00 | 0.2360 | 0.2360 | CRIT |

Takenouchi, S. - Kennedy, G. C., The binary system H2O-CO2 at high temperatures and pressures, American Journal of Science 9 (1964) 1055-1074. doi:10.2475/ajs.262.9.1055

**T / K = 598.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 150.00 | 0.0100 | 0.1060 | |
| 200.00 | 0.0260 | 0.2460 | |
| 250.01 | 0.0430 | 0.3210 | |
| 300.00 | 0.0610 | 0.3420 | |
| 350.00 | 0.0820 | 0.3340 | |
| 399.99 | 0.1120 | 0.2860 | |
| 435.00 | 0.1300 | 0.1300 | CRIT |

Takenouchi, S. - Kennedy, G. C., The binary system H2O-CO2 at high temperatures and pressures, American Journal of Science 9 (1964) 1055-1074. doi:10.2475/ajs.262.9.1055

**T / K = 623.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 200.00 | 0.0150 | 0.0900 | |
| 250.01 | 0.0400 | 0.1620 | |
| 300.00 | 0.0640 | 0.1660 | |
| 325.00 | 0.1050 | 0.1050 | CRIT |

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**Isobaric phase equilibrium data**

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Gillespie, P.C. - Wilson, G.M., Vapor-Liquid and Liquid-Liquid Equilibria: Water - Methane, Water - Carbon Dioxide, Water - Hydrogen Sulfide, Water - n-Pentane, Water - Methane - n-Pentane, GPA Research Report (1982) 1-73.

**P / bar = 101.35**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 288.71 | 0.0242 | 0.9972 |
| 298.15 | 0.0249 | 0.9966 |
| 302.59 | 0.0239 | 0.9961 |
| 304.21 | 0.0241 | 0.9959 |

Gillespie, P.C. - Wilson, G.M., Vapor-Liquid and Liquid-Liquid Equilibria: Water - Methane, Water - Carbon Dioxide, Water - Hydrogen Sulfide, Water - n-Pentane, Water - Methane - n-Pentane, GPA Research Report (1982) 1-73.

**P / bar = 202.71**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 288.71 | 0.0261 | 0.9971 |
| 298.15 | 0.0257 | 0.9962 |
| 302.59 | 0.0263 | 0.9956 |
| 304.21 | 0.0262 | 0.9955 |

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**Enthalpy of mixing**

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Pérez, Eduardo - Sánchez-Vicente, Yolanda - Cabañas, Albertina - Pando, Concepción - Renuncio, Juan A.R., Excess molar enthalpies for mixtures of supercritical carbon dioxide and water+ethanol solutions, The Journal of Supercritical Fluids 1 (2005) 23-30. doi:10.1016/j.supflu.2005.03.006

**T / K = 308.15**

**P / bar = 76.40**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -94.00 | 0.0060 |
| -207.00 | 0.0110 |
| -231.00 | 0.0300 |
| -220.00 | 0.0500 |
| -215.00 | 0.0720 |
| -212.00 | 0.1050 |
| -201.00 | 0.1170 |
| -187.00 | 0.1550 |
| -184.00 | 0.1710 |
| -179.00 | 0.2020 |
| -172.00 | 0.2160 |
| -168.00 | 0.2380 |
| -159.00 | 0.2590 |
| -137.00 | 0.3560 |
| -98.00 | 0.5130 |
| -67.00 | 0.6280 |
| -33.00 | 0.7290 |
| -20.00 | 0.8120 |
| 15.00 | 0.9370 |

Xuemin Chen - Gillespie, Sue E. - Oscarson, John L. - Izatt, Reed M., Calorimetric determination of thermodynamic quantities for chemical reactions in the system CO2-NaOH-H2O from 225 to 325°C, Journal of Solution Chemistry 8 (1992) 825-848. doi:10.1007/BF00651511

**T / K = 498.15**

**P / bar = 124.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 546.00 | 0.0508 |
| 715.00 | 0.0666 |
| 960.00 | 0.0869 |
| 1737.0 | 0.1599 |
| 2481.0 | 0.2222 |
| 2881.0 | 0.2631 |
| 3842.0 | 0.3487 |
| 4560.0 | 0.4166 |
| 5265.0 | 0.4716 |
| 5747.0 | 0.5171 |
| 6582.0 | 0.5881 |
| 7595.0 | 0.6817 |
| 7782.0 | 0.7281 |
| 7302.0 | 0.7407 |
| 6117.0 | 0.7812 |
| 5338.0 | 0.8107 |
| 4371.0 | 0.8510 |
| 3555.0 | 0.8771 |
| 2652.0 | 0.9049 |
| 1858.0 | 0.9346 |
| 1396.0 | 0.9501 |

Xuemin Chen - Gillespie, Sue E. - Oscarson, John L. - Izatt, Reed M., Calorimetric determination of thermodynamic quantities for chemical reactions in the system CO2-NaOH-H2O from 225 to 325°C, Journal of Solution Chemistry 8 (1992) 825-848. doi:10.1007/BF00651511

**T / K = 548.15**

**P / bar = 104.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 306.00 | 0.0112 |
| 802.00 | 0.0223 |

| | |
|---|---|
| 1667.0 | 0.0340 |
| 2108.0 | 0.0489 |
| 2638.0 | 0.0642 |
| 3527.0 | 0.0789 |
| 4016.0 | 0.0935 |
| 5103.0 | 0.1143 |
| 5397.0 | 0.1252 |
| 6487.0 | 0.1403 |
| 6654.0 | 0.1473 |
| 8237.0 | 0.1845 |
| 11436.0 | 0.2551 |
| 11811.0 | 0.2710 |
| 14357.0 | 0.3116 |
| 15441.0 | 0.3407 |
| 15217.0 | 0.4045 |
| 14370.0 | 0.4250 |
| 13600.0 | 0.4741 |
| 12158.0 | 0.5048 |
| 11990.0 | 0.5289 |
| 11168.0 | 0.5906 |
| 8414.0 | 0.6711 |
| 6954.0 | 0.7403 |
| 5123.0 | 0.8032 |
| 4475.0 | 0.8323 |
| 3203.0 | 0.8715 |
| 1594.0 | 0.9395 |

Xuemin Chen - Gillespie, Sue E. - Oscarson, John L. - Izatt, Reed M., Calorimetric determination of thermodynamic quantities for chemical reactions in the system CO2-NaOH-H2O from 225 to 325°C, Journal of Solution Chemistry 8 (1992) 825-848. doi:10.1007/BF00651511

**T / K = 573.15**

**P / bar = 110.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 543.00 | 0.0085 |
| 803.00 | 0.0113 |
| 1482.0 | 0.0169 |
| 2018.0 | 0.0224 |
| 2776.0 | 0.0279 |
| 3339.0 | 0.0332 |
| 3827.0 | 0.0399 |
| 5154.0 | 0.0491 |
| 6532.0 | 0.0644 |
| 8137.0 | 0.0789 |
| 10128.0 | 0.0936 |
| 12053.0 | 0.1146 |
| 13872.0 | 0.1250 |
| 15744.0 | 0.1474 |
| 18379.0 | 0.1848 |
| 17141.0 | 0.2553 |
| 15497.0 | 0.3119 |
| 13796.0 | 0.4047 |
| 11557.0 | 0.5049 |
| 9054.0 | 0.6047 |
| 7691.0 | 0.6710 |
| 6241.0 | 0.7328 |
| 4480.0 | 0.8031 |
| 3024.0 | 0.8718 |
| 1448.0 | 0.9391 |

Wormald, C.J. - Lancaster, N.M. - Sellars, A.J., The excess molar enthalpies of {xH2O + (1 − x)CO}(g) and {xH2O + (1 − x)CO2}(g) at high temperatures and pressures, The Journal of Chemical Thermodynamics 2 (1986) 135-147. doi:10.1016/0021-9614(86)90128-X

**T / K = 648.20**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 260.00 | 0.3030 |
| 295.00 | 0.4010 |
| 308.00 | 0.4970 |
| 292.00 | 0.5970 |
| 251.00 | 0.6980 |

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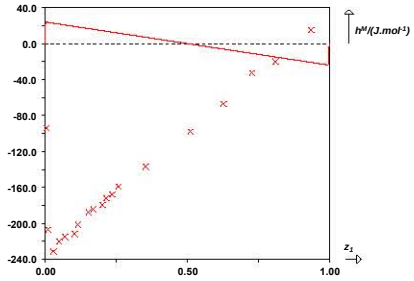
**Critical point**

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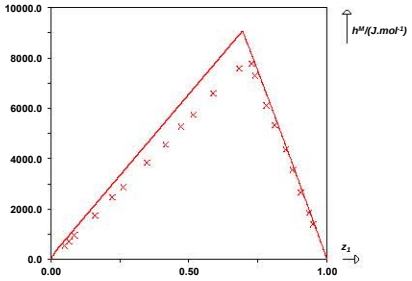
Tödheide, K. - Franck, E. U., Das Zweiphasengebiet und die kritische Kurve im System Kohlendioxid–Wasser bis zu Drucken von 3500 bar, Zeitschrift für Physikalische Chemie 5_6 (1963) 387-401. doi:10.1524/zpch.1963.37.5_6.387

| T / K | P / bar | $x_1$ |
|---|---|---|
| 633.15 | 279.00 | 0.0750 |
| 613.15 | 373.00 | 0.1550 |
| 603.15 | 427.00 | 0.1900 |
| 593.15 | 485.00 | 0.2200 |
| 583.15 | 539.00 | 0.2420 |
| 563.15 | 716.00 | 0.2950 |
| 553.15 | 917.00 | 0.3300 |
| 542.15 | 1470.0 | 0.3750 |
| 539.15 | 2450.0 | 0.4150 |
| 540.15 | 3140.0 | 0.4300 |
| 541.15 | 3600.0 | 0.4350 |
| 304.65 | 74.00 | 0.9965 |
| 304.65 | 74.10 | 0.9965 |

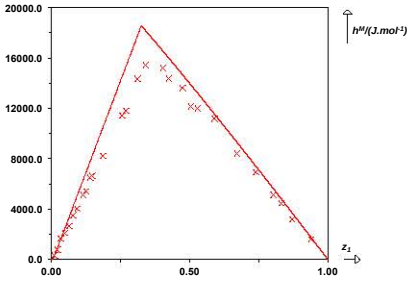
T/K = 308.15 - P/bar = 76.400



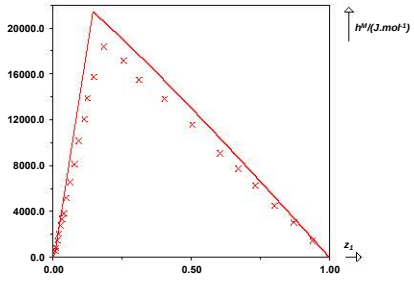

T/K = 498.15 - P/bar = 124.00



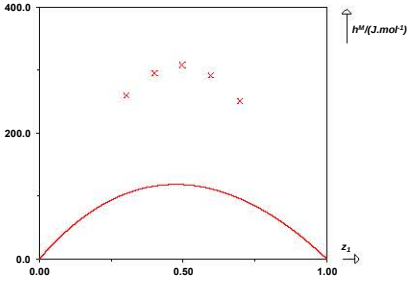

T/K = 548.15 - P/bar = 104.00



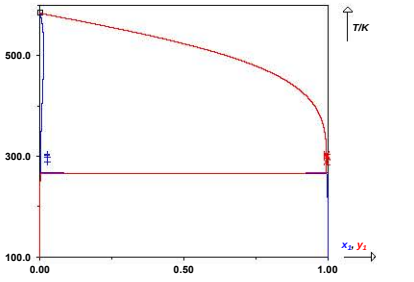

T/K = 573.15 - P/bar = 110.00



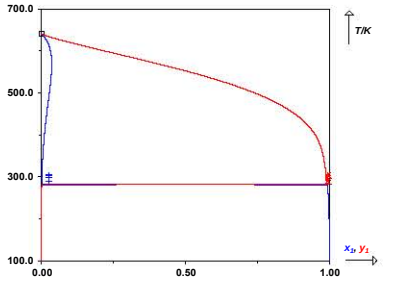

T/K = 648.20 - P/bar = 50.00



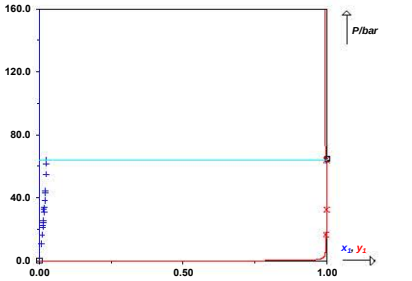

P/bar = 101.35000



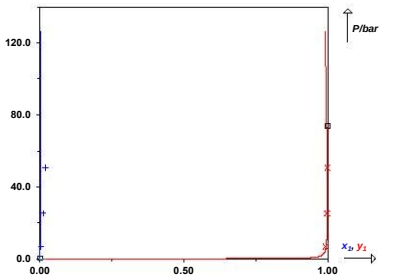

P/bar = 202.71000



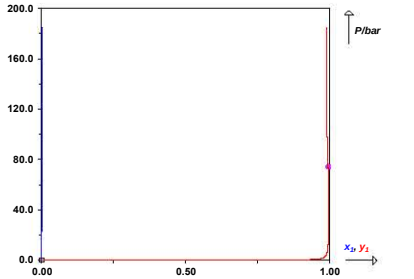

T/K = 298.15



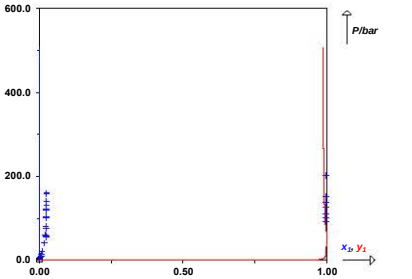

T/K = 304.21



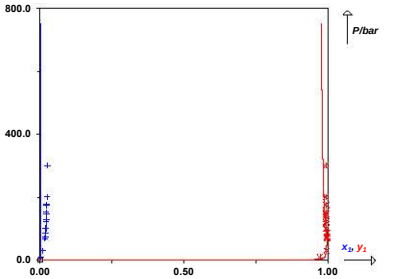

T/K = 304.65



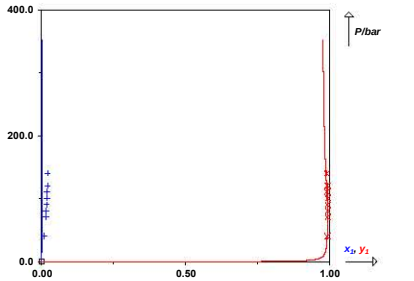

T/K = 308.15



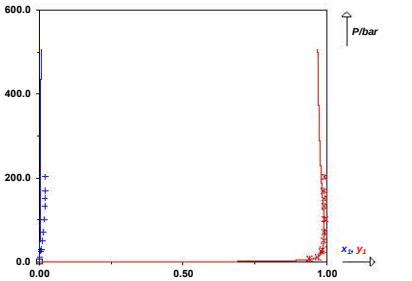

T/K = 323.15



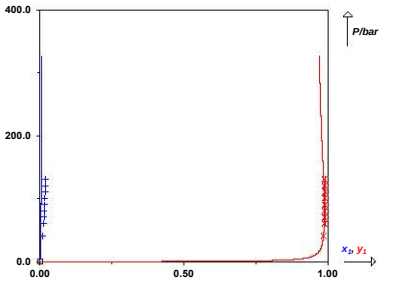

T/K = 333.20



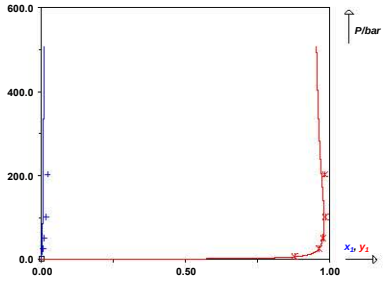

T/K = 348.15



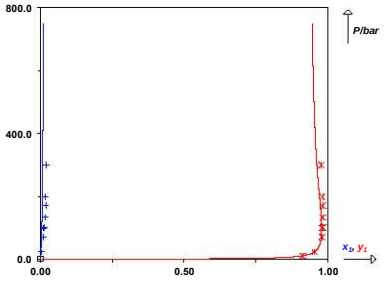

T/K = 353.10



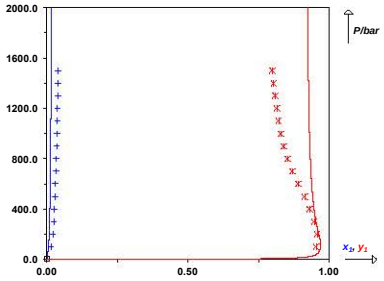
T/K = 366.48



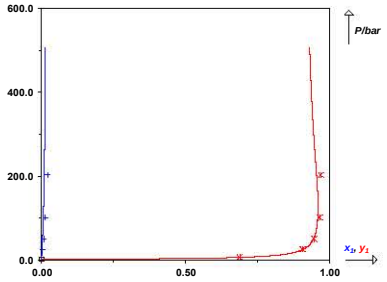

T/K = 373.15



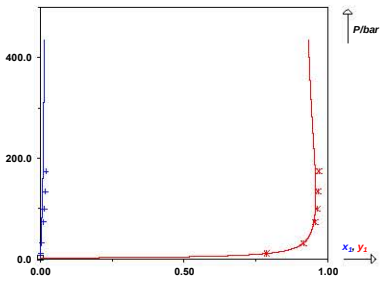

T/K = 383.15



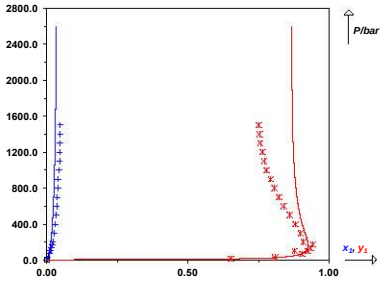

T/K = 394.26



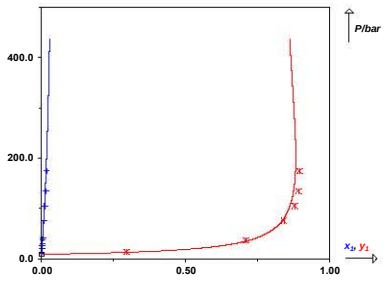

T/K = 398.15



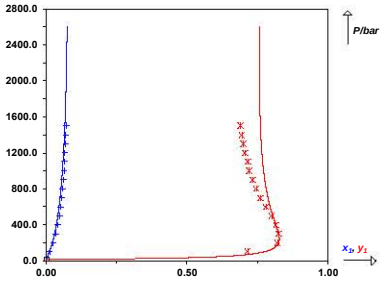

T/K = 423.15



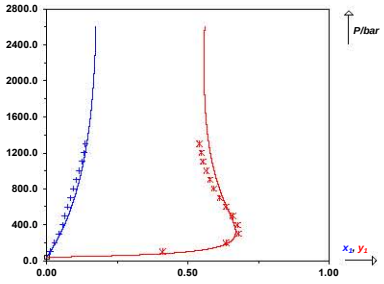

T/K = 448.15



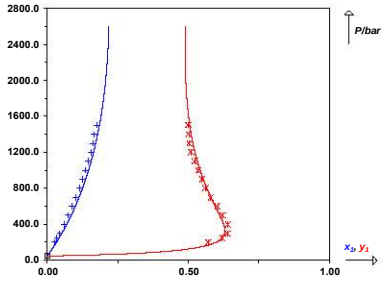

T/K = 473.15



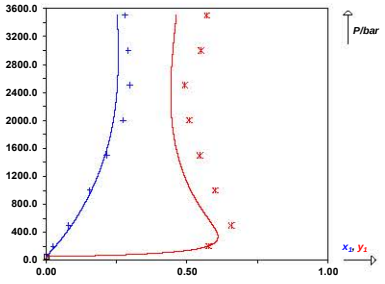

T/K = 523.15



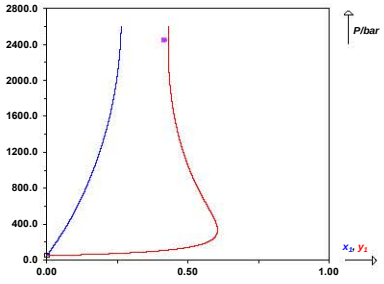

T/K = 533.15



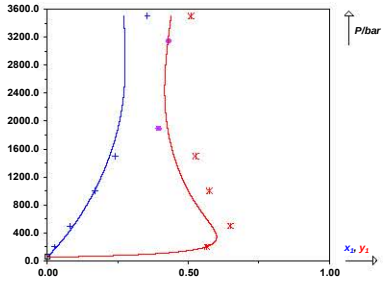

T/K = 538.15



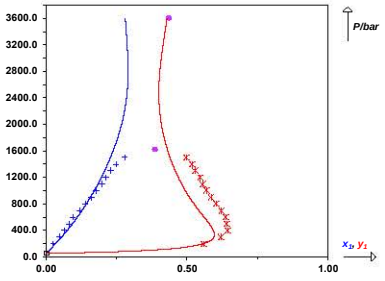

T/K = 539.15



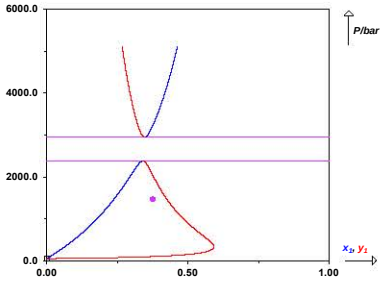

T/K = 540.15



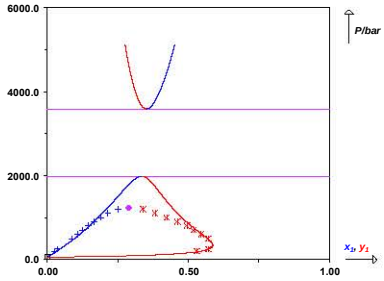

T/K = 541.15



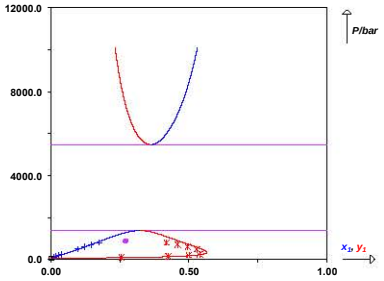

T/K = 542.15



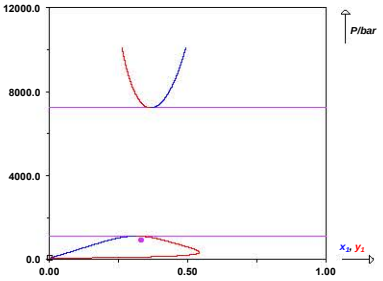
T/K = 543.15



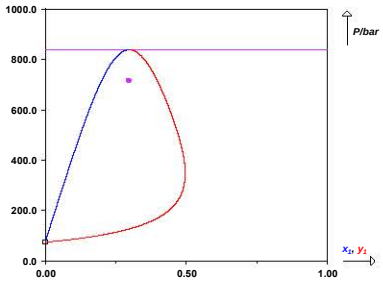

T/K = 548.15



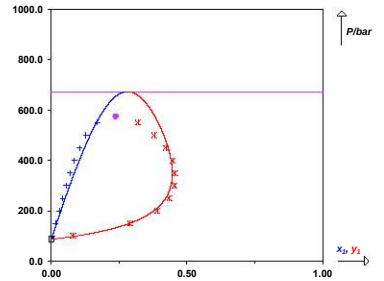

T/K = 553.15



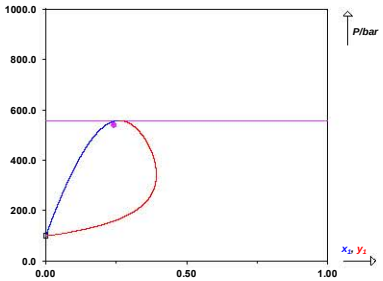

T/K = 563.15



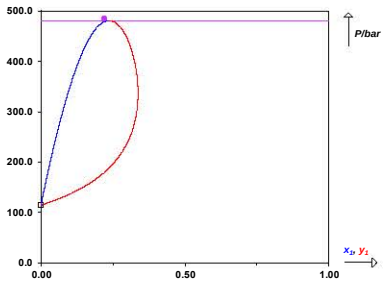

T/K = 573.15



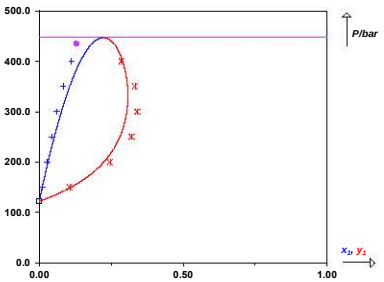

T/K = 583.15



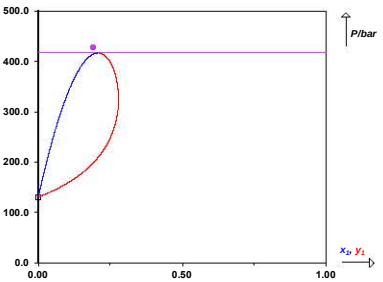

T/K = 593.15



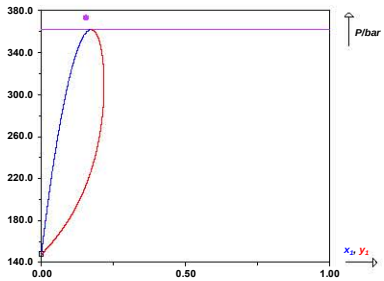

T/K = 598.15



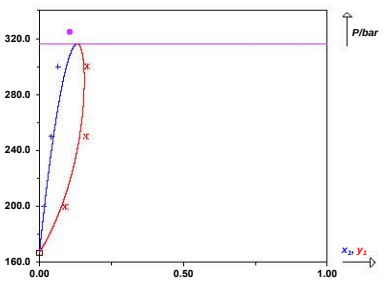

T/K = 603.15



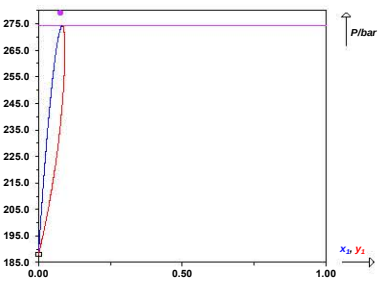

T/K = 613.15




T/K = 623.15




T/K = 633.15



## CARBON DIOXIDE (1) + ETHANOL (2)

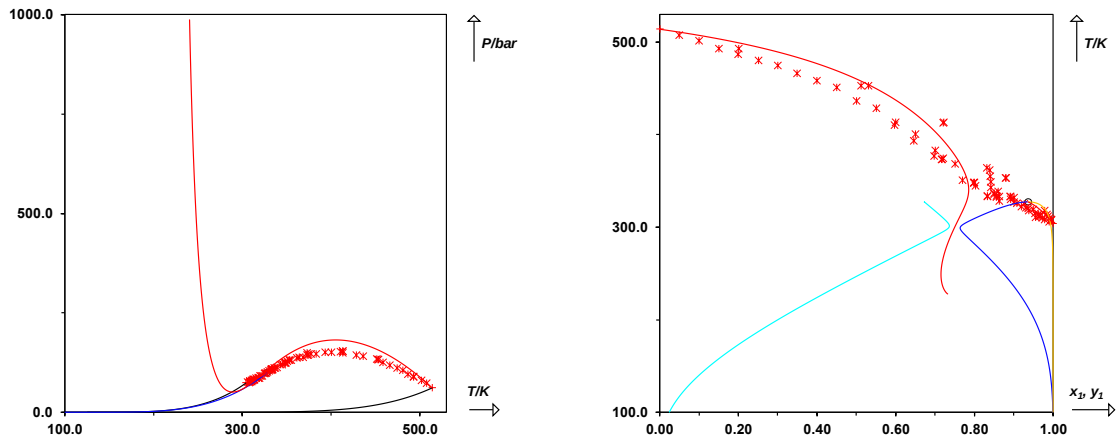
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 64-17-5 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | LFQSCWFLJHTTHZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 514.00 |
| **$P_c$ / bar** | 73.83 | 61.37 |
| **ω** | 0.2240 | 0.644 |

Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 395
B/MPa = 501

*Deviations*
MAPE on x = 12 %
MAPE on y = 16 %
MAPE on $x_c$ = 40 %
MAPE on $P_c$ = 10 %
MAPE on $h^M$ = 140 %



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**Isothermal phase equilibrium data**

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Guo, L. - Wu, X.-H. - Zheng, D.-X. - Deng, W., Measurement and Correlation of Vapor−Liquid Equilibrium for the Carbon Dioxide + 1-Butoxy Butane System, Journal of Chemical & Engineering Data 1 (2010) 476-478. doi:10.1021/je900231r

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.500 | 0.0555 | 0.9886 |
| 16.00 | 0.1292 | 0.9948 |
| 22.20 | 0.1755 | 0.9972 |

Secuianu, Catinca - Feroiu, Viorel - Geană, Dan, Phase behavior for carbon dioxide+ethanol system: Experimental measurements and modeling with a cubic equation of state, The Journal of Supercritical Fluids 2 (2008) 109-116. doi:10.1016/j.supflu.2008.08.004

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.800 | 0.0497 | 0.9879 |
| 16.70 | 0.1315 | 0.9950 |
| 21.40 | 0.1692 | 0.9967 |
| 28.70 | 0.2417 | 0.9978 |
| 35.40 | 0.3062 | 0.9983 |
| 46.20 | 0.4870 | 0.9978 |

Day, Chany-Yih - Chang, Chiehming J. - Chen, Chiu-Yang, Phase Equilibrium of Ethanol + CO2 and Acetone + CO2 at Elevated Pressures, Journal of Chemical & Engineering Data 4 (1996) 839-843. doi:10.1021/je960049d

**T / K = 298.17**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.60 | 0.1305 | 0.9855 |
| 16.20 | 0.1865 | 0.9873 |
| 22.80 | 0.2624 | 0.9895 |
| 29.60 | 0.3273 | 0.9906 |
| 36.50 | 0.4103 | 0.9918 |
| 43.40 | 0.5172 | 0.9905 |
| 53.90 | 0.6866 | 0.9879 |
| 58.20 | 0.8139 | 0.9860 |

Yao, S. - Liu, F. - Han, Z. - Zhu, Z., Vapor-liquid equilibria of binary systems of alcohols, water-carbon dioxide at supercritical or near critical condition, Gaoxiao Huaxue Gongcheng Xuebao 3 (1989) 9-15.

**T / K = 304.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 22.20 | 0.1834 | 0.9959 |
| 28.40 | 0.2420 | 0.9963 |
| 35.90 | 0.3050 | 0.9966 |
| 40.80 | 0.3540 | 0.9960 |
| 45.30 | 0.3999 | 0.9963 |
| 49.80 | 0.4610 | 0.9962 |
| 53.70 | 0.5161 | 0.9959 |
| 58.80 | 0.6169 | 0.9952 |
| 62.40 | 0.6719 | 0.9950 |
| 65.70 | 0.7326 | 0.9943 |
| 68.20 | 0.7866 | 0.9913 |
| 69.80 | 0.8855 | 0.9904 |

Tanaka, Hiroyuki - Kato, Masahiro, Vapor-liquid equilibrium properties of carbon dioxide + ethanol mixture at high pressures., JOURNAL OF CHEMICAL ENGINEERING OF JAPAN 3 (1995) 263-266. doi:10.1252/jcej.28.263

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 15.52 | 0.1098 | 0.9833 | |
| 26.16 | 0.1904 | 0.9892 | |
| 49.41 | 0.3755 | 0.9942 | |
| 57.32 | 0.4587 | 0.9915 | |
| 59.92 | 0.5160 | 0.9952 | |
| 65.95 | 0.6152 | 0.9953 | |
| 66.15 | 0.6415 | 0.9954 | |
| 68.65 | 0.7206 | 0.9924 | |
| 69.18 | 0.7511 | 0.9898 | |
| 70.12 | 0.8010 | 0.9956 | |
| 70.63 | 0.8376 | 0.9978 | |
| 72.46 | 0.9289 | 0.9971 | |
| 74.28 | 0.9687 | 0.9978 | |
| 74.73 | 0.9752 | 0.9951 | |
| 76.04 | 0.9926 | 0.9963 | |
| 77.94 | 0.9940 | 0.9940 | CRIT |
| 77.12 | 0.9944 | 0.9964 | |
| 77.48 | 0.9945 | 0.9960 | |

Tochigi, Katsumi - Namae, Tooru - Suga, Tooru - Matsuda, Hiroyuki - Kurihara, Kiyofumi - dos Ramos, M. Carolina - McCabe, Clare, Measurement and prediction of high-pressure vapor–liquid equilibria for binary mixtures of carbon dioxide+n-octane, methanol, ethanol, and perfluorohexane, The Journal of Supercritical Fluids 2 (2010) 682-689. doi:10.1016/j.supflu.2010.10.016

**T / K = 313.14**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.130 | 0.0480 | 0.9685 |
| 10.54 | 0.0751 | 0.9813 |
| 15.46 | 0.1031 | 0.9859 |
| 20.51 | 0.1375 | 0.9922 |

| | | |
|---|---|---|
| 25.82 | 0.1710 | 0.9916 |
| 30.41 | 0.1933 | 0.9942 |
| 35.55 | 0.2267 | 0.9948 |
| 40.37 | 0.2606 | 0.9942 |
| 45.52 | 0.2832 | 0.9948 |
| 50.44 | 0.3313 | 0.9947 |
| 55.33 | 0.3709 | 0.9943 |
| 60.61 | 0.4123 | 0.9938 |
| 65.58 | 0.4550 | 0.9928 |
| 70.87 | 0.5236 | 0.9926 |
| 74.27 | 0.6095 | 0.9925 |
| 77.16 | 0.7261 | 0.9890 |

Day, Chany-Yih - Chang, Chiehming J. - Chen, Chiu-Yang, Phase Equilibrium of Ethanol + CO2 and Acetone + CO2 at Elevated Pressures, Journal of Chemical & Engineering Data 4 (1996) 839-843. doi:10.1021/je960049d

**T / K = 313.14**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 9.100 | 0.0529 | 0.9849 |
| 18.40 | 0.1009 | 0.9864 |
| 29.20 | 0.1718 | 0.9877 |
| 39.30 | 0.2280 | 0.9894 |
| 45.00 | 0.2800 | 0.9905 |
| 49.70 | 0.3200 | 0.9912 |
| 54.90 | 0.3609 | 0.9918 |
| 59.00 | 0.3999 | 0.9922 |
| 63.10 | 0.4398 | 0.9912 |
| 66.50 | 0.4897 | 0.9900 |
| 70.20 | 0.5399 | 0.9886 |
| 73.10 | 0.5844 | 0.9865 |
| 76.00 | 0.6593 | 0.9823 |
| 77.30 | 0.7492 | 0.9770 |
| 79.20 | 0.8210 | 0.9725 |

Joung, Seung Nam - Yoo, Chang Woo - Shin, Hun Yong - Kim, Sun Young - Yoo, Ki-Pung - Lee, Chul Soo - Huh, Wan Soo, Measurements and correlation of high-pressure VLE of binary CO2–alcohol systems (methanol, ethanol, 2-methoxyethanol and 2-ethoxyethanol), Fluid Phase Equilibria 1-2 (2001) 219-230. doi:10.1016/S0378-3812(01)00472-1

**T / K = 322.50**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.700 | 0.0302 | 0.9406 | |
| 25.60 | 0.1272 | 0.9804 | |
| 38.10 | 0.1908 | 0.9844 | |
| 48.50 | 0.2514 | 0.9853 | |
| 58.60 | 0.3180 | 0.9855 | |
| 77.40 | 0.4887 | 0.9809 | |
| 84.60 | 0.6091 | 0.9753 | |
| 87.90 | 0.7056 | 0.9704 | |
| 89.80 | 0.7878 | 0.9645 | |
| 91.40 | 0.9162 | 0.9470 | |
| 91.80 | 0.9192 | 0.9297 | |
| 92.10 | 0.9198 | 0.9198 | CRIT |

Brandt, L., Einsatz überkritischer Fluide für die Trenntechnik, Thesis (2011) 1-128.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.57 | 0.0420 | 0.9160 |
| 19.75 | 0.0940 | 0.9630 |
| 31.25 | 0.1560 | 0.9730 |
| 43.33 | 0.2180 | 0.9740 |
| 45.74 | 0.2300 | 0.9800 |
| 79.87 | 0.4780 | 0.9720 |
| 90.05 | 0.5830 | 0.9760 |
| 93.83 | 0.6520 | 0.9590 |
| 98.91 | 0.8170 | 0.9450 |

Suzuki, Kazuhiko - Sue, Haruhusa - Itou, Masahiro - Smith, Richard L. - Inomata, Hiroshi - Arai, Kunio - Saito, Shozaburo, Isothermal vapor-liquid equilibrium data for binary systems at high pressures: carbon dioxide-methanol, carbon dioxide-ethanol, carbon dioxide-1-propanol, methane-ethanol, methane-1-propanol, ethane-ethanol, and ethane-1-propanol systems, Journal of Chemical & Engineering Data 1 (1990) 63-66. doi:10.1021/je00059a020

**T / K = 333.40**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.440 | 0.0200 | 0.9050 |
| 9.910 | 0.0380 | 0.9470 |
| 21.10 | 0.0880 | 0.9720 |
| 30.30 | 0.1290 | 0.9780 |
| 40.43 | 0.1690 | 0.9810 |
| 49.93 | 0.2170 | 0.9820 |
| 60.94 | 0.2780 | 0.9810 |
| 75.29 | 0.3720 | 0.9790 |
| 90.24 | 0.4940 | 0.9720 |
| 99.49 | 0.6100 | 0.9540 |
| 105.18 | 0.7260 | 0.9340 |
| 105.80 | 0.7630 | 0.9230 |
| 106.54 | 0.8170 | 0.9080 |

Joung, Seung Nam - Yoo, Chang Woo - Shin, Hun Yong - Kim, Sun Young - Yoo, Ki-Pung - Lee, Chul Soo - Huh, Wan Soo, Measurements and correlation of high-pressure VLE of binary CO2–alcohol systems

(methanol, ethanol, 2-methoxyethanol and 2-ethoxyethanol), Fluid Phase Equilibria 1-2 (2001) 219-230. doi:10.1016/S0378-3812(01)00472-1

**T / K = 333.40**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 6.600 | 0.0285 | 0.9141 | |
| 27.30 | 0.1172 | 0.9716 | |
| 37.50 | 0.1618 | 0.9750 | |
| 58.30 | 0.2666 | 0.9778 | |
| 71.80 | 0.3456 | 0.9780 | |
| 87.00 | 0.4629 | 0.9707 | |
| 95.40 | 0.5534 | 0.9647 | |
| 103.70 | 0.7091 | 0.9373 | |
| 104.50 | 0.7333 | 0.9299 | |
| 106.10 | 0.8323 | 0.8906 | |
| 106.40 | 0.8633 | 0.8633 | CRIT |

Joung, Seung Nam - Yoo, Chang Woo - Shin, Hun Yong - Kim, Sun Young - Yoo, Ki-Pung - Lee, Chul Soo - Huh, Wan Soo, Measurements and correlation of high-pressure VLE of binary CO2–alcohol systems (methanol, ethanol, 2-methoxyethanol and 2-ethoxyethanol), Fluid Phase Equilibria 1-2 (2001) 219-230. doi:10.1016/S0378-3812(01)00472-1

**T / K = 344.75**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 8.000 | 0.0307 | 0.8727 | |
| 28.30 | 0.1082 | 0.9543 | |
| 38.80 | 0.1492 | 0.9617 | |
| 60.30 | 0.2448 | 0.9678 | |
| 70.60 | 0.2941 | 0.9679 | |
| 92.80 | 0.4253 | 0.9614 | |
| 102.70 | 0.5024 | 0.9523 | |
| 114.00 | 0.6346 | 0.9252 | |
| 116.30 | 0.6720 | 0.9076 | |
| 119.00 | 0.7734 | 0.8494 | |
| 119.30 | 0.8008 | 0.8068 | |
| 119.70 | 0.8020 | 0.8020 | CRIT |

Galicia-Luna, Luis A. - Ortega-Rodriguez, A. - Richon, D., New Apparatus for the Fast Determination of High-Pressure Vapor−Liquid Equilibria of Mixtures and of Accurate Critical Pressures, Journal of Chemical & Engineering Data 2 (2000) 265-271. doi:10.1021/je990187d

**T / K = 348.40**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 15.15 | 0.0576 | 0.9176 | |
| 35.15 | 0.1391 | 0.9606 | |
| 55.18 | 0.2213 | 0.9618 | |
| 76.34 | 0.3285 | 0.9599 | |
| 106.07 | 0.5193 | 0.9425 | |
| 120.02 | 0.6718 | 0.9003 | |
| 123.01 | 0.7273 | 0.8851 | |
| 124.60 | 0.7980 | 0.7980 | CRIT |

Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 55.00 | 0.2097 | 0.9825 | |
| 70.00 | 0.2798 | 0.9854 | |
| 80.00 | 0.3184 | 0.9840 | |
| 90.00 | 0.3682 | 0.9890 | |
| 110.00 | 0.4926 | 0.9637 | |
| 120.00 | 0.5714 | 0.9510 | |
| 131.00 | 0.8784 | 0.8784 | CRIT |

Secuianu, Catinca - Feroiu, Viorel - Geană, Dan, Phase behavior for carbon dioxide+ethanol system: Experimental measurements and modeling with a cubic equation of state, The Journal of Supercritical Fluids 2 (2008) 109-116. doi:10.1016/j.supflu.2008.08.004

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.200 | 0.0187 | 0.7819 |
| 14.50 | 0.0596 | 0.8933 |
| 30.00 | 0.1096 | 0.9464 |
| 41.50 | 0.1536 | 0.9604 |
| 52.70 | 0.2037 | 0.9656 |
| 64.20 | 0.2471 | 0.9695 |
| 74.80 | 0.2948 | 0.9703 |
| 79.70 | 0.3185 | 0.9704 |
| 85.30 | 0.3439 | 0.9692 |
| 95.50 | 0.4077 | 0.9650 |
| 100.80 | 0.4359 | 0.9610 |
| 110.80 | 0.4951 | 0.9471 |

Galicia-Luna, Luis A. - Ortega-Rodriguez, A. - Richon, D., New Apparatus for the Fast Determination of High-Pressure Vapor−Liquid Equilibria of Mixtures and of Accurate Critical Pressures, Journal of Chemical & Engineering Data 2 (2000) 265-271. doi:10.1021/je990187d

**T / K = 373.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 21.76 | 0.0649 | 0.8827 |
| 42.20 | 0.1350 | 0.9165 |
| 61.51 | 0.2054 | 0.9328 |
| 91.65 | 0.3358 | 0.9161 |
| 120.24 | 0.4790 | 0.9120 |

| | | | |
|---|---|---|---|
| 128.21 | 0.5303 | 0.8980 | |
| 141.14 | 0.6593 | 0.8297 | |
| 143.45 | 0.7181 | 0.7181 | CRIT |

Mendoza de la Cruz, J.L. - Galicia-Luna, L.A., High-pressure vapor-liquid equilibria for the carbon dioxide + ethanol and carbon dioxide + 1-propanol systems at temperatures from 322.36 K to 391.96 K, ELDATA Int. Electron. J. Phys. Chem. Data 3 (1999) 157-164.

**T / K = 391.96**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 13.20 | 0.0290 | 0.6670 |
| 30.30 | 0.0820 | 0.7940 |
| 46.70 | 0.1340 | 0.8480 |
| 60.20 | 0.1800 | 0.8640 |
| 79.30 | 0.2440 | 0.8730 |
| 103.61 | 0.3330 | 0.8830 |
| 120.31 | 0.4150 | 0.8730 |
| 141.11 | 0.5390 | 0.8310 |
| 146.21 | 0.5960 | 0.8040 |

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**Enthalpy of mixing**

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Hauser, Raul A. - Zhao, Jian Ping - Tremaine, Peter R. - Mather, Alan E., Excess molar enthalpies of six (carbon dioxide + a polar solvent) mixtures at the temperatures 298.15 K and 308.15 K and pressures from 7.5 MPa to 12.6 MPa, The Journal of Chemical Thermodynamics 11 (1996) 1303-1317. doi:10.1006/jcht.1996.0115

**T / K = 298.15**

**P / bar = 75.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -78.80 | 0.0508 |
| -131.90 | 0.1006 |
| -171.70 | 0.1495 |
| -200.00 | 0.1975 |
| -214.20 | 0.2447 |
| -220.60 | 0.2909 |
| -218.90 | 0.3363 |
| -215.40 | 0.3810 |
| -195.50 | 0.4248 |
| -179.60 | 0.4678 |
| -159.70 | 0.5102 |
| -139.00 | 0.5517 |
| -117.30 | 0.5926 |
| -92.40 | 0.6328 |
| -67.90 | 0.6723 |
| -41.70 | 0.7111 |
| -15.40 | 0.7493 |
| 11.90 | 0.7869 |
| 38.10 | 0.8239 |
| 60.50 | 0.8602 |
| 80.50 | 0.8960 |
| 89.00 | 0.9312 |
| 84.50 | 0.9659 |

Cordray, D.R. - Izatt, R.M. - Christensen, J.J. - Oscarson, J.L., The excess enthalpies of (carbon dioxide + ethanol) at 308.15, 325.15, 373.15, 413.15, and 473.15 K from 5.00 to 14.91 MPa, The Journal of Chemical Thermodynamics 6 (1988) 655-663. doi:10.1016/0021-9614(88)90016-X

**T / K = 308.15**

**P / bar = 125.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -54.20 | 0.0435 |
| -75.60 | 0.0651 |
| -117.00 | 0.1081 |
| -143.00 | 0.1508 |
| -156.00 | 0.1932 |
| -160.00 | 0.2143 |
| -163.00 | 0.2353 |
| -159.00 | 0.2562 |
| -163.00 | 0.2771 |
| -153.00 | 0.2979 |
| -151.00 | 0.2979 |
| -151.00 | 0.3186 |
| -139.00 | 0.3598 |
| -136.00 | 0.3598 |
| -118.00 | 0.4007 |
| -95.80 | 0.4414 |
| -68.80 | 0.4817 |
| -42.20 | 0.5218 |
| -16.60 | 0.5616 |
| -14.70 | 0.5616 |
| 13.10 | 0.6011 |
| 39.20 | 0.6403 |
| 45.90 | 0.6403 |
| 79.20 | 0.6793 |
| 132.00 | 0.7564 |
| 166.00 | 0.7946 |
| 183.00 | 0.8325 |
| 195.00 | 0.8514 |
| 204.00 | 0.8702 |
| 206.00 | 0.8889 |
| 210.00 | 0.9076 |
| 210.00 | 0.9262 |
| 195.00 | 0.9447 |

| | |
|---|---|
| 166.00 | 0.9632 |
| 108.00 | 0.9816 |

Cordray, D.R. - Izatt, R.M. - Christensen, J.J. - Oscarson, J.L., The excess enthalpies of (carbon dioxide + ethanol) at 308.15, 325.15, 373.15, 413.15, and 473.15 K from 5.00 to 14.91 MPa, The Journal of Chemical Thermodynamics 6 (1988) 655-663. doi:10.1016/0021-9614(88)90016-X

**T / K = 373.15**

**P / bar = 125.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -101.00 | 0.0449 |
| -171.00 | 0.0672 |
| -248.00 | 0.1114 |
| -346.00 | 0.1552 |
| -454.00 | 0.1985 |
| -420.00 | 0.1985 |
| -474.00 | 0.2414 |
| -473.00 | 0.2414 |
| -542.00 | 0.2839 |
| -577.00 | 0.3259 |
| -615.00 | 0.3676 |
| -647.00 | 0.4088 |
| -673.00 | 0.4496 |
| -667.00 | 0.4496 |
| -657.00 | 0.4496 |
| -631.00 | 0.4901 |
| -454.00 | 0.5301 |
| -309.00 | 0.5698 |
| -170.00 | 0.6091 |
| -11.20 | 0.6480 |
| 127.00 | 0.6865 |
| 331.00 | 0.7247 |
| 478.00 | 0.7625 |
| 633.00 | 0.8000 |
| 687.00 | 0.8186 |
| 762.00 | 0.8371 |
| 837.00 | 0.8555 |
| 860.00 | 0.8555 |
| 936.00 | 0.8739 |
| 961.00 | 0.8739 |
| 977.00 | 0.8739 |
| 977.00 | 0.8922 |
| 916.00 | 0.9103 |
| 936.00 | 0.9103 |
| 838.00 | 0.9284 |
| 731.00 | 0.9465 |
| 544.00 | 0.9644 |

Cordray, D.R. - Izatt, R.M. - Christensen, J.J. - Oscarson, J.L., The excess enthalpies of (carbon dioxide + ethanol) at 308.15, 325.15, 373.15, 413.15, and 473.15 K from 5.00 to 14.91 MPa, The Journal of Chemical Thermodynamics 6 (1988) 655-663. doi:10.1016/0021-9614(88)90016-X

**T / K = 473.15**

**P / bar = 100.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 431.00 | 0.0643 |
| 440.00 | 0.0643 |
| 798.00 | 0.1068 |
| 1180.0 | 0.1490 |
| 1420.0 | 0.1701 |
| 1710.0 | 0.1910 |
| 2070.0 | 0.2119 |
| 2490.0 | 0.2328 |
| 4210.0 | 0.3155 |
| 5240.0 | 0.3566 |
| 6530.0 | 0.4176 |
| 6710.0 | 0.4379 |
| 7050.0 | 0.4581 |
| 7110.0 | 0.4782 |
| 7280.0 | 0.4982 |
| 7350.0 | 0.5182 |
| 7310.0 | 0.5382 |
| 7400.0 | 0.5581 |
| 7410.0 | 0.5581 |
| 7100.0 | 0.5977 |
| 6680.0 | 0.6370 |
| 6200.0 | 0.6762 |
| 5020.0 | 0.7538 |
| 4290.0 | 0.7923 |
| 3620.0 | 0.8305 |
| 2880.0 | 0.8686 |
| 2080.0 | 0.9064 |
| 1290.0 | 0.9440 |
| 861.00 | 0.9627 |

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**Critical point**

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Gurdial, Gurdev S. - Foster, Neil R. - Yun, S. L. Jimmy - Tilly, Kevin D., Phase Behavior of Supercritical Fluid—Entrainer Systems, Supercritical Fluid Engineering Science (1992) 34-45.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 305.80 | 76.50 | 0.9905 |
| 308.40 | 78.30 | 0.9786 |

| | | |
|---|---|---|
| 310.30 | 80.70 | 0.9722 |
| 312.10 | 82.50 | 0.9634 |
| 315.20 | 86.10 | 0.9536 |
| 320.10 | 91.90 | 0.9362 |
| 325.10 | 97.40 | 0.9268 |

Joung, Seung Nam - Yoo, Chang Woo - Shin, Hun Yong - Kim, Sun Young - Yoo, Ki-Pung - Lee, Chul Soo - Huh, Wan Soo, Measurements and correlation of high-pressure VLE of binary CO2–alcohol systems (methanol, ethanol, 2-methoxyethanol and 2-ethoxyethanol), Fluid Phase Equilibria 1-2 (2001) 219-230. doi:10.1016/S0378-3812(01)00472-1

| T / K | P / bar | $x_1$ |
|---|---|---|
| 313.40 | 81.60 | 0.9630 |
| 338.80 | 113.10 | 0.8601 |

Sun, M. - Ye, R. - Liu, T. - Liu, H., Measurements of the Critical Temperature and Pressure of Ethylene+ Benzene+ Ethylbenzene Mixture, Chin. J. Chem. Eng. 4 (2002) 469-472.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 311.72 | 80.75 | 0.9669 |
| 332.80 | 106.50 | 0.8562 |
| 332.91 | 108.05 | 0.8323 |
| 347.45 | 123.65 | 0.7980 |

Galicia-Luna, Luis A. - Ortega-Rodriguez, A. - Richon, D., New Apparatus for the Fast Determination of High-Pressure Vapor−Liquid Equilibria of Mixtures and of Accurate Critical Pressures, Journal of Chemical & Engineering Data 2 (2000) 265-271. doi:10.1021/je990187d

| T / K | P / bar | $x_1$ |
|---|---|---|
| 312.82 | 81.54 | 0.9669 |
| 333.75 | 107.60 | 0.8562 |
| 333.82 | 108.78 | 0.8323 |

Zhang, J.C. - Wu, X.Y. - Cao, W.L., Phase Equilibrium Properties of Supercritical Carbon Dioxide in Binary System, Gaodeng Xuexiao Huaxue Xuebao 1 (2002) 10-13.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 307.85 | 75.10 | 0.9958 |
| 308.35 | 76.20 | 0.9954 |
| 310.25 | 77.60 | 0.9909 |
| 311.65 | 80.10 | 0.9876 |
| 313.75 | 82.30 | 0.9844 |
| 317.85 | 86.60 | 0.9777 |

Yi-Ling Tian - Ming Han - Li Chen - Ji-Jun Feng - Ying Qin, Study on Vapor-Liquid Phase Equilibria for CO2-C2H5OH System, Wuli Huaxue Xuebao 2 (2001) 155-160.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 333.00 | 108.00 | 0.8900 |
| 353.00 | 131.00 | 0.8800 |
| 413.00 | 153.00 | 0.7200 |
| 453.00 | 133.00 | 0.5300 |

Sima, Sergiu - Feroiu, Viorel - Geană, Dan, New High Pressure Vapor−Liquid Equilibrium and Density Predictions for the Carbon Dioxide + Ethanol System, Journal of Chemical & Engineering Data 12 (2011) 5052-5059. doi:10.1021/je2008186

| T / K | P / bar | $x_1$ |
|---|---|---|
| 364.20 | 138.60 | 0.8315 |
| 361.65 | 137.00 | 0.8380 |
| 355.05 | 131.10 | 0.8401 |
| 348.65 | 125.40 | 0.8409 |
| 342.65 | 120.00 | 0.8420 |
| 335.65 | 111.70 | 0.8507 |
| 332.20 | 106.00 | 0.9010 |
| 330.20 | 104.50 | 0.8920 |
| 325.70 | 98.40 | 0.9080 |
| 321.20 | 91.00 | 0.9310 |

Pfohl, O. - Avramova, Pavlina - Brunner, Gerd, Two- and three-phase equilibria in systems containing benzene derivatives, carbon dioxide, and water at 373.15 K and 10-30 MPa, Fluid Phase Equilibria (1998) 179-206. doi:10.1016/S0378-3812(97)00210-0

| T / K | P / bar | $x_1$ |
|---|---|---|
| 373.15 | 150.00 | 0.7158 |

Gil, Laura - Blanco, Sofía T. - Rivas, Clara - Laga, Eduardo - Fernández, Javier - Artal, Manuela - Velasco, Inmaculada, Experimental determination of the critical loci for {n-C6H14 or CO2+alkan-1-ol} mixtures. Evaluation of their critical and subcritical behavior using PC-SAFT EoS, The Journal of Supercritical Fluids (2012) 26-44. doi:10.1016/j.supflu.2012.07.008

| T / K | P / bar | $x_1$ |
|---|---|---|
| 507.29 | 73.09 | 0.0500 |
| 501.54 | 80.64 | 0.1000 |
| 493.23 | 90.52 | 0.1500 |
| 486.84 | 95.79 | 0.1998 |
| 480.48 | 105.09 | 0.2504 |
| 474.58 | 110.56 | 0.3000 |
| 466.35 | 118.65 | 0.3496 |
| 458.40 | 125.78 | 0.3999 |
| 451.14 | 133.90 | 0.4496 |
| 436.22 | 140.86 | 0.5002 |
| 428.65 | 144.39 | 0.5505 |

| | | |
|---|---|---|
| 413.32 | 149.29 | 0.6001 |
| 400.57 | 150.77 | 0.6504 |
| 374.38 | 144.00 | 0.7199 |
| 368.18 | 138.42 | 0.7506 |
| 348.47 | 124.29 | 0.8002 |
| 336.96 | 110.88 | 0.8504 |
| 326.90 | 98.17 | 0.9000 |
| 319.07 | 86.05 | 0.9501 |

Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 333.15 | 108.00 | 0.8920 |
| 413.15 | 153.00 | 0.7213 |
| 453.15 | 133.00 | 0.5117 |

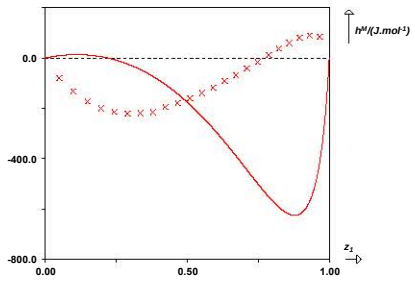
Yeo, Sang-Do - Park, Su-Jin - Kim, Jin-Woo - Kim, Jae-Chang, Critical Properties of Carbon Dioxide + Methanol, + Ethanol, + 1-Propanol, and + 1-Butanol, Journal of Chemical & Engineering Data 5 (2000) 932-935. doi:10.1021/je000104p

| T / K | P / bar | $x_1$ |
|---|---|---|
| 310.58 | 77.73 | 0.9560 |
| 318.24 | 86.35 | 0.9380 |
| 328.36 | 100.89 | 0.8630 |
| 350.62 | 128.04 | 0.7690 |
| 377.17 | 146.30 | 0.6970 |
| 393.08 | 151.54 | 0.6460 |
| 410.32 | 151.67 | 0.5970 |

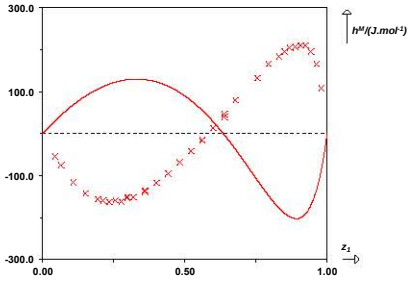
Wu, Weize - Ke, Jie - Poliakoff, Martyn, Phase Boundaries of CO2 + Toluene, CO2 + Acetone, and CO2 + Ethanol at High Temperatures and High Pressures, Journal of Chemical & Engineering Data 4 (2006) 1398-1403. doi:10.1021/je060099a

| T / K | P / bar | $x_1$ |
|---|---|---|
| 383.20 | 147.20 | 0.7000 |
| 493.00 | 88.70 | 0.2000 |

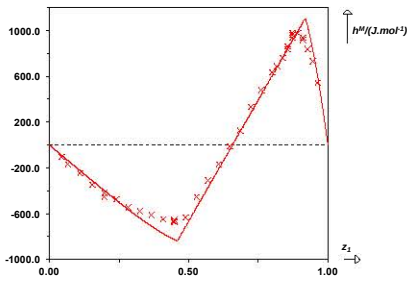
T/K = 298.15 - P/bar = 75.00



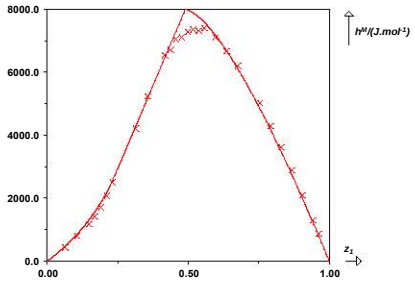

T/K = 308.15 - P/bar = 125.00



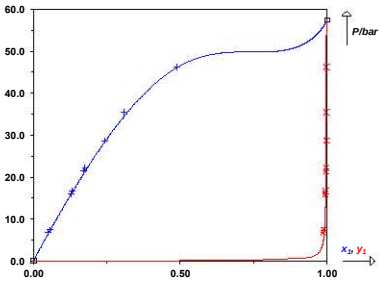

T/K = 373.15 - P/bar = 125.00



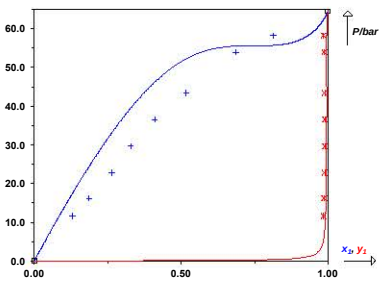

T/K = 473.15 - P/bar = 100.00



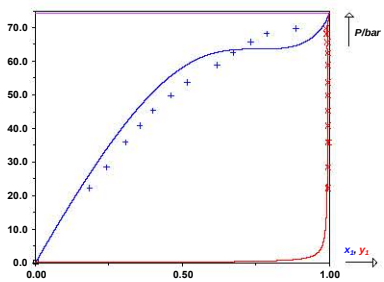

T/K = 293.15



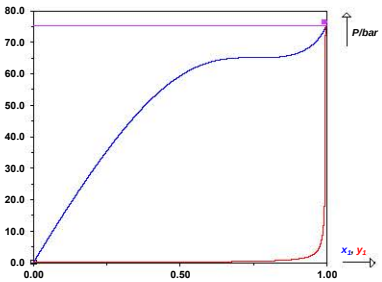

T/K = 298.17



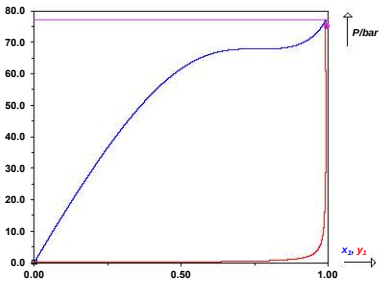

T/K = 304.65



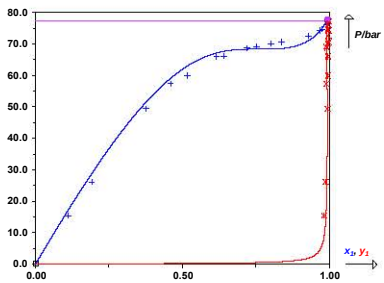

T/K = 305.80



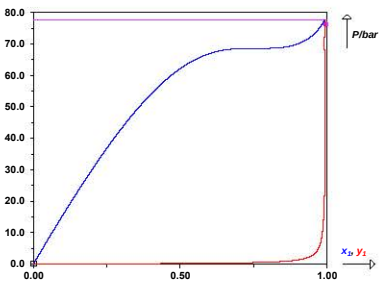

T/K = 307.85



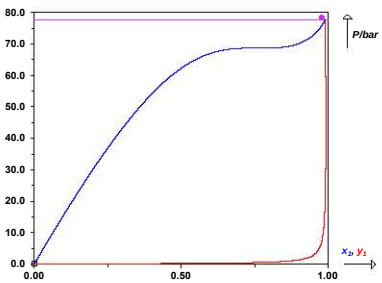

T/K = 308.15



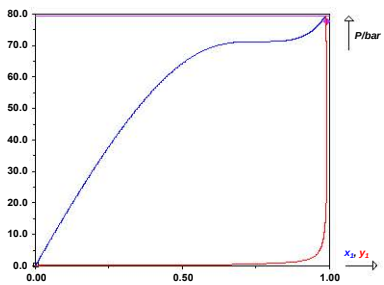

T/K = 308.35



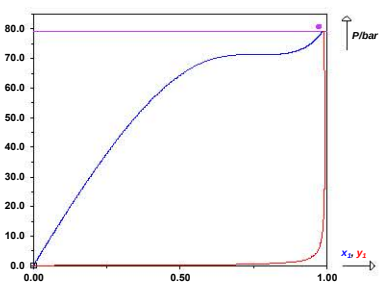

T/K = 308.40



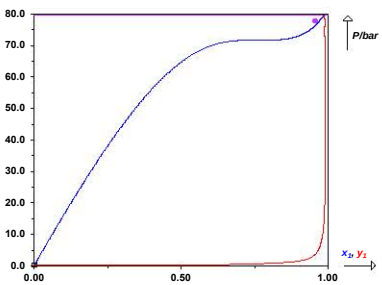

T/K = 310.25



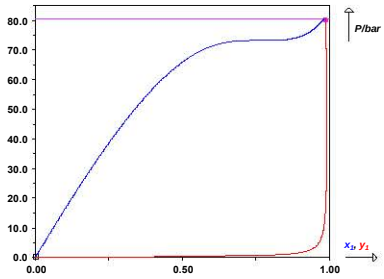

T/K = 310.30



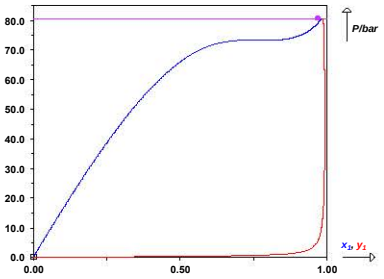

T/K = 310.58



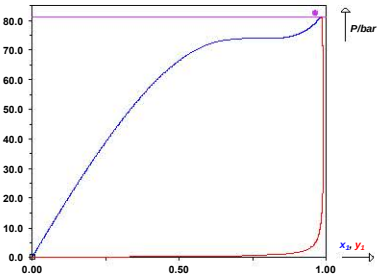
T/K = 311.65



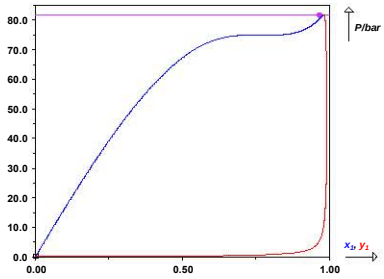

T/K = 311.72



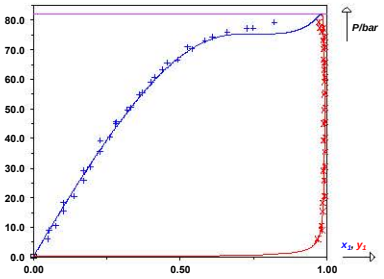

T/K = 312.10



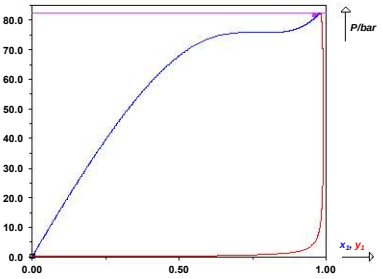

T/K = 312.82



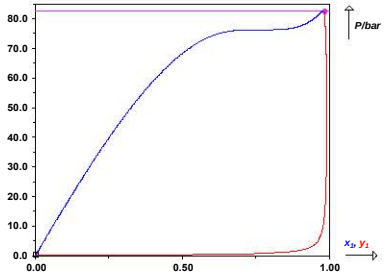

T/K = 313.14



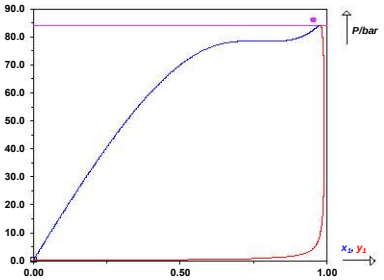

T/K = 313.40



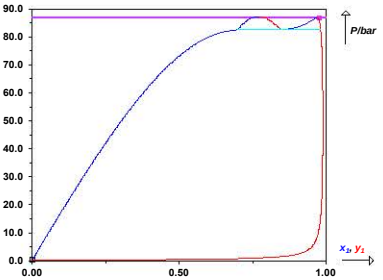

T/K = 313.75



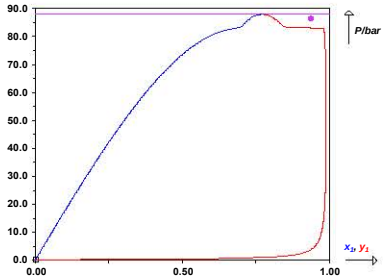

T/K = 315.20



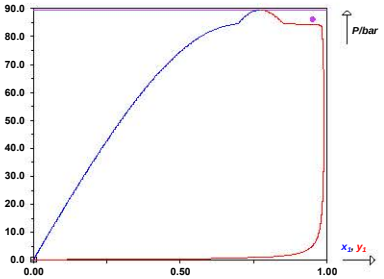

T/K = 317.85



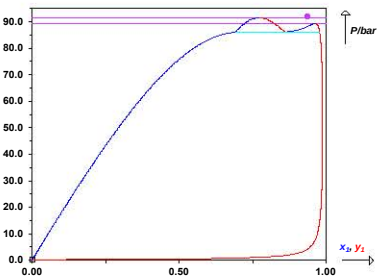

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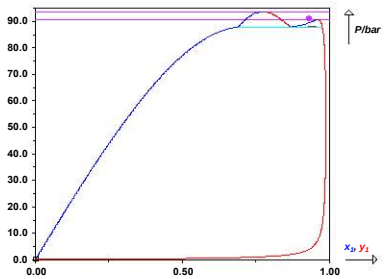

T/K = 319.07



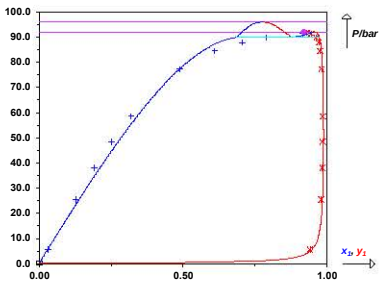

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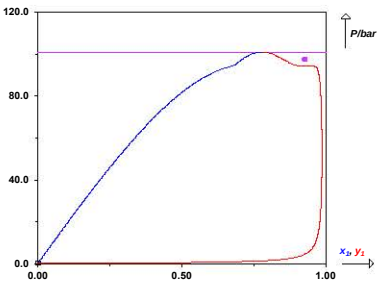

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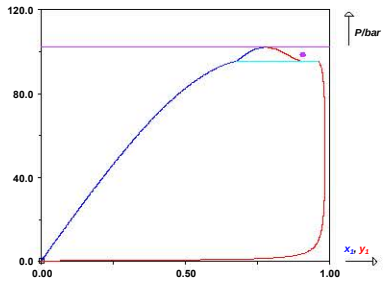

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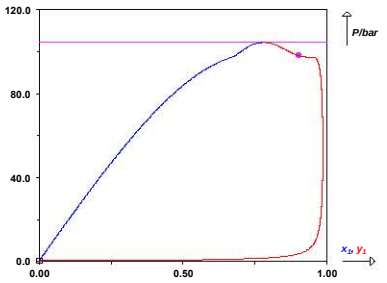

T/K = 325.10



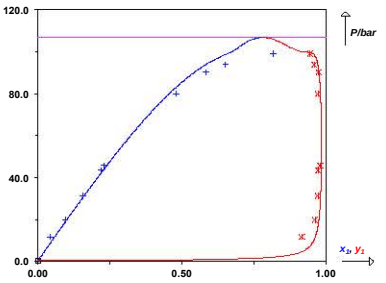
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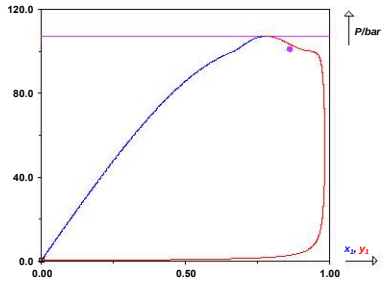

T/K = 326.90



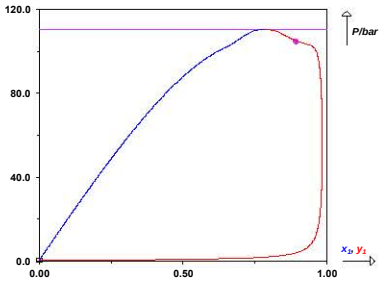

T/K = 328.15



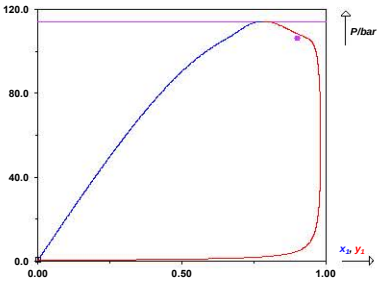

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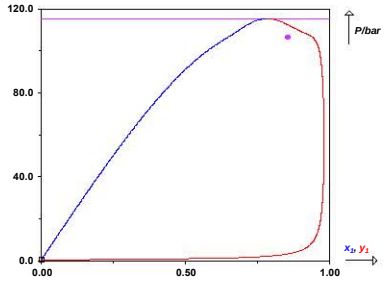

T/K = 330.20



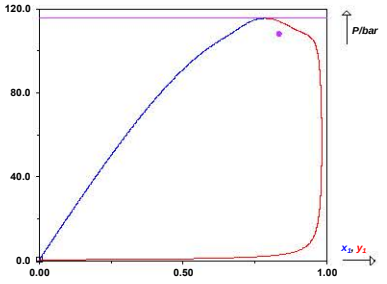

T/K = 332.20



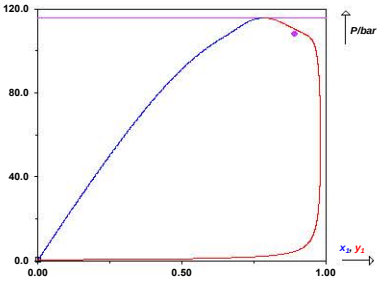

T/K = 332.80



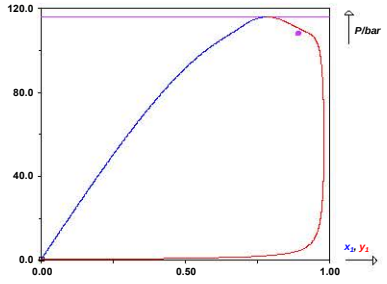

T/K = 332.91



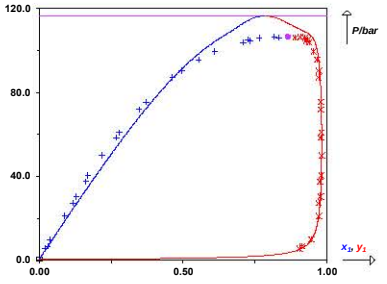

T/K = 333.00



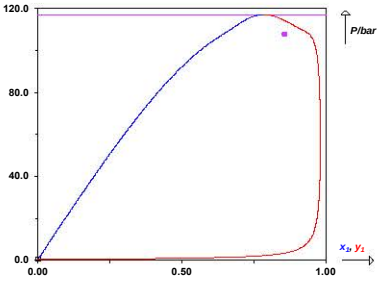

T/K = 333.15



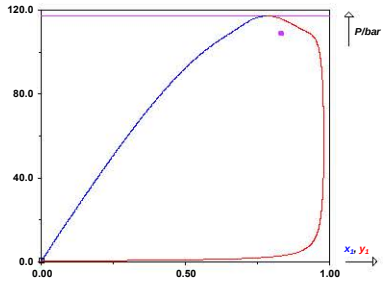

T/K = 333.40



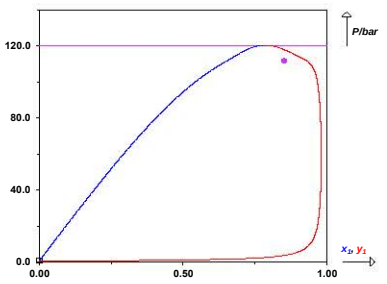

T/K = 333.75



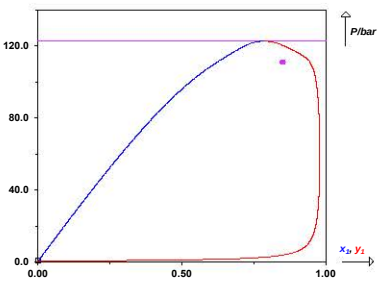

T/K = 333.82



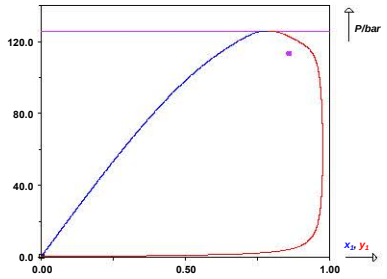

T/K = 335.65



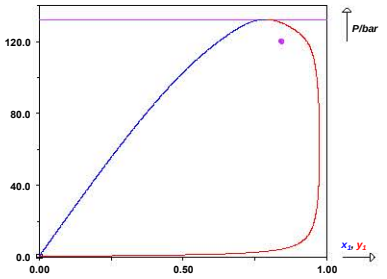

T/K = 336.96



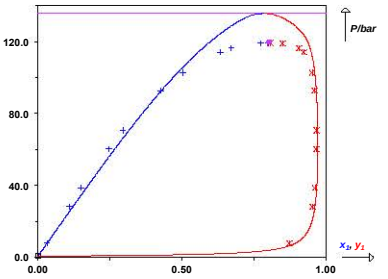
T/K = 338.80



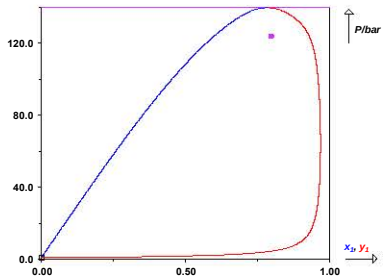

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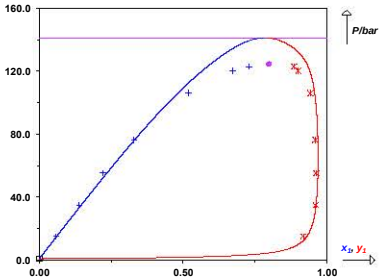

T/K = 344.75



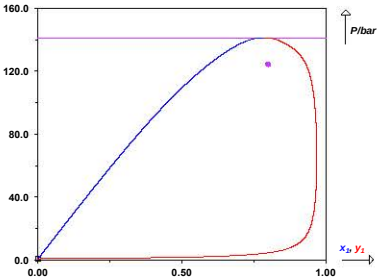

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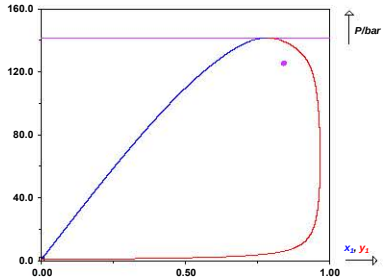

T/K = 348.40



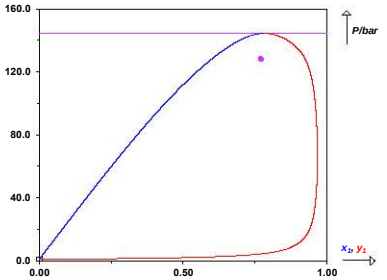

T/K = 348.47



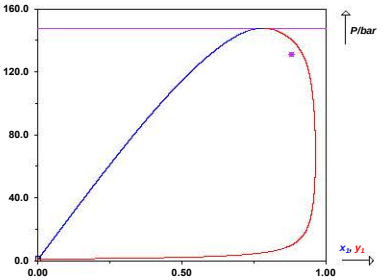

T/K = 348.65



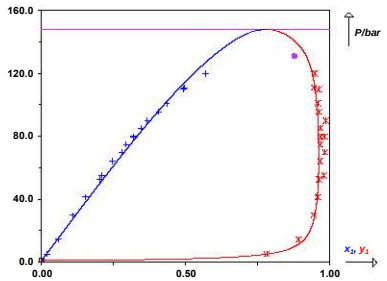

T/K = 350.62



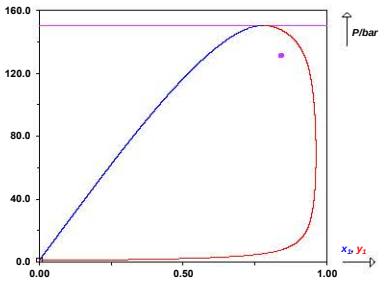

T/K = 353.00



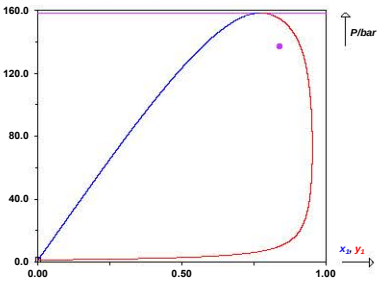

T/K = 353.15



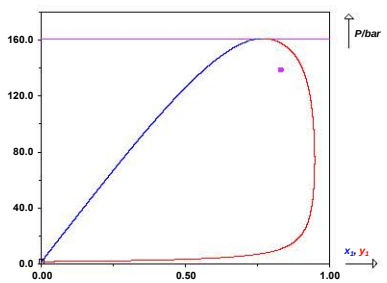

T/K = 355.05



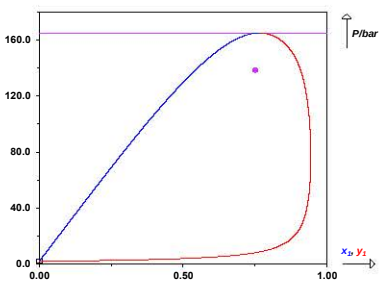

T/K = 361.65



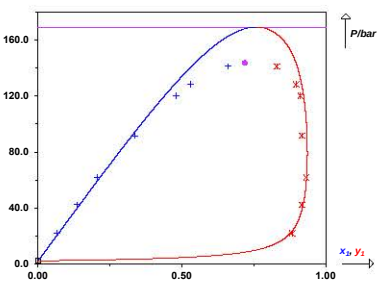

T/K = 364.20



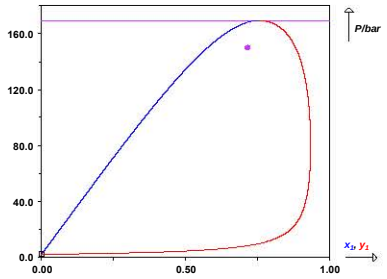

T/K = 368.18



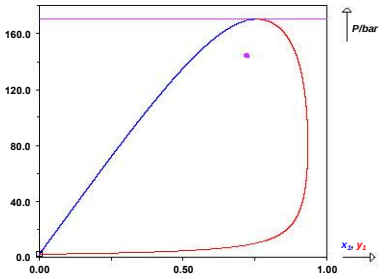

T/K = 373.00



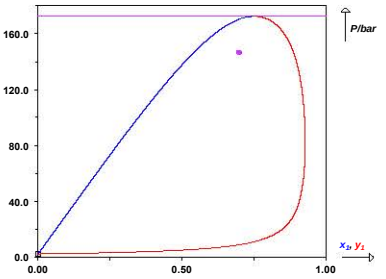
T/K = 373.15



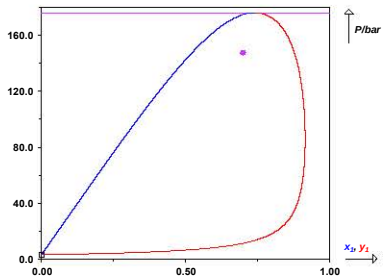

T/K = 374.38



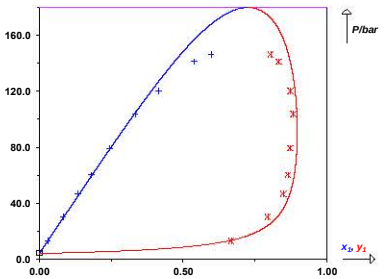

T/K = 377.17



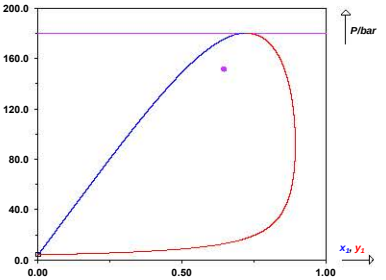

T/K = 383.20



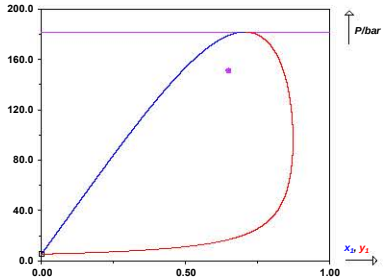

T/K = 391.96



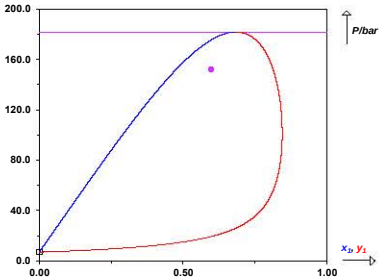

T/K = 393.08



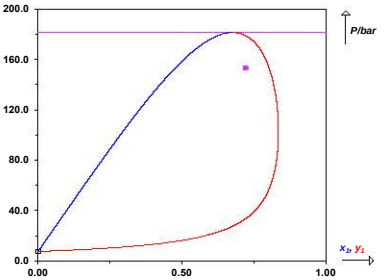

T/K = 400.57



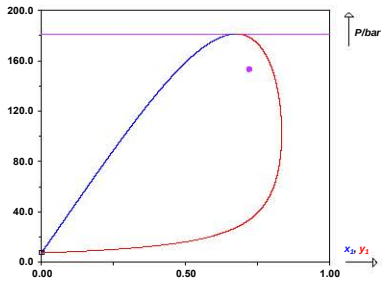

T/K = 410.32



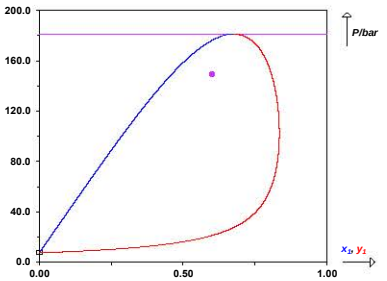

T/K = 413.00



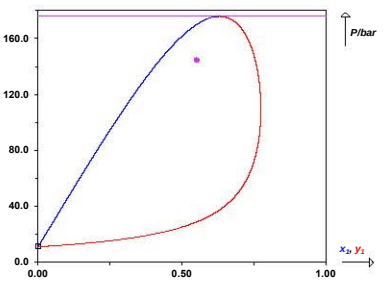

T/K = 413.15



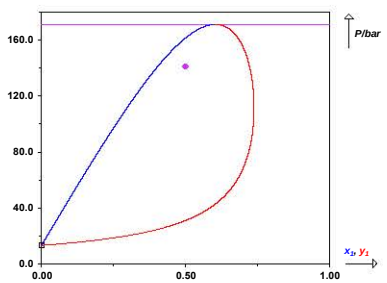

T/K = 413.32



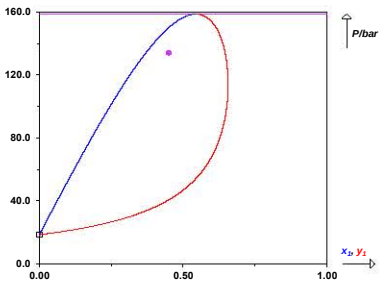

T/K = 428.65



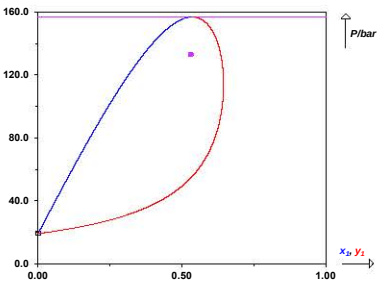

T/K = 436.22



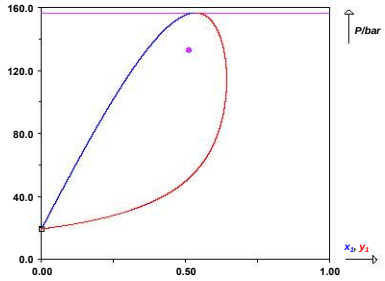

T/K = 451.14



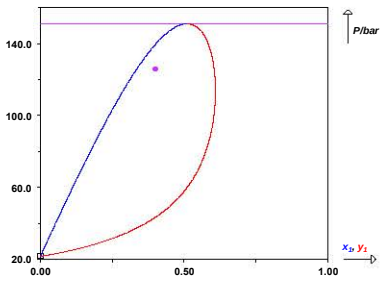

T/K = 453.00



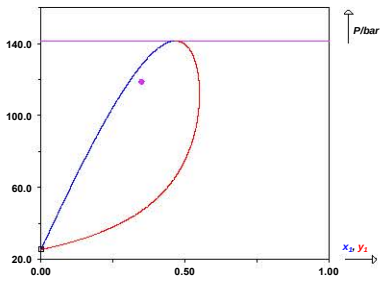
T/K = 453.15



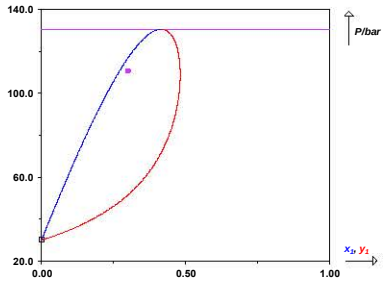

T/K = 458.40



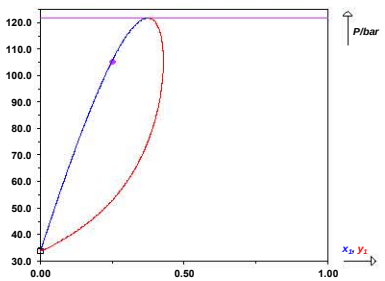

T/K = 466.35



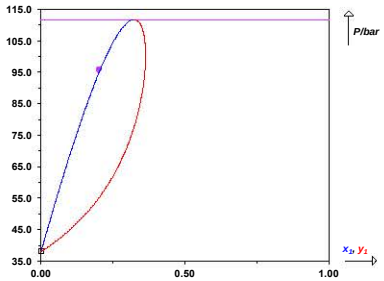

T/K = 474.58



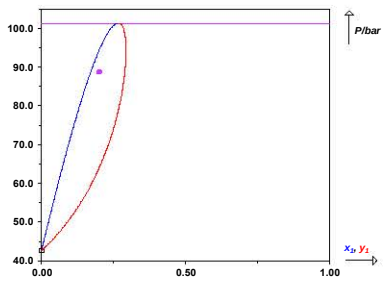

T/K = 480.48



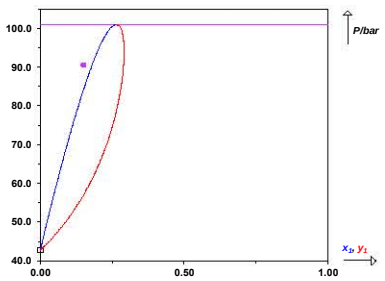

T/K = 486.84



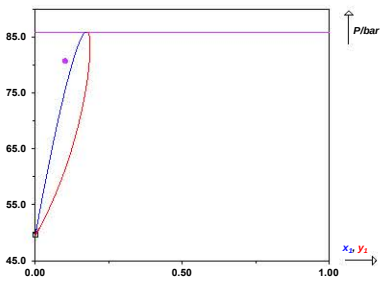

T/K = 493.00



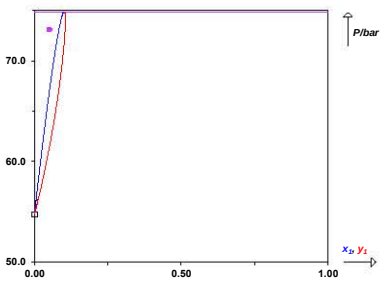

T/K = 493.23




T/K = 501.54




T/K = 507.29



## ETHANOL (1) + METHYL tert-BUTYL ETHER (2)

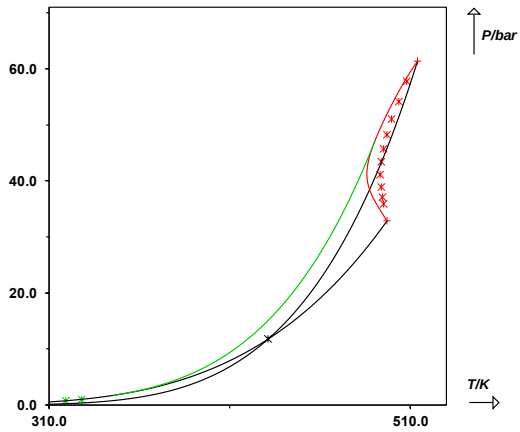
| | | |
|---|---|---|
| **CAS** | 64-17-5 | 1634-04-4 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | BZLVMXJERCGZMT-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 497.10 |
| **$P_c$ / bar** | 61.37 | 32.86 |
| **ω** | 0.6440 | 0.2470 |

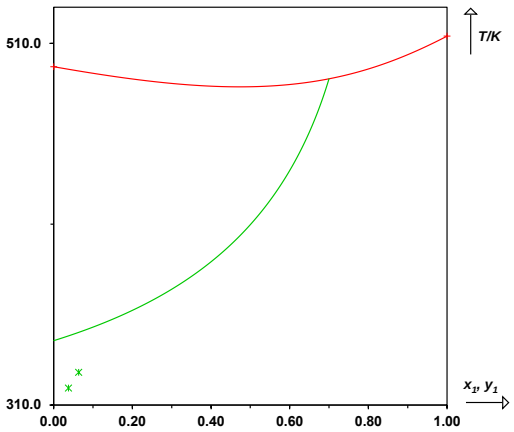
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 232
B/MPa = 30.2

*Deviations*
MAPE on x = 17 %
MAPE on y = 9.2 %
MAPE on $x_c$ = 34 %
MAPE on $P_c$ = 4.3 %
MAPE on $h^M$ = 35 %



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**Isobaric phase equilibrium data**

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Mejía, Andrés - Segura, Hugo - Cartes, Marcela, Vapor−Liquid Equilibria and Interfacial Tensions of the System Ethanol + 2-Methoxy-2-methylpropane, Journal of Chemical & Engineering Data 1 (2010) 428-434. doi:10.1021/je9004068

**P / bar = 0.5000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 330.45 | 0.9600 | 0.7970 |
| 327.90 | 0.9300 | 0.6820 |
| 324.74 | 0.8850 | 0.5630 |
| 321.92 | 0.8340 | 0.4710 |
| 319.54 | 0.7830 | 0.3980 |
| 316.99 | 0.7100 | 0.3270 |
| 315.54 | 0.6550 | 0.2900 |
| 314.44 | 0.6080 | 0.2620 |
| 313.62 | 0.5600 | 0.2400 |
| 312.90 | 0.5150 | 0.2240 |
| 312.14 | 0.4640 | 0.2050 |
| 311.26 | 0.4130 | 0.1830 |
| 310.93 | 0.3680 | 0.1710 |
| 310.41 | 0.3140 | 0.1540 |
| 309.94 | 0.2680 | 0.1410 |
| 309.47 | 0.2130 | 0.1210 |
| 308.96 | 0.1450 | 0.0940 |
| 308.58 | 0.0830 | 0.0630 |
| 308.40 | 0.0460 | 0.0390 |

Mejía, Andrés - Segura, Hugo - Cartes, Marcela, Vapor−Liquid Equilibria and Interfacial Tensions of the System Ethanol + 2-Methoxy-2-methylpropane, Journal of Chemical & Engineering Data 1 (2010) 428-434. doi:10.1021/je9004068

**P / bar = 0.7500**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 339.48 | 0.9570 | 0.7970 |
| 337.38 | 0.9290 | 0.7080 |
| 334.68 | 0.8890 | 0.6090 |
| 332.22 | 0.8380 | 0.5120 |
| 329.79 | 0.7940 | 0.4430 |
| 327.54 | 0.7140 | 0.3620 |
| 326.14 | 0.6590 | 0.3230 |
| 324.53 | 0.6080 | 0.2910 |
| 324.14 | 0.5620 | 0.2710 |
| 323.42 | 0.5170 | 0.2490 |
| 322.80 | 0.4720 | 0.2310 |
| 321.40 | 0.4160 | 0.2080 |
| 320.92 | 0.3680 | 0.1910 |
| 320.64 | 0.3140 | 0.1740 |
| 320.66 | 0.2710 | 0.1590 |
| 320.18 | 0.2160 | 0.1370 |
| 319.79 | 0.1530 | 0.1090 |
| 319.47 | 0.0830 | 0.0700 |
| 319.37 | 0.0460 | 0.0430 |

Arce, Alberto - Martínez-Ageitos, José - Soto, Ana, VLE Measurements of Binary Mixtures of Methanol, Ethanol, 2-Methoxy-2-methylpropane, and 2-Methoxy-2-methylbutane at 101.32 kPa, Journal of Chemical & Engineering Data 4 (1996) 718-723. doi:10.1021/je950323o

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 351.34 | 0.9994 | 0.9966 |
| 351.21 | 0.9981 | 0.9909 |
| 351.18 | 0.9980 | 0.9901 |
| 351.05 | 0.9966 | 0.9837 |
| 350.86 | 0.9952 | 0.9763 |
| 350.73 | 0.9938 | 0.9695 |
| 350.59 | 0.9923 | 0.9624 |
| 350.33 | 0.9895 | 0.9508 |
| 350.11 | 0.9869 | 0.9390 |
| 349.81 | 0.9830 | 0.9255 |
| 348.59 | 0.9689 | 0.8692 |
| 347.97 | 0.9624 | 0.8422 |
| 347.40 | 0.9551 | 0.8162 |
| 346.90 | 0.9478 | 0.7929 |
| 346.24 | 0.9376 | 0.7639 |
| 345.47 | 0.9302 | 0.7323 |
| 344.65 | 0.9167 | 0.6998 |
| 344.26 | 0.9092 | 0.6832 |
| 343.68 | 0.9014 | 0.6607 |
| 342.92 | 0.8871 | 0.6299 |
| 342.18 | 0.8754 | 0.6063 |
| 341.28 | 0.8566 | 0.5700 |
| 340.56 | 0.8422 | 0.5452 |
| 339.30 | 0.8145 | 0.4963 |
| 337.86 | 0.7776 | 0.4457 |
| 336.94 | 0.7482 | 0.4185 |
| 336.24 | 0.7234 | 0.3979 |
| 335.69 | 0.7071 | 0.3840 |
| 335.13 | 0.6851 | 0.3676 |
| 334.09 | 0.6377 | 0.3345 |
| 333.33 | 0.6024 | 0.3153 |
| 332.85 | 0.5782 | 0.3009 |
| 332.29 | 0.5432 | 0.2839 |
| 331.79 | 0.5093 | 0.2692 |

| | | |
|---|---|---|
| 331.35 | 0.4789 | 0.2545 |
| 330.95 | 0.4479 | 0.2421 |
| 330.56 | 0.4117 | 0.2298 |
| 330.18 | 0.3793 | 0.2162 |
| 329.89 | 0.3511 | 0.2037 |
| 329.49 | 0.3057 | 0.1850 |
| 329.28 | 0.2839 | 0.1775 |
| 329.06 | 0.2569 | 0.1662 |
| 328.90 | 0.2323 | 0.1561 |
| 328.68 | 0.2070 | 0.1455 |
| 328.54 | 0.1847 | 0.1347 |
| 328.37 | 0.1523 | 0.1188 |
| 328.24 | 0.1272 | 0.1048 |
| 328.15 | 0.1058 | 0.0921 |
| 328.12 | 0.0937 | 0.0844 |
| 328.11 | 0.0864 | 0.0804 |
| 328.09 | 0.0035 | 0.0082 |

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**Enthalpy of mixing**

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Letcher, Trevor M. - Govender, Penny U., Excess Molar Enthalpies of an Alkanol + a Branched Chain Ether at the Temperature 298.15 K, Journal of Chemical & Engineering Data 4 (1995) 997-1000. doi:10.1021/je00020a060

**T / K =** **298.15**

**P / bar =** **1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 14.00 | 0.9820 |
| 79.40 | 0.9230 |
| 135.50 | 0.8810 |
| 183.00 | 0.8300 |
| 198.90 | 0.8250 |
| 266.10 | 0.7660 |
| 304.00 | 0.7320 |
| 350.40 | 0.6860 |
| 361.00 | 0.6780 |
| 440.60 | 0.5910 |
| 448.70 | 0.5810 |
| 470.10 | 0.5260 |
| 478.10 | 0.5250 |
| 515.80 | 0.4510 |
| 525.60 | 0.3590 |
| 460.10 | 0.2220 |
| 300.80 | 0.1200 |
| 214.90 | 0.0770 |

Cebreiro, S.M. - Illobre, M. - Mato, M.M. - Verdes, P.V. - Legido, J.L. - Paz Andrade, M.I., Excess molar enthalpies at 298.15 K of the binary mixtures. tert-butyl methyl ether + alcohol (n = 1,2,3,5), J. Therm. Anal. Calorim. 1 (2002) 251-254. doi:10.1023/A:1020634507355

**T / K =** **298.15**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 34.00 | 0.9677 |
| 76.00 | 0.9353 |
| 115.00 | 0.8998 |
| 164.00 | 0.8618 |
| 216.00 | 0.8248 |
| 223.00 | 0.8163 |
| 272.00 | 0.7763 |
| 285.00 | 0.7589 |
| 317.00 | 0.7324 |
| 461.00 | 0.5340 |
| 492.00 | 0.4757 |
| 527.00 | 0.4090 |
| 529.00 | 0.3157 |
| 522.00 | 0.2910 |
| 493.00 | 0.2301 |
| 449.00 | 0.1873 |
| 461.00 | 0.1870 |
| 376.00 | 0.1320 |
| 337.00 | 0.1098 |
| 138.00 | 0.0372 |
| 97.00 | 0.0252 |

Mato, Marta M. - Illobre, M. - Verdes, Pedro V. - Legido, José Luis - Andrade, María Inmaculada Paz, Study on the effect of increasing the chain length of the alkanol in excess molar enthalpies of mixtures containing 2-methoxy-2-methylpropane, 1-alkanol, decane, Fluid Phase Equilibria 1 (2010) 37-41. doi:10.1016/j.fluid.2010.02.012

**T / K =** **298.15**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 288.00 | 0.7522 |
| 486.00 | 0.5044 |
| 512.00 | 0.2582 |

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**Critical point**

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Han, Kewei - Xia, Shuqian - Ma, Peisheng - Yan, Fangyou - Liu, Tao, Measurement of critical temperatures and critical pressures for binary mixtures

of methyl tert-butyl ether (MTBE)+alcohol and MTBE+alkane, The Journal of Chemical Thermodynamics (2013) 111-117. doi:10.1016/j.jct.2013.03.002

| T / K | P / bar | $x_1$ |
|---|---|---|
| 495.00 | 35.86 | 0.0620 |
| 494.60 | 37.12 | 0.1005 |
| 493.80 | 38.90 | 0.2007 |
| 493.30 | 41.10 | 0.3011 |
| 493.90 | 43.38 | 0.4005 |
| 495.00 | 45.72 | 0.5003 |
| 497.10 | 48.20 | 0.5997 |
| 499.50 | 51.01 | 0.7005 |
| 503.50 | 54.12 | 0.7999 |
| 508.10 | 57.74 | 0.9000 |

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**Azeotropic point**

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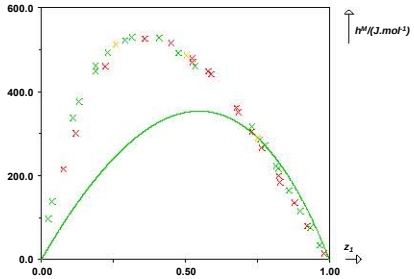
Arce, Alberto - Martínez-Ageitos, José - Soto, Ana, VLE Measurements of Binary Mixtures of Methanol, Ethanol, 2-Methoxy-2-methylpropane, and 2-Methoxy-2-methylbutane at 101.32 kPa, Journal of Chemical & Engineering Data 4 (1996) 718-723. doi:10.1021/je950323o

| T / K | P / bar | $x_1$ |
|---|---|---|
| 328.06 | 1.013 | 0.0630 |

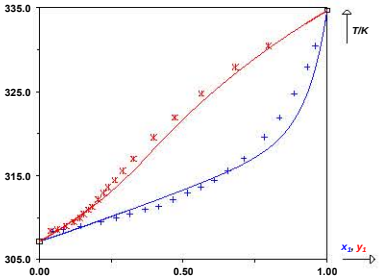
Mejía, Andrés - Segura, Hugo - Cartes, Marcela, Vapor−Liquid Equilibria and Interfacial Tensions of the System Ethanol + 2-Methoxy-2-methylpropane, Journal of Chemical & Engineering Data 1 (2010) 428-434. doi:10.1021/je9004068

| T / K | P / bar | $x_1$ |
|---|---|---|
| 319.32 | 0.7500 | 0.0370 |

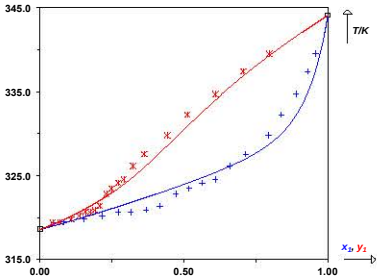
T/K = 298.15 - P/bar = 1.0100 1.0132 1.0132



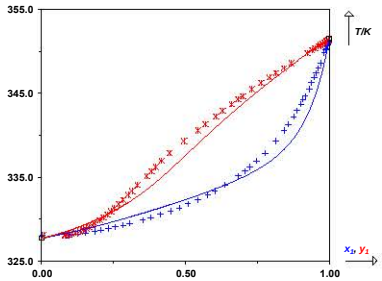

P/bar = 0.50000



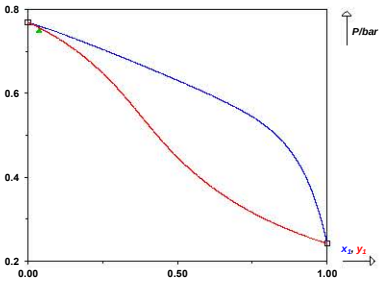

P/bar = 0.75001



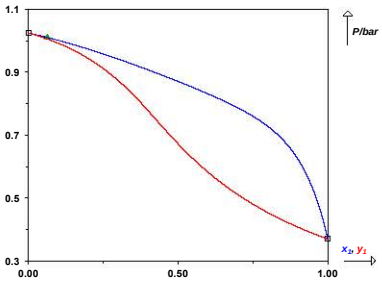

P/bar = 1.01320



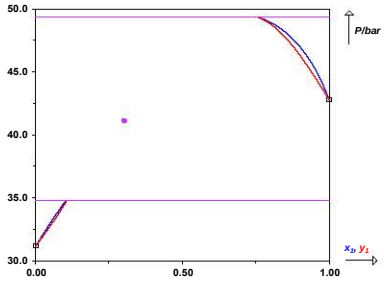

T/K = 319.32



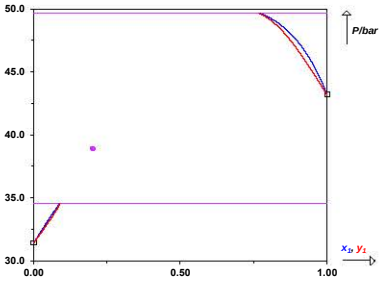

T/K = 328.06



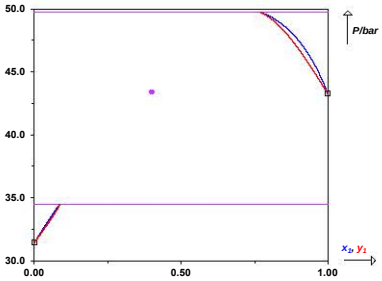

T/K = 493.30



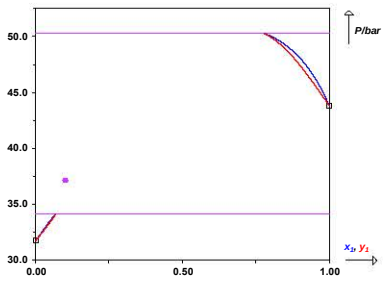

T/K = 493.80



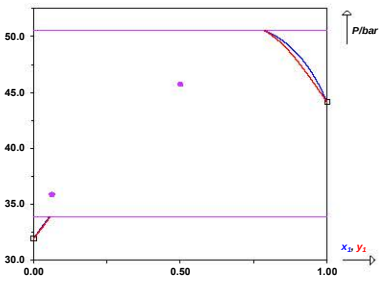

T/K = 493.90



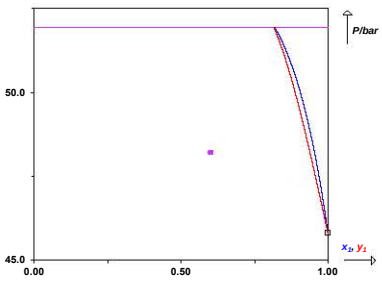

T/K = 494.60



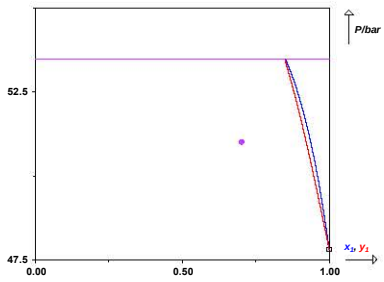

T/K = 495.00



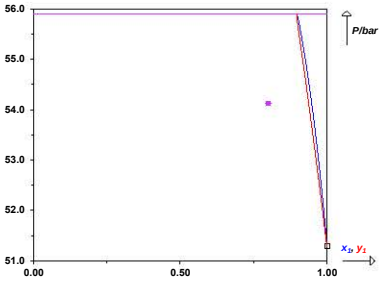

T/K = 497.10



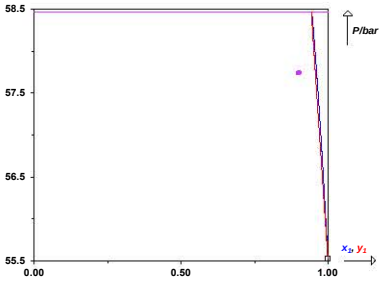

T/K = 499.50




T/K = 503.50




T/K = 508.10



## CARBON DIOXIDE (1) + 2-METHYL-1-PROPANOL (2)

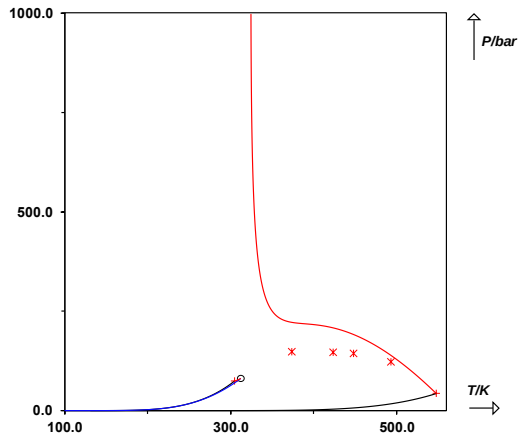
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 78-83-1 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | ZXEKIIBDNHEJCQ-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 547.80 |
| **$P_c$ / bar** | 73.83 | 42.95 |
| **ω** | 0.2240 | 0.5860 |

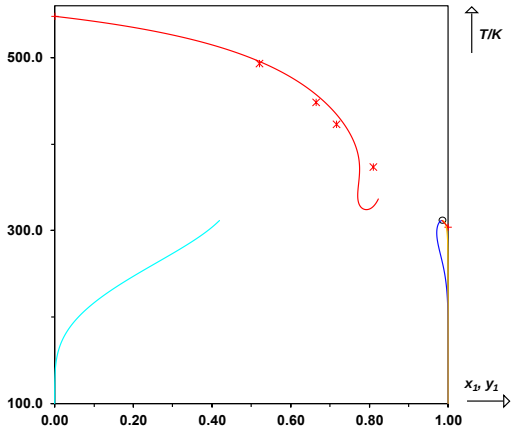
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 544
B/MPa = 1190

*Deviations*
MAPE on x = 28 %
MAPE on y = 18 %
MAPE on $x_c$ = 6 %
MAPE on $P_c$ = 35 %
MAPE on $h^M$ = 80 %



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**Isothermal phase equilibrium data**

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da Silva, Marta Vázquez - Barbosa, Domingos, High pressure vapor–liquid equilibrium data for the systems carbon dioxide/2-methyl-1-propanol and carbon dioxide/3-methyl-1-butanol at 288.2, 303.2 and 313.2 K, Fluid Phase Equilibria 2 (2002) 229-237. doi:10.1016/S0378-3812(01)00766-X

**T / K = 288.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 40.20 | 0.5500 | 0.9950 |
| 34.70 | 0.4530 | 0.9940 |
| 31.50 | 0.3680 | 0.9930 |
| 26.70 | 0.3080 | 0.9950 |
| 21.00 | 0.2340 | 0.9910 |

Yun, Z. - Shi, M. - Shi, J., High Pressure Vapor-Liquid Phase Equilibrium For Carbon Dioxide-n-Butanol And Carbon Dioxide-i-Butanol, Ranliao Huaxue Xuebao (1996) 87-92.

**T / K = 298.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 46.00 | 0.4190 | 0.9881 |
| 52.50 | 0.6292 | 0.9883 |
| 59.00 | 0.8900 | 0.9901 |

Gutiérrez, Jorge E. - Bejarano, Arturo - Fuente, Juan C. de la, Measurement and modeling of high-pressure (vapour+liquid) equilibria of (CO2+alcohol) binary systems, The Journal of Chemical Thermodynamics 5 (2010) 591-596. doi:10.1016/j.jct.2009.11.015

**T / K = 313.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 21.10 | 0.1230 | 0.9710 |
| 30.90 | 0.1940 | 0.9800 |
| 35.60 | 0.2350 | 0.9900 |
| 44.00 | 0.2890 | 0.9850 |
| 53.40 | 0.3670 | 0.9810 |
| 63.90 | 0.5060 | 0.9890 |
| 71.00 | 0.6210 | 0.9910 |
| 74.40 | 0.7250 | 0.9920 |

Gutiérrez, Jorge E. - Bejarano, Arturo - Fuente, Juan C. de la, Measurement and modeling of high-pressure (vapour+liquid) equilibria of (CO2+alcohol) binary systems, The Journal of Chemical Thermodynamics 5 (2010) 591-596. doi:10.1016/j.jct.2009.11.015

**T / K = 323.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 23.20 | 0.1120 | 0.9610 |
| 30.20 | 0.1540 | 0.9730 |
| 39.00 | 0.2130 | 0.9790 |
| 50.20 | 0.2970 | 0.9750 |
| 56.60 | 0.3390 | 0.9830 |
| 68.80 | 0.4370 | 0.9900 |
| 73.40 | 0.4860 | 0.9930 |
| 78.50 | 0.5590 | 0.9900 |
| 83.10 | 0.6270 | 0.9910 |
| 85.40 | 0.6780 | 0.9890 |
| 87.80 | 0.7210 | 0.9880 |
| 89.10 | 0.7540 | 0.9870 |
| 90.70 | 0.7940 | 0.9850 |

Yun, Z. - Shi, M. - Shi, J., High Pressure Vapor-Liquid Phase Equilibrium For Carbon Dioxide-n-Butanol And Carbon Dioxide-i-Butanol, Ranliao Huaxue Xuebao (1996) 87-92.

**T / K = 328.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.300 | 0.0286 | 0.7957 |
| 12.40 | 0.0594 | 0.9116 |
| 21.40 | 0.1018 | 0.9430 |
| 29.70 | 0.1448 | 0.9700 |
| 38.30 | 0.1987 | 0.9784 |
| 47.30 | 0.2524 | 0.9779 |
| 57.20 | 0.3219 | 0.9775 |
| 66.60 | 0.4023 | 0.9820 |
| 74.90 | 0.4789 | 0.9854 |
| 83.30 | 0.5797 | 0.9844 |
| 90.00 | 0.6733 | 0.9818 |
| 95.20 | 0.7662 | 0.9793 |
| 98.20 | 0.8409 | 0.9735 |
| 99.40 | 0.8733 | 0.9684 |

Gutiérrez, Jorge E. - Bejarano, Arturo - Fuente, Juan C. de la, Measurement and modeling of high-pressure (vapour+liquid) equilibria of (CO2+alcohol) binary systems, The Journal of Chemical Thermodynamics 5 (2010) 591-596. doi:10.1016/j.jct.2009.11.015

**T / K = 333.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 22.10 | 0.0940 | 0.9790 |
| 31.00 | 0.1410 | 0.9800 |
| 40.20 | 0.1870 | 0.9870 |
| 51.20 | 0.2670 | 0.9850 |
| 60.30 | 0.3260 | 0.9870 |
| 99.20 | 0.7000 | 0.9880 |
| 105.60 | 0.7790 | 0.9820 |
| 107.90 | 0.8360 | 0.9640 |

Chen, Huey-Ing - Chen, Po-Hung - Chang, Hung-Yi, High-Pressure Vapor-Liquid Equilibria for CO2 + 2-Butanol, CO2 + Isobutanol, and CO2 + tert-Butanol Systems, Journal of Chemical & Engineering Data 6 (2003) 1407-1412. doi:10.1021/je020214r

**T / K = 341.60**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 50.10 | 0.2481 | 0.9929 |
| 60.80 | 0.3027 | 0.9862 |
| 69.60 | 0.3551 | 0.9844 |
| 80.20 | 0.4189 | 0.9839 |
| 89.90 | 0.4805 | 0.9806 |
| 99.70 | 0.5625 | 0.9767 |
| 110.40 | 0.6640 | 0.9763 |
| 120.10 | 0.7443 | 0.9602 |

Chen, Huey-Ing - Chen, Po-Hung - Chang, Hung-Yi, High-Pressure Vapor-Liquid Equilibria for CO2 + 2-Butanol, CO2 + Isobutanol, and CO2 + tert-Butanol Systems, Journal of Chemical & Engineering Data 6 (2003) 1407-1412. doi:10.1021/je020214r

**T / K = 351.30**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 50.10 | 0.2369 | 0.9853 |
| 60.80 | 0.2838 | 0.9818 |
| 69.60 | 0.3310 | 0.9793 |
| 80.20 | 0.3888 | 0.9787 |
| 89.90 | 0.4421 | 0.9764 |
| 99.70 | 0.4997 | 0.9703 |
| 110.40 | 0.5642 | 0.9658 |
| 120.10 | 0.6290 | 0.9650 |

Semenova, A.I. - Emel'yanova, E.A. - Tsimmerman, S.S. - Tsiklis, D.S., Phase equilibriums in the isobutyl alcohol-carbon dioxide system, Russ. J. Phys. Chem. 5 (1978) 1149-1152.

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.000 | 0.0180 | 0.8460 | |
| 10.00 | 0.0380 | 0.9060 | |
| 20.00 | 0.0810 | 0.9520 | |
| 30.00 | 0.1240 | 0.9730 | |
| 40.00 | 0.1660 | 0.9760 | |
| 50.00 | 0.2080 | 0.9750 | |
| 120.00 | 0.5220 | 0.9730 | |
| 130.00 | 0.5800 | 0.9680 | |
| 140.00 | 0.6470 | 0.9300 | |
| 147.40 | 0.8100 | 0.8100 | CRIT |

Semenova, A.I. - Emel'yanova, E.A. - Tsimmerman, S.S. - Tsiklis, D.S., Phase equilibriums in the isobutyl alcohol-carbon dioxide system, Russ. J. Phys. Chem. 5 (1978) 1149-1152.

**T / K = 423.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 10.00 | 0.0210 | 0.6180 | |
| 20.00 | 0.0580 | 0.7710 | |
| 30.00 | 0.0960 | 0.8420 | |
| 40.00 | 0.1340 | 0.8740 | |
| 50.00 | 0.1720 | 0.8860 | |
| 60.00 | 0.2090 | 0.8910 | |
| 70.00 | 0.2470 | 0.8970 | |
| 80.00 | 0.2860 | 0.8980 | |
| 90.00 | 0.3260 | 0.9000 | |
| 100.00 | 0.3640 | 0.8980 | |
| 110.00 | 0.4020 | 0.8960 | |
| 120.00 | 0.4400 | 0.8930 | |
| 130.00 | 0.4890 | 0.8740 | |
| 140.00 | 0.5770 | 0.8320 | |
| 147.00 | 0.7160 | 0.7160 | CRIT |

Semenova, A.I. - Emel'yanova, E.A. - Tsimmerman, S.S. - Tsiklis, D.S., Phase equilibriums in the isobutyl alcohol-carbon dioxide system, Russ. J. Phys. Chem. 5 (1978) 1149-1152.

**T / K = 448.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 10.00 | 0.0030 | 0.3450 | |
| 20.00 | 0.0420 | 0.6180 | |
| 30.00 | 0.0760 | 0.7180 | |
| 40.00 | 0.1110 | 0.7640 | |
| 50.00 | 0.1470 | 0.7860 | |
| 60.00 | 0.1820 | 0.8010 | |
| 70.00 | 0.2170 | 0.8080 | |
| 80.00 | 0.2520 | 0.8120 | |
| 90.00 | 0.2890 | 0.8170 | |
| 100.00 | 0.3260 | 0.8210 | |
| 110.00 | 0.3660 | 0.8270 | |
| 120.00 | 0.4070 | 0.8320 | |
| 130.00 | 0.4570 | 0.8150 | |
| 140.00 | 0.5400 | 0.7470 | |
| 143.60 | 0.6640 | 0.6640 | CRIT |

Semenova, A.I. - Emel'yanova, E.A. - Tsimmerman, S.S. - Tsiklis, D.S., Phase equilibriums in the isobutyl alcohol-carbon dioxide system, Russ. J. Phys. Chem. 5 (1978) 1149-1152.

**T / K = 493.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 30.00 | 0.0230 | 0.4960 |
| 40.00 | 0.0630 | 0.5940 |

| | | | |
|---|---|---|---|
| 50.00 | 0.1010 | 0.6360 | |
| 60.00 | 0.1400 | 0.6660 | |
| 70.00 | 0.1780 | 0.6920 | |
| 80.00 | 0.2180 | 0.7050 | |
| 110.00 | 0.3490 | 0.6920 | |
| 120.00 | 0.4550 | 0.6130 | |
| 122.00 | 0.5200 | 0.5200 | CRIT |

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**Enthalpy of mixing**

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Ochi, Kenji - Dai, Wenbin - Wada, Yutaka - Hayashi, Hiroyuki - Kurihara, Kiyofumi - Kojima, Kazuo, Measurement and correlation of excess molar enthalpies for the systems containing supercritical carbon dioxide and alcohols, Fluid Phase Equilibria (2002) 919-928. doi:10.1016/S0378-3812(01)00704-X

**T / K =** **308.15**

**P / bar =** **75.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -113.00 | 0.0825 |
| -281.00 | 0.1596 |
| -444.00 | 0.2317 |
| -691.00 | 0.2993 |
| -953.00 | 0.3629 |
| -1308.0 | 0.4227 |
| -1686.0 | 0.4792 |
| -2030.0 | 0.5325 |
| -2351.0 | 0.5830 |
| -2718.0 | 0.6308 |
| -2992.0 | 0.6762 |
| -3306.0 | 0.7193 |
| -3566.0 | 0.7604 |
| -3804.0 | 0.7995 |
| -4034.0 | 0.8368 |
| -4212.0 | 0.8724 |
| -4362.0 | 0.9064 |
| -4091.0 | 0.9389 |
| -2110.0 | 0.9701 |

Ochi, Kenji - Dai, Wenbin - Wada, Yutaka - Hayashi, Hiroyuki - Kurihara, Kiyofumi - Kojima, Kazuo, Measurement and correlation of excess molar enthalpies for the systems containing supercritical carbon dioxide and alcohols, Fluid Phase Equilibria (2002) 919-928. doi:10.1016/S0378-3812(01)00704-X

**T / K =** **308.15**

**P / bar =** **80.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 19.00 | 0.0424 |
| 34.00 | 0.0833 |
| 39.00 | 0.1228 |
| 32.00 | 0.1610 |
| 18.00 | 0.2335 |
| -18.00 | 0.3015 |
| -58.00 | 0.3653 |
| -122.00 | 0.4253 |
| -194.00 | 0.4818 |
| -278.00 | 0.5351 |
| -370.00 | 0.5855 |
| -472.00 | 0.6333 |
| -586.00 | 0.6785 |
| -706.00 | 0.7214 |
| -815.00 | 0.7623 |
| -925.00 | 0.8011 |
| -1039.0 | 0.8382 |
| -1148.0 | 0.8735 |
| -1183.0 | 0.9073 |
| -1198.0 | 0.9395 |
| -932.00 | 0.9704 |
| -487.00 | 0.9854 |

Ochi, Kenji - Dai, Wenbin - Wada, Yutaka - Hayashi, Hiroyuki - Kurihara, Kiyofumi - Kojima, Kazuo, Measurement and correlation of excess molar enthalpies for the systems containing supercritical carbon dioxide and alcohols, Fluid Phase Equilibria (2002) 919-928. doi:10.1016/S0378-3812(01)00704-X

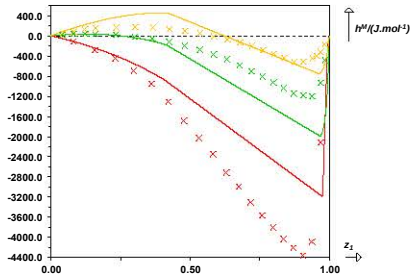
**T / K =** **308.15**

**P / bar =** **85.00**

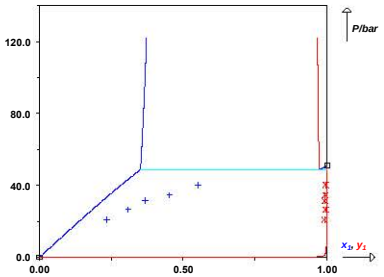
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 45.00 | 0.0428 |
| 87.00 | 0.0840 |
| 122.00 | 0.1238 |
| 144.00 | 0.1622 |
| 165.00 | 0.2352 |
| 169.00 | 0.3035 |
| 165.00 | 0.3675 |
| 132.00 | 0.4275 |
| 96.00 | 0.4841 |
| 49.00 | 0.5374 |
| -10.00 | 0.5878 |
| -66.00 | 0.6354 |
| -132.00 | 0.6805 |
| -200.00 | 0.7233 |
| -288.00 | 0.7640 |
| -360.00 | 0.8026 |

| | |
|---|---|
| -441.00 | 0.8394 |
| -515.00 | 0.8745 |
| -513.00 | 0.9080 |
| -448.00 | 0.9401 |
| -400.00 | 0.9555 |
| -317.00 | 0.9707 |
| -173.00 | 0.9855 |

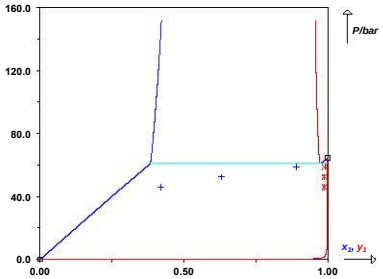
T/K = 308.15 - P/bar = 75.00 80.00 85.00



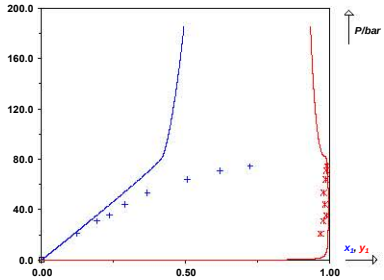

T/K = 288.20



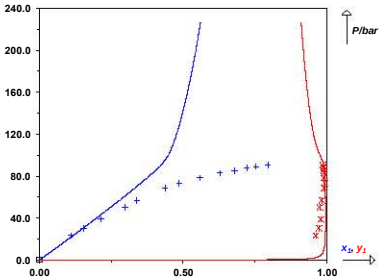

T/K = 298.20



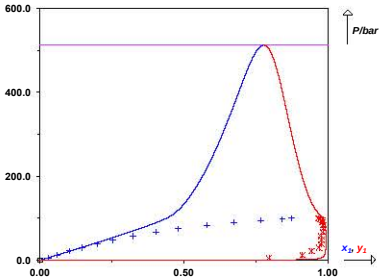

T/K = 313.00



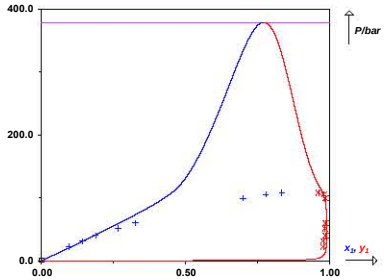

T/K = 323.00



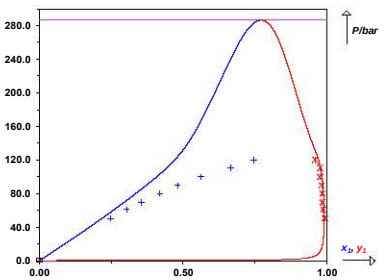

T/K = 328.20



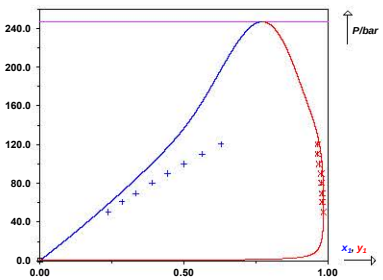

T/K = 333.00



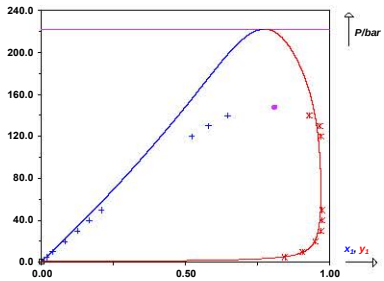

T/K = 341.60



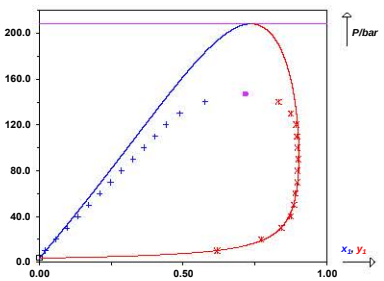

T/K = 351.30



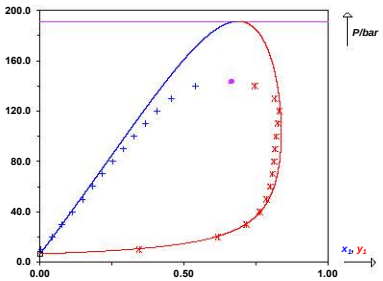

T/K = 373.15



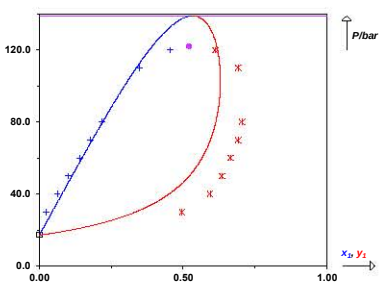

T/K = 423.15




T/K = 448.15




T/K = 493.15



## CARBON MONOXIDE (1) + METHANOL (2)

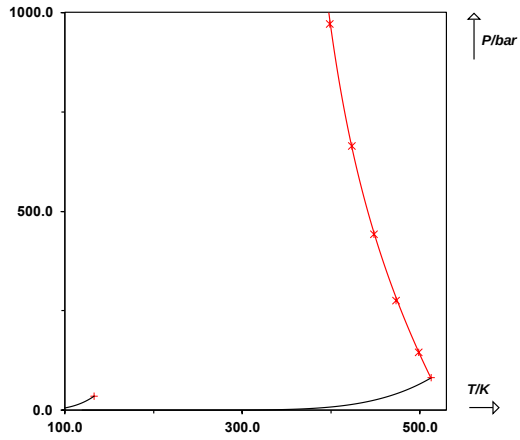
| | | |
|---|---|---|
| **CAS** | 630-08-0 | 67-56-1 |
| **InChiKey** | WSFSSNUMVMOOMR-UHFFFAOYSA-N | OKKJLVBELUTLKV-UHFFFAOYSA-N |
| **$T_c$ / K** | 132.92 | 512.50 |
| **$P_c$ / bar** | 34.99 | 80.84 |
| **ω** | 0.0480 | 0.5660 |

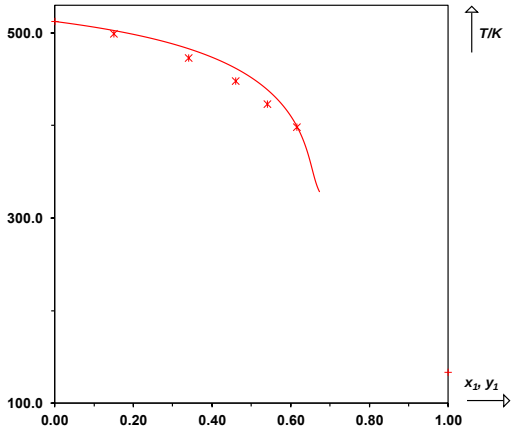
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 834
B/MPa = 1790

**Deviations**
MAPE on x = 250 %
MAPE on $x_c$ = 10 %
MAPE on $P_c$ = 1.4 %



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**Isothermal phase equilibrium data**

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Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

| **T / K =** | **298.15** |
|---|---|
| P / bar | $x_1$ |
| 24.00 | 0.9911 |
| 36.00 | 0.9934 |
| 50.00 | 0.9948 |
| 55.00 | 0.9950 |
| 100.00 | 0.9964 |
| 600.00 | 0.9945 |
| 800.00 | 0.9891 |
| 1000.0 | 0.9862 |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

| **T / K =** | **298.15** |
|---|---|
| P / bar | $x_1$ |
| 22.82 | 0.0082 |
| 45.43 | 0.0164 |
| 68.79 | 0.0246 |
| 93.41 | 0.0327 |
| 144.90 | 0.0484 |
| 244.30 | 0.0768 |
| 331.00 | 0.0988 |
| 469.00 | 0.1298 |
| 849.00 | 0.2030 |
| 1007.0 | 0.2323 |

Li, N. - Ma, P. - Xia, S., Determination of Solubility of Carbon Monoxide in Methanol-Dimethyl Carbonate under High Pressure, Shiyou Huagong 1 (2005) 60-64.

| **T / K =** | **298.15** |
|---|---|
| P / bar | $x_1$ |
| 80.30 | 0.0267 |
| 61.30 | 0.0207 |
| 40.00 | 0.0140 |
| 20.20 | 0.0088 |

Krichevskii, I.R. - Zhavoronkov, N.M. - Tsiklis, D.S., Solubility of hydrogen, carbon monoxide and of their mixtures in methanol at high pressures, Zh. Fiz. Khim. (1937) 317-328.

| **T / K =** | **298.15** |
|---|---|
| P / bar | $x_1$ |
| 60.80 | 0.0191 |
| 67.89 | 0.0217 |
| 111.46 | 0.0358 |
| 182.39 | 0.0556 |
| 188.46 | 0.0559 |
| 244.19 | 0.0757 |
| 246.22 | 0.0769 |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

| **T / K =** | **323.15** |
|---|---|
| P / bar | $x_1$ |
| 50.00 | 0.9842 |
| 100.00 | 0.9895 |
| 200.00 | 0.9909 |
| 400.00 | 0.9883 |
| 600.00 | 0.9841 |
| 800.00 | 0.9792 |
| 1000.0 | 0.9742 |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

| **T / K =** | **323.15** |
|---|---|
| P / bar | $x_1$ |
| 43.57 | 0.0156 |
| 65.28 | 0.0233 |
| 87.13 | 0.0310 |
| 112.40 | 0.0394 |
| 237.80 | 0.0779 |
| 373.00 | 0.1155 |
| 577.00 | 0.1667 |
| 817.00 | 0.2158 |
| 990.00 | 0.2539 |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase

equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

**T / K = 373.15**

| P / bar | $x_1$ |
|---|---|
| 100.00 | 0.9395 |
| 200.00 | 0.9538 |
| 300.00 | 0.9544 |
| 400.00 | 0.9504 |
| 600.00 | 0.9371 |
| 800.00 | 0.9191 |
| 1000.0 | 0.8944 |
| 914.00 | 0.7653 |
| 830.00 | 0.8098 |
| 762.00 | 0.8359 |
| 718.00 | 0.8459 |
| 667.00 | 0.8570 |
| 601.00 | 0.8705 |
| 477.00 | 0.8980 |
| 403.80 | 0.9023 |
| 311.10 | 0.9076 |
| 195.50 | 0.9019 |
| 109.90 | 0.8846 |
| 72.80 | 0.8517 |
| 971.00 | 0.6161 CRIT |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

**T / K = 373.15**

| P / bar | $x_1$ |
|---|---|
| 21.35 | 0.0072 |
| 40.06 | 0.0147 |
| 57.85 | 0.0216 |
| 76.68 | 0.0287 |
| 93.80 | 0.0356 |
| 113.10 | 0.0430 |
| 150.10 | 0.0568 |
| 186.40 | 0.0737 |
| 286.50 | 0.1064 |
| 379.00 | 0.1400 |
| 530.50 | 0.1900 |
| 738.00 | 0.2599 |
| 893.00 | 0.3132 |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

**T / K = 398.15**

| P / bar | $x_1$ |
|---|---|
| 971.00 | 0.6278 |
| 970.00 | 0.6429 |
| 965.00 | 0.6777 |
| 961.00 | 0.7049 |
| 934.00 | 0.7430 |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

**T / K = 398.15**

| P / bar | $x_1$ |
|---|---|
| 72.00 | 0.0291 |
| 161.80 | 0.0672 |
| 276.50 | 0.1174 |
| 444.00 | 0.1807 |
| 582.00 | 0.2402 |
| 707.00 | 0.3028 |
| 862.00 | 0.3961 |
| 904.00 | 0.4338 |
| 931.00 | 0.4636 |
| 954.00 | 0.4851 |
| 960.00 | 0.5036 |
| 967.00 | 0.5485 |
| 969.00 | 0.5942 |
| 968.00 | 0.5994 |
| 971.00 | 0.6161 CRIT |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

**T / K = 423.15**

| P / bar | $x_1$ |
|---|---|
| 664.00 | 0.5538 |
| 663.00 | 0.5650 |
| 658.00 | 0.6306 |

| | | |
|---|---|---|
| 653.00 | 0.6512 | |
| 549.00 | 0.7723 | |
| 450.00 | 0.8160 | |
| 331.00 | 0.8361 | |
| 273.30 | 0.8435 | |
| 220.00 | 0.8375 | |
| 121.50 | 0.8043 | |
| 116.60 | 0.7964 | |
| 86.20 | 0.7519 | |
| 48.60 | 0.6320 | |
| 664.00 | 0.5400 | CRIT |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

**T / K = 423.15**

| P / bar | $x_1$ | |
|---|---|---|
| 71.50 | 0.0280 | |
| 158.00 | 0.0702 | |
| 236.00 | 0.1123 | |
| 311.00 | 0.1518 | |
| 403.00 | 0.1992 | |
| 457.00 | 0.2370 | |
| 510.00 | 0.2800 | |
| 559.00 | 0.3246 | |
| 607.20 | 0.3886 | |
| 632.00 | 0.4238 | |
| 661.00 | 0.4875 | |
| 664.00 | 0.5398 | |
| 664.00 | 0.5400 | CRIT |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

**T / K = 448.15**

| P / bar | $x_1$ |
|---|---|
| 440.00 | 0.5025 |
| 434.80 | 0.5541 |
| 402.30 | 0.6264 |
| 352.00 | 0.6805 |
| 302.10 | 0.7020 |
| 245.00 | 0.7150 |
| 185.20 | 0.7093 |
| 132.20 | 0.6750 |
| 93.10 | 0.6176 |
| 59.70 | 0.4924 |
| 442.00 | 0.4600 CRIT |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

**T / K = 448.15**

| P / bar | $x_1$ | |
|---|---|---|
| 113.00 | 0.0518 | |
| 184.70 | 0.0987 | |
| 271.00 | 0.1571 | |
| 362.40 | 0.2451 | |
| 421.00 | 0.3368 | |
| 433.30 | 0.3768 | |
| 434.40 | 0.3861 | |
| 439.10 | 0.4240 | |
| 442.00 | 0.4600 | CRIT |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

**T / K = 473.15**

| P / bar | $x_1$ | |
|---|---|---|
| 243.00 | 0.4906 | |
| 167.20 | 0.5143 | |
| 121.00 | 0.4718 | |
| 78.30 | 0.3408 | |
| 276.00 | 0.3400 | CRIT |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

**T / K = 473.15**

| P / bar | $x_1$ |
|---|---|
| 160.00 | 0.0919 |
| 219.00 | 0.1604 |
| 263.00 | 0.2469 |
| 275.00 | 0.2684 |

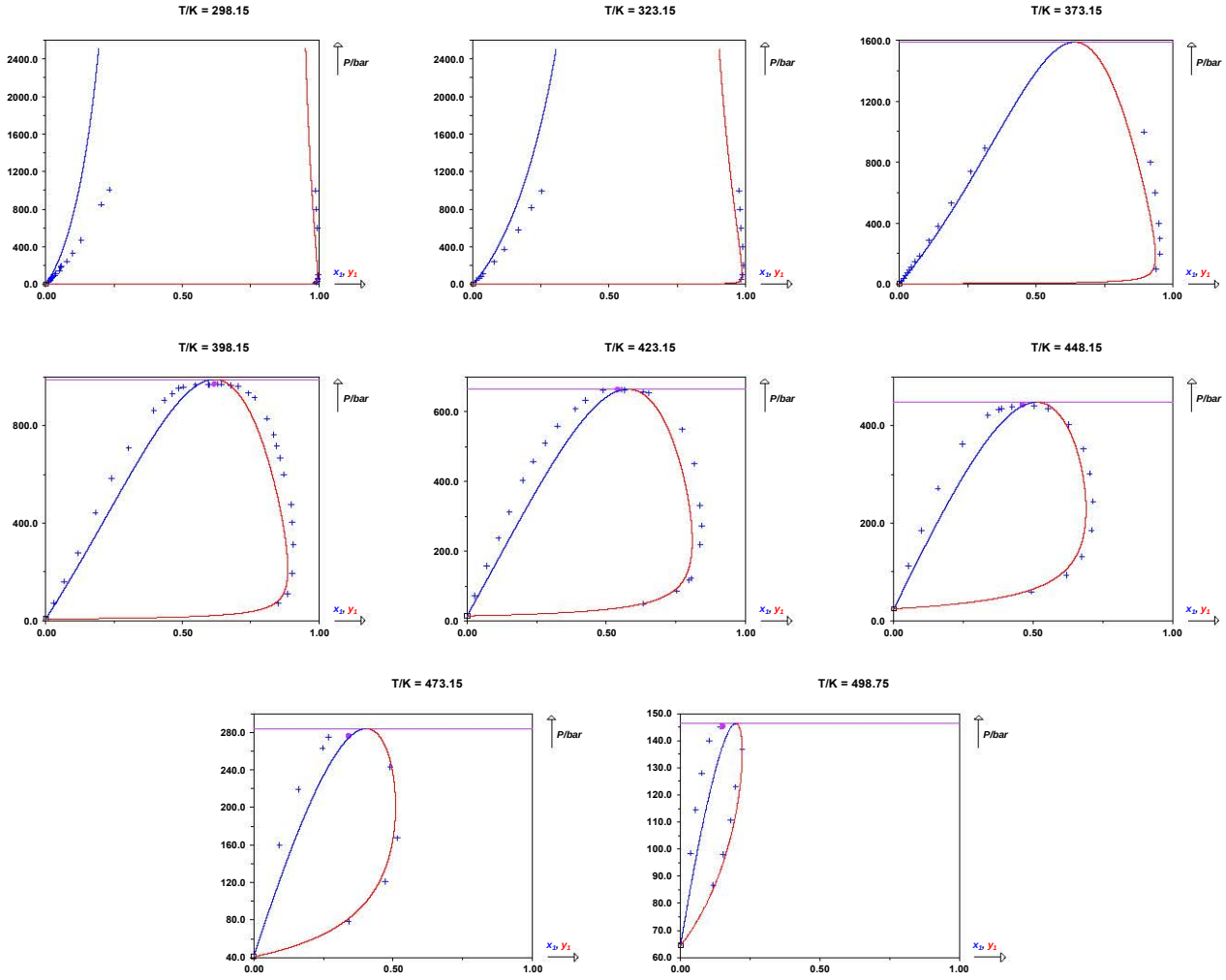
| | | |
|---|---|---|
| 276.00 | 0.3400 | CRIT |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

| **T / K =** | **498.75** | |
|---|---|---|
| P / bar | $x_1$ | |
| 86.60 | 0.1167 | |
| 98.00 | 0.1523 | |
| 110.50 | 0.1784 | |
| 123.00 | 0.1970 | |
| 136.70 | 0.2201 | |
| 145.20 | 0.1500 | CRIT |

Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

| **T / K =** | **498.75** | |
|---|---|---|
| P / bar | $x_1$ | |
| 98.50 | 0.0355 | |
| 114.50 | 0.0542 | |
| 128.00 | 0.0750 | |
| 140.00 | 0.1023 | |
| 145.20 | 0.1415 | |
| 145.20 | 0.1500 | CRIT |


T/K = 298.15
T/K = 323.15
T/K = 373.15
T/K = 398.15
T/K = 423.15
T/K = 448.15
T/K = 473.15
T/K = 498.75
P/bar
x1, y1

## CARBON DIOXIDE (1) + 1-PENTANOL (2)

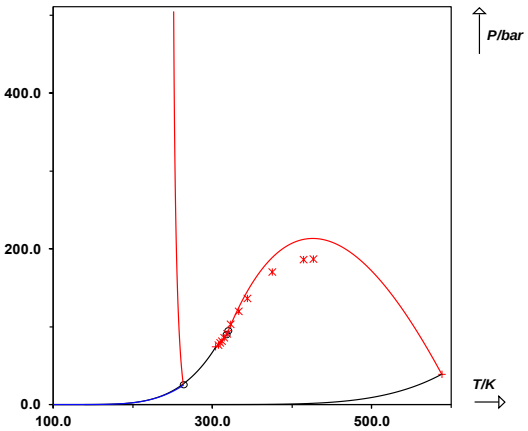
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 71-41-0 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | AMQJEAYHLZJPGS-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 588.10 |
| **$P_c$ / bar** | 73.83 | 38.97 |
| **ω** | 0.2240 | 0.5750 |

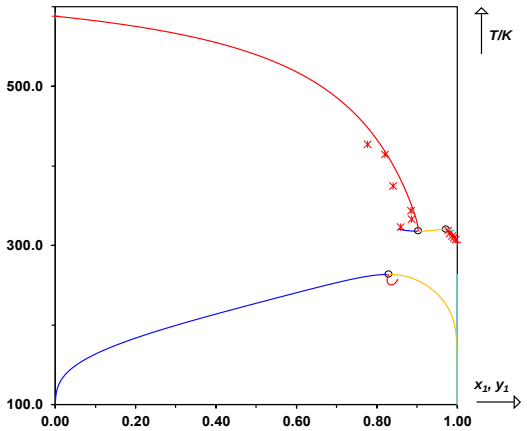
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 252
B/MPa = 618

*Deviations*
MAPE on $x_c$ = 10 %
MAPE on $P_c$ = 5.1 %



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**Critical point**

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Gurdial, Gurdev S. - Foster, Neil R. - Yun, S. L. Jimmy - Tilly, Kevin D., Phase Behavior of Supercritical Fluid—Entrainer Systems, Supercritical Fluid Engineering Science (1992) 34-45.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 307.50 | 76.60 | 0.9955 |
| 309.70 | 78.90 | 0.9916 |
| 312.00 | 81.50 | 0.9872 |
| 315.00 | 85.50 | 0.9818 |
| 318.50 | 90.80 | 0.9763 |

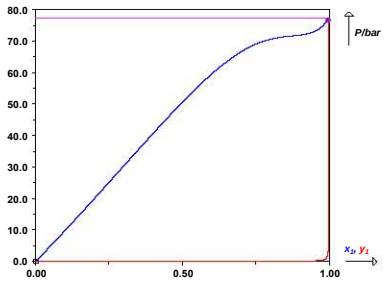
Raeissi, S - Peters, C.J, Double retrograde vaporization in a multi-component system: ethane+orange peel oil, The Journal of Supercritical Fluids 1-2 (2004) 69-75. doi:10.1016/S0896-8446(03)00068-8

| T / K | P / bar | $x_1$ |
|---|---|---|
| 333.08 | 119.36 | 0.8866 |
| 343.69 | 136.09 | 0.8850 |
| 374.93 | 170.34 | 0.8401 |
| 414.23 | 186.10 | 0.8198 |
| 426.86 | 186.65 | 0.7765 |

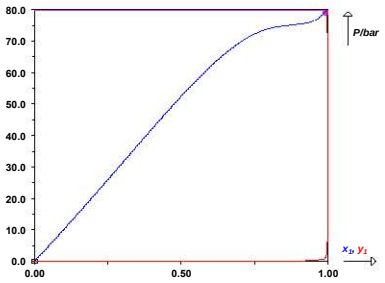
Gutiérrez, Jorge E. - Bejarano, Arturo - Fuente, Juan C. de la, Measurement and modeling of high-pressure (vapour+liquid) equilibria of (CO2+alcohol) binary systems, The Journal of Chemical Thermodynamics 5 (2010) 591-596. doi:10.1016/j.jct.2009.11.015

| T / K | P / bar | $x_1$ |
|---|---|---|
| 323.00 | 103.20 | 0.8590 |

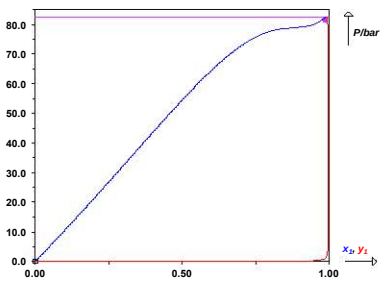
T/K = 307.50



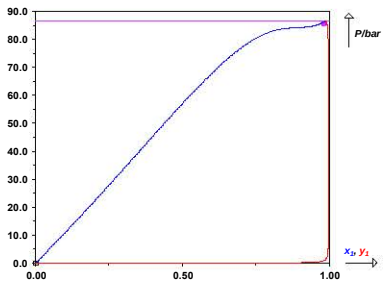

T/K = 309.70



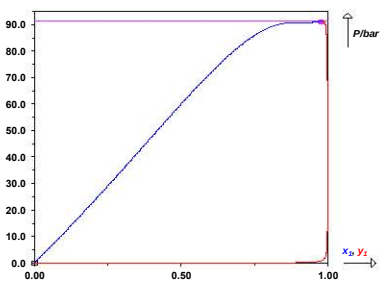

T/K = 312.00



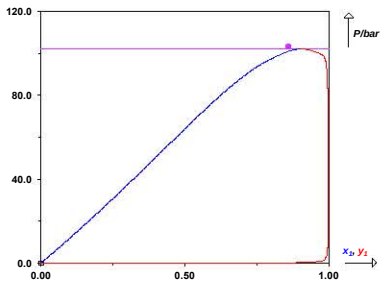

T/K = 315.00



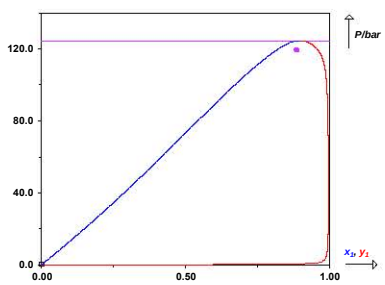

T/K = 318.50



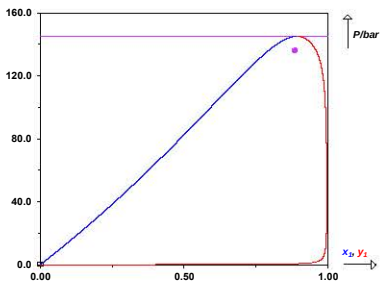

T/K = 323.00



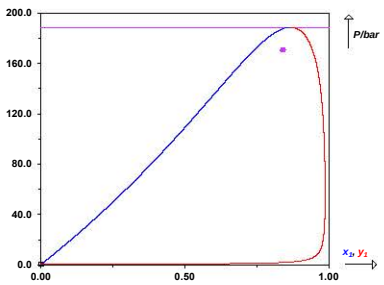

T/K = 333.08



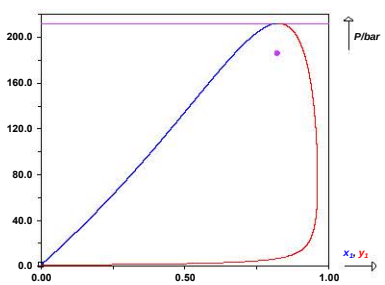

T/K = 343.69



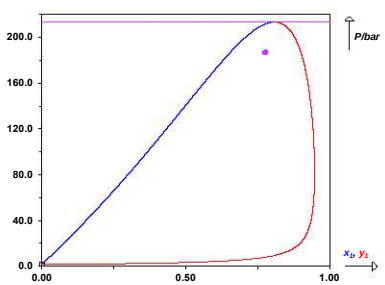

T/K = 374.93




T/K = 414.23




T/K = 426.86



## DIETHYLAMINE (1) + ETHYL ACETATE (2)

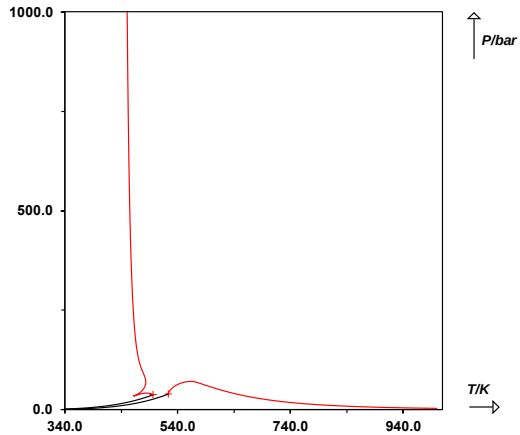
| | | |
|---|---|---|
| **CAS** | 109-89-7 | 141-78-6 |
| **InChiKey** | HPNMFZURTQLUMO-UHFFFAOYSA-N | XEKOWRVHYACXOJ-UHFFFAOYSA-N |
| **$T_c$ / K** | 496.60 | 523.30 |
| **$P_c$ / bar** | 37.10 | 38.80 |
| **ω** | 0.3040 | 0.3660 |

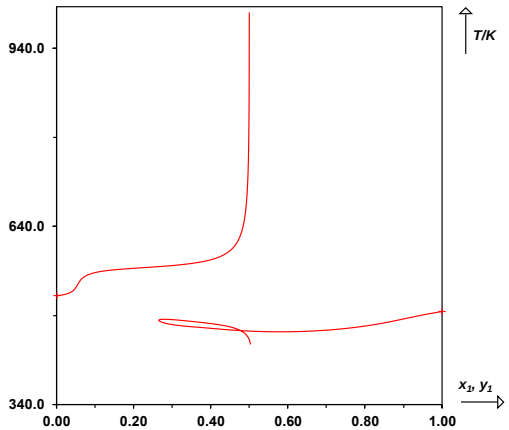
Ideal

**PPR78 results**

*Parameters*
A/MPa = 17.7
B/MPa = -123

*Deviations*
MAPE on x = 5.3 %
MAPE on y = 4.8 %



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**Isobaric phase equilibrium data**

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Engelmann, K. - Bittrich, H.J., Isobaric liquid-vapor equilibriums of the system diethylamine-ethyl acetate, diethylamine-1,4-dioxane and ethyl acetate-1,4-dioxane at reduced pressures, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 289-291.

**P / bar = 0.3333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 319.20 | 0.0200 | 0.0550 |
| 318.75 | 0.0320 | 0.0790 |
| 318.20 | 0.0430 | 0.1120 |
| 317.55 | 0.0600 | 0.1460 |
| 316.35 | 0.0930 | 0.2170 |
| 315.60 | 0.1140 | 0.2530 |
| 314.65 | 0.1380 | 0.3010 |
| 314.20 | 0.1540 | 0.3270 |
| 313.40 | 0.1800 | 0.3650 |
| 312.65 | 0.2020 | 0.4000 |
| 312.15 | 0.2200 | 0.4250 |
| 311.55 | 0.2460 | 0.4580 |
| 310.75 | 0.2720 | 0.4920 |
| 309.95 | 0.3090 | 0.5320 |
| 308.90 | 0.3520 | 0.5810 |
| 308.10 | 0.3930 | 0.6190 |
| 306.95 | 0.4570 | 0.6660 |
| 306.25 | 0.5060 | 0.7020 |
| 305.30 | 0.5650 | 0.7420 |
| 304.70 | 0.6100 | 0.7740 |
| 303.90 | 0.6650 | 0.8090 |
| 303.30 | 0.7110 | 0.8360 |
| 302.85 | 0.7440 | 0.8570 |
| 301.95 | 0.8150 | 0.9000 |
| 301.15 | 0.8820 | 0.9370 |
| 300.45 | 0.9410 | 0.9690 |

Engelmann, K. - Bittrich, H.J., Isobaric liquid-vapor equilibriums of the system diethylamine-ethyl acetate, diethylamine-1,4-dioxane and ethyl acetate-1,4-dioxane at reduced pressures, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 289-291.

**P / bar = 0.5999**

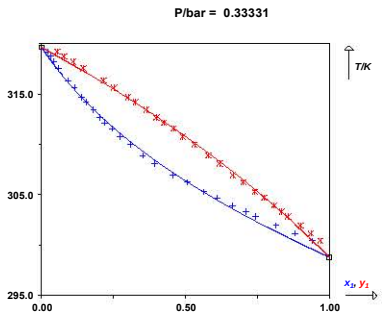
| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 334.65 | 0.0080 | 0.0270 |
| 334.25 | 0.0160 | 0.0490 |
| 333.80 | 0.0260 | 0.0760 |
| 333.25 | 0.0380 | 0.1080 |
| 332.65 | 0.0520 | 0.1420 |
| 331.35 | 0.0860 | 0.2080 |
| 330.30 | 0.1140 | 0.2620 |
| 329.40 | 0.1420 | 0.3060 |
| 328.15 | 0.1840 | 0.3660 |
| 326.70 | 0.2400 | 0.4400 |
| 325.75 | 0.2780 | 0.4790 |
| 324.75 | 0.3180 | 0.5300 |
| 323.55 | 0.3760 | 0.5810 |
| 322.55 | 0.4220 | 0.6270 |
| 321.50 | 0.4840 | 0.6720 |
| 320.75 | 0.5320 | 0.7060 |
| 320.15 | 0.5710 | 0.7330 |
| 319.00 | 0.6450 | 0.7850 |
| 318.00 | 0.7080 | 0.8260 |
| 317.00 | 0.7810 | 0.8720 |
| 316.20 | 0.8380 | 0.9080 |
| 315.45 | 0.8920 | 0.9380 |
| 315.00 | 0.9310 | 0.9620 |
| 314.55 | 0.9660 | 0.9800 |

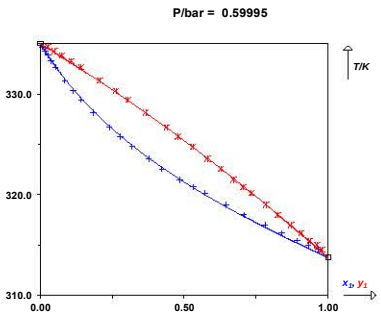
Engelmann, K. - Bittrich, H.J., Isobaric liquid-vapor equilibriums of the systems diethylamine/ethyl acetate, diethylamine/1,4-dioxane, and ethyl acetate /1,4-dioxane at 760 mm, Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg (1966) 148-153.

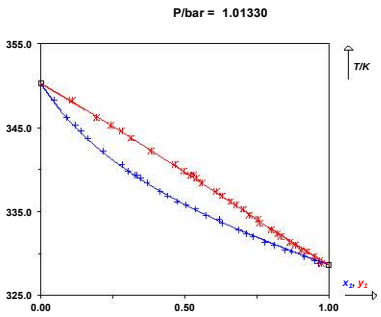
**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 348.25 | 0.0450 | 0.1080 |
| 346.20 | 0.0880 | 0.1920 |
| 345.25 | 0.1180 | 0.2420 |
| 344.60 | 0.1380 | 0.2810 |
| 343.75 | 0.1620 | 0.3120 |
| 342.20 | 0.2170 | 0.3820 |
| 340.60 | 0.2810 | 0.4650 |
| 339.80 | 0.3030 | 0.4960 |
| 339.35 | 0.3330 | 0.5300 |
| 339.30 | 0.3270 | 0.5210 |
| 338.95 | 0.3460 | 0.5410 |
| 338.45 | 0.3670 | 0.5600 |
| 337.40 | 0.4130 | 0.6090 |
| 336.85 | 0.4400 | 0.6300 |
| 336.20 | 0.4710 | 0.6590 |
| 335.80 | 0.5040 | 0.6780 |
| 335.25 | 0.5380 | 0.7030 |
| 334.55 | 0.5730 | 0.7230 |
| 334.05 | 0.6180 | 0.7550 |
| 333.60 | 0.6290 | 0.7600 |
| 332.80 | 0.6880 | 0.8000 |
| 332.35 | 0.7130 | 0.8210 |
| 332.00 | 0.7360 | 0.8330 |

| | | |
|---|---|---|
| 331.35 | 0.7770 | 0.8640 |
| 331.00 | 0.8110 | 0.8830 |
| 330.35 | 0.8460 | 0.9050 |
| 330.20 | 0.8710 | 0.9230 |
| 329.60 | 0.9150 | 0.9490 |
| 329.15 | 0.9490 | 0.9680 |
| 328.85 | 0.9620 | 0.9750 |


P/bar = 0.33331
T/K
315.0
305.0
295.0
0.00
0.50
1.00
x1, y1


P/bar = 0.59995
T/K
330.0
320.0
310.0
0.00
0.50
1.00
x1, y1


P/bar = 1.01330
T/K
355.0
345.0
335.0
325.0
0.00
0.50
1.00
x1, y1

## DIETHYLAMINE (1) + TRIETHYLAMINE (2)

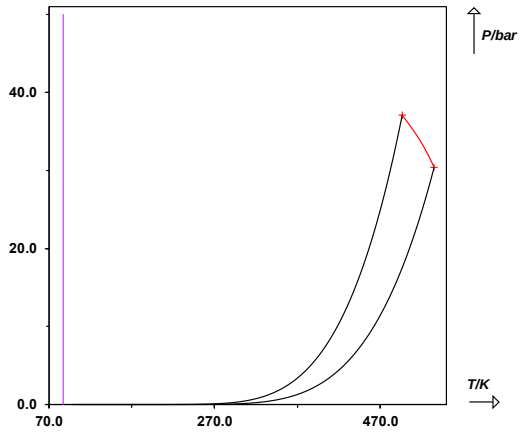
| | | |
|---|---|---|
| **CAS** | 109-89-7 | 121-44-8 |
| **InChiKey** | HPNMFZURTQLUMO-UHFFFAOYSA-N | ZMANZCXQSJIPKH-UHFFFAOYSA-N |
| **$T_c$ / K** | 496.6 | 535.15 |
| **$P_c$ / bar** | 37.1 | 30.4 |
| **ω** | 0.304 | 0.316 |

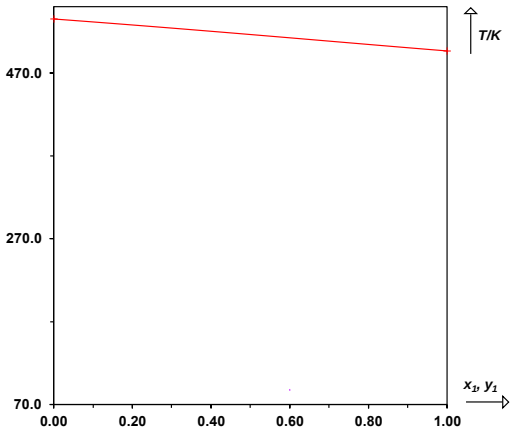
Ideal

**PPR78 results**

*Parameters*
A/MPa = 27.8
B/MPa = 48.6

*Deviations*
MAPE on x = 6.1 %
MAPE on y = 8.8 %
MAPE on $h^M$ = 23 %
MAPE on $c_P^M$ = 120 %



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**Isothermal phase equilibrium data**

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Ratkovics, F. - Liszi, J. - Laszlo-Parragi, M. - Szeiler, B. - Devay, J., Mixing properties of the ethanol-diethylamine-triethylamine system, Acta Chim. Acad. Sci. Hung. 3 (1973) 249-265.

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2600 | 0.1090 | 0.2180 |
| 0.2826 | 0.1790 | 0.3410 |
| 0.3160 | 0.2750 | 0.4800 |
| 0.3493 | 0.3720 | 0.6020 |
| 0.3840 | 0.4750 | 0.6950 |
| 0.4146 | 0.5610 | 0.7680 |
| 0.4266 | 0.6010 | 0.7920 |
| 0.4733 | 0.7390 | 0.8720 |
| 0.5133 | 0.8550 | 0.9340 |
| 0.5280 | 0.9020 | 0.9630 |

Bittrich, H.J. - Kauer, E., Thermodynamics of the system diethylamine-triethylamine. I. The liquid-vapor equilibrium, Z. Phys. Chem. Leipzig 3-4 (1962) 224-238.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2773 | 0.0200 | 0.0813 |
| 0.3013 | 0.0500 | 0.1801 |
| 0.3333 | 0.1000 | 0.2937 |
| 0.3900 | 0.2000 | 0.4571 |
| 0.4460 | 0.3000 | 0.5799 |
| 0.5013 | 0.4000 | 0.6792 |
| 0.5580 | 0.5000 | 0.7569 |
| 0.6133 | 0.6000 | 0.8235 |
| 0.6700 | 0.7000 | 0.8773 |
| 0.7253 | 0.8000 | 0.9244 |
| 0.7813 | 0.9000 | 0.9640 |
| 0.8086 | 0.9500 | 0.9824 |
| 0.8253 | 0.9800 | 0.9917 |

Bittrich, H.J. - Kauer, E., Thermodynamics of the system diethylamine-triethylamine. I. The liquid-vapor equilibrium, Z. Phys. Chem. Leipzig 3-4 (1962) 224-238.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3360 | 0.0200 | 0.0775 |
| 0.3640 | 0.0500 | 0.1723 |
| 0.4026 | 0.1000 | 0.2865 |
| 0.4693 | 0.2000 | 0.4523 |
| 0.5360 | 0.3000 | 0.5768 |
| 0.6040 | 0.4000 | 0.6747 |
| 0.6706 | 0.5000 | 0.7543 |
| 0.7379 | 0.6000 | 0.8194 |
| 0.8033 | 0.7000 | 0.8758 |
| 0.8693 | 0.8000 | 0.9222 |
| 0.9346 | 0.9000 | 0.9627 |
| 0.9659 | 0.9500 | 0.9811 |
| 0.9839 | 0.9800 | 0.9917 |

Bittrich, H.J. - Kauer, E., Thermodynamics of the system diethylamine-triethylamine. I. The liquid-vapor equilibrium, Z. Phys. Chem. Leipzig 3-4 (1962) 224-238.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4073 | 0.0200 | 0.0731 |
| 0.4386 | 0.0500 | 0.1625 |
| 0.4813 | 0.1000 | 0.2726 |
| 0.5586 | 0.2000 | 0.4415 |
| 0.6386 | 0.3000 | 0.5668 |
| 0.7159 | 0.4000 | 0.6695 |
| 0.7939 | 0.5000 | 0.7515 |
| 0.8726 | 0.6000 | 0.8181 |
| 0.9506 | 0.7000 | 0.8742 |
| 1.027 | 0.8000 | 0.9219 |
| 1.104 | 0.9000 | 0.9629 |
| 1.142 | 0.9500 | 0.9822 |
| 1.163 | 0.9800 | 0.9920 |

Bittrich, H.J. - Kauer, E., Thermodynamics of the system diethylamine-triethylamine. I. The liquid-vapor equilibrium, Z. Phys. Chem. Leipzig 3-4 (1962) 224-238.

**T / K = 338.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4940 | 0.0200 | 0.0720 |
| 0.5266 | 0.0500 | 0.1546 |
| 0.5733 | 0.1000 | 0.2608 |
| 0.6666 | 0.2000 | 0.4318 |
| 0.7593 | 0.3000 | 0.5613 |
| 0.8506 | 0.4000 | 0.6630 |
| 0.9413 | 0.5000 | 0.7456 |
| 1.033 | 0.6000 | 0.8135 |
| 1.123 | 0.7000 | 0.8709 |
| 1.212 | 0.8000 | 0.9193 |
| 1.301 | 0.9000 | 0.9606 |
| 1.343 | 0.9500 | 0.9803 |
| 1.367 | 0.9800 | 0.9920 |

Bittrich, H.J. - Kauer, E., Thermodynamics of the system diethylamine-triethylamine. I. The liquid-vapor equilibrium, Z. Phys. Chem. Leipzig 3-4 (1962) 224-238.

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5840 | 0.0200 | 0.0696 |
| 0.6226 | 0.0500 | 0.1531 |
| 0.6799 | 0.1000 | 0.2613 |
| 0.7873 | 0.2000 | 0.4307 |
| 0.8959 | 0.3000 | 0.5587 |
| 1.003 | 0.4000 | 0.6611 |
| 1.109 | 0.5000 | 0.7438 |
| 1.216 | 0.6000 | 0.8125 |
| 1.323 | 0.7000 | 0.8696 |
| 1.427 | 0.8000 | 0.9201 |
| 1.533 | 0.9000 | 0.9621 |
| 1.585 | 0.9500 | 0.9816 |
| 1.612 | 0.9800 | 0.9918 |

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**Isobaric phase equilibrium data**

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Bittrich, H.J. - Kauer, E., Thermodynamics of the system diethylamine-triethylamine. I. The liquid-vapor equilibrium, Z. Phys. Chem. Leipzig 3-4 (1962) 224-238.

**P / bar = 0.4666**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 336.35 | 0.0230 | 0.0680 |
| 334.65 | 0.0520 | 0.1500 |
| 332.45 | 0.0940 | 0.2600 |
| 329.65 | 0.1570 | 0.3820 |
| 323.65 | 0.3220 | 0.6040 |
| 319.40 | 0.4660 | 0.7270 |
| 315.85 | 0.5940 | 0.8220 |
| 310.85 | 0.8310 | 0.9380 |
| 308.70 | 0.9350 | 0.9780 |

Bittrich, H.J. - Kauer, E., Thermodynamics of the system diethylamine-triethylamine. I. The liquid-vapor equilibrium, Z. Phys. Chem. Leipzig 3-4 (1962) 224-238.

**P / bar = 0.7999**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 352.85 | 0.0210 | 0.0450 |
| 350.70 | 0.0600 | 0.1480 |
| 348.15 | 0.1000 | 0.2670 |
| 343.05 | 0.2180 | 0.4540 |
| 339.40 | 0.3230 | 0.5740 |
| 336.85 | 0.3860 | 0.6510 |
| 329.15 | 0.6550 | 0.8480 |
| 324.75 | 0.8510 | 0.9430 |
| 322.45 | 0.9630 | 0.9850 |

Bittrich, H.J. - Kauer, E., Thermodynamics of the system diethylamine-triethylamine. I. The liquid-vapor equilibrium, Z. Phys. Chem. Leipzig 3-4 (1962) 224-238.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 360.50 | 0.0200 | 0.0420 |
| 358.35 | 0.0520 | 0.1240 |
| 357.55 | 0.0650 | 0.1530 |
| 356.32 | 0.0900 | 0.2250 |
| 356.00 | 0.0920 | 0.2430 |
| 353.65 | 0.1400 | 0.3160 |
| 350.30 | 0.2150 | 0.4490 |
| 342.45 | 0.4300 | 0.6780 |
| 337.45 | 0.6010 | 0.8020 |
| 333.00 | 0.7820 | 0.9100 |
| 331.35 | 0.8530 | 0.9480 |
| 329.85 | 0.9320 | 0.9700 |
| 328.90 | 0.9850 | 0.9930 |

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**Enthalpy of mixing**

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Bittrich, H.J. - Kulanek, M. - Duering, G., Thermodynamics of the system diethylamine-triethylamine. Enthalpies of mixing at 14, 18, and 25°, Z. Phys. Chem. Leipzig (1962) 387-395.

**T / K = 287.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 103.00 | 0.1000 |
| 152.00 | 0.2000 |
| 205.00 | 0.3000 |
| 258.00 | 0.4000 |
| 281.00 | 0.5000 |
| 260.00 | 0.6000 |
| 209.00 | 0.7000 |
| 160.00 | 0.8000 |
| 96.00 | 0.9000 |

Ratkovics, F. - Liszi, J. - Laszlo-Parragi, M. - Szeiler, B. - Devay, J., Mixing properties of the ethanol-diethylamine-triethylamine system, Acta Chim. Acad. Sci. Hung. 3 (1973) 249-265.

**T / K = 293.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 113.88 | 0.0840 |
| 248.28 | 0.2070 |
| 356.72 | 0.3440 |
| 385.60 | 0.4730 |
| 356.72 | 0.6240 |
| 293.49 | 0.7520 |
| 235.72 | 0.8190 |
| 148.63 | 0.9010 |
| 72.01 | 0.9540 |

Bittrich, H.J. - Kulanek, M. - Duering, G., Thermodynamics of the system diethylamine-triethylamine. Enthalpies of mixing at 14, 18, and 25°, Z. Phys. Chem. Leipzig (1962) 387-395.

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 151.00 | 0.1000 |
| 216.00 | 0.2000 |
| 267.00 | 0.3000 |
| 325.00 | 0.4000 |
| 360.00 | 0.5000 |
| 332.00 | 0.6000 |
| 281.00 | 0.7000 |
| 210.00 | 0.8000 |
| 139.00 | 0.9000 |

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**Heat capacity of mixing**

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Kauer, E. - Grote, L. - Bittrich, H.- J., Zur Thermodynamik des Systems Diäthylamin-Triäthylamin. IV, Zeitschrift für Physikalische Chemie 1 (1966) doi:10.1515/zpch-1966-23231

**T / K =** **293.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 1.623 | 0.0800 |
| 2.336 | 0.1810 |
| 4.260 | 0.5780 |
| 2.558 | 0.8030 |
| 1.511 | 0.9070 |

Kauer, E. - Grote, L. - Bittrich, H.- J., Zur Thermodynamik des Systems Diäthylamin-Triäthylamin. IV, Zeitschrift für Physikalische Chemie 1 (1966) doi:10.1515/zpch-1966-23231

**T / K =** **303.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 2.926 | 0.1560 |
| 4.385 | 0.5580 |
| 2.888 | 0.8030 |
| 1.326 | 0.9070 |

Kauer, E. - Grote, L. - Bittrich, H.- J., Zur Thermodynamik des Systems Diäthylamin-Triäthylamin. IV, Zeitschrift für Physikalische Chemie 1 (1966) doi:10.1515/zpch-1966-23231

**T / K =** **313.15**

**P / bar =** **UNKNOWN (1.0132)**

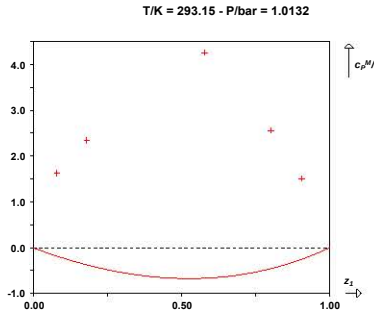
| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 1.705 | 0.1390 |
| 3.503 | 0.4920 |
| 3.636 | 0.5310 |
| 2.283 | 0.7890 |
| 1.377 | 0.9040 |

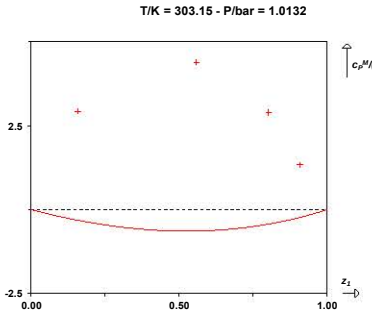
Kauer, E. - Grote, L. - Bittrich, H.- J., Zur Thermodynamik des Systems Diäthylamin-Triäthylamin. IV, Zeitschrift für Physikalische Chemie 1 (1966) doi:10.1515/zpch-1966-23231

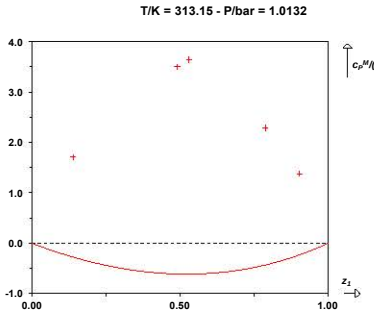
**T / K =** **323.15**

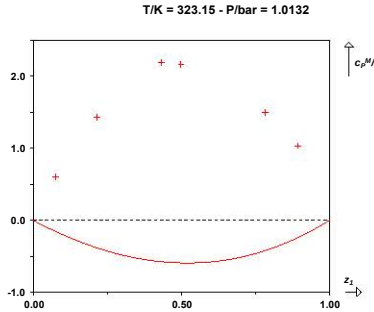
**P / bar =** **UNKNOWN (1.0132)**

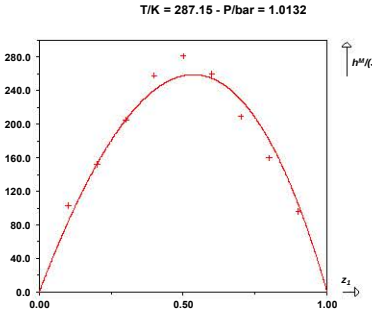
| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.6045 | 0.0750 |
| 1.430 | 0.2140 |
| 2.190 | 0.4320 |
| 2.165 | 0.4990 |
| 1.500 | 0.7840 |
| 1.035 | 0.8940 |

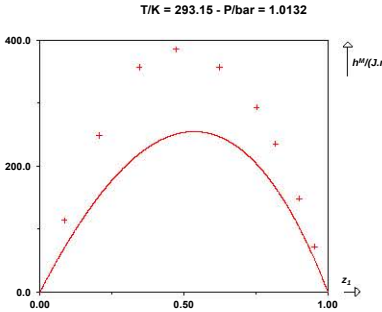

T/K = 293.15 - P/bar = 1.0132
$c_p^M$/(J.mol$^{-1}$.K$^{-1}$)
$z_1$

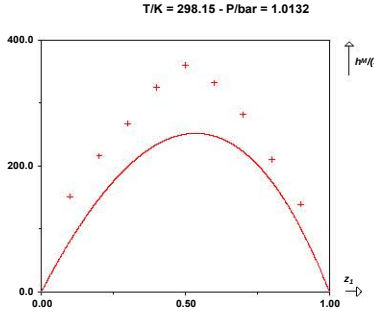

T/K = 303.15 - P/bar = 1.0132
$c_p^M$/(J.mol$^{-1}$.K$^{-1}$)
$z_1$

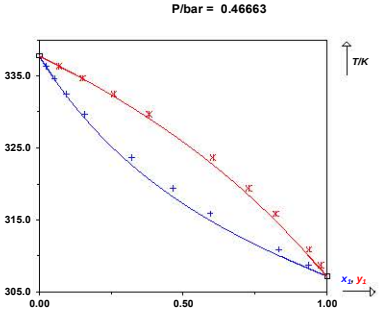

T/K = 313.15 - P/bar = 1.0132
$c_p^M$/(J.mol$^{-1}$.K$^{-1}$)
$z_1$

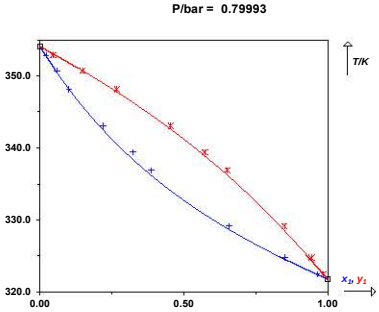

T/K = 323.15 - P/bar = 1.0132
$c_p^M$/(J.mol$^{-1}$.K$^{-1}$)
$z_1$

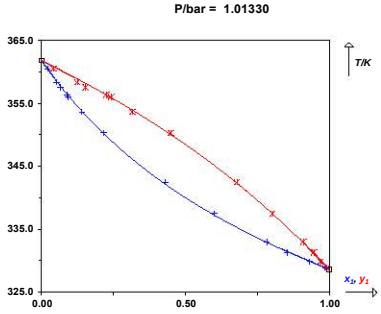

T/K = 287.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
$z_1$

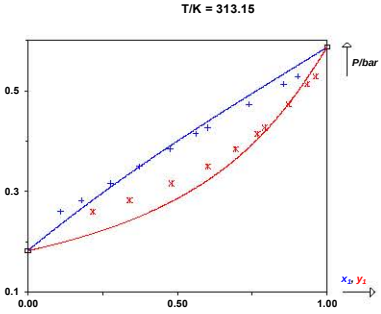

T/K = 293.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
$z_1$

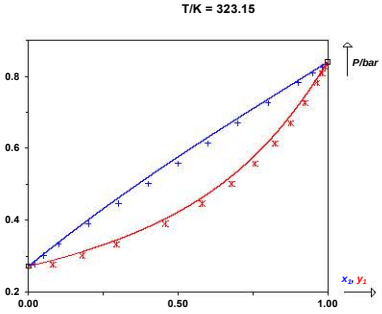

T/K = 298.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
$z_1$

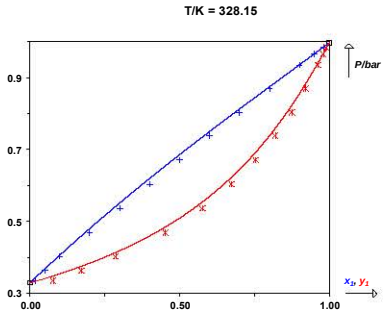

P/bar = 0.46663
T/K
$x_1$, $y_1$

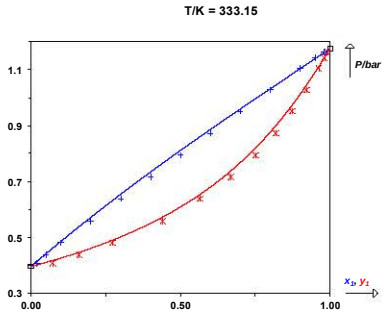

P/bar = 0.79993
T/K
$x_1$, $y_1$

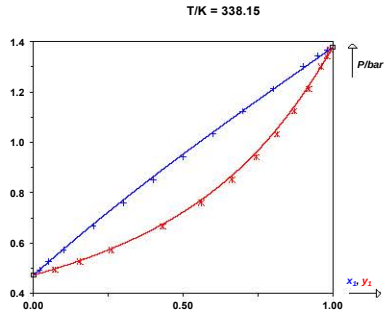

P/bar = 1.01330
T/K
$x_1$, $y_1$

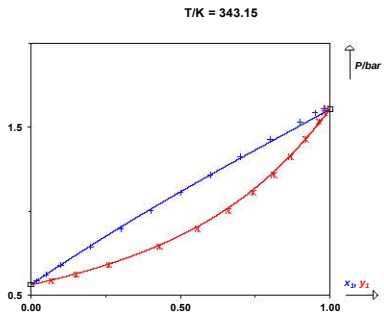

T/K = 313.15
P/bar
$x_1$, $y_1$


T/K = 323.15
P/bar
$x_1$, $y_1$


T/K = 328.15
P/bar
0.9
0.7
0.5
0.3
0.00
0.50
1.00
x1, y1


T/K = 333.15
P/bar
1.1
0.9
0.7
0.5
0.3
0.00
0.50
1.00
x1, y1


T/K = 338.15
P/bar
1.4
1.2
1.0
0.8
0.6
0.4
0.00
0.50
1.00
x1, y1


T/K = 343.15
P/bar
1.5
0.5
0.00
0.50
1.00
x1, y1

## ACETIC ACID (1) + ACETIC ANHYDRIDE (2)

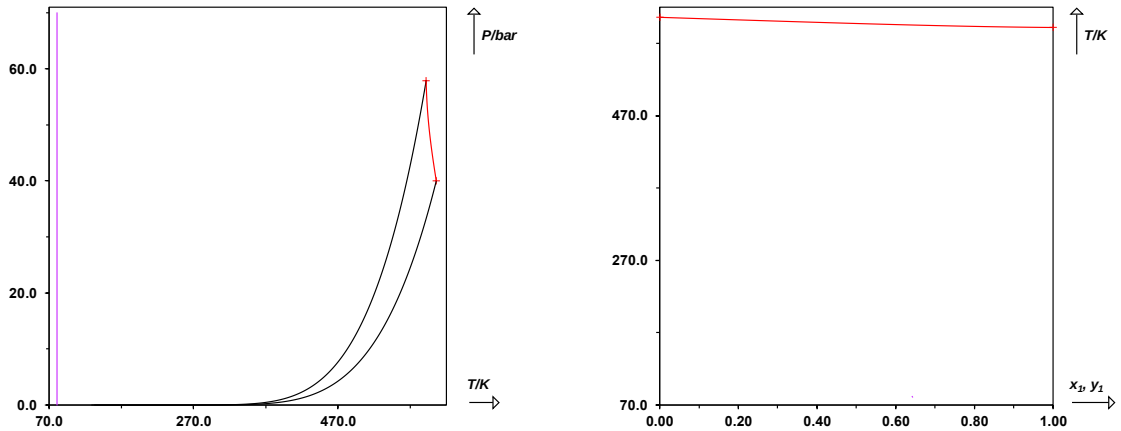
| | | |
|---|---|---|
| **CAS** | 64-19-7 | 108-24-7 |
| **InChiKey** | QTBSBXVTEAMEQO-UHFFFAOYSA-N | WFDIJRYMOXRFFG-UHFFFAOYSA-N |
| **$T_c$ / K** | 591.95 | 606.00 |
| **$P_c$ / bar** | 57.86 | 40.00 |
| **ω** | 0.4670 | 0.4550 |

Ideal

**PPR78 results**

*Parameters*
A/MPa = 51.1
B/MPa = 68.7

*Deviations*
MAPE on x = 8.1 %
MAPE on y = 6.5 %
MAPE on $h^M$ = 27 %



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**Isobaric phase equilibrium data**

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Jones, H. E., Vapor-Liquid Equilibria for Eight Binary Mixtures., Journal of Chemical & Engineering Data 1 (1962) 13-18. doi:10.1021/je60012a004

**P / bar = 0.1333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 352.45 | 0.1000 | 0.1990 |
| 350.05 | 0.2000 | 0.3600 |
| 347.95 | 0.3000 | 0.4950 |
| 342.45 | 0.6000 | 0.7800 |
| 340.75 | 0.7000 | 0.8450 |
| 339.05 | 0.8000 | 0.9020 |
| 337.35 | 0.9000 | 0.9530 |
| 336.55 | 0.9500 | 0.9780 |
| 336.15 | 0.9750 | 0.9890 |

Jones, H. E., Vapor-Liquid Equilibria for Eight Binary Mixtures., Journal of Chemical & Engineering Data 1 (1962) 13-18. doi:10.1021/je60012a004

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 409.45 | 0.1000 | 0.1800 |
| 406.45 | 0.2000 | 0.3300 |
| 403.75 | 0.3000 | 0.4600 |
| 401.45 | 0.4000 | 0.5660 |
| 399.35 | 0.5000 | 0.6600 |
| 397.65 | 0.6000 | 0.7400 |
| 395.75 | 0.7000 | 0.8150 |
| 394.15 | 0.8000 | 0.8800 |
| 392.65 | 0.9000 | 0.9400 |
| 391.65 | 0.9500 | 0.9700 |
| 391.35 | 0.9750 | 0.9850 |

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**Enthalpy of mixing**

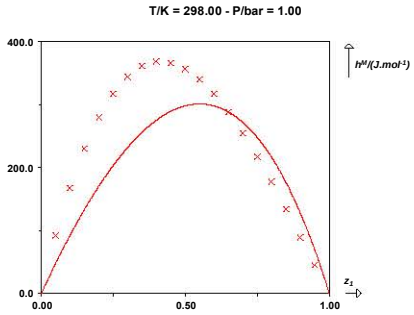
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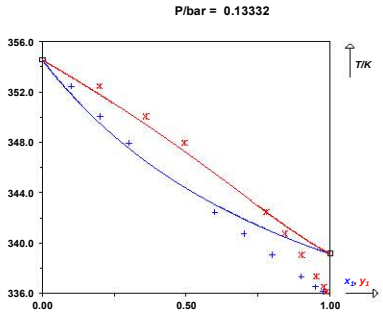
Balland, Laurent - Ben Talouba, Imed - Mouhab, Nordine - Abdelghani-Idrissi, Ahmed, Evaluation of Excess Molar Enthalpies for a Quaternary Mixture System of Acetic Anhydride, Ethanol, Acetic Acid, and Ethyl Acetate, Journal of Chemical & Engineering Data 3 (2012) 811-816. doi:10.1021/je200595b

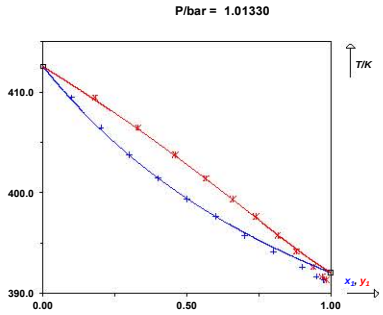
**T / K = 298.00**

**P / bar = 1.0000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 45.00 | 0.9500 |
| 89.00 | 0.9000 |
| 134.00 | 0.8500 |
| 177.00 | 0.8000 |
| 217.00 | 0.7500 |
| 254.00 | 0.7000 |
| 288.00 | 0.6500 |
| 317.00 | 0.6000 |
| 340.00 | 0.5500 |
| 356.00 | 0.5000 |
| 366.00 | 0.4500 |
| 368.00 | 0.4000 |
| 361.00 | 0.3500 |
| 344.00 | 0.3000 |
| 317.00 | 0.2500 |
| 280.00 | 0.2000 |
| 230.00 | 0.1500 |
| 168.00 | 0.1000 |
| 92.00 | 0.0500 |


T/K = 298.00 - P/bar = 1.00
400.0
200.0
0.0
0.00
0.50
1.00
hᴱ/(J.mol⁻¹)
z₁


P/bar = 0.13332
356.0
352.0
348.0
344.0
340.0
336.0
0.00
0.50
1.00
T/K
x₁, y₁


P/bar = 1.01330
410.0
400.0
390.0
0.00
0.50
1.00
T/K
x₁, y₁

## 2-METHYL-2-PROPANOL (1) + METHYL tert-BUTYL ETHER (2)

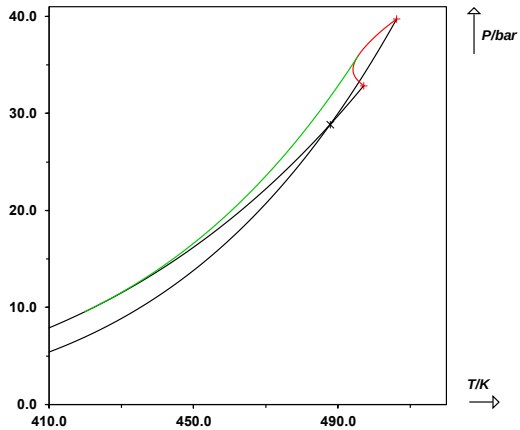
| | | |
|---|---|---|
| **CAS** | 75-65-0 | 1634-04-4 |
| **InChiKey** | DKGAVHZHDRPRBM-UHFFFAOYSA-N | BZLVMXJERCGZMT-UHFFFAOYSA-N |
| **$T_c$ / K** | 506.20 | 497.10 |
| **$P_c$ / bar** | 39.72 | 32.86 |
| **ω** | 0.6150 | 0.2470 |

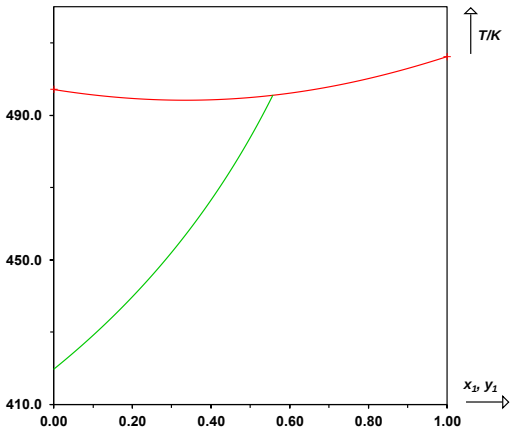
Ideal

**PPR78 results**

*Parameters*
A/MPa = 52
B/MPa = -7.92

*Deviations*
MAPE on x = 8.9 %
MAPE on y = 8.5 %



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**Isothermal phase equilibrium data**

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Fuangfoo, Surajit - Kersting, Mark - Viswanath, Dabir S., Isothermal Vapor−Liquid Equilibria for Methyl-2,2-dimethylethyl Ether + 2-Methylpropan-2-ol, Diethyl Ether + Ethyl-2,2-dimethylethyl Ether, 2-Methyl-2-butene + (2-Methylbutan-2-ol), and Diisopropyl Ether + Octane, Journal of Chemical & Engineering Data 3 (1999) 405-410. doi:10.1021/je980248s

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1504 | 0.9777 | 0.8965 |
| 0.2180 | 0.8446 | 0.5448 |
| 0.3018 | 0.6725 | 0.3272 |
| 0.3953 | 0.4747 | 0.1735 |
| 0.4813 | 0.2832 | 0.0861 |
| 0.5361 | 0.1581 | 0.0507 |
| 0.5606 | 0.0986 | 0.0308 |

Bernatová, Svatoslava - Wichterle, Ivan, Isothermal vapour–liquid equilibria in the ternary system tert-butyl methyl ether + tert-butanol + 2,2,4-trimethylpentane and the three binary subsystems, Fluid Phase Equilibria 1-2 (2001) 235-245. doi:10.1016/S0378-3812(01)00349-1

**T / K = 328.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3741 | 0.9370 | 0.7664 |
| 0.4089 | 0.9075 | 0.6809 |
| 0.4488 | 0.8721 | 0.6028 |
| 0.5054 | 0.8170 | 0.4996 |
| 0.5622 | 0.7562 | 0.4221 |
| 0.6235 | 0.6887 | 0.3526 |
| 0.6852 | 0.6079 | 0.2926 |
| 0.7468 | 0.5187 | 0.2375 |
| 0.7888 | 0.4529 | 0.2035 |
| 0.8416 | 0.3615 | 0.1635 |
| 0.8961 | 0.2572 | 0.1202 |
| 0.9426 | 0.1599 | 0.0793 |
| 0.9772 | 0.0877 | 0.0465 |
| 0.9976 | 0.0413 | 0.0228 |
| 1.011 | 0.0114 | 0.0064 |

Bernatová, Svatoslava - Wichterle, Ivan, Isothermal vapour–liquid equilibria in the ternary system tert-butyl methyl ether + tert-butanol + 2,2,4-trimethylpentane and the three binary subsystems, Fluid Phase Equilibria 1-2 (2001) 235-245. doi:10.1016/S0378-3812(01)00349-1

**T / K = 339.28**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5913 | 0.9305 | 0.7759 |
| 0.6275 | 0.9047 | 0.7130 |
| 0.6930 | 0.8583 | 0.6165 |
| 0.7643 | 0.8024 | 0.5254 |
| 0.8369 | 0.7434 | 0.4502 |
| 0.9137 | 0.6734 | 0.3797 |
| 0.9963 | 0.5899 | 0.3131 |
| 1.050 | 0.5267 | 0.2742 |

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**Isobaric phase equilibrium data**

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Perrotin-Brunel, Helene - Perez, Pablo Cabeza - van Roosmalen, Maaike J.E. - van Spronsen, Jaap - Witkamp, Geert-Jan - Peters, Cor J., Solubility of Δ9-tetrahydrocannabinol in supercritical carbon dioxide: Experiments and modeling, The Journal of Supercritical Fluids 1 (2010) 6-10. doi:10.1016/j.supflu.2009.12.001

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 354.05 | 0.9720 | 0.9140 |
| 352.45 | 0.9410 | 0.8300 |
| 350.05 | 0.8930 | 0.7100 |
| 347.85 | 0.8440 | 0.6100 |
| 345.85 | 0.7940 | 0.5240 |
| 343.75 | 0.7400 | 0.4610 |
| 341.95 | 0.6890 | 0.3940 |
| 340.45 | 0.6410 | 0.3460 |
| 339.15 | 0.5950 | 0.3080 |
| 338.15 | 0.5610 | 0.2810 |
| 336.95 | 0.5120 | 0.2460 |
| 335.85 | 0.4620 | 0.2170 |
| 334.75 | 0.4130 | 0.1910 |
| 333.85 | 0.3630 | 0.1680 |
| 332.75 | 0.3120 | 0.1440 |
| 331.95 | 0.2570 | 0.1200 |
| 331.15 | 0.2070 | 0.0980 |
| 330.25 | 0.1540 | 0.0740 |
| 329.55 | 0.1020 | 0.0510 |
| 328.75 | 0.0510 | 0.0270 |
| 328.45 | 0.0200 | 0.0110 |

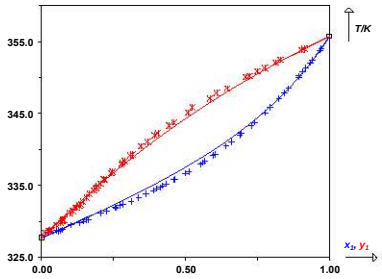
Hiaki, Toshihiko - Tatsuhana, Kazuteru - Tsuji, Tomoya - Hongo, Masaru, Vapor–liquid equilibria for binary and ternary systems composed of 2-methoxy-2-methyl propane, 2-methyl-2-propanol, and octane at 101.3 kPa, Fluid Phase Equilibria 1-2 (1999) 161-171. doi:10.1016/S0378-3812(99)00026-6

**P / bar = 1.013**

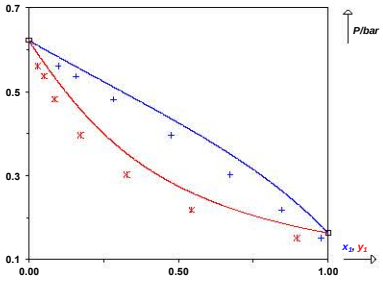
| T / K | $x_1$ | $y_1$ |
|---|---|---|

| | | |
|---|---|---|
| 353.82 | 0.9680 | 0.9047 |
| 352.07 | 0.9331 | 0.8142 |
| 351.34 | 0.9194 | 0.7763 |
| 350.81 | 0.9077 | 0.7503 |
| 350.23 | 0.8945 | 0.7233 |
| 348.49 | 0.8583 | 0.6454 |
| 347.09 | 0.8249 | 0.5861 |
| 345.14 | 0.7770 | 0.5095 |
| 343.33 | 0.7287 | 0.4434 |
| 342.24 | 0.6952 | 0.4056 |
| 341.06 | 0.6596 | 0.3692 |
| 339.33 | 0.6043 | 0.3166 |
| 338.38 | 0.5671 | 0.2896 |
| 337.95 | 0.5520 | 0.2789 |
| 336.72 | 0.4997 | 0.2426 |
| 335.78 | 0.4590 | 0.2202 |
| 335.22 | 0.4322 | 0.2050 |
| 334.95 | 0.4203 | 0.1983 |
| 334.56 | 0.4007 | 0.1889 |
| 334.31 | 0.3889 | 0.1832 |
| 333.32 | 0.3378 | 0.1580 |
| 332.41 | 0.2845 | 0.1366 |
| 332.24 | 0.2731 | 0.1313 |
| 331.90 | 0.2583 | 0.1226 |
| 331.45 | 0.2249 | 0.1094 |
| 330.24 | 0.1612 | 0.0788 |
| 330.02 | 0.1473 | 0.0722 |
| 329.80 | 0.1334 | 0.0664 |
| 328.84 | 0.0724 | 0.0371 |
| 328.73 | 0.0662 | 0.0339 |
| 328.65 | 0.0601 | 0.0313 |

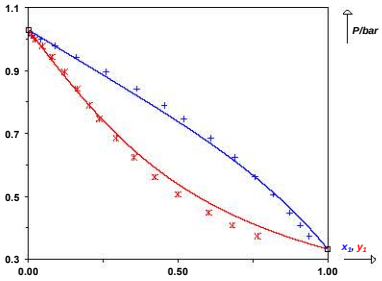
P/bar = 1.01300



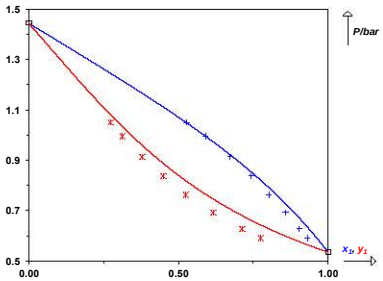

T/K = 313.15




T/K = 328.20




T/K = 339.28



## ACETONITRILE (1) + 1,4-DIOXANE (2)

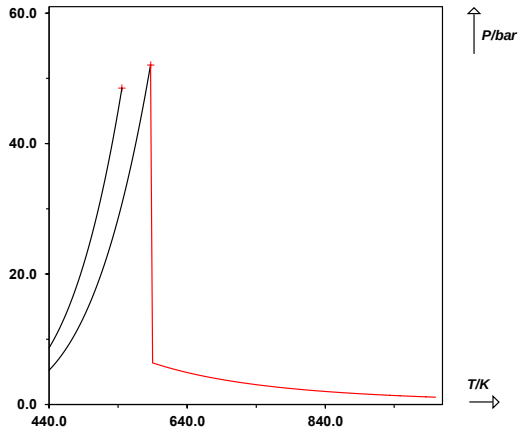
| | | |
|---|---|---|
| **CAS** | 75-05-8 | 123-91-1 |
| **InChiKey** | WEVYAHXRMPXWCK-UHFFFAOYSA-N | RYHBNJHYFVUHQT-UHFFFAOYSA-N |
| **$T_c$ / K** | 545.50 | 587.00 |
| **$P_c$ / bar** | 48.50 | 52.08 |
| **ω** | 0.3420 | 0.2790 |

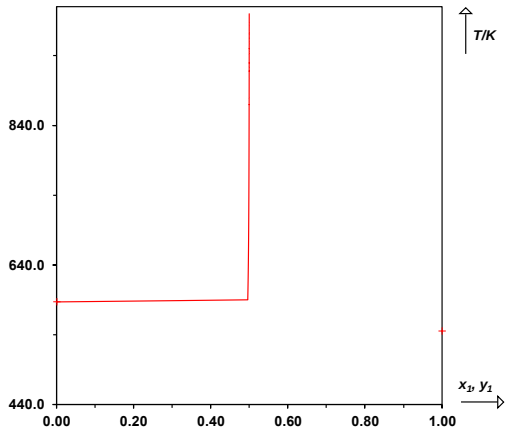
Ideal

**PPR78 results**

*Parameters*
A/MPa = 1620
B/MPa = -7000

*Deviations*
MAPE on x = 140 %
MAPE on y = 93 %
MAPE on $h^M$ = 92 %
MAPE on $c_P^M$ = 38 %



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**Isothermal phase equilibrium data**

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Davolio, Franco - Pedrosa, Graciela C. - Katz, Miguel, Vapor-liquid equilibrium for the p-dioxane-acetonitrile system at 298.15 K, Journal of Chemical & Engineering Data 1 (1981) 26-27. doi:10.1021/je00023a011

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0569 | 0.0700 | 0.2035 |
| 0.0605 | 0.1012 | 0.2738 |
| 0.0694 | 0.1870 | 0.4188 |
| 0.0752 | 0.2535 | 0.5029 |
| 0.0827 | 0.3530 | 0.5987 |
| 0.0891 | 0.4494 | 0.6765 |
| 0.0914 | 0.4830 | 0.6998 |
| 0.0981 | 0.5995 | 0.7728 |
| 0.1030 | 0.6930 | 0.8285 |
| 0.1090 | 0.8000 | 0.8875 |
| 0.1133 | 0.8875 | 0.9360 |

Francesconi, Romolo - Comelli, Fabio, Excess thermodynamic properties for the binary system 1,4-dioxane-acetonitrile at 40.degree.C, Journal of Chemical & Engineering Data 2 (1988) 80-83. doi:10.1021/je00052a004

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2200 | 0.9010 | 0.9380 |
| 0.2151 | 0.8490 | 0.9060 |
| 0.2091 | 0.7890 | 0.8710 |
| 0.2040 | 0.7320 | 0.8370 |
| 0.1960 | 0.6570 | 0.7890 |
| 0.1895 | 0.5950 | 0.7460 |
| 0.1851 | 0.5500 | 0.7180 |
| 0.1771 | 0.4830 | 0.6610 |
| 0.1651 | 0.3780 | 0.5870 |
| 0.1571 | 0.3130 | 0.5300 |
| 0.1511 | 0.2630 | 0.4790 |
| 0.1400 | 0.1840 | 0.3900 |
| 0.1311 | 0.1280 | 0.3090 |
| 0.1280 | 0.1100 | 0.2820 |
| 0.1175 | 0.0600 | 0.1800 |
| 0.1091 | 0.0260 | 0.0940 |

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**Enthalpy of mixing**

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Francesconi, Romolo - Comelli, Fabio, Excess thermodynamic properties for the binary system 1,4-dioxane-acetonitrile at 40.degree.C, Journal of Chemical & Engineering Data 2 (1988) 80-83. doi:10.1021/je00052a004

**T / K = 313.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 11.40 | 0.0200 |
| 22.70 | 0.0390 |
| 25.50 | 0.0480 |
| 30.20 | 0.0630 |
| 35.60 | 0.0920 |
| 38.70 | 0.1190 |
| 37.70 | 0.1680 |
| 33.20 | 0.2120 |
| 21.80 | 0.2880 |
| 9.400 | 0.3500 |
| 3.900 | 0.3770 |
| -7.600 | 0.4470 |
| -23.40 | 0.5480 |
| -28.80 | 0.6180 |
| -31.60 | 0.6860 |
| -32.00 | 0.7080 |
| -31.10 | 0.7640 |
| -23.60 | 0.8660 |
| -15.60 | 0.9060 |
| -5.500 | 0.9510 |
| -1.900 | 0.9750 |
| -2.100 | 0.9850 |

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**Heat capacity of mixing**

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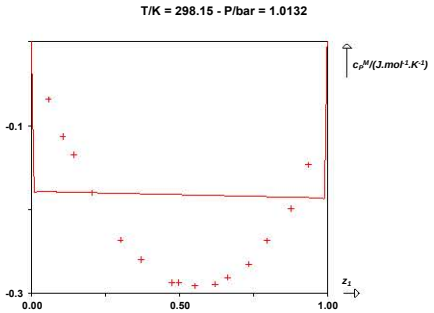
Zegers, H.C. - Somsen, G., Volumes and heat capacities of mixtures of dimethylformamide with several dialkylacetamides, Fluid Phase Equilibria 3 (1984) 299-311. doi:10.1016/0378-3812(84)85013-X

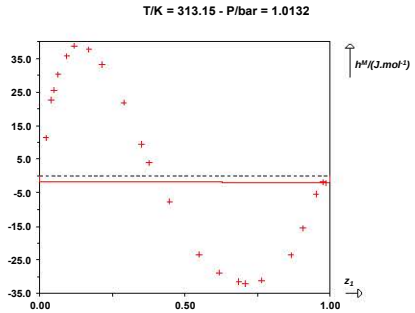
**T / K = 298.15**

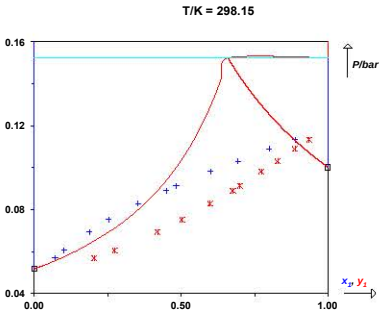
**P / bar = UNKNOWN (1.0132)**

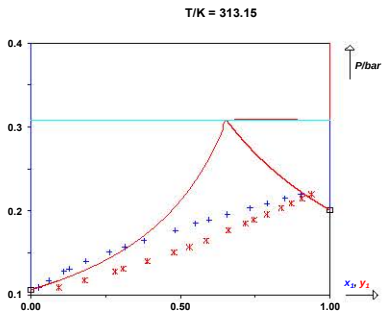
| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.0690 | 0.0572 |
| -0.1130 | 0.1063 |
| -0.1350 | 0.1438 |
| -0.1800 | 0.2048 |
| -0.2360 | 0.3013 |
| -0.2600 | 0.3708 |
| -0.2870 | 0.4751 |
| -0.2870 | 0.4982 |
| -0.2910 | 0.5532 |
| -0.2890 | 0.6205 |

| | |
|---|---|
| -0.2810 | 0.6633 |
| -0.2650 | 0.7355 |
| -0.2370 | 0.7953 |
| -0.1990 | 0.8774 |
| -0.1470 | 0.9354 |


T/K = 298.15 - P/bar = 1.0132
$c_p^M$/(J.mol$^{-1}$.K$^{-1}$)
-0.1
-0.3
0.00
0.50
1.00
$z_1$


T/K = 313.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
35.0
25.0
15.0
5.0
-5.0
-15.0
-25.0
-35.0
0.00
0.50
1.00
$z_1$


T/K = 298.15
P/bar
0.16
0.12
0.08
0.04
0.00
0.50
1.00
$x_1$, $y_1$


T/K = 313.15
P/bar
0.4
0.3
0.2
0.1
0.00
0.50
1.00
$x_1$, $y_1$

## DIMETHYL ETHER (1) + WATER (2)

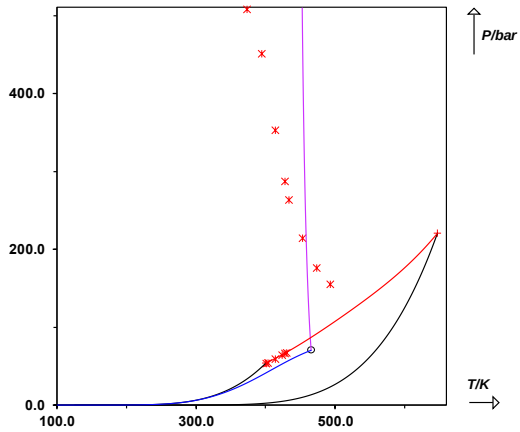
| | | |
|---|---|---|
| **CAS** | 115-10-6 | 7732-18-5 |
| **InChiKey** | LCGLNKUTAGEVQW-UHFFFAOYSA-N | XLYOFNOQVPJJNP-UHFFFAOYSA-N |
| **$T_c$ / K** | 400.10 | 647.10 |
| **$P_c$ / bar** | 53.70 | 220.64 |
| **ω** | 0.200 | 0.345 |

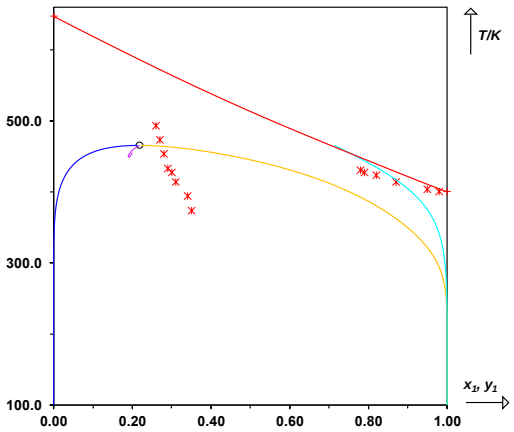
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 2740
B/MPa = 7160

*Deviations*
MAPE on x = 49 %
MAPE on y = 17 %
MAPE on $x_c$ = 55 %
MAPE on $P_c$ = 400 %
MAPE on $h^M$ = 510 %



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**Isothermal phase equilibrium data**

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Song, H.J. - Zhang, H.T. - Ying, W.Y., Study on vapor-liquid equilibrium for dimethyl ether/methanol binary system, Tianranqi Huagong 6 (2005) 67-71.

**T / K = 309.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.260 | 0.0137 | 0.9345 |
| 1.580 | 0.0175 | 0.9465 |
| 1.950 | 0.0218 | 0.9516 |
| 2.260 | 0.0264 | 0.9547 |
| 2.580 | 0.0306 | 0.9585 |
| 2.890 | 0.0354 | 0.9619 |
| 3.160 | 0.0398 | 0.9658 |
| 3.420 | 0.0443 | 0.9704 |
| 3.630 | 0.0486 | 0.9756 |
| 4.050 | 0.0573 | 0.9815 |

Song, H.J. - Zhang, H.T. - Ying, W.Y., Study on vapor-liquid equilibrium for dimethyl ether/methanol binary system, Tianranqi Huagong 6 (2005) 67-71.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.530 | 0.0094 | 0.9012 |
| 1.890 | 0.0123 | 0.9167 |
| 2.420 | 0.0182 | 0.9328 |
| 2.890 | 0.0247 | 0.9408 |
| 3.420 | 0.0326 | 0.9485 |
| 3.890 | 0.0381 | 0.9539 |
| 4.890 | 0.0480 | 0.9594 |
| 5.740 | 0.0562 | 0.9639 |
| 6.320 | 0.0631 | 0.9646 |
| 7.050 | 0.0756 | 0.9648 |
| 7.680 | 0.0854 | 0.9652 |

Song, H.J. - Zhang, H.T. - Ying, W.Y., Study on vapor-liquid equilibrium for dimethyl ether/methanol binary system, Tianranqi Huagong 6 (2005) 67-71.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.370 | 0.0066 | 0.7846 |
| 1.790 | 0.0093 | 0.8384 |
| 2.050 | 0.0111 | 0.8625 |
| 2.530 | 0.0148 | 0.8747 |
| 2.890 | 0.0188 | 0.8956 |
| 4.740 | 0.0355 | 0.9351 |
| 5.950 | 0.0416 | 0.9448 |
| 6.320 | 0.0459 | 0.9485 |
| 7.160 | 0.0554 | 0.9496 |
| 7.740 | 0.0628 | 0.9513 |
| 8.530 | 0.0746 | 0.9551 |
| 9.260 | 0.0891 | 0.9606 |

Pozo, Maria E. - Streett, William B., Fluid phase equilibria for the system dimethyl ether/water from 50 to 220.degree.C and pressures to 50.9 MPa, Journal of Chemical & Engineering Data 3 (1984) 324-329. doi:10.1021/je00037a030

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.240 | 0.0110 | 0.8500 |
| 4.000 | 0.0150 | 0.8780 |
| 5.520 | 0.0190 | 0.9130 |
| 8.070 | 0.0280 | 0.9330 |
| 9.450 | 0.0430 | 0.9410 |
| 13.24 | 0.0710 | 0.9560 |
| 15.93 | 0.0870 | 0.9570 |
| 18.00 | 0.7810 | 0.9580 |
| 18.82 | 0.9070 | 0.9720 |
| 20.20 | 0.9910 | 0.9940 |

Song, H.J. - Zhang, H.T. - Ying, W.Y., Study on vapor-liquid equilibrium for dimethyl ether/methanol binary system, Tianranqi Huagong 6 (2005) 67-71.

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.530 | 0.0048 | 0.6756 |
| 2.000 | 0.0069 | 0.7508 |
| 2.530 | 0.0093 | 0.7948 |
| 3.740 | 0.0137 | 0.8713 |
| 3.890 | 0.0146 | 0.8752 |
| 5.160 | 0.0180 | 0.9049 |
| 6.370 | 0.0216 | 0.9223 |
| 7.420 | 0.0247 | 0.9280 |
| 8.680 | 0.0336 | 0.9368 |
| 9.680 | 0.0453 | 0.9423 |
| 10.63 | 0.0539 | 0.9466 |
| 11.68 | 0.0615 | 0.9499 |
| 12.32 | 0.0655 | 0.9524 |

Song, H.J. - Zhang, H.T. - Ying, W.Y., Study on vapor-liquid equilibrium for dimethyl ether/methanol binary system, Tianranqi Huagong 6 (2005) 67-71.

**T / K = 358.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.050 | 0.0052 | 0.6436 |
| 2.580 | 0.0068 | 0.7203 |
| 3.050 | 0.0103 | 0.7678 |

| | | |
|---|---|---|
| 4.160 | 0.0126 | 0.8236 |
| 4.580 | 0.0135 | 0.8408 |
| 5.370 | 0.0146 | 0.8649 |
| 7.000 | 0.0225 | 0.8897 |
| 7.740 | 0.0243 | 0.8988 |
| 8.950 | 0.0306 | 0.9083 |
| 10.37 | 0.0398 | 0.9181 |
| 11.42 | 0.0469 | 0.9248 |
| 12.74 | 0.0533 | 0.9317 |
| 14.16 | 0.0605 | 0.9370 |

Song, H.J. - Zhang, H.T. - Ying, W.Y., Study on vapor-liquid equilibrium for dimethyl ether/methanol binary system, Tianranqi Huagong 6 (2005) 67-71.

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.790 | 0.0065 | 0.6166 |
| 3.740 | 0.0071 | 0.7003 |
| 3.890 | 0.0072 | 0.7116 |
| 4.580 | 0.0075 | 0.7554 |
| 5.320 | 0.0079 | 0.7926 |
| 5.950 | 0.0097 | 0.8136 |
| 6.320 | 0.0125 | 0.8242 |
| 7.370 | 0.0191 | 0.8449 |
| 8.260 | 0.0198 | 0.8632 |
| 9.110 | 0.0204 | 0.8653 |
| 10.58 | 0.0223 | 0.8801 |
| 11.35 | 0.0250 | 0.8876 |
| 12.95 | 0.0313 | 0.8996 |

Pozo, Maria E. - Streett, William B., Fluid phase equilibria for the system dimethyl ether/water from 50 to 220.degree.C and pressures to 50.9 MPa, Journal of Chemical & Engineering Data 3 (1984) 324-329. doi:10.1021/je00037a030

**T / K = 373.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.450 | 0.0070 | 0.6840 | |
| 5.650 | 0.0080 | 0.8030 | |
| 7.170 | 0.0180 | 0.8410 | |
| 9.790 | 0.0210 | 0.8720 | |
| 13.72 | 0.0340 | 0.9050 | |
| 17.44 | 0.0440 | 0.9150 | |
| 20.62 | 0.0540 | 0.9250 | |
| 24.41 | 0.0650 | 0.9310 | |
| 508.00 | 0.3500 | 0.3500 | CRIT |
| 28.61 | 0.7770 | 0.9410 | |
| 29.58 | 0.8550 | 0.9500 | |
| 31.10 | 0.9340 | 0.9670 | |
| 28.48 | 0.7550 | 0.9360 | |
| 28.61 | 0.7770 | 0.9410 | |
| 29.58 | 0.8550 | 0.9500 | |
| 31.10 | 0.9340 | 0.9670 | |

Song, H.J. - Zhang, H.T. - Ying, W.Y., Study on vapor-liquid equilibrium for dimethyl ether/methanol binary system, Tianranqi Huagong 6 (2005) 67-71.

**T / K = 393.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.950 | 0.0024 | 0.4629 |
| 4.370 | 0.0032 | 0.5148 |
| 4.680 | 0.0035 | 0.5446 |
| 5.110 | 0.0045 | 0.5762 |
| 5.740 | 0.0050 | 0.6156 |
| 7.890 | 0.0081 | 0.7352 |
| 9.630 | 0.0126 | 0.7629 |
| 11.58 | 0.0137 | 0.7931 |
| 13.00 | 0.0169 | 0.8136 |
| 15.68 | 0.0226 | 0.8411 |
| 17.16 | 0.0253 | 0.8521 |
| 18.42 | 0.0271 | 0.8568 |
| 21.68 | 0.0305 | 0.8697 |

Pozo, Maria E. - Streett, William B., Fluid phase equilibria for the system dimethyl ether/water from 50 to 220.degree.C and pressures to 50.9 MPa, Journal of Chemical & Engineering Data 3 (1984) 324-329. doi:10.1021/je00037a030

**T / K = 394.21**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 4.960 | 0.0040 | 0.5630 | |
| 7.310 | 0.0070 | 0.6970 | |
| 9.100 | 0.0120 | 0.7490 | |
| 11.10 | 0.0130 | 0.7850 | |
| 13.79 | 0.0190 | 0.8180 | |
| 17.79 | 0.0260 | 0.8520 | |
| 22.20 | 0.0310 | 0.8710 | |
| 26.20 | 0.0430 | 0.8810 | |
| 28.61 | 0.0480 | 0.8840 | |
| 35.65 | 0.0690 | 0.8990 | |
| 451.00 | 0.3400 | 0.3400 | CRIT |
| 41.51 | 0.8060 | 0.9180 | |
| 42.20 | 0.8510 | 0.9220 | |
| 43.99 | 0.8980 | 0.9380 | |
| 46.06 | 0.9490 | 0.9690 | |
| 40.54 | 0.7270 | 0.9100 | |
| 41.51 | 0.8060 | 0.9180 | |
| 42.20 | 0.8510 | 0.9220 | |

| | | |
|---|---|---|
| 43.99 | 0.8980 | 0.9380 |
| 46.06 | 0.9490 | 0.9690 |

Pozo, Maria E. - Streett, William B., Fluid phase equilibria for the system dimethyl ether/water from 50 to 220.degree.C and pressures to 50.9 MPa, Journal of Chemical & Engineering Data 3 (1984) 324-329. doi:10.1021/je00037a030

**T / K = 403.26**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.860 | 0.0030 | 0.5180 | |
| 7.240 | 0.0050 | 0.6110 | |
| 8.480 | 0.0060 | 0.6620 | |
| 9.450 | 0.0080 | 0.6870 | |
| 10.14 | 0.0100 | 0.7050 | |
| 12.82 | 0.0120 | 0.7450 | |
| 17.72 | 0.0200 | 0.8110 | |
| 24.27 | 0.0290 | 0.8350 | |
| 31.16 | 0.0400 | 0.8630 | |
| 37.09 | 0.0530 | 0.8750 | |
| 41.23 | 0.0670 | 0.8770 | |
| 46.61 | 0.7210 | 0.8790 | |
| 47.09 | 0.7780 | 0.8900 | |
| 48.13 | 0.8190 | 0.8950 | |
| 50.81 | 0.8550 | 0.9190 | |
| 50.12 | 0.8710 | 0.9150 | |
| 50.81 | 0.8850 | 0.9190 | |
| 52.26 | 0.9170 | 0.9360 | |
| 53.30 | 0.9360 | 0.9480 | |
| 54.00 | 0.9500 | 0.9500 | CRIT |

Pozo, Maria E. - Streett, William B., Fluid phase equilibria for the system dimethyl ether/water from 50 to 220.degree.C and pressures to 50.9 MPa, Journal of Chemical & Engineering Data 3 (1984) 324-329. doi:10.1021/je00037a030

**T / K = 414.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.790 | 0.0010 | 0.3550 |
| 6.620 | 0.0020 | 0.4410 |
| 7.580 | 0.0030 | 0.5080 |
| 9.790 | 0.0040 | 0.5900 |
| 13.38 | 0.0100 | 0.6830 |
| 16.55 | 0.0110 | 0.7410 |
| 21.37 | 0.0170 | 0.7840 |
| 30.61 | 0.0270 | 0.8170 |
| 37.09 | 0.0350 | 0.8450 |
| 43.51 | 0.0510 | 0.8540 |
| 48.95 | 0.0670 | 0.8590 |
| 54.54 | 0.7050 | 0.8620 |
| 56.81 | 0.8030 | 0.8740 |
| 58.05 | 0.8290 | 0.8760 |
| 59.09 | 0.8520 | 0.8730 |
| 59.29 | 0.8660 | 0.8720 |
| 59.00 | 0.8700 | 0.8700 CRIT |

Pozo, Maria E. - Streett, William B., Fluid phase equilibria for the system dimethyl ether/water from 50 to 220.degree.C and pressures to 50.9 MPa, Journal of Chemical & Engineering Data 3 (1984) 324-329. doi:10.1021/je00037a030

**T / K = 423.50**

| P / bar | $x_1$ | |
|---|---|---|
| 6.140 | 0.2110 | |
| 6.830 | 0.2970 | |
| 7.450 | 0.3420 | |
| 8.410 | 0.4040 | |
| 64.00 | 0.8200 | CRIT |

Pozo, Maria E. - Streett, William B., Fluid phase equilibria for the system dimethyl ether/water from 50 to 220.degree.C and pressures to 50.9 MPa, Journal of Chemical & Engineering Data 3 (1984) 324-329. doi:10.1021/je00037a030

**T / K = 423.50**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 10.34 | 0.0050 | 0.4930 | |
| 11.17 | 0.0060 | 0.5200 | |
| 13.51 | 0.0080 | 0.5920 | |
| 15.86 | 0.0120 | 0.6430 | |
| 20.55 | 0.0170 | 0.7100 | |
| 22.06 | 0.0180 | 0.7240 | |
| 25.58 | 0.0250 | 0.7570 | |
| 31.72 | 0.0330 | 0.7830 | |
| 37.65 | 0.0400 | 0.8080 | |
| 43.99 | 0.0540 | 0.8120 | |
| 51.30 | 0.0560 | 0.8290 | |
| 58.19 | 0.0820 | 0.8390 | |
| 62.19 | 0.7360 | 0.8440 | |
| 62.81 | 0.7640 | 0.8450 | |
| 63.91 | 0.7940 | 0.8410 | |
| 64.19 | 0.8150 | 0.8340 | |
| 64.00 | 0.8200 | 0.8200 | CRIT |

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**Enthalpy of mixing**

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Park, So-Jin - Han, Kyu-Jin - Gmehling, Jürgen, Isothermal Phase Equilibria and Excess Molar Enthalpies for Binary Systems with Dimethyl Ether at

323.15 K, Journal of Chemical & Engineering Data 5 (2007) 1814-1818. doi:10.1021/je700174h

**T / K = 323.15**

**P / bar = 18.93**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -131.64 | 0.0137 |
| -316.77 | 0.0363 |
| -542.52 | 0.0808 |
| -646.32 | 0.1366 |
| -547.04 | 0.2087 |
| -399.40 | 0.3054 |
| -187.92 | 0.4418 |
| -14.71 | 0.5543 |
| 132.12 | 0.6487 |
| 215.55 | 0.7036 |
| 307.98 | 0.7649 |
| 412.57 | 0.8337 |
| 399.51 | 0.8713 |
| 348.00 | 0.9114 |
| 242.54 | 0.9542 |

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**Critical point**

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Pozo, Maria E. - Streett, William B., Fluid phase equilibria for the system dimethyl ether/water from 50 to 220.degree.C and pressures to 50.9 MPa, Journal of Chemical & Engineering Data 3 (1984) 324-329. doi:10.1021/je00037a030

| T / K | P / bar | $x_1$ |
|---|---|---|
| 414.01 | 353.00 | 0.3100 |
| 427.40 | 287.00 | 0.3000 |
| 433.20 | 263.00 | 0.2900 |
| 453.30 | 214.00 | 0.2800 |
| 473.60 | 176.00 | 0.2700 |
| 493.16 | 155.00 | 0.2600 |
| 400.49 | 53.00 | 0.9800 |
| 427.40 | 66.00 | 0.7900 |
| 430.15 | 67.20 | 0.7800 |

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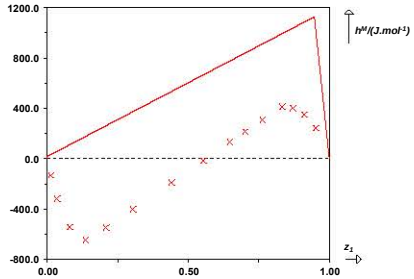
**Three-phase line**

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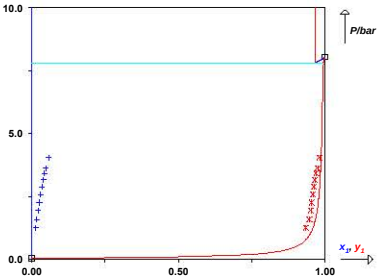
M.E. Pozo, W.B. Streett, Fluid phase equilibria for the system dimethyl ether/water from 50 to 220.degree.C and pressures to 50.9 MPa, Journal of Chemical & Engineering Data. 29 (1984) 324–329. doi:10.1021/je00037a030.

| T / K | P / bar | $x_{1a}$ | $x_{1b}$ | $y_1$ |
|---|---|---|---|---|
| 323.15 | 10.2700 | 0.1550 | 0.8140 | 0.9770 |
| 348.15 | 18.0000 | 0.1280 | 0.7810 | 0.9580 |
| 373.26 | 28.4800 | 0.1040 | 0.7550 | 0.9360 |
| 394.21 | 40.5400 | 0.0900 | 0.7270 | 0.9100 |
| 400.49 | 44.4000 | 0.0890 | 0.7250 | 0.9010 |
| 403.26 | 46.6100 | 0.0870 | 0.7210 | 0.8790 |
| 414.00 | 54.5400 | 0.0810 | 0.7050 | 0.8620 |
| 423.50 | 62.1900 | 0.0930 | 0.7360 | 0.8440 |
| 427.40 | 66.0500 | 0.1040 | 0.7550 | 0.8320 |

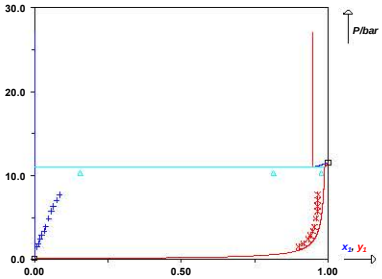
T/K = 323.15 - P/bar = 18.9300



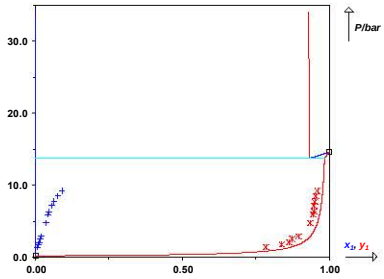

T/K = 309.15



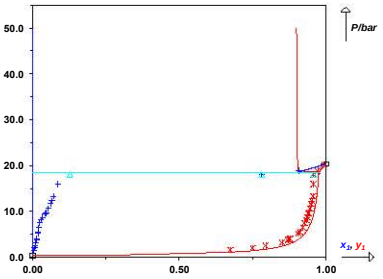

T/K = 323.15



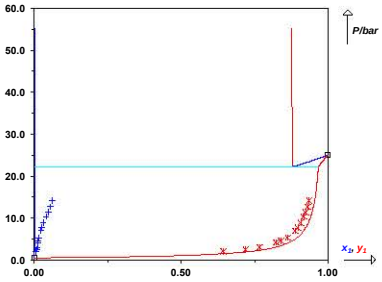

T/K = 333.15



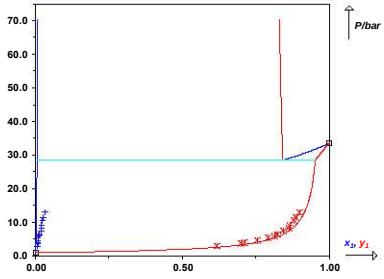

T/K = 348.15



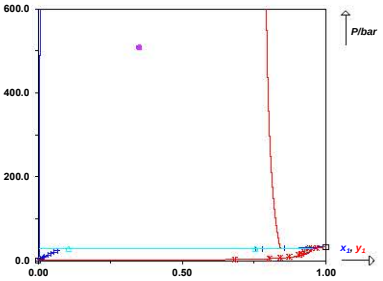

T/K = 358.15



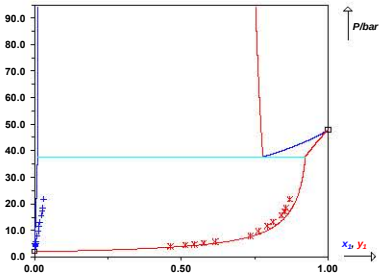

T/K = 373.15



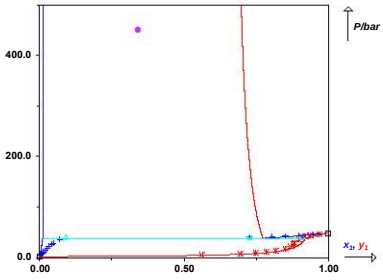

T/K = 373.26



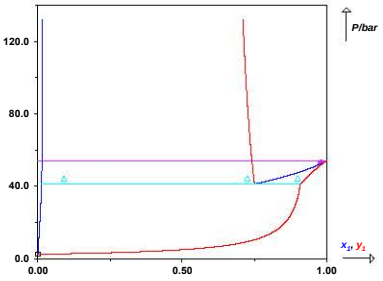

T/K = 393.15



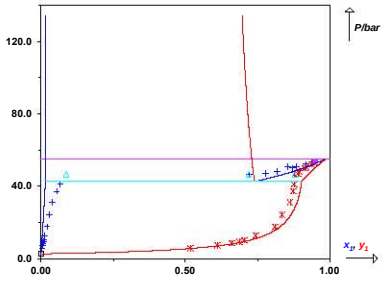

T/K = 394.21



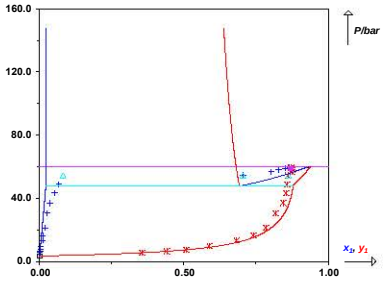

T/K = 400.49



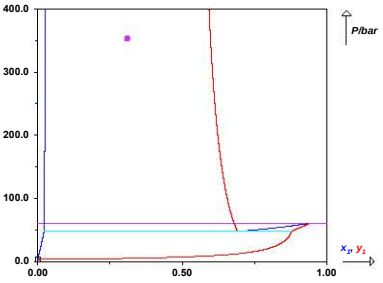

T/K = 403.26



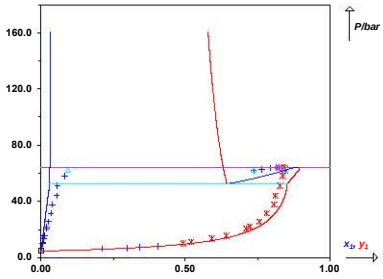

T/K = 414.00



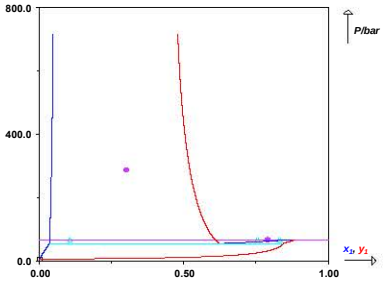

T/K = 414.01



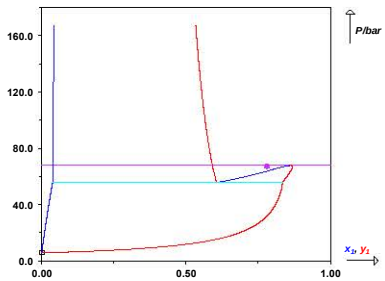

T/K = 423.50



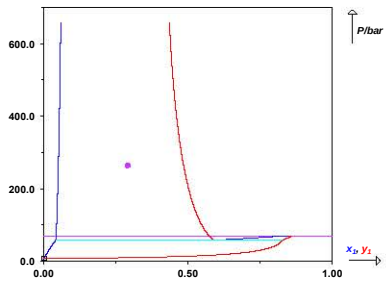
T/K = 427.40



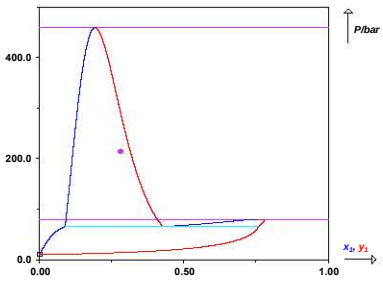

T/K = 430.15



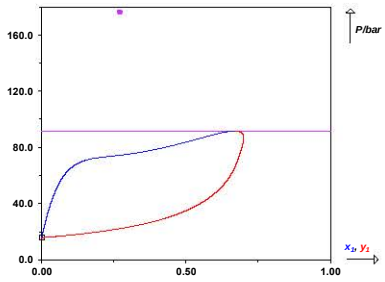

T/K = 433.20



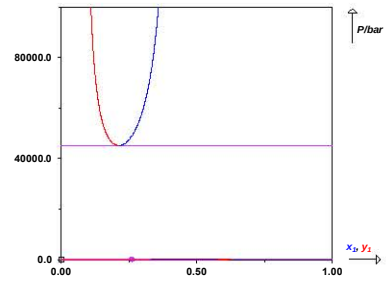

T/K = 453.30




T/K = 473.60




T/K = 493.16



## CARBON DIOXIDE (1) + METHANOL (2)

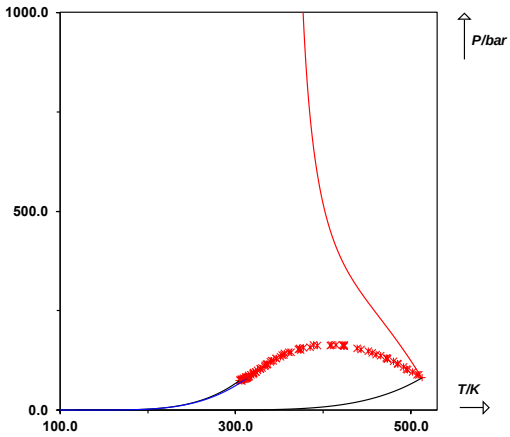
| | | |
|---|---|---|
| **CAS** | 124-38-9 | 67-56-1 |
| **InChiKey** | CURLTUGMZLYLDI-UHFFFAOYSA-N | OKKJLVBELUTLKV-UHFFFAOYSA-N |
| **$T_c$ / K** | 304.21 | 512.50 |
| **$P_c$ / bar** | 73.83 | 80.84 |
| **ω** | 0.224 | 0.566 |

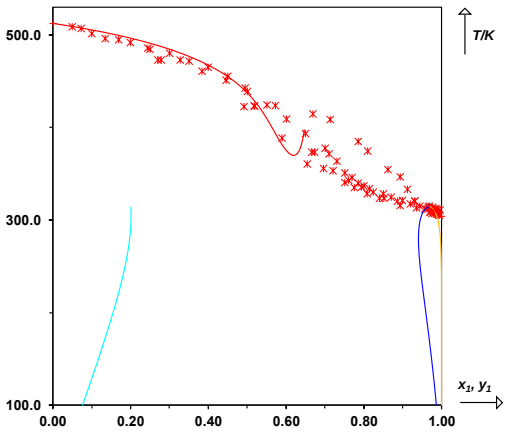
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 768
B/MPa = 265

*Deviations*
MAPE on x = 70 %
MAPE on y = 9.1 %
MAPE on $x_c$ = 16 %
MAPE on $P_c$ = 39 %
MAPE on $h^M$ = 94 %



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**Isothermal phase equilibrium data**

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Naidoo, Paramespri - Ramjugernath, Deresh - Raal, Johan David, A new high-pressure vapour–liquid equilibrium apparatus, Fluid Phase Equilibria 1-2 (2008) 104-112. doi:10.1016/j.fluid.2008.05.002

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.910 | 0.1106 | 0.9908 |
| 17.92 | 0.2315 | 0.9943 |
| 26.81 | 0.4155 | 0.9968 |
| 32.73 | 0.6753 | 0.9975 |

Hong, Jane H. - Kobayashi, Riki, Vapor—liquid equilibrium studies for the carbon dioxide—methanol system, Fluid Phase Equilibria 3 (1988) 269-276. doi:10.1016/0378-3812(88)80011-6

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0828 | 0.9942 |
| 13.79 | 0.1692 | 0.9969 |
| 17.24 | 0.2210 | 0.9975 |
| 20.68 | 0.2710 | 0.9979 |
| 27.58 | 0.4163 | 0.9984 |
| 30.82 | 0.5394 | 0.9985 |
| 33.03 | 0.7680 | 0.9985 |
| 33.23 | 0.8160 | 0.9986 |

Hong, Jane H. - Kobayashi, Riki, Vapor—liquid equilibrium studies for the carbon dioxide—methanol system, Fluid Phase Equilibria 3 (1988) 269-276. doi:10.1016/0378-3812(88)80011-6

**T / K = 290.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0550 | 0.9844 |
| 13.79 | 0.1159 | 0.9910 |
| 17.24 | 0.1475 | 0.9925 |
| 27.58 | 0.2475 | 0.9948 |
| 41.37 | 0.4310 | 0.9959 |
| 48.26 | 0.6671 | 0.9959 |
| 50.06 | 0.8454 | 0.9960 |
| 50.33 | 0.8964 | 0.9961 |
| 51.64 | 0.9694 | 0.9971 |

Ohgaki, Kazunari - Katayama, Takashi, Isothermal vapor-liquid equilibrium data for binary systems containing carbon dioxide at high pressures: methanol-carbon dioxide, n-hexane-carbon dioxide, and benzene-carbon dioxide systems, Journal of Chemical & Engineering Data 1 (1976) 53-55. doi:10.1021/je60068a015

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 7.895 | 0.0596 | 0.9761 |
| 19.06 | 0.1548 | 0.9907 |
| 30.65 | 0.2601 | 0.9920 |
| 40.03 | 0.3495 | 0.9929 |
| 49.31 | 0.4886 | 0.9930 |
| 55.74 | 0.6451 | 0.9931 |

Katayama, Takashi - Ohgaki, Kazunari - Maekawa, Goro - Goto, Motojiro - Nagano, Tamon, Isothermal Vapor-Liquid Equilibria Of Acetone-Carbon Dioxide And Methanol-Carbon Dioxide Systems At High Pressures, Journal of Chemical Engineering of Japan 2 (1975) 89-92. doi:10.1252/jcej.8.89

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.186 | 0.0150 | 0.9202 |
| 5.652 | 0.0410 | 0.9685 |
| 9.511 | 0.0700 | 0.9797 |
| 17.31 | 0.1310 | 0.9878 |
| 30.01 | 0.2560 | 0.9917 |
| 41.34 | 0.3610 | 0.9928 |
| 47.59 | 0.4500 | 0.9930 |
| 54.59 | 0.6100 | 0.9929 |
| 56.51 | 0.6620 | 0.9922 |
| 58.54 | 0.8100 | 0.9926 |
| 59.83 | 0.9225 | 0.9930 |
| 60.25 | 0.9325 | 0.9926 |
| 61.28 | 0.9573 | 0.9937 |

Chang, Chiehming J. - Day, Chany-Yih - Ko, Ching-Ming - Chiu, Kou-Lung, Densities and P-x-y diagrams for carbon dioxide dissolution in methanol, ethanol, and acetone mixtures, Fluid Phase Equilibria 1-2 (1997) 243-258. doi:10.1016/S0378-3812(96)03208-6

**T / K = 303.18**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.900 | 0.0689 | 0.9766 |
| 13.10 | 0.0924 | 0.9807 |
| 16.50 | 0.1204 | 0.9825 |
| 20.10 | 0.1509 | 0.9848 |
| 24.30 | 0.1814 | 0.9859 |
| 29.10 | 0.2154 | 0.9866 |
| 34.20 | 0.2571 | 0.9877 |
| 38.90 | 0.2972 | 0.9985 |
| 42.50 | 0.3245 | 0.9906 |
| 45.60 | 0.3507 | 0.9912 |
| 49.40 | 0.4005 | 0.9918 |
| 53.10 | 0.4777 | 0.9901 |

| | | |
|---|---|---|
| 55.80 | 0.5455 | 0.9885 |
| 59.30 | 0.6219 | 0.9867 |
| 61.70 | 0.7083 | 0.9834 |
| 63.20 | 0.8833 | 0.9740 |

Hong, Jane H. - Kobayashi, Riki, Vapor—liquid equilibrium studies for the carbon dioxide—methanol system, Fluid Phase Equilibria 3 (1988) 269-276. doi:10.1016/0378-3812(88)80011-6

**T / K = 310.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0373 | 0.9516 |
| 10.34 | 0.0573 | 0.9665 |
| 13.79 | 0.0779 | 0.9751 |
| 20.68 | 0.1214 | 0.9826 |
| 27.58 | 0.1648 | 0.9863 |
| 41.37 | 0.2628 | 0.9891 |
| 55.16 | 0.3831 | 0.9894 |
| 68.95 | 0.5954 | 0.9874 |
| 71.15 | 0.6458 | 0.9862 |
| 72.40 | 0.7248 | 0.9856 |
| 73.77 | 0.8493 | 0.9847 |
| 74.33 | 0.8931 | 0.9846 |
| 74.39 | 0.9184 | 0.9844 |
| 74.46 | 0.9065 | 0.9846 |
| 74.81 | 0.9348 | 0.9835 |
| 76.67 | 0.9703 | 0.9833 |
| 77.22 | 0.9736 | 0.9823 |
| 77.29 | 0.9745 | 0.9820 |
| 77.43 | 0.9750 | 0.9814 |

Naidoo, Paramespri - Ramjugernath, Deresh - Raal, Johan David, A new high-pressure vapour–liquid equilibrium apparatus, Fluid Phase Equilibria 1-2 (2008) 104-112. doi:10.1016/j.fluid.2008.05.002

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 12.91 | 0.0653 | 0.9732 |
| 23.13 | 0.1233 | 0.9825 |
| 31.45 | 0.1856 | 0.9856 |
| 43.39 | 0.2516 | 0.9826 |
| 51.92 | 0.3227 | 0.9845 |
| 55.46 | 0.3470 | 0.9860 |
| 61.31 | 0.3968 | 0.9849 |
| 67.58 | 0.4736 | 0.9866 |

Joung, Seung Nam - Yoo, Chang Woo - Shin, Hun Yong - Kim, Sun Young - Yoo, Ki-Pung - Lee, Chul Soo - Huh, Wan Soo, Measurements and correlation of high-pressure VLE of binary CO2–alcohol systems (methanol, ethanol, 2-methoxyethanol and 2-ethoxyethanol), Fluid Phase Equilibria 1-2 (2001) 219-230. doi:10.1016/S0378-3812(01)00472-1

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 27.30 | 0.1479 | 0.9781 | |
| 37.80 | 0.2199 | 0.9832 | |
| 56.00 | 0.3546 | 0.9857 | |
| 65.70 | 0.4555 | 0.9846 | |
| 78.40 | 0.7651 | 0.9757 | |
| 79.30 | 0.8218 | 0.9743 | |
| 79.90 | 0.8968 | 0.9745 | |
| 80.60 | 0.9147 | 0.9688 | |
| 81.00 | 0.9298 | 0.9635 | |
| 81.20 | 0.9350 | 0.9452 | |
| 81.50 | 0.9351 | 0.9351 | CRIT |

Laursen, T. - Rasmussen, P. - Andersen, S.I., VLE and VLLE Measurements of Dimethyl Ether Containing Systems, J. Chem. Eng. Data 2 (2002) 198-202. doi:10.1021/je010154+

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 15.90 | 0.0887 | 0.9799 |
| 28.80 | 0.1693 | 0.9871 |
| 41.40 | 0.2486 | 0.9889 |
| 53.80 | 0.3448 | 0.9894 |
| 63.40 | 0.4251 | 0.9883 |

Ohgaki, Kazunari - Katayama, Takashi, Isothermal vapor-liquid equilibrium data for binary systems containing carbon dioxide at high pressures: methanol-carbon dioxide, n-hexane-carbon dioxide, and benzene-carbon dioxide systems, Journal of Chemical & Engineering Data 1 (1976) 53-55. doi:10.1021/je60068a015

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.773 | 0.0285 | 0.9363 |
| 17.70 | 0.1023 | 0.9774 |
| 30.05 | 0.1641 | 0.9847 |
| 40.87 | 0.2339 | 0.9868 |
| 57.06 | 0.3655 | 0.9882 |
| 62.72 | 0.4201 | 0.9880 |
| 70.93 | 0.5429 | 0.9866 |
| 77.03 | 0.6892 | 0.9840 |
| 80.58 | 0.8970 | 0.9748 |

Kodama, Daisuke - Kubota, Nobuo - Yamaki, Yoshikazu - Tanaka, Hiroyuki - Kato, Masahiro, High Pressure Vapor-Liquid Equilibria and Density Behaviors for Carbon Dioxide+Methanol System at 313.15 K., Netsu Bussei 1 (1996) 16-20. doi:10.2963/jjtp.10.16

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 20.11 | 0.1060 | 0.9750 |
| 50.35 | 0.2980 | 0.9780 |
| 59.69 | 0.3750 | 0.9770 |
| 65.07 | 0.4260 | 0.9800 |
| 70.22 | 0.4920 | 0.9890 |
| 75.06 | 0.5850 | 0.9810 |

Joung, Seung Nam - Yoo, Chang Woo - Shin, Hun Yong - Kim, Sun Young - Yoo, Ki-Pung - Lee, Chul Soo - Huh, Wan Soo, Measurements and correlation of high-pressure VLE of binary CO2–alcohol systems (methanol, ethanol, 2-methoxyethanol and 2-ethoxyethanol), Fluid Phase Equilibria 1-2 (2001) 219-230. doi:10.1016/S0378-3812(01)00472-1

**T / K = 320.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 6.000 | 0.0326 | 0.9150 | |
| 26.90 | 0.1371 | 0.9717 | |
| 37.00 | 0.1913 | 0.9778 | |
| 57.20 | 0.3166 | 0.9815 | |
| 65.00 | 0.3750 | 0.9804 | |
| 81.40 | 0.5505 | 0.9738 | |
| 86.20 | 0.6757 | 0.9662 | |
| 88.50 | 0.8053 | 0.9484 | |
| 88.80 | 0.8287 | 0.9441 | |
| 89.30 | 0.8791 | 0.9010 | |
| 89.50 | 0.8860 | 0.8860 | CRIT |

Joung, Seung Nam - Yoo, Chang Woo - Shin, Hun Yong - Kim, Sun Young - Yoo, Ki-Pung - Lee, Chul Soo - Huh, Wan Soo, Measurements and correlation of high-pressure VLE of binary CO2–alcohol systems (methanol, ethanol, 2-methoxyethanol and 2-ethoxyethanol), Fluid Phase Equilibria 1-2 (2001) 219-230. doi:10.1016/S0378-3812(01)00472-1

**T / K = 330.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 7.800 | 0.0346 | 0.8857 | |
| 22.40 | 0.0960 | 0.9537 | |
| 31.20 | 0.1342 | 0.9610 | |
| 51.70 | 0.2365 | 0.9717 | |
| 60.70 | 0.2845 | 0.9725 | |
| 89.00 | 0.4836 | 0.9647 | |
| 94.20 | 0.5382 | 0.9584 | |
| 102.20 | 0.6779 | 0.9438 | |
| 104.80 | 0.7401 | 0.8777 | |
| 105.50 | 0.7694 | 0.8619 | |
| 105.70 | 0.8215 | 0.8572 | |
| 105.90 | 0.8243 | 0.8243 | CRIT |

Hong, Jane H. - Kobayashi, Riki, Vapor—liquid equilibrium studies for the carbon dioxide—methanol system, Fluid Phase Equilibria 3 (1988) 269-276. doi:10.1016/0378-3812(88)80011-6

**T / K = 330.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 6.895 | 0.0245 | 0.8791 |
| 13.79 | 0.0558 | 0.9403 |
| 20.68 | 0.0874 | 0.9572 |
| 27.58 | 0.1183 | 0.9668 |
| 41.37 | 0.1850 | 0.9746 |
| 55.16 | 0.2597 | 0.9772 |
| 68.95 | 0.3448 | 0.9773 |
| 82.74 | 0.4415 | 0.9735 |
| 96.53 | 0.5830 | 0.9621 |
| 103.42 | 0.7127 | 0.9347 |
| 104.80 | 0.7475 | 0.9203 |
| 106.18 | 0.8195 | 0.8903 |
| 106.45 | 0.8460 | 0.8759 |

Joung, Seung Nam - Yoo, Chang Woo - Shin, Hun Yong - Kim, Sun Young - Yoo, Ki-Pung - Lee, Chul Soo - Huh, Wan Soo, Measurements and correlation of high-pressure VLE of binary CO2–alcohol systems (methanol, ethanol, 2-methoxyethanol and 2-ethoxyethanol), Fluid Phase Equilibria 1-2 (2001) 219-230. doi:10.1016/S0378-3812(01)00472-1

**T / K = 335.65**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 8.400 | 0.0336 | 0.8592 | |
| 30.80 | 0.1208 | 0.9502 | |
| 44.10 | 0.1768 | 0.9620 | |
| 65.20 | 0.2760 | 0.9671 | |
| 74.40 | 0.3247 | 0.9664 | |
| 93.20 | 0.4471 | 0.9583 | |
| 102.80 | 0.5330 | 0.9466 | |
| 111.50 | 0.6651 | 0.8948 | |
| 112.50 | 0.6762 | 0.8901 | |
| 114.40 | 0.7759 | 0.8250 | |
| 114.50 | 0.7925 | 0.8059 | |
| 114.60 | 0.7940 | 0.7940 | CRIT |

Joung, Seung Nam - Yoo, Chang Woo - Shin, Hun Yong - Kim, Sun Young - Yoo, Ki-Pung - Lee, Chul Soo - Huh, Wan Soo, Measurements and correlation of high-pressure VLE of binary CO2–alcohol systems (methanol, ethanol, 2-methoxyethanol and 2-ethoxyethanol), Fluid Phase Equilibria 1-2 (2001) 219-230. doi:10.1016/S0378-3812(01)00472-1

**T / K = 342.80**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|

| | | | |
|---|---|---|---|
| 6.700 | 0.0247 | 0.7999 | |
| 31.30 | 0.1145 | 0.9403 | |
| 42.00 | 0.1553 | 0.9510 | |
| 52.30 | 0.1961 | 0.9559 | |
| 73.70 | 0.2909 | 0.9586 | |
| 84.00 | 0.3427 | 0.9574 | |
| 104.10 | 0.4664 | 0.9432 | |
| 111.00 | 0.5234 | 0.9312 | |
| 116.40 | 0.5806 | 0.9108 | |
| 122.30 | 0.6792 | 0.8498 | |
| 122.10 | 0.6719 | 0.8526 | |
| 123.70 | 0.7311 | 0.8026 | |
| 123.90 | 0.7603 | 0.7720 | |
| 124.00 | 0.7610 | 0.7610 | CRIT |

Semenova, A.I. - Emel'yanova, E.A. - Tsimmerman, S.S. - Tsiklis, D.S., Phase equilibriums in the methanol-carbon dioxide system, Zh. Fiz. Khim. 10 (1979) 2502-2505.

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.000 | 0.0110 | 0.6180 |
| 10.00 | 0.0300 | 0.8150 |
| 15.00 | 0.0490 | 0.8780 |
| 20.00 | 0.0680 | 0.9080 |
| 25.00 | 0.0860 | 0.9240 |
| 30.00 | 0.1040 | 0.9350 |
| 45.00 | 0.1580 | 0.9460 |
| 50.00 | 0.1740 | 0.9480 |
| 60.00 | 0.2120 | 0.9530 |
| 70.00 | 0.2520 | 0.9580 |
| 80.00 | 0.2960 | 0.9520 |
| 90.00 | 0.3420 | 0.9460 |
| 100.00 | 0.3860 | 0.9400 |
| 110.00 | 0.4310 | 0.9360 |

Leu, Ah-Dong - Chung, Samuel Y.-K. - Robinson, Donald B., The equilibrium phase properties of (carbon dioxide + methanol), The Journal of Chemical Thermodynamics 10 (1991) 979-985. doi:10.1016/S0021-9614(05)80178-8

**T / K = 352.60**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.250 | 0.0187 | 0.7554 |
| 21.51 | 0.0615 | 0.8917 |
| 45.57 | 0.1409 | 0.9332 |
| 76.68 | 0.2535 | 0.9422 |
| 113.28 | 0.4238 | 0.9224 |
| 126.73 | 0.5273 | 0.8885 |

Naidoo, Paramespri - Ramjugernath, Deresh - Raal, Johan David, A new high-pressure vapour–liquid equilibrium apparatus, Fluid Phase Equilibria 1-2 (2008) 104-112. doi:10.1016/j.fluid.2008.05.002

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 21.57 | 0.0451 | 0.8042 |
| 30.89 | 0.0697 | 0.8629 |
| 38.73 | 0.0887 | 0.8837 |
| 50.94 | 0.1258 | 0.9053 |
| 68.22 | 0.1783 | 0.9138 |
| 75.28 | 0.2033 | 0.9127 |
| 90.67 | 0.2531 | 0.9118 |
| 105.94 | 0.3103 | 0.9100 |
| 120.68 | 0.3611 | 0.8927 |

Semenova, A.I. - Emel'yanova, E.A. - Tsimmerman, S.S. - Tsiklis, D.S., Phase equilibriums in the methanol-carbon dioxide system, Zh. Fiz. Khim. 10 (1979) 2502-2505.

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.000 | 0.0050 | 0.3500 |
| 10.00 | 0.0180 | 0.6300 |
| 15.00 | 0.0320 | 0.7350 |
| 20.00 | 0.0470 | 0.7890 |
| 25.00 | 0.0610 | 0.8270 |
| 30.00 | 0.0750 | 0.8550 |
| 35.00 | 0.0900 | 0.8760 |
| 40.00 | 0.1040 | 0.8910 |
| 45.00 | 0.1180 | 0.9010 |
| 50.00 | 0.1320 | 0.9070 |
| 90.00 | 0.2500 | 0.9100 |
| 100.00 | 0.2830 | 0.9080 |
| 110.00 | 0.3160 | 0.9040 |

Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 85.00 | 0.2395 | 0.9010 | |
| 90.00 | 0.2487 | 0.9117 | |
| 120.00 | 0.3534 | 0.8989 | |
| 130.00 | 0.4018 | 0.8801 | |
| 150.00 | 0.5212 | 0.8092 | |
| 155.00 | 0.6654 | 0.6654 | CRIT |
| 155.00 | 0.6654 | 0.6621 | |

Leu, Ah-Dong - Chung, Samuel Y.-K. - Robinson, Donald B., The equilibrium phase properties of (carbon

dioxide + methanol), The Journal of Chemical Thermodynamics 10 (1991) 979-985. doi:10.1016/S0021-9614(05)80178-8

**T / K = 394.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.30 | 0.0087 | 0.3328 |
| 26.80 | 0.0446 | 0.6590 |
| 37.00 | 0.0680 | 0.7458 |
| 60.10 | 0.1243 | 0.8202 |
| 100.50 | 0.2307 | 0.8407 |
| 139.10 | 0.3693 | 0.7916 |
| 152.80 | 0.4469 | 0.7613 |
| 162.90 | 0.5493 | 0.6621 |

Semenova, A.I. - Emel'yanova, E.A. - Tsimmerman, S.S. - Tsiklis, D.S., Phase equilibriums in the methanol-carbon dioxide system, Zh. Fiz. Khim. 10 (1979) 2502-2505.

**T / K = 398.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 10.00 | 0.0070 | 0.2680 |
| 15.00 | 0.0190 | 0.4500 |
| 20.00 | 0.0320 | 0.6000 |
| 25.00 | 0.0440 | 0.6600 |
| 30.00 | 0.0560 | 0.7100 |
| 35.00 | 0.0680 | 0.7340 |
| 40.00 | 0.0800 | 0.7620 |
| 45.00 | 0.0940 | 0.7840 |
| 50.00 | 0.1050 | 0.8020 |
| 60.00 | 0.1290 | 0.8240 |
| 70.00 | 0.1540 | 0.8380 |
| 80.00 | 0.1800 | 0.8450 |
| 90.00 | 0.2040 | 0.8480 |
| 120.00 | 0.2920 | 0.8480 |
| 130.00 | 0.3150 | 0.8400 |

Leu, Ah-Dong - Chung, Samuel Y.-K. - Robinson, Donald B., The equilibrium phase properties of (carbon dioxide + methanol), The Journal of Chemical Thermodynamics 10 (1991) 979-985. doi:10.1016/S0021-9614(05)80178-8

**T / K = 477.60**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 52.90 | 0.0173 | 0.1283 |
| 54.40 | 0.0179 | 0.1452 |
| 63.30 | 0.0384 | 0.1854 |
| 83.60 | 0.0769 | 0.3001 |
| 109.40 | 0.1422 | 0.3378 |
| 121.00 | 0.1842 | 0.3112 |
| 125.10 | 0.2131 | 0.2928 |

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**Enthalpy of mixing**

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Hauser, Raul A. - Zhao, Jian Ping - Tremaine, Peter R. - Mather, Alan E., Excess molar enthalpies of six (carbon dioxide + a polar solvent) mixtures at the temperatures 298.15 K and 308.15 K and pressures from 7.5 MPa to 12.6 MPa, The Journal of Chemical Thermodynamics 11 (1996) 1303-1317. doi:10.1006/jcht.1996.0115

**T / K = 298.15**

**P / bar = 75.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -111.20 | 0.0420 |
| -202.80 | 0.0840 |
| -398.20 | 0.1700 |
| -555.60 | 0.2600 |
| -654.20 | 0.3530 |
| -640.60 | 0.5510 |
| -542.40 | 0.6560 |
| -397.90 | 0.7650 |
| -172.50 | 0.8790 |
| -39.00 | 0.9380 |

Hauser, Raul A. - Zhao, Jian Ping - Tremaine, Peter R. - Mather, Alan E., Excess molar enthalpies of six (carbon dioxide + a polar solvent) mixtures at the temperatures 298.15 K and 308.15 K and pressures from 7.5 MPa to 12.6 MPa, The Journal of Chemical Thermodynamics 11 (1996) 1303-1317. doi:10.1006/jcht.1996.0115

**T / K = 298.15**

**P / bar = 126.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -70.30 | 0.0430 |
| -145.50 | 0.0860 |
| -306.70 | 0.1750 |
| -456.60 | 0.2660 |
| -511.60 | 0.3600 |
| -465.50 | 0.4580 |
| -331.30 | 0.5580 |
| -206.50 | 0.6630 |
| -54.80 | 0.7700 |
| 113.00 | 0.8820 |
| 151.00 | 0.9400 |

Dai, W. - Kojima, K. - Ochi, K., Measurement and Correlation of Excess Molar Enthalpies of CO2 + CH3OH System in the Vicinity of Critical Point of Carbon Dioxide, J. Chem. Eng. Data 1 (1999) 161-164. doi:10.1021/je980191+

**T / K = 303.15**

**P / bar = 80.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -36.00 | 0.0190 |
| -165.00 | 0.0382 |
| -288.00 | 0.0774 |
| -424.00 | 0.1176 |
| -540.00 | 0.1588 |
| -622.00 | 0.2011 |
| -702.00 | 0.2445 |
| -768.00 | 0.2891 |
| -829.00 | 0.3349 |
| -857.00 | 0.3819 |
| -868.00 | 0.4303 |
| -866.00 | 0.4800 |
| -863.00 | 0.5311 |
| -831.00 | 0.5838 |
| -785.00 | 0.6380 |
| -701.00 | 0.6938 |
| -610.00 | 0.7513 |
| -449.00 | 0.8106 |
| -270.00 | 0.8717 |
| -142.00 | 0.9349 |

Dai, W. - Kojima, K. - Ochi, K., Measurement and Correlation of Excess Molar Enthalpies of CO2 + CH3OH System in the Vicinity of Critical Point of Carbon Dioxide, J. Chem. Eng. Data 1 (1999) 161-164. doi:10.1021/je980191+

**T / K = 303.15**

**P / bar = 70.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -262.00 | 0.0374 |
| -627.00 | 0.0758 |
| -895.00 | 0.1153 |
| -1151.0 | 0.1559 |
| -1430.0 | 0.1975 |
| -1705.0 | 0.2404 |
| -1963.0 | 0.2845 |
| -2245.0 | 0.3299 |
| -2540.0 | 0.3767 |
| -2773.0 | 0.4248 |
| -2990.0 | 0.4744 |
| -3157.0 | 0.5256 |
| -3315.0 | 0.5783 |
| -3489.0 | 0.6328 |
| -3524.0 | 0.6890 |
| -3500.0 | 0.7471 |
| -1313.0 | 0.8194 |
| 190.00 | 0.8692 |
| 94.00 | 0.9335 |

Dai, Wenbin - Ochi, Kenji - Kurihara, Kiyofumi - Kojima, Kazuo - Hongo, Masaru, Measurement and Correlation of Excess Enthalpy for the System(CO2+CH3OH) Containing Supercritical Carbon Dioxide., Netsu Bussei 2 (1998) 64-69. doi:10.2963/jjtp.12.64

**T / K = 308.15**

**P / bar = 75.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -578.19 | 0.0756 |
| -872.37 | 0.1150 |
| -1236.6 | 0.1554 |
| -1452.8 | 0.1970 |
| -1708.6 | 0.2398 |
| -1996.2 | 0.2838 |
| -2324.4 | 0.3292 |
| -2592.2 | 0.3759 |
| -2893.2 | 0.4240 |
| -3129.4 | 0.4736 |
| -3428.2 | 0.5247 |
| -3648.1 | 0.5775 |
| -3918.9 | 0.6320 |
| -4200.8 | 0.6883 |
| -4308.8 | 0.7465 |
| -4429.6 | 0.8066 |
| -4280.1 | 0.8688 |
| -3319.9 | 0.9333 |
| -2895.5 | 0.9464 |
| -2276.8 | 0.9597 |
| -1524.8 | 0.9730 |

Dai, Wenbin - Ochi, Kenji - Kurihara, Kiyofumi - Kojima, Kazuo - Hongo, Masaru, Measurement and Correlation of Excess Enthalpy for the System(CO2+CH3OH) Containing Supercritical Carbon Dioxide., Netsu Bussei 2 (1998) 64-69. doi:10.2963/jjtp.12.64

**T / K = 308.15**

**P / bar = 77.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -199.62 | 0.1554 |
| -277.63 | 0.1970 |
| -533.39 | 0.2398 |
| -803.45 | 0.2838 |
| -1083.1 | 0.3292 |
| -1384.0 | 0.3759 |
| -1656.1 | 0.4240 |
| -2038.1 | 0.4736 |
| -2266.5 | 0.5247 |
| -2489.2 | 0.5775 |

| | |
|---|---|
| -2656.8 | 0.6320 |
| -2887.3 | 0.6883 |
| -3010.3 | 0.7465 |
| -2855.0 | 0.8066 |
| -2367.7 | 0.8688 |
| -1488.6 | 0.9333 |
| -839.63 | 0.9663 |

Dai, Wenbin - Ochi, Kenji - Kurihara, Kiyofumi - Kojima, Kazuo - Hongo, Masaru, Measurement and Correlation of Excess Enthalpy for the System(CO2+CH3OH) Containing Supercritical Carbon Dioxide., Netsu Bussei 2 (1998) 64-69. doi:10.2963/jjtp.12.64

| **T / K =** | **308.15** |
|---|---|
| **P / bar =** | **79.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| -242.23 | 0.3292 |
| -349.88 | 0.3759 |
| -545.77 | 0.4240 |
| -867.68 | 0.4736 |
| -1307.7 | 0.5247 |
| -1644.8 | 0.5775 |
| -1778.8 | 0.6320 |
| -1867.2 | 0.6883 |
| -1679.4 | 0.7465 |
| -1366.2 | 0.8066 |
| -697.48 | 0.8688 |
| -388.15 | 0.9008 |
| -136.38 | 0.9333 |

Christensen, J.J - Cordray, D.R - Oscarson, J.L - Izatt, R.M, The excess enthalpies of four (carbon dioxide + an alkanol) mixtures from 308.15 to 573.15 K at 7.50 to 12.50 MPa, The Journal of Chemical Thermodynamics 7 (1988) 867-875. doi:10.1016/0021-9614(88)90076-6

| **T / K =** | **473.15** |
|---|---|
| **P / bar =** | **75.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 127.00 | 0.0139 |
| 376.00 | 0.0423 |
| 616.00 | 0.0568 |
| 1180.0 | 0.0714 |
| 1440.0 | 0.0863 |
| 2090.0 | 0.1013 |
| 3360.0 | 0.1319 |
| 5920.0 | 0.1794 |
| 6320.0 | 0.1956 |
| 7130.0 | 0.2121 |
| 8240.0 | 0.2288 |
| 9610.0 | 0.2629 |
| 10000.0 | 0.2802 |
| 11200.0 | 0.3158 |
| 11200.0 | 0.3339 |
| 11700.0 | 0.3523 |
| 11800.0 | 0.3709 |
| 11700.0 | 0.3899 |
| 11900.0 | 0.4091 |
| 11300.0 | 0.4285 |
| 10900.0 | 0.4483 |
| 10100.0 | 0.5304 |
| 9480.0 | 0.5733 |
| 8690.0 | 0.6176 |
| 7400.0 | 0.6633 |
| 6570.0 | 0.7105 |
| 5650.0 | 0.7592 |
| 4650.0 | 0.8096 |
| 3360.0 | 0.8617 |

Christensen, J.J - Cordray, D.R - Oscarson, J.L - Izatt, R.M, The excess enthalpies of four (carbon dioxide + an alkanol) mixtures from 308.15 to 573.15 K at 7.50 to 12.50 MPa, The Journal of Chemical Thermodynamics 7 (1988) 867-875. doi:10.1016/0021-9614(88)90076-6

| **T / K =** | **573.15** |
|---|---|
| **P / bar =** | **125.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 224.00 | 0.0155 |
| 716.00 | 0.0469 |
| 1110.0 | 0.0789 |
| 1280.0 | 0.1115 |
| 1290.0 | 0.1115 |
| 1480.0 | 0.1281 |
| 1560.0 | 0.1448 |
| 1860.0 | 0.1958 |
| 1910.0 | 0.2132 |
| 2080.0 | 0.2484 |
| 2160.0 | 0.2843 |
| 2240.0 | 0.3209 |
| 2300.0 | 0.3583 |
| 2290.0 | 0.3964 |
| 2260.0 | 0.4354 |
| 2220.0 | 0.4751 |
| 2200.0 | 0.5157 |
| 2010.0 | 0.5571 |
| 1930.0 | 0.5782 |
| 1800.0 | 0.5995 |
| 1780.0 | 0.6210 |

| | | |
|---|---|---|
| 1800.0 | 0.6427 | |
| 1640.0 | 0.6647 | |
| 1600.0 | 0.6870 | |
| 1440.0 | 0.7094 | |
| 1310.0 | 0.7322 | |
| 1170.0 | 0.7784 | |
| 910.00 | 0.8257 | |
| 673.00 | 0.8740 | |
| 380.00 | 0.9235 | |
| 146.00 | 0.9742 | |

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**Critical point**

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Gurdial, Gurdev S. - Foster, Neil R. - Yun, S. L. Jimmy - Tilly, Kevin D., Phase Behavior of Supercritical Fluid—Entrainer Systems, Supercritical Fluid Engineering Science (1992) 34-45.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 305.00 | 76.20 | 0.9924 |
| 306.20 | 76.60 | 0.9874 |
| 307.20 | 77.40 | 0.9811 |
| 309.10 | 79.70 | 0.9693 |
| 311.70 | 82.70 | 0.9562 |
| 314.90 | 86.50 | 0.9432 |
| 320.50 | 93.50 | 0.9307 |

Zhang, J.C. - Wu, X.Y. - Cao, W.L., Phase Equilibrium Properties of Supercritical Carbon Dioxide in Binary System, Gaodeng Xuexiao Huaxue Xuebao 1 (2002) 10-13.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 310.45 | 78.00 | 0.9951 |
| 311.35 | 79.10 | 0.9916 |
| 312.05 | 80.00 | 0.9869 |
| 312.75 | 81.10 | 0.9826 |
| 313.75 | 82.10 | 0.9764 |
| 314.85 | 83.40 | 0.9689 |

Gil, Laura - Blanco, Sofía T. - Rivas, Clara - Laga, Eduardo - Fernández, Javier - Artal, Manuela - Velasco, Inmaculada, Experimental determination of the critical loci for {n-C6H14 or CO2+alkan-1-ol} mixtures. Evaluation of their critical and subcritical behavior using PC-SAFT EoS, The Journal of Supercritical Fluids (2012) 26-44. doi:10.1016/j.supflu.2012.07.008

| T / K | P / bar | $x_1$ |
|---|---|---|
| 508.63 | 88.07 | 0.0501 |
| 501.64 | 95.82 | 0.0995 |
| 495.95 | 101.33 | 0.1351 |
| 491.70 | 108.30 | 0.1997 |
| 484.72 | 117.12 | 0.2501 |
| 480.24 | 122.49 | 0.3000 |
| 471.87 | 130.58 | 0.3505 |
| 465.25 | 136.14 | 0.4001 |
| 455.58 | 143.89 | 0.4494 |
| 438.84 | 154.80 | 0.4999 |
| 424.25 | 160.96 | 0.5503 |
| 408.98 | 163.88 | 0.6006 |
| 393.20 | 162.66 | 0.6505 |
| 377.29 | 156.23 | 0.7000 |
| 371.44 | 151.69 | 0.7101 |
| 363.32 | 144.87 | 0.7301 |
| 350.96 | 134.39 | 0.7502 |
| 346.18 | 129.64 | 0.7695 |
| 339.82 | 121.12 | 0.7853 |
| 336.81 | 116.14 | 0.7998 |
| 333.74 | 112.86 | 0.8144 |
| 328.42 | 103.45 | 0.8503 |
| 324.92 | 100.16 | 0.8701 |
| 320.75 | 94.19 | 0.8989 |
| 317.10 | 88.78 | 0.9198 |
| 311.86 | 80.09 | 0.9601 |
| 306.25 | 75.03 | 0.9901 |
| 305.06 | 74.02 | 0.9949 |

Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 323.15 | 96.00 | 0.8510 |
| 423.15 | 162.00 | 0.5184 |
| 473.15 | 130.00 | 0.2779 |

Yeo, Sang-Do - Park, Su-Jin - Kim, Jin-Woo - Kim, Jae-Chang, Critical Properties of Carbon Dioxide + Methanol, + Ethanol, + 1-Propanol, and + 1-Butanol, Journal of Chemical & Engineering Data 5 (2000) 932-935. doi:10.1021/je000104p

| T / K | P / bar | $x_1$ |
|---|---|---|
| 307.26 | 73.52 | 0.9760 |
| 308.12 | 76.63 | 0.9710 |
| 315.67 | 84.49 | 0.8940 |
| 328.21 | 103.92 | 0.8090 |
| 335.19 | 115.56 | 0.7750 |
| 340.65 | 124.04 | 0.7510 |
| 353.15 | 138.37 | 0.7210 |
| 355.65 | 141.68 | 0.6960 |
| 360.65 | 145.33 | 0.6540 |
| 388.65 | 163.66 | 0.5890 |
| 422.32 | 164.15 | 0.4920 |

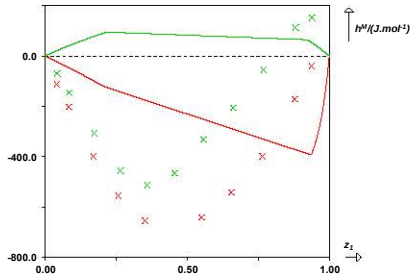
Brunner, E - Hültenschmidt, W - Schlichthärle, G, Fluid mixtures at high pressures IV. Isothermal phase equilibria in binary mixtures consisting of (methanol + hydrogen or nitrogen or methane or carbon monoxide or carbon dioxide), The Journal of Chemical Thermodynamics 3 (1987) 273-291. doi:10.1016/0021-9614(87)90135-2

| T / K | P / bar | $x_1$ |
|---|---|---|
| 323.15 | 95.50 | 0.8404 |
| 373.15 | 154.20 | 0.6735 |
| 423.15 | 161.30 | 0.5178 |
| 473.15 | 129.30 | 0.2700 |

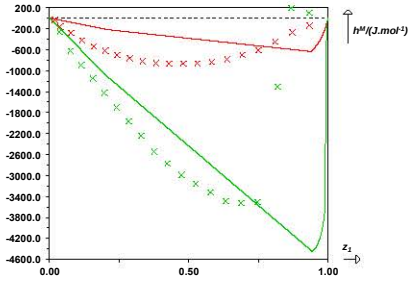
Liu, Jianguo - Qin, Zhangfeng - Wang, Guofu - Hou, Xianglin - Wang, Jianguo, Critical Properties of Binary and Ternary Mixtures of Hexane + Methanol, Hexane + Carbon Dioxide, Methanol + Carbon Dioxide, and Hexane + Carbon Dioxide + Methanol, Journal of Chemical & Engineering Data 6 (2003) 1610-1613. doi:10.1021/je034127q

| T / K | P / bar | $x_1$ |
|---|---|---|
| 507.20 | 88.00 | 0.0720 |
| 494.60 | 103.30 | 0.1690 |
| 485.40 | 115.40 | 0.2440 |
| 473.20 | 128.40 | 0.3270 |
| 460.50 | 140.00 | 0.3830 |
| 451.10 | 147.40 | 0.4460 |
| 442.80 | 152.70 | 0.4950 |
| 423.90 | 163.20 | 0.5720 |
| 414.30 | 163.40 | 0.6680 |
| 408.20 | 162.60 | 0.7130 |
| 384.80 | 157.60 | 0.7860 |
| 374.30 | 150.70 | 0.8100 |
| 354.70 | 137.50 | 0.8620 |
| 346.70 | 129.50 | 0.8930 |
| 333.30 | 110.40 | 0.9120 |
| 313.40 | 82.90 | 0.9650 |

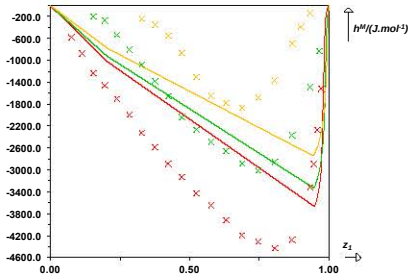
T/K = 298.15 - P/bar = 75.00 126.00



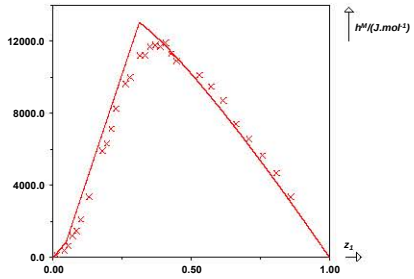

T/K = 303.15 - P/bar = 80.00 70.00



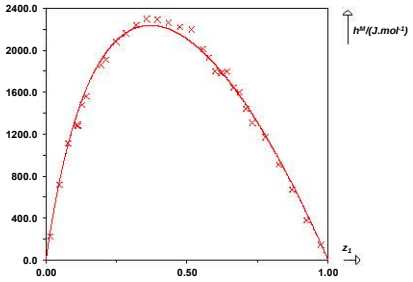

T/K = 308.15 - P/bar = 75.00 77.00 79.00



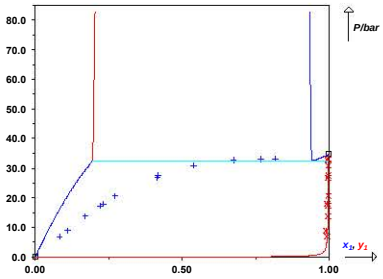

T/K = 473.15 - P/bar = 75.00



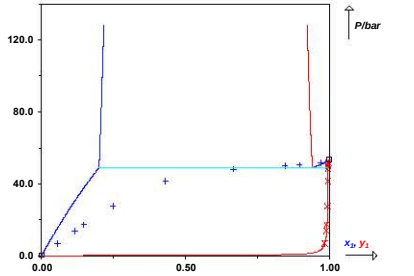

T/K = 573.15 - P/bar = 125.00



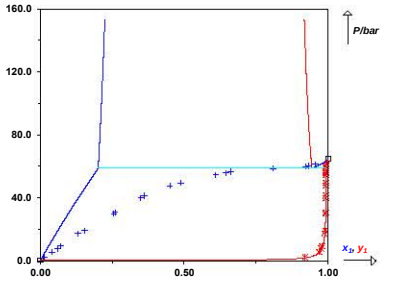

T/K = 273.15



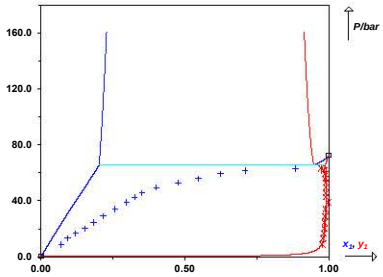

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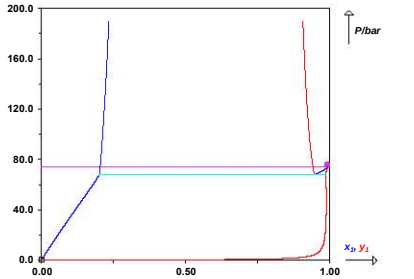

T/K = 298.15



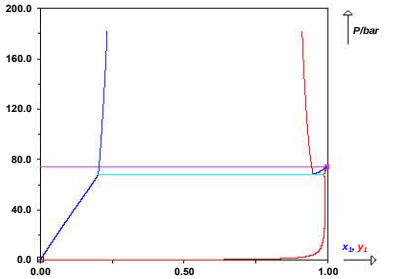

T/K = 303.18



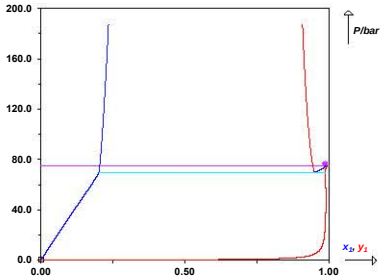

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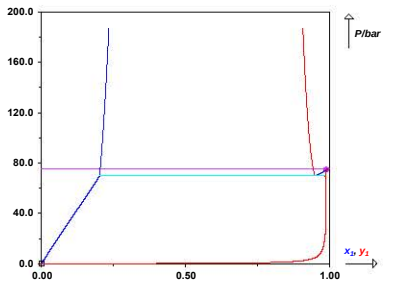

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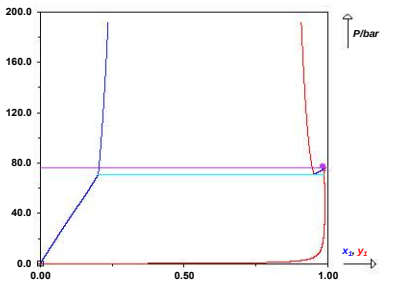

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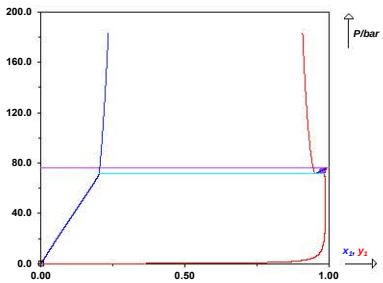

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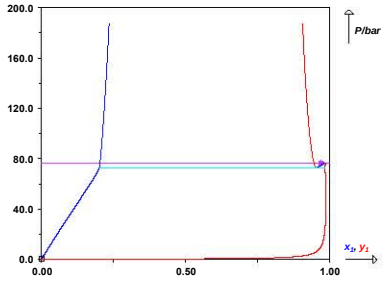

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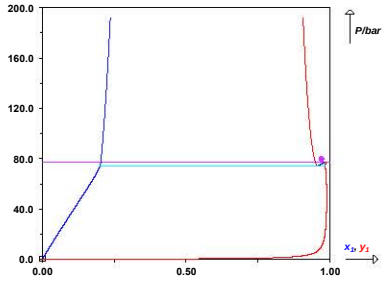

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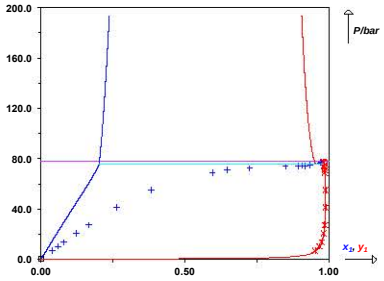
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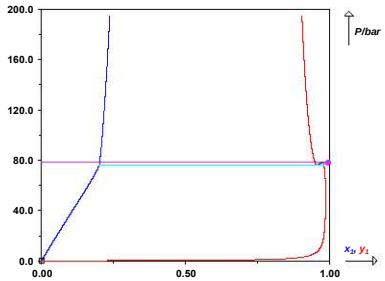

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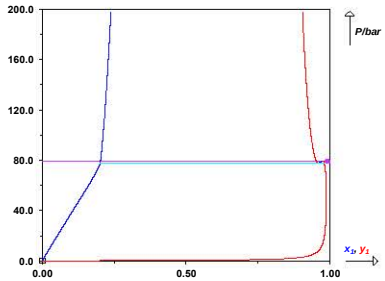

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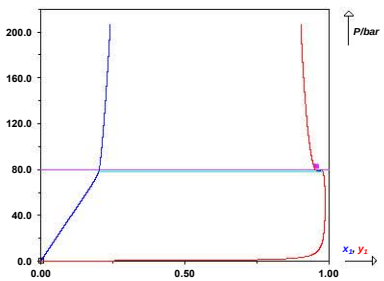

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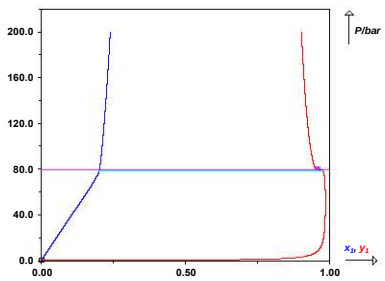

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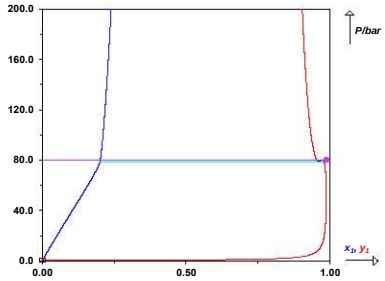

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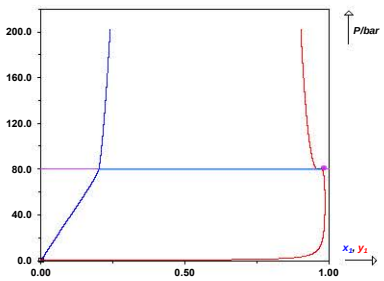

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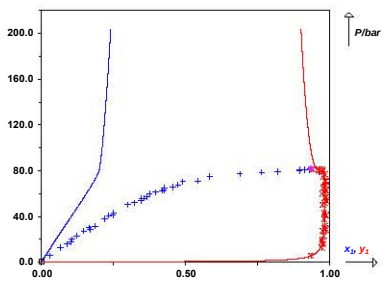

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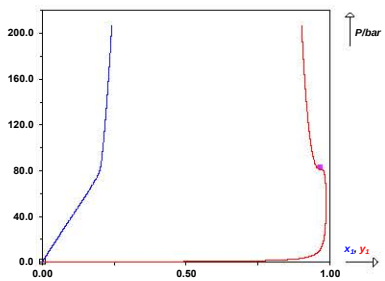

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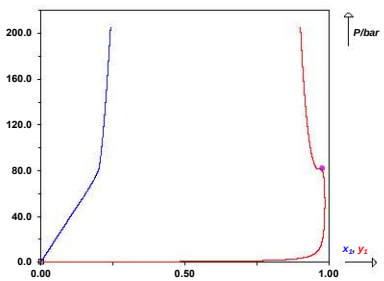

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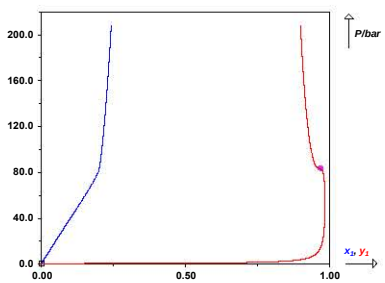

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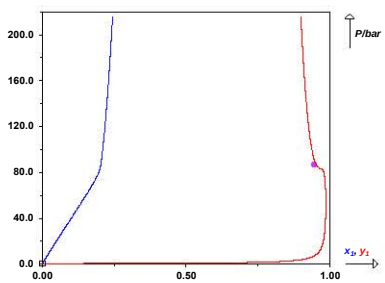

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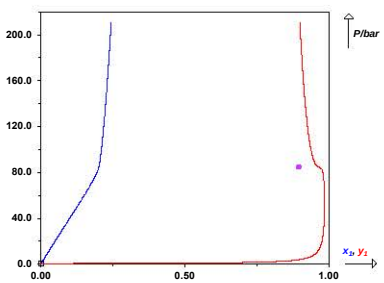

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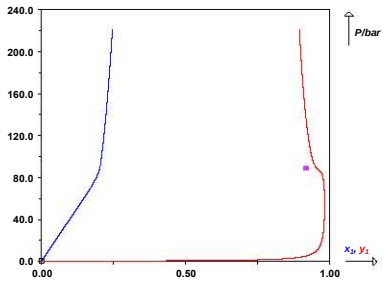

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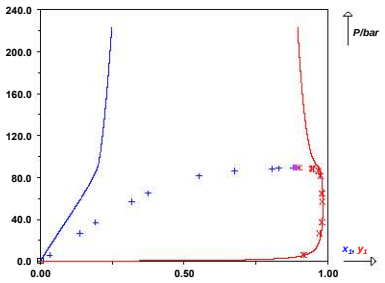

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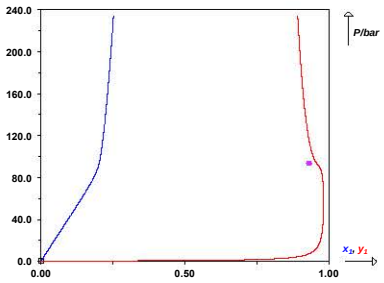
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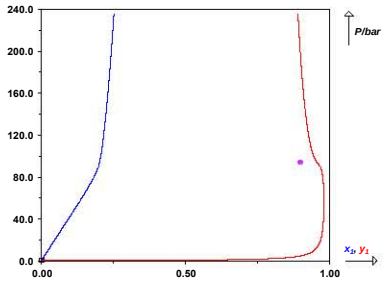

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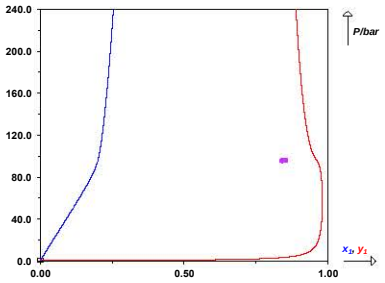

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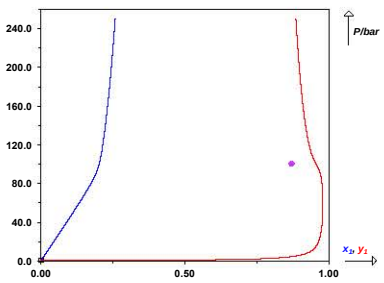

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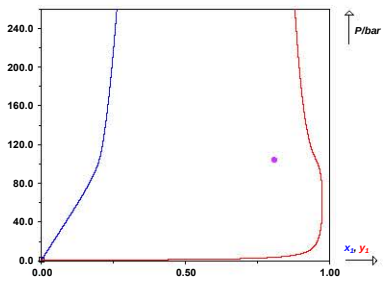

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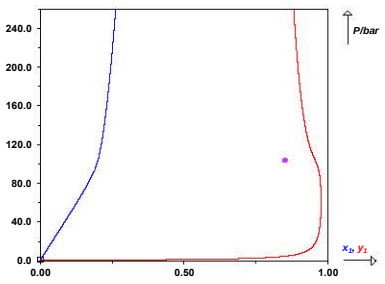

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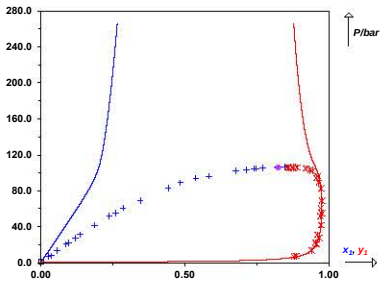

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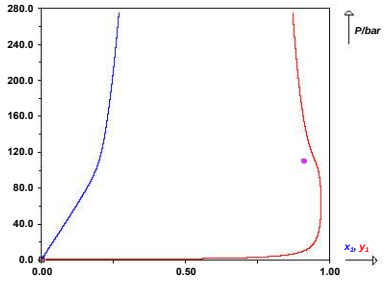

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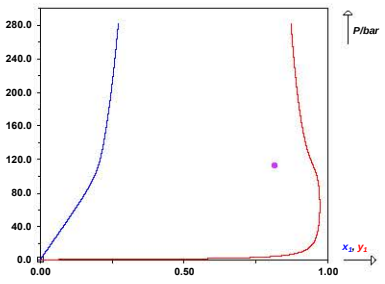

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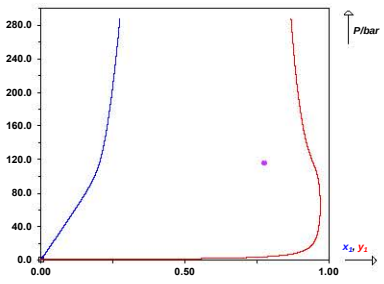

T/K = 333.30



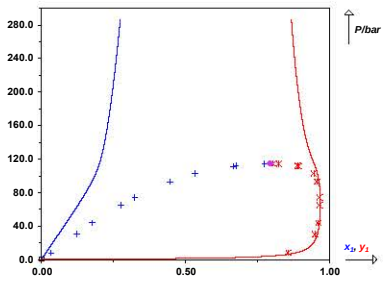

T/K = 333.74



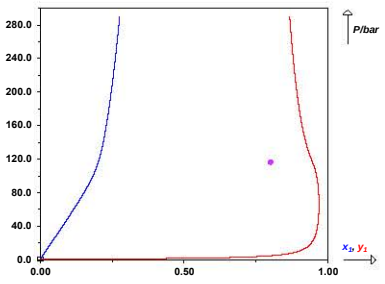

T/K = 335.19



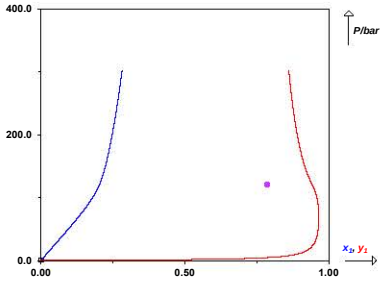

T/K = 335.65



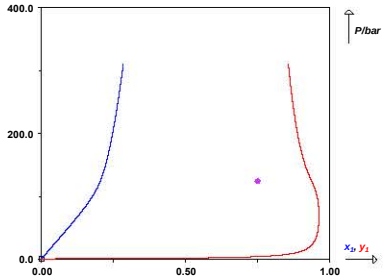

T/K = 336.81



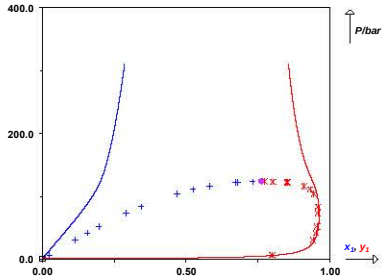

T/K = 339.82



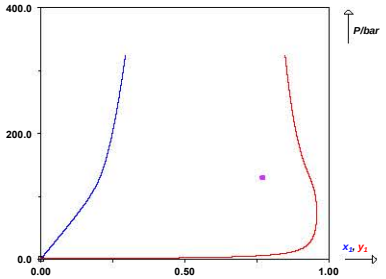
T/K = 340.65



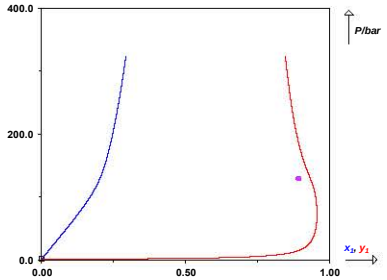

T/K = 342.80



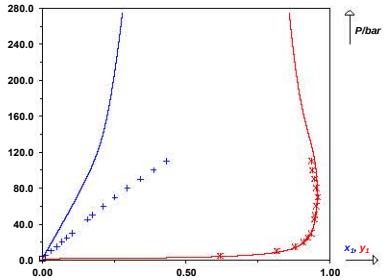

T/K = 346.18



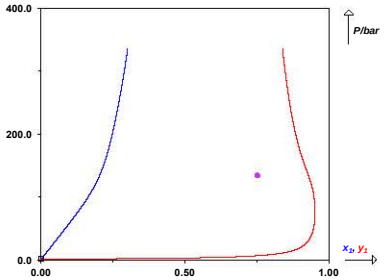

T/K = 346.70



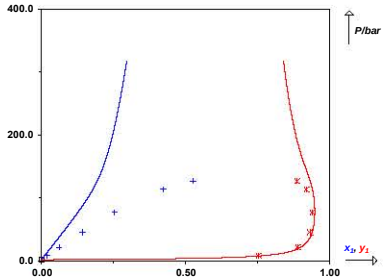

T/K = 348.15



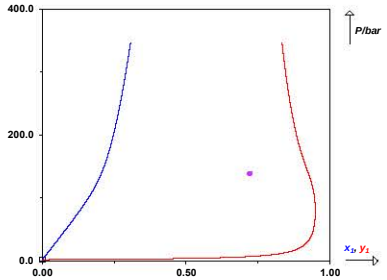

T/K = 350.96



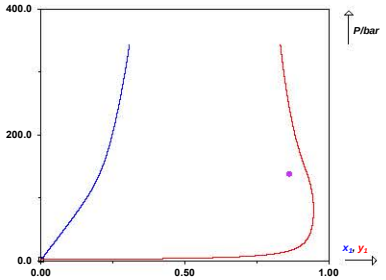

T/K = 352.60



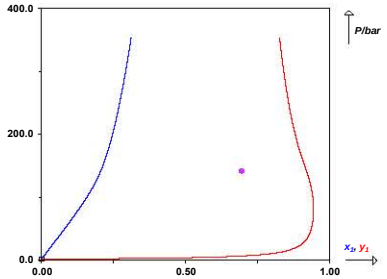

T/K = 353.15



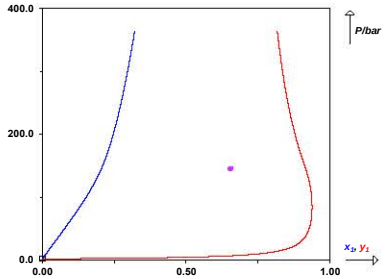

T/K = 354.70



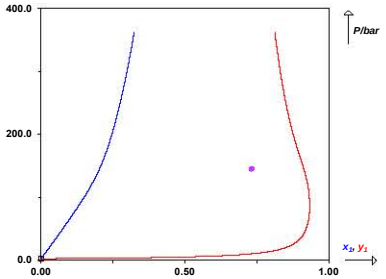

T/K = 355.65



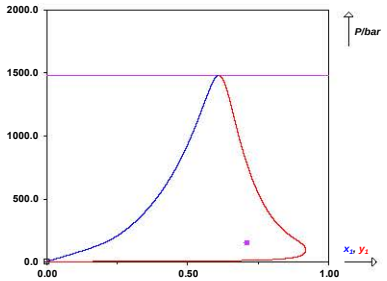

T/K = 360.65



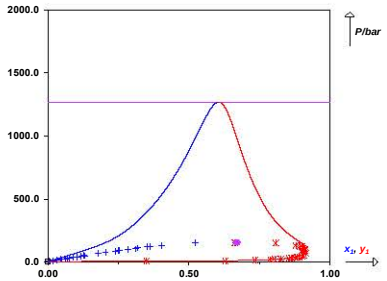

T/K = 363.32



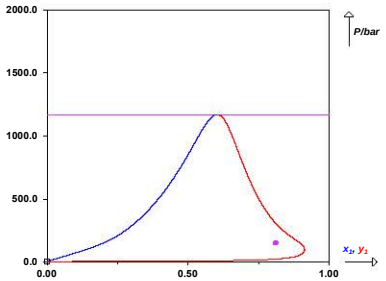

T/K = 371.44



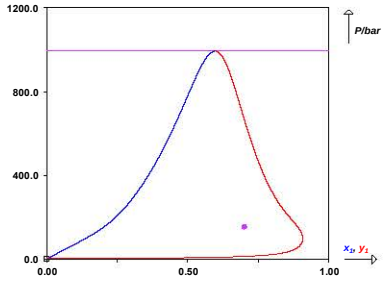

T/K = 373.15



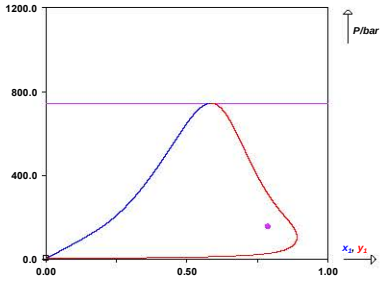

T/K = 374.30



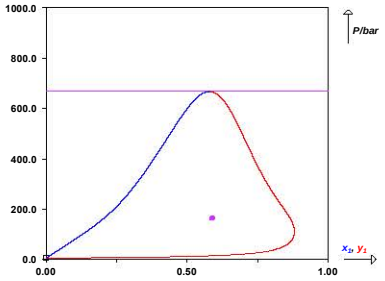
T/K = 377.29



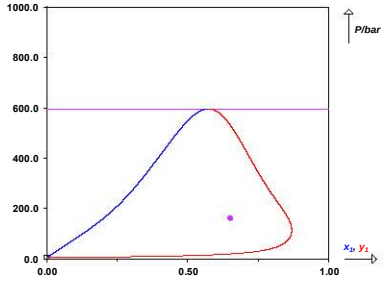

T/K = 384.80



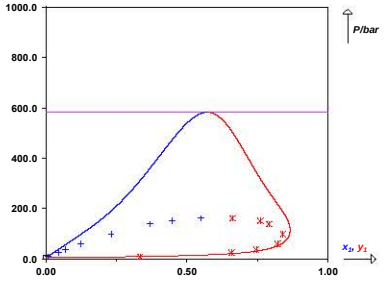

T/K = 388.65



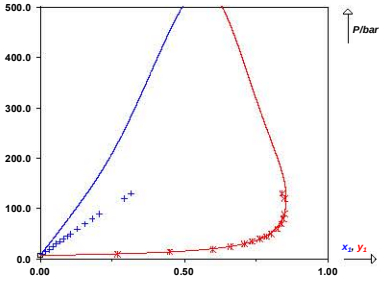

T/K = 393.20



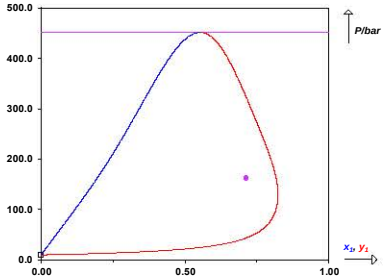

T/K = 394.20



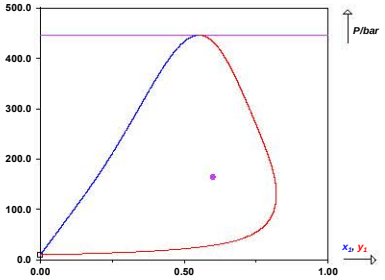

T/K = 398.15



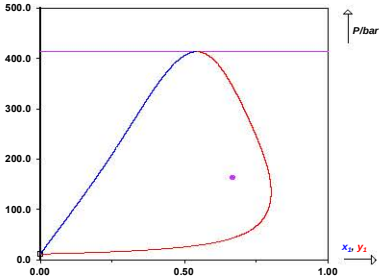

T/K = 408.20



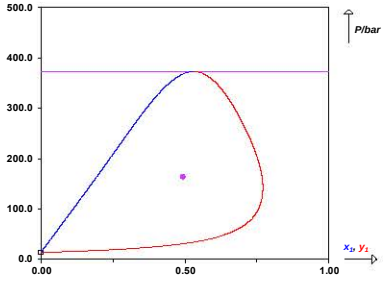

T/K = 408.98



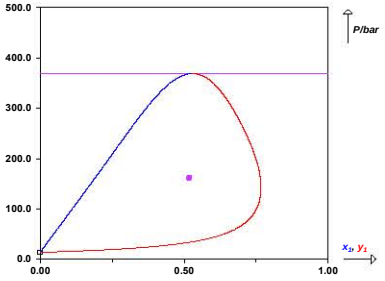

T/K = 414.30



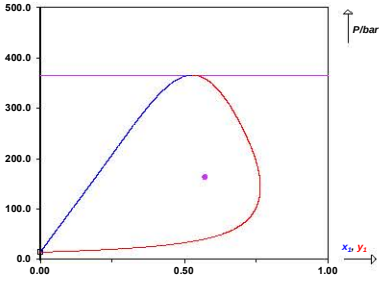

T/K = 422.32



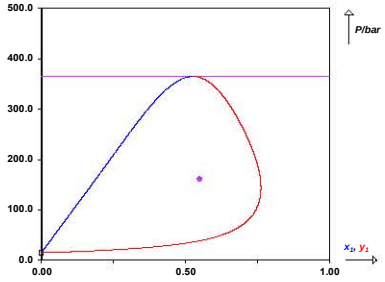

T/K = 423.15



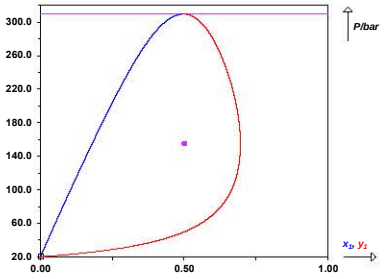

T/K = 423.90



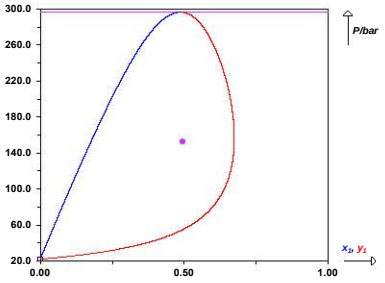

T/K = 424.25



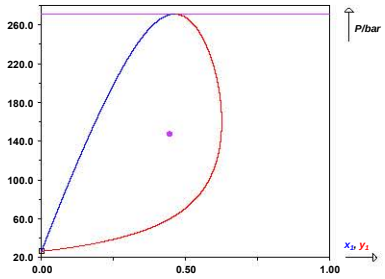

T/K = 438.84



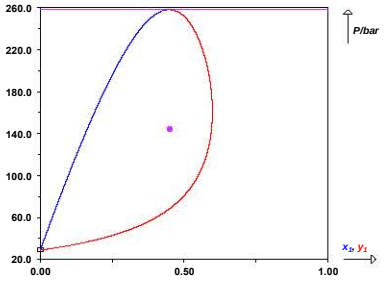

T/K = 442.80



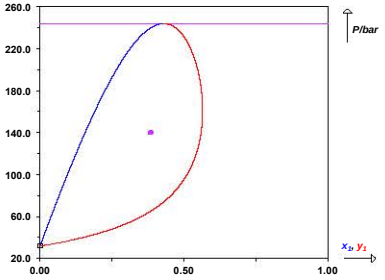
T/K = 451.10



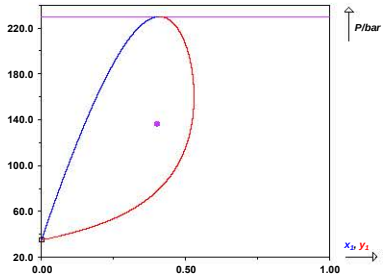

T/K = 455.58



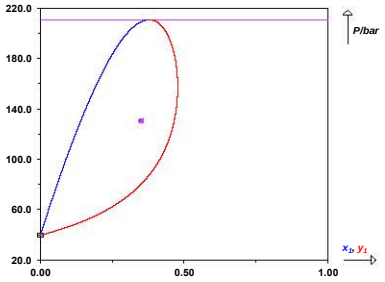

T/K = 460.50



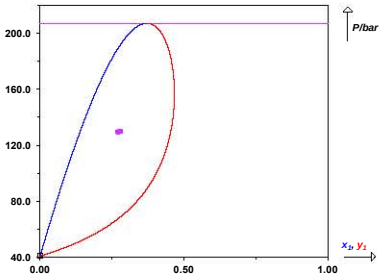

T/K = 465.25



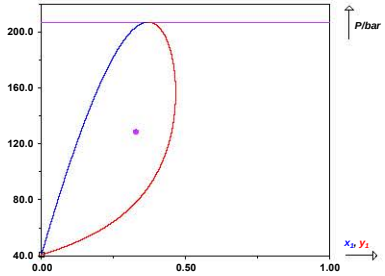

T/K = 471.87



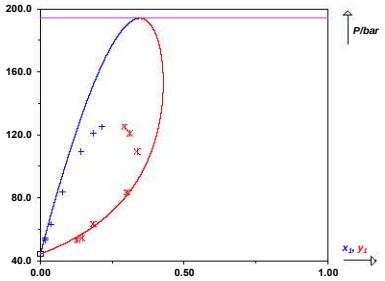

T/K = 473.15



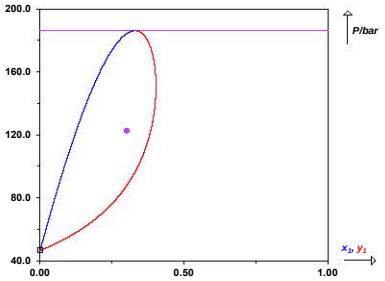

T/K = 473.20



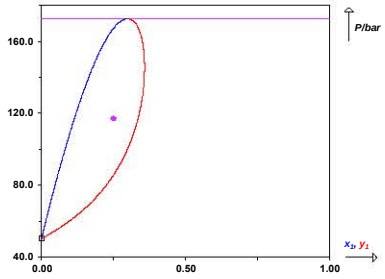

T/K = 477.60



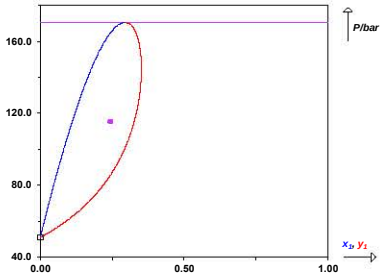

T/K = 480.24



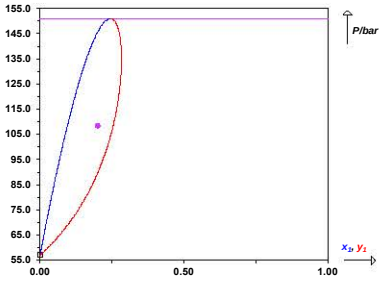

T/K = 484.72

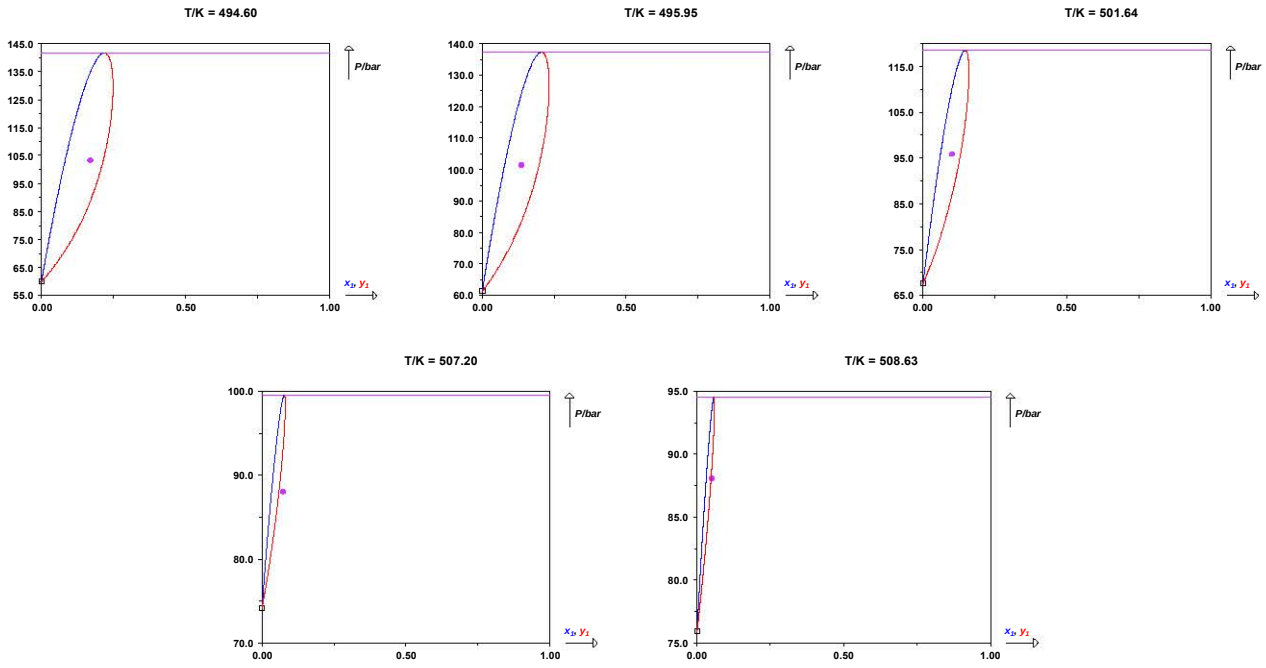



T/K = 485.40




T/K = 491.70




T/K = 494.60
P/bar
x1, y1
T/K = 495.95
P/bar
x1, y1
T/K = 501.64
P/bar
x1, y1
T/K = 507.20
P/bar
x1, y1
T/K = 508.63
P/bar
x1, y1

## METHANOL (1) + ETHYL ACETATE (2)

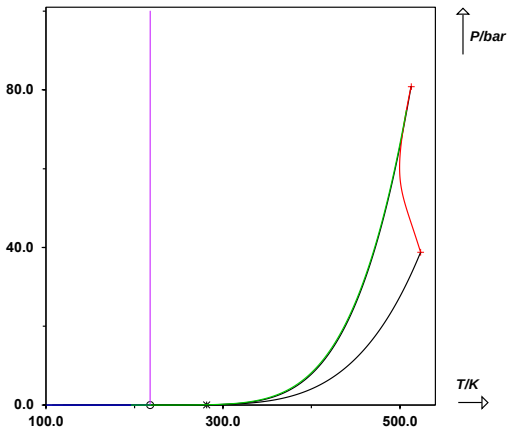
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 141-78-6 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | XEKOWRVHYACXOJ-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.50 | 523.30 |
| **$P_c$ / bar** | 80.84 | 38.80 |
| **ω** | 0.566 | 0.366 |

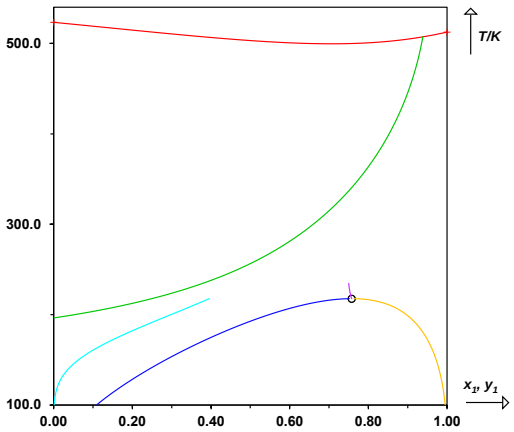
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 337
B/MPa = 257

*Deviations*
MAPE on x = 19 %
MAPE on y = 12 %
MAPE on $x_{az}$ = 5.8 %
MAPE on $P_{az}$ = 0.62 %
MAPE on $h^M$ = 30 %



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**Isothermal phase equilibrium data**

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Batiu, I. - Jimenez Esteller, L., Vapor-liquid equilibria in the binary system (+)-carvone + (+)-limonene at temperatures between 365 and 411 K, ELDATA: The International Electronic Journal of Physico-Chemical Data 2 (1996) 59-66.

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1351 | 0.0258 | 0.0937 |
| 0.1532 | 0.0825 | 0.2450 |
| 0.1584 | 0.1091 | 0.2832 |
| 0.1703 | 0.1652 | 0.3613 |
| 0.1740 | 0.1956 | 0.3852 |
| 0.1835 | 0.2719 | 0.4519 |
| 0.1904 | 0.3454 | 0.4907 |
| 0.1952 | 0.4495 | 0.5492 |
| 0.1987 | 0.5487 | 0.5913 |
| 0.1977 | 0.7425 | 0.6892 |
| 0.1944 | 0.8196 | 0.7490 |
| 0.1927 | 0.8448 | 0.7698 |
| 0.1883 | 0.8922 | 0.8137 |
| 0.1803 | 0.9509 | 0.8958 |
| 0.1772 | 0.9624 | 0.9206 |
| 0.1737 | 0.9811 | 0.9591 |

Kumełan, Jacek - Pérez-Salado Kamps, Álvaro - Tuma, Dirk - Maurer, Gerd, Solubility of the single gases H2 and CO in the ionic liquid [bmim][CH3SO4], Fluid Phase Equilibria 1 (2007) 3-8. doi:10.1016/j.fluid.2006.06.010

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4406 | 0.0525 | 0.1700 |
| 0.4980 | 0.1260 | 0.3375 |
| 0.5406 | 0.2315 | 0.4360 |
| 0.5800 | 0.3435 | 0.5125 |
| 0.6073 | 0.4500 | 0.5685 |
| 0.6126 | 0.5425 | 0.6170 |
| 0.6140 | 0.5680 | 0.6325 |
| 0.6153 | 0.6350 | 0.6640 |
| 0.6173 | 0.7060 | 0.6975 |
| 0.6153 | 0.7580 | 0.7290 |
| 0.6100 | 0.8215 | 0.7655 |
| 0.6033 | 0.8755 | 0.8100 |
| 0.5926 | 0.9250 | 0.8550 |

Nagata, Isamu - Yamada, Toshiro - Nakagawa, Shigeo, Excess Gibbs free energies and heats of mixing for binary systems ethyl acetate with methanol, ethanol, 1-propanol, and 2-propanol, Journal of Chemical & Engineering Data 3 (1975) 271-275. doi:10.1021/je60066a007

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5080 | 0.0310 | 0.1160 |
| 0.6368 | 0.1660 | 0.3640 |
| 0.6581 | 0.2060 | 0.4060 |
| 0.7125 | 0.3390 | 0.5130 |
| 0.7394 | 0.4550 | 0.5730 |
| 0.7518 | 0.5410 | 0.6150 |
| 0.7574 | 0.6040 | 0.6490 |
| 0.7614 | 0.6600 | 0.6750 |
| 0.7622 | 0.7390 | 0.7250 |
| 0.7497 | 0.8620 | 0.8150 |
| 0.7379 | 0.9000 | 0.8560 |

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**Isobaric phase equilibrium data**

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Susial, Pedro - Sosa-Rosario, Aday - Rios-Santana, Raul, Vapor−Liquid Equilibria for Ethyl Acetate + Methanol at (0.1, 0.5, and 0.7) MPa. Measurements with a New Ebulliometer, Journal of Chemical & Engineering Data 12 (2010) 5701-5706. doi:10.1021/je100614r

**P / bar = 1.0000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 337.65 | 0.9870 | 0.9740 |
| 337.35 | 0.9740 | 0.9510 |
| 336.85 | 0.9330 | 0.8990 |
| 336.65 | 0.9190 | 0.8830 |
| 336.35 | 0.8890 | 0.8510 |
| 335.95 | 0.8340 | 0.7990 |
| 335.85 | 0.8110 | 0.7800 |
| 335.75 | 0.6730 | 0.6960 |
| 335.95 | 0.6030 | 0.6640 |
| 336.15 | 0.5540 | 0.6390 |
| 336.25 | 0.5220 | 0.6210 |
| 336.45 | 0.4870 | 0.6030 |
| 336.75 | 0.4500 | 0.5840 |
| 337.05 | 0.4090 | 0.5640 |
| 337.95 | 0.3330 | 0.5220 |
| 338.45 | 0.2990 | 0.4990 |
| 339.65 | 0.2270 | 0.4360 |
| 342.75 | 0.1280 | 0.3160 |
| 343.95 | 0.0880 | 0.2450 |
| 344.85 | 0.0680 | 0.2070 |
| 345.95 | 0.0480 | 0.1680 |
| 347.05 | 0.0280 | 0.1080 |

Blanco, Ana M. - Ortega, Juan, Densities and Vapor−Liquid Equilibrium Values for Binary Mixtures Composed of Methanol + an Ethyl Ester at 141.3 kPa with Application of an Extended Correlation Equation for Isobaric VLE Data, Journal of Chemical & Engineering Data 4 (1998) 638-645. doi:10.1021/je980012o

**P / bar = 1.413**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 358.69 | 0.0200 | 0.0780 |
| 357.55 | 0.0430 | 0.1340 |
| 356.19 | 0.0630 | 0.1900 |
| 355.14 | 0.0820 | 0.2340 |
| 354.16 | 0.1010 | 0.2700 |
| 352.66 | 0.1290 | 0.3250 |
| 350.14 | 0.1840 | 0.4090 |
| 348.66 | 0.2330 | 0.4650 |
| 347.51 | 0.2850 | 0.5060 |
| 346.74 | 0.3310 | 0.5360 |
| 346.05 | 0.3710 | 0.5650 |
| 345.68 | 0.4110 | 0.5790 |
| 345.02 | 0.4640 | 0.6120 |
| 344.65 | 0.5160 | 0.6360 |
| 344.32 | 0.5660 | 0.6600 |
| 344.07 | 0.6280 | 0.6860 |
| 343.90 | 0.6910 | 0.7160 |
| 343.85 | 0.7320 | 0.7330 |
| 344.01 | 0.8220 | 0.7910 |
| 344.18 | 0.8590 | 0.8210 |
| 344.67 | 0.9200 | 0.8810 |
| 344.95 | 0.9420 | 0.9070 |
| 345.21 | 0.9610 | 0.9300 |
| 345.58 | 0.9750 | 0.9490 |
| 345.88 | 0.9910 | 0.9810 |

Susial, Pedro - Sosa-Rosario, Aday - Rios-Santana, Raul, Vapor−Liquid Equilibria for Ethyl Acetate + Methanol at (0.1, 0.5, and 0.7) MPa. Measurements with a New Ebulliometer, Journal of Chemical & Engineering Data 12 (2010) 5701-5706. doi:10.1021/je100614r

**P / bar = 5.000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 384.85 | 0.9780 | 0.9660 |
| 384.75 | 0.9710 | 0.9560 |
| 384.65 | 0.9610 | 0.9450 |
| 384.55 | 0.9550 | 0.9370 |
| 384.45 | 0.9420 | 0.9230 |
| 384.35 | 0.9280 | 0.9080 |
| 384.25 | 0.9080 | 0.8880 |
| 384.15 | 0.8870 | 0.8700 |
| 384.15 | 0.7600 | 0.7920 |
| 384.35 | 0.7110 | 0.7660 |
| 384.65 | 0.6560 | 0.7390 |
| 384.85 | 0.6300 | 0.7250 |
| 385.05 | 0.6120 | 0.7110 |
| 385.85 | 0.5330 | 0.6720 |
| 386.35 | 0.4990 | 0.6560 |
| 387.75 | 0.4090 | 0.6120 |
| 388.35 | 0.3800 | 0.5940 |
| 392.35 | 0.2270 | 0.4620 |
| 396.65 | 0.1280 | 0.3330 |
| 400.65 | 0.0680 | 0.2270 |
| 407.45 | 0.0090 | 0.0480 |

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**Enthalpy of mixing**

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Ortega, J., Excess enthalpy. Ethanol-ethyl ethanoate system, Int. Data Ser. Sel. Data Mixtures Ser. A 3 (1995)

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 563.90 | 0.1260 |
| 858.90 | 0.2414 |
| 1041.3 | 0.3429 |
| 1102.8 | 0.4294 |
| 1094.4 | 0.5023 |
| 1044.6 | 0.5543 |
| 991.70 | 0.5940 |
| 935.30 | 0.6238 |
| 883.50 | 0.6578 |
| 810.70 | 0.6944 |
| 731.90 | 0.7305 |
| 641.90 | 0.7682 |
| 561.10 | 0.8057 |
| 476.00 | 0.8411 |
| 378.80 | 0.8786 |
| 277.90 | 0.9141 |
| 174.70 | 0.9484 |
| 83.00 | 0.9772 |

Zhang, Rui - Yan, Weidong - Wang, Xu - Lin, Ruisen, Molar excess enthalpies of ethyl acetate+alkanols at T=298.15K, p=10.0MPa, Thermochimica Acta 2 (2005) 155-161. doi:10.1016/j.tca.2005.03.009

**T / K = 298.15**

**P / bar = 100.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 182.60 | 0.9430 |

| | |
|---|---|
| 272.50 | 0.9140 |
| 333.80 | 0.8870 |
| 523.20 | 0.8120 |
| 680.30 | 0.7430 |
| 809.40 | 0.6810 |
| 897.10 | 0.6230 |
| 968.30 | 0.5700 |
| 995.80 | 0.5220 |
| 1013.3 | 0.4760 |
| 1009.1 | 0.4340 |
| 987.00 | 0.3950 |
| 977.40 | 0.3590 |
| 945.30 | 0.3250 |
| 910.20 | 0.2930 |
| 869.60 | 0.2620 |
| 821.80 | 0.2340 |
| 767.60 | 0.2070 |
| 711.30 | 0.1820 |
| 651.30 | 0.1580 |
| 585.40 | 0.1360 |
| 518.10 | 0.1140 |
| 446.50 | 0.0940 |
| 367.70 | 0.0740 |
| 284.60 | 0.0560 |
| 200.10 | 0.0380 |
| 105.90 | 0.0210 |

Rajendran, M. - Renganarayanan, S. - Madhavan, P.R. - Srinivasan, D., Effect Of Dissolved Inorganic Salts On The Vapor-Liquid Equilibria And Enthalpy Of Mixing Of The Methanol-Ethyl Acetate System, Chemical Engineering Communications 1 (1988) 179-193. doi:10.1080/00986448808940458

| **T / K =** | **303.15** |
|---|---|
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| 389.37 | 0.0650 |
| 780.54 | 0.1700 |
| 898.57 | 0.2300 |
| 1047.9 | 0.3210 |
| 1111.8 | 0.4080 |
| 1097.8 | 0.4940 |
| 1029.4 | 0.5720 |
| 937.59 | 0.6530 |
| 608.80 | 0.7800 |
| 468.08 | 0.8370 |
| 302.20 | 0.9000 |
| 69.84 | 0.9810 |

Nagata, Isamu - Yamada, Toshiro - Nakagawa, Shigeo, Excess Gibbs free energies and heats of mixing for binary systems ethyl acetate with methanol, ethanol, 1-propanol, and 2-propanol, Journal of Chemical & Engineering Data 3 (1975) 271-275. doi:10.1021/je60066a007

| **T / K =** | **308.15** |
|---|---|
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| 308.15 | 0.0569 |
| 487.34 | 0.1065 |
| 785.44 | 0.2057 |
| 974.27 | 0.3030 |
| 983.06 | 0.3056 |
| 1013.2 | 0.3986 |
| 1031.2 | 0.4850 |
| 998.55 | 0.5610 |
| 916.07 | 0.6414 |
| 767.44 | 0.7314 |
| 549.73 | 0.8370 |
| 188.41 | 0.9569 |
| 180.45 | 0.9576 |

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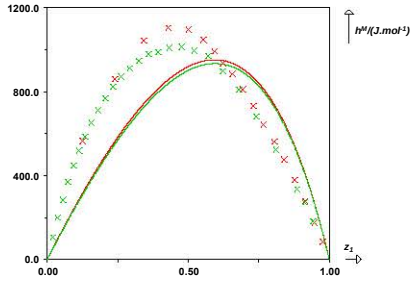
**Azeotropic point**

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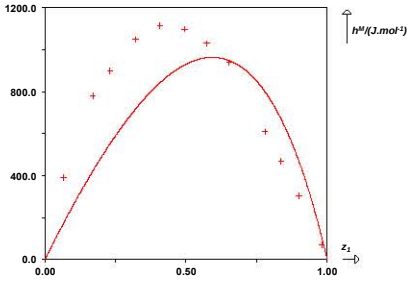
Blanco, Ana M. - Ortega, Juan, Densities and Vapor−Liquid Equilibrium Values for Binary Mixtures Composed of Methanol + an Ethyl Ester at 141.3 kPa with Application of an Extended Correlation Equation for Isobaric VLE Data, Journal of Chemical & Engineering Data 4 (1998) 638-645. doi:10.1021/je980012o

| T / K | P / bar | $x_1$ |
|---|---|---|
| 343.80 | 1.413 | 0.7420 |

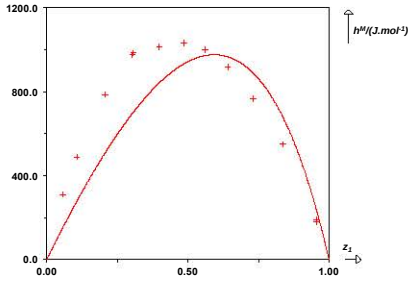
T/K = 298.15 - P/bar = 1.0100 100.00



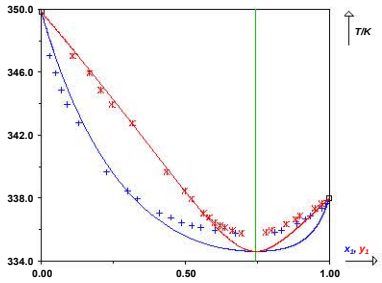

T/K = 303.15 - P/bar = 1.0132



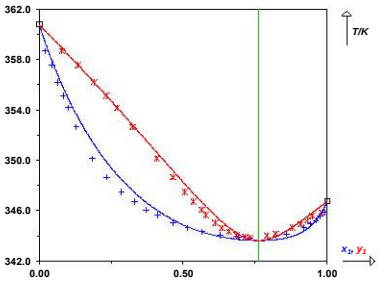

T/K = 308.15 - P/bar = 1.0132



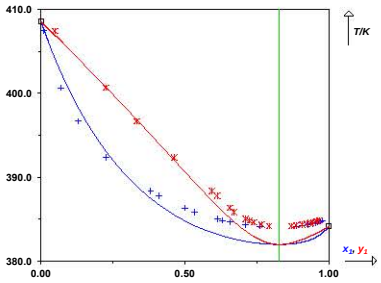

P/bar = 1.00000



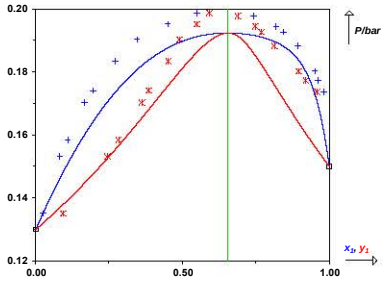

P/bar = 1.41300



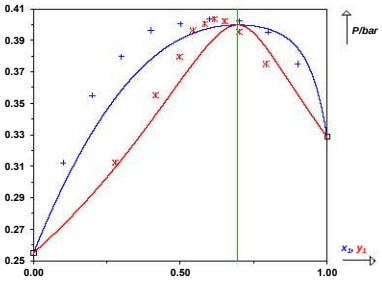

P/bar = 5.00000



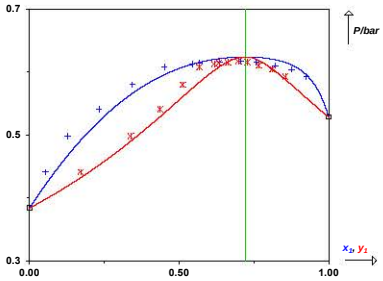

T/K = 298.15



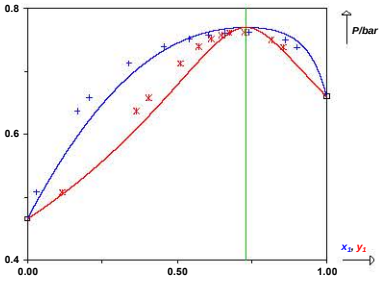

T/K = 313.15



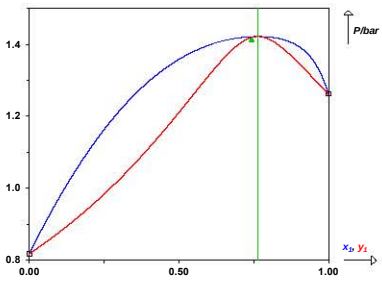

T/K = 323.15




T/K = 328.15




T/K = 343.80



## ISOPROPANOL (1) + DIISOPROPYL ETHER (2)

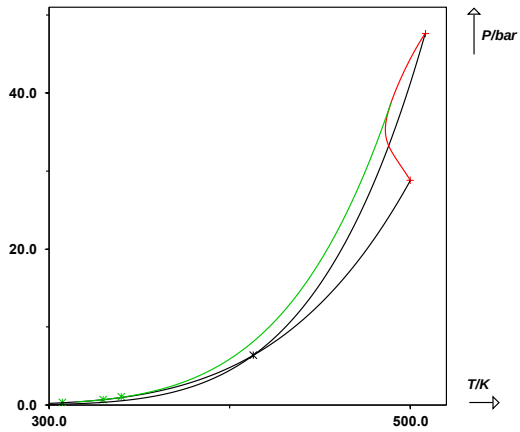
| | | |
|---|---|---|
| **CAS** | 67-63-0 | 108-20-3 |
| **InChiKey** | KFZMGEQAYNKOFK-UHFFFAOYSA-N | ZAFNJMIOTHYJRJ-UHFFFAOYSA-N |
| **$T_c$ / K** | 508.30 | 500.05 |
| **$P_c$ / bar** | 47.65 | 28.80 |
| **ω** | 0.663 | 0.339 |

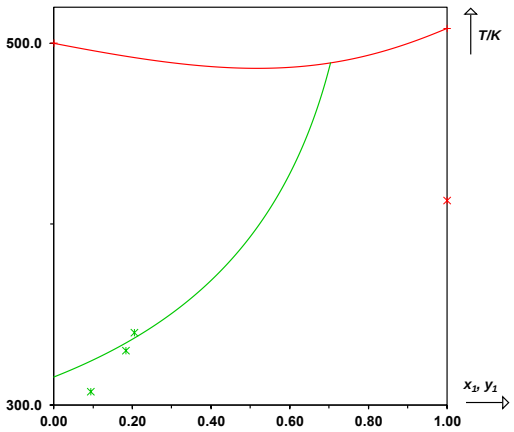
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 186
B/MPa = 47.8

*Deviations*
MAPE on x = 19 %
MAPE on y = 11 %
MAPE on $x_{az}$ = 9.6 %
MAPE on $P_{az}$ = 3.9 %
MAPE on $h^M$ = 34 %



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**Isothermal phase equilibrium data**

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Wichterle, I., Isothermal vapor-liquid equilibria in the ternary system propan-2-ol + diisopropyl ether + 2,2, 4-trimethylpentane and the three binary subsystems at 330 K and 340 K, ELDATA Int. Electron. J. Phys. Chem. Data 4 (1999) 179-189.

**T / K = 330.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.3354 | 0.9992 | 0.9912 | |
| 0.3436 | 0.9949 | 0.9634 | |
| 0.3545 | 0.9872 | 0.9261 | |
| 0.3685 | 0.9780 | 0.8818 | |
| 0.3887 | 0.9676 | 0.8289 | |
| 0.4144 | 0.9449 | 0.7623 | |
| 0.4456 | 0.9187 | 0.6936 | |
| 0.4773 | 0.8893 | 0.6319 | |
| 0.5123 | 0.8535 | 0.5710 | |
| 0.5443 | 0.8149 | 0.5201 | |
| 0.5771 | 0.7661 | 0.4718 | |
| 0.6334 | 0.6592 | 0.3950 | |
| 0.6567 | 0.5970 | 0.3610 | |
| 0.6757 | 0.5359 | 0.3318 | |
| 0.6882 | 0.4827 | 0.3111 | |
| 0.6925 | 0.4653 | 0.3029 | |
| 0.7009 | 0.4225 | 0.2911 | |
| 0.7057 | 0.3957 | 0.2767 | |
| 0.7153 | 0.3346 | 0.2524 | |
| 0.7180 | 0.3123 | 0.2423 | |
| 0.7235 | 0.2479 | 0.2184 | |
| 0.7271 | 0.1840 | 0.1840 | AZEO |
| 0.7234 | 0.1094 | 0.1334 | |
| 0.7137 | 0.0556 | 0.0820 | |

Wichterle, I., Isothermal vapor-liquid equilibria in the ternary system propan-2-ol + diisopropyl ether + 2,2, 4-trimethylpentane and the three binary subsystems at 330 K and 340 K, ELDATA Int. Electron. J. Phys. Chem. Data 4 (1999) 179-189.

**T / K = 340.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.5340 | 0.9988 | 0.9913 | |
| 0.5470 | 0.9933 | 0.9618 | |
| 0.5634 | 0.9875 | 0.9250 | |
| 0.5864 | 0.9719 | 0.8836 | |
| 0.6147 | 0.9606 | 0.8294 | |
| 0.6516 | 0.9349 | 0.7639 | |
| 0.6930 | 0.9070 | 0.7015 | |
| 0.7359 | 0.8752 | 0.6439 | |
| 0.7803 | 0.8389 | 0.5886 | |
| 0.8208 | 0.8000 | 0.5400 | |
| 0.8617 | 0.7523 | 0.4944 | |
| 0.8975 | 0.6992 | 0.4582 | |
| 0.9297 | 0.6415 | 0.4202 | |
| 0.9584 | 0.5782 | 0.3859 | |
| 0.9804 | 0.5209 | 0.3397 | |
| 0.9957 | 0.4674 | 0.3387 | |
| 1.000 | 0.4516 | 0.3272 | |
| 1.015 | 0.3855 | 0.2989 | |
| 1.025 | 0.3255 | 0.2727 | |
| 1.027 | 0.3039 | 0.2652 | |
| 1.033 | 0.2414 | 0.2390 | |
| 1.034 | 0.2050 | 0.2050 | AZEO |
| 1.021 | 0.1073 | 0.1439 | |
| 1.003 | 0.0551 | 0.0881 | |

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**Isobaric phase equilibrium data**

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Lladosa, Estela - Montón, Juan B. - Burguet, MªCruz - Muñoz, Rosa, Effect of pressure and the capability of 2-methoxyethanol as a solvent in the behaviour of a diisopropyl ether–isopropyl alcohol azeotropic mixture, Fluid Phase Equilibria 1-2 (2007) 271-279. doi:10.1016/j.fluid.2007.09.014

**P / bar = 0.3000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 324.48 | 0.9750 | 0.8790 |
| 320.62 | 0.9240 | 0.6830 |
| 317.83 | 0.8730 | 0.5700 |
| 315.41 | 0.8140 | 0.4650 |
| 313.47 | 0.7530 | 0.3940 |
| 312.10 | 0.6910 | 0.3470 |
| 310.82 | 0.6180 | 0.3070 |
| 309.98 | 0.5530 | 0.2710 |
| 309.31 | 0.4920 | 0.2460 |
| 308.75 | 0.4340 | 0.2250 |
| 308.32 | 0.3740 | 0.2060 |
| 307.89 | 0.3160 | 0.1870 |
| 307.60 | 0.2540 | 0.1700 |
| 307.37 | 0.2040 | 0.1490 |
| 307.20 | 0.1530 | 0.1270 |
| 307.18 | 0.1020 | 0.0990 |
| 307.25 | 0.0590 | 0.0670 |
| 307.47 | 0.0230 | 0.0310 |

Zhang, Zhigang - Yang, Lei - Xing, Yuan - Li, Wenxiu, Vapor–Liquid Equilibrium for Ternary and Binary Mixtures of 2-Isopropoxypropane, 2-Propanol, and

N,N-Dimethylacetamide at 101.3 kPa, Journal of Chemical & Engineering Data 2 (2013) 357-363. doi:10.1021/je300994y

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 352.94 | 0.9710 | 0.8940 |
| 350.39 | 0.9340 | 0.7870 |
| 348.39 | 0.8980 | 0.7050 |
| 346.61 | 0.8580 | 0.6320 |
| 345.02 | 0.8110 | 0.5660 |
| 343.92 | 0.7680 | 0.5170 |
| 342.97 | 0.7190 | 0.4710 |
| 342.23 | 0.6690 | 0.4330 |
| 341.63 | 0.6180 | 0.4000 |
| 341.10 | 0.5610 | 0.3680 |
| 340.57 | 0.5010 | 0.3400 |
| 340.13 | 0.4450 | 0.3150 |
| 339.73 | 0.3870 | 0.2910 |
| 339.39 | 0.3280 | 0.2670 |
| 339.18 | 0.2720 | 0.2430 |
| 339.13 | 0.2150 | 0.2160 |
| 339.30 | 0.1580 | 0.1830 |
| 339.71 | 0.1060 | 0.1440 |
| 340.37 | 0.0530 | 0.0880 |

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**Enthalpy of mixing**

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Letcher, Trevor M. - Govender, Penny U., Excess Molar Enthalpies of an Alkanol + a Branched Chain Ether at the Temperature 298.15 K, Journal of Chemical & Engineering Data 4 (1995) 997-1000. doi:10.1021/je00020a060

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 120.60 | 0.9260 |
| 192.40 | 0.8790 |
| 257.60 | 0.8370 |
| 326.40 | 0.7870 |
| 386.30 | 0.7480 |
| 456.30 | 0.7090 |
| 547.60 | 0.6260 |
| 626.20 | 0.5400 |
| 672.10 | 0.4520 |
| 688.30 | 0.3480 |
| 670.70 | 0.2870 |
| 628.70 | 0.2320 |
| 520.20 | 0.1490 |
| 479.00 | 0.1310 |
| 379.40 | 0.0870 |

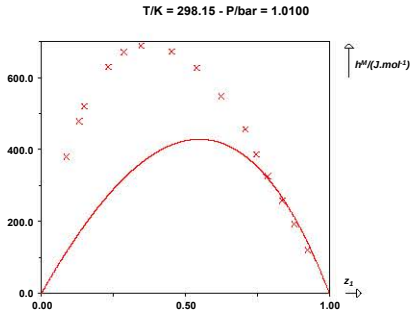
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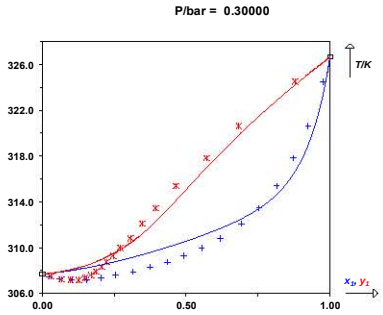
**Azeotropic point**

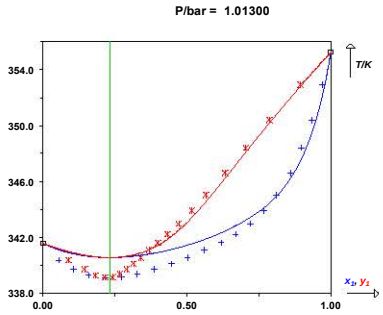
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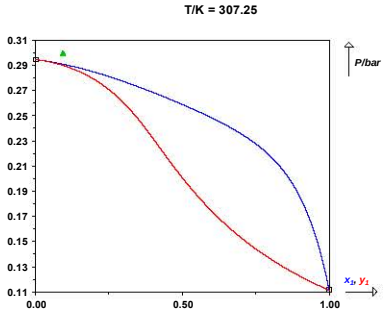
Lladosa, Estela - Montón, Juan B. - Burguet, MªCruz - Muñoz, Rosa, Effect of pressure and the capability of 2-methoxyethanol as a solvent in the behaviour of a diisopropyl ether–isopropyl alcohol azeotropic mixture, Fluid Phase Equilibria 1-2 (2007) 271-279. doi:10.1016/j.fluid.2007.09.014

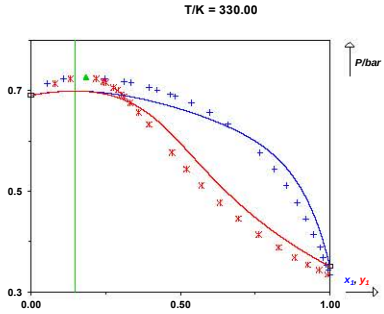
| T / K | P / bar | $x_1$ |
|---|---|---|
| 307.25 | 0.3000 | 0.0936 |

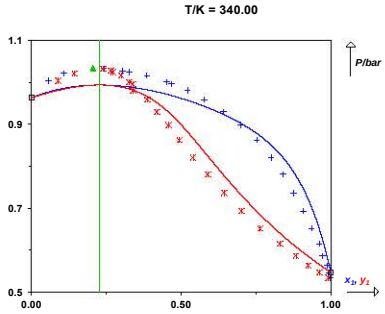

T/K = 298.15 - P/bar = 1.0100
$h^M$/(J.mol$^{-1}$)
600.0
400.0
200.0
0.0
0.00
0.50
1.00
$z_1$


P/bar = 0.30000
T/K
326.0
322.0
318.0
314.0
310.0
306.0
0.00
0.50
1.00
$x_1$, $y_1$


P/bar = 1.01300
T/K
354.0
350.0
346.0
342.0
338.0
0.00
0.50
1.00
$x_1$, $y_1$


T/K = 307.25
P/bar
0.31
0.29
0.27
0.25
0.23
0.21
0.19
0.17
0.15
0.13
0.11
0.00
0.50
1.00
$x_1$, $y_1$


T/K = 330.00
P/bar
0.7
0.5
0.3
0.00
0.50
1.00
$x_1$, $y_1$


T/K = 340.00
P/bar
1.1
0.9
0.7
0.5
0.00
0.50
1.00
$x_1$, $y_1$

## METHANOL (1) + n-BUTYL ACETATE (2)

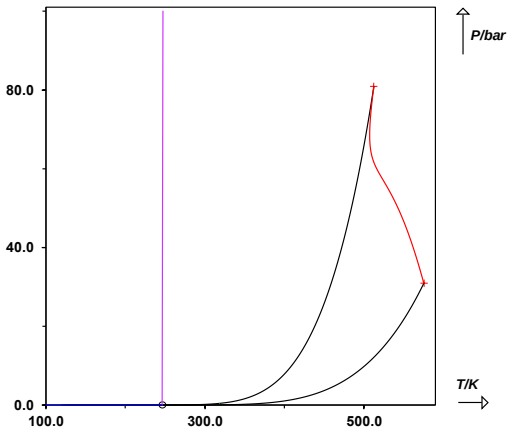
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 123-86-4 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | DKPFZGUDAPQIHT-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.5 | 575.4 |
| **$P_c$ / bar** | 80.84 | 30.9 |
| **ω** | 0.566 | 0.439 |

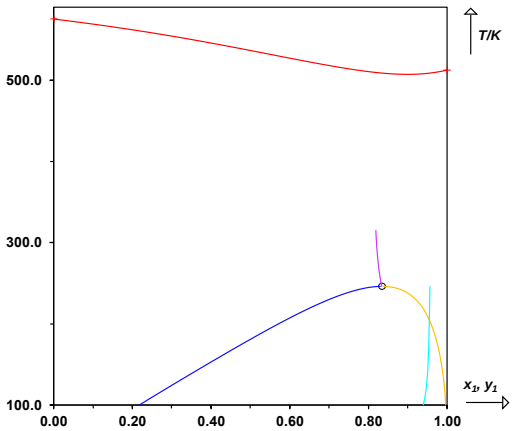
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 346
B/MPa = 193

*Deviations*
MAPE on x = 17 %
MAPE on y = 6.5 %
MAPE on $h^M$ = 30 %



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**Isothermal phase equilibrium data**

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Sieg, L. - Cruetzen, J.L. - Jost, W., Zur Thermodynamik von Mischphasen VIII. Über das Verdampfungsgleichgewicht Methanol-n-Butylazetat, Z. Elektrochem. Angew. Phys. Chem. 3 (1951) 199-201. doi:10.1002/bbpc.19510550307

**T / K = 296.65**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0365 | 0.0500 | 0.6000 |
| 0.0589 | 0.1060 | 0.7510 |
| 0.0781 | 0.2000 | 0.8330 |
| 0.1087 | 0.4030 | 0.8980 |
| 0.1181 | 0.5400 | 0.9100 |
| 0.1325 | 0.7450 | 0.9430 |
| 0.1396 | 0.8310 | 0.9570 |
| 0.1513 | 0.9480 | 0.9860 |

Sieg, L. - Cruetzen, J.L. - Jost, W., Zur Thermodynamik von Mischphasen VIII. Über das Verdampfungsgleichgewicht Methanol-n-Butylazetat, Z. Elektrochem. Angew. Phys. Chem. 3 (1951) 199-201. doi:10.1002/bbpc.19510550307

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1213 | 0.1060 | 0.7520 |
| 0.1413 | 0.1380 | 0.7810 |
| 0.1731 | 0.2000 | 0.8270 |
| 0.2091 | 0.2960 | 0.8650 |
| 0.2277 | 0.3780 | 0.8810 |
| 0.2476 | 0.4720 | 0.8970 |
| 0.2596 | 0.5430 | 0.9090 |
| 0.2706 | 0.5880 | 0.9160 |
| 0.2740 | 0.6140 | 0.9200 |
| 0.2897 | 0.7000 | 0.9340 |
| 0.2978 | 0.7490 | 0.9440 |
| 0.3098 | 0.8180 | 0.9540 |
| 0.3160 | 0.8590 | 0.9570 |

Sieg, L. - Cruetzen, J.L. - Jost, W., Zur Thermodynamik von Mischphasen VIII. Über das Verdampfungsgleichgewicht Methanol-n-Butylazetat, Z. Elektrochem. Angew. Phys. Chem. 3 (1951) 199-201. doi:10.1002/bbpc.19510550307

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2477 | 0.0760 | 0.6500 |
| 0.3466 | 0.1450 | 0.7520 |
| 0.4486 | 0.2510 | 0.8270 |
| 0.4942 | 0.3060 | 0.8520 |
| 0.5896 | 0.4780 | 0.8930 |
| 0.6470 | 0.6060 | 0.9120 |
| 0.7002 | 0.7180 | 0.9350 |
| 0.7331 | 0.7930 | 0.9410 |
| 0.7845 | 0.9000 | 0.9660 |

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**Isobaric phase equilibrium data**

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Park, W.K., Vapor-liquid equilibriums of ester-alcohol systems. III, Hwahak Konghak 4 (1971) 181-190.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 379.15 | 0.0500 | 0.5050 |
| 367.15 | 0.1000 | 0.6750 |
| 361.25 | 0.1500 | 0.7530 |
| 356.95 | 0.2000 | 0.7970 |
| 353.75 | 0.2500 | 0.8290 |
| 351.15 | 0.3000 | 0.8510 |
| 349.25 | 0.3500 | 0.8670 |
| 347.65 | 0.4000 | 0.8800 |
| 346.35 | 0.4500 | 0.8910 |
| 345.15 | 0.5000 | 0.9010 |
| 344.15 | 0.5500 | 0.9100 |
| 343.35 | 0.6000 | 0.9180 |
| 342.65 | 0.6500 | 0.9270 |
| 342.05 | 0.7000 | 0.9360 |
| 341.35 | 0.7500 | 0.9430 |
| 340.65 | 0.8000 | 0.9520 |
| 339.95 | 0.8500 | 0.9620 |
| 339.35 | 0.9000 | 0.9720 |
| 338.55 | 0.9500 | 0.9850 |

Nebig, Silke - Gmehling, Jürgen, Prediction of phase equilibria and excess properties for systems with ionic liquids using modified UNIFAC: Typical results and present status of the modified UNIFAC matrix for ionic liquids, Fluid Phase Equilibria 1-2 (2011) 220-225. doi:10.1016/j.fluid.2010.09.021

**P / bar = 1.413**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 407.30 | 0.0074 | 0.1137 |
| 401.98 | 0.0198 | 0.2483 |
| 397.67 | 0.0318 | 0.3359 |
| 393.88 | 0.0426 | 0.4098 |
| 387.50 | 0.0658 | 0.5229 |
| 383.43 | 0.0837 | 0.5800 |
| 378.35 | 0.1151 | 0.6549 |
| 373.23 | 0.1476 | 0.7135 |
| 368.85 | 0.1853 | 0.7601 |

| | | |
|---|---|---|
| 365.34 | 0.2239 | 0.7970 |
| 361.80 | 0.2755 | 0.8281 |
| 358.65 | 0.3377 | 0.8505 |
| 356.45 | 0.3906 | 0.8686 |
| 353.95 | 0.4587 | 0.8896 |
| 352.61 | 0.5307 | 0.9015 |
| 351.55 | 0.5937 | 0.9126 |
| 350.39 | 0.6716 | 0.9249 |
| 349.25 | 0.7249 | 0.9343 |
| 348.55 | 0.7650 | 0.9425 |
| 348.07 | 0.8114 | 0.9500 |
| 347.57 | 0.8672 | 0.9585 |
| 347.11 | 0.8901 | 0.9668 |
| 346.78 | 0.9234 | 0.9758 |
| 346.35 | 0.9519 | 0.9838 |
| 346.10 | 0.9721 | 0.9913 |

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**Enthalpy of mixing**

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Sieg, L. - Cruetzen, J.L. - Jost, W., Zur Thermodynamik von Mischphasen VIII. Über das Verdampfungsgleichgewicht Methanol-n-Butylazetat, Z. Elektrochem. Angew. Phys. Chem. 3 (1951) 199-201. doi:10.1002/bbpc.19510550307

**T / K = 293.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 502.42 | 0.1010 |
| 816.43 | 0.1890 |
| 1113.7 | 0.3330 |
| 1172.3 | 0.4480 |
| 1118.7 | 0.5420 |
| 1000.6 | 0.6300 |
| 602.06 | 0.8130 |
| 440.03 | 0.8670 |

Ortega, J., Excess enthalpy. Ethanol-ethyl ethanoate system, Int. Data Ser. Sel. Data Mixtures Ser. A 3 (1995)

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 647.60 | 0.1201 |
| 930.30 | 0.2117 |
| 1086.7 | 0.2807 |
| 1159.3 | 0.3369 |
| 1200.2 | 0.3953 |
| 1203.1 | 0.4478 |
| 1186.7 | 0.4973 |
| 1150.0 | 0.5414 |
| 1103.5 | 0.5825 |
| 1051.2 | 0.6137 |
| 966.90 | 0.6669 |
| 869.20 | 0.7055 |
| 792.60 | 0.7447 |
| 681.10 | 0.7860 |
| 556.30 | 0.8274 |
| 451.70 | 0.8683 |
| 326.20 | 0.9055 |
| 238.50 | 0.9338 |
| 153.60 | 0.9598 |
| 70.80 | 0.9812 |

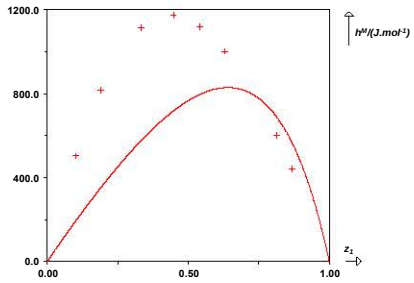
Mainar, Ana M. - García-Abarrio, Sandra M. - Palavra, Antonio M. F. - Urieta, José S. - Pardo, Juan I., Excess Molar Enthalpies of Mixtures of (±)-Linalool with Several Alkanols, Journal of Chemical & Engineering Data 10 (2011) 3818-3822. doi:10.1021/je200457q

**T / K = 318.15**

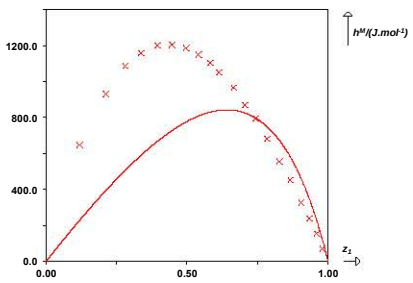
**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 360.00 | 0.0956 |
| 658.00 | 0.1761 |
| 932.00 | 0.2722 |
| 1077.0 | 0.3517 |
| 1143.0 | 0.4208 |
| 1152.0 | 0.4831 |
| 1141.0 | 0.5375 |
| 1102.0 | 0.5894 |
| 1052.0 | 0.6350 |
| 991.00 | 0.6767 |
| 922.00 | 0.7139 |
| 852.00 | 0.7483 |
| 779.00 | 0.7771 |
| 710.00 | 0.8031 |
| 641.00 | 0.8247 |
| 582.00 | 0.8445 |
| 522.00 | 0.8617 |

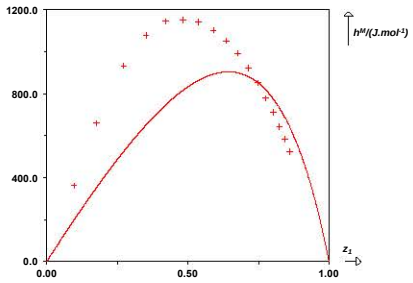
T/K = 293.15 - P/bar = 1.0132



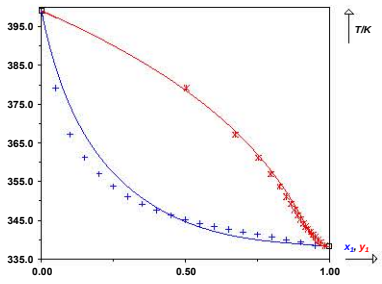

T/K = 298.15 - P/bar = 1.0100



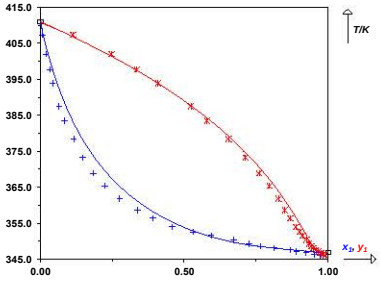

T/K = 318.15 - P/bar = 1.0132



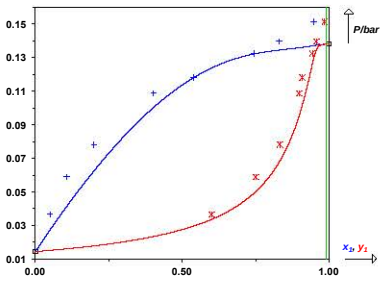

P/bar = 1.01330



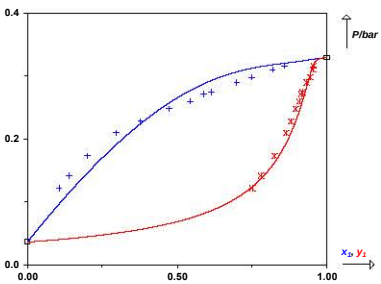

P/bar = 1.41300



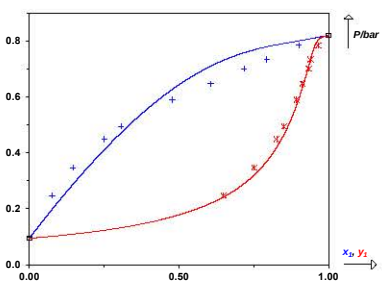

T/K = 296.65




T/K = 313.15




T/K = 333.15



## DIETHYL ETHER (1) + ETHANOL (2)

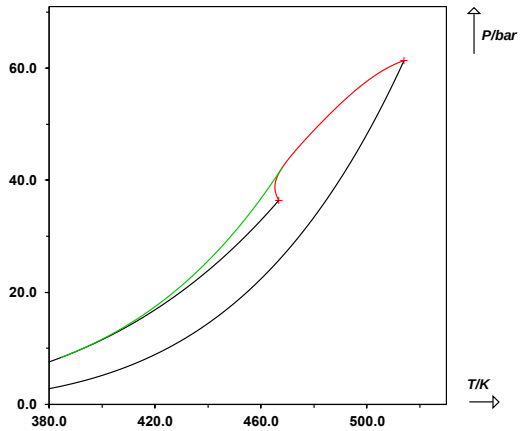
| | | |
|---|---|---|
| **CAS** | 60-29-7 | 64-17-5 |
| **InChiKey** | RTZKZFJDLAIYFH-UHFFFAOYSA-N | LFQSCWFLJHTTHZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 466.70 | 514.00 |
| **$P_c$ / bar** | 36.40 | 61.37 |
| **ω** | 0.281 | 0.644 |

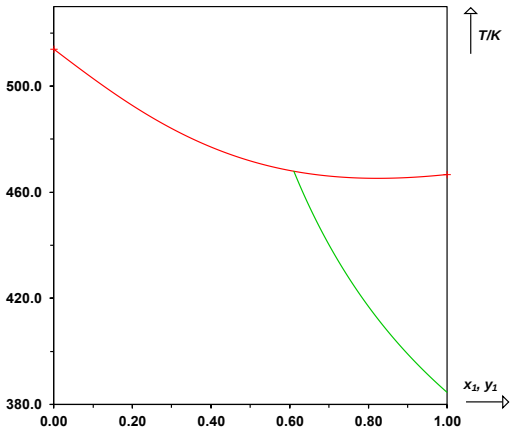
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 271
B/MPa = 54

*Deviations*
MAPE on x = 17 %
MAPE on y = 6.1 %
MAPE on $h^M$ = 37 %



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**Isothermal phase equilibrium data**

---

Nagai, J. - Isii, N., Volatility of fuels containing ethyl alcohol. I. Partial pressures of ethyl alcohol and ethyl ether in their mixtures and calculation of heat of mixture, J. Soc. Chem. Ind. Jpn. 1 (1935) 8B-12B.

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0491 | 0.0500 | 0.6787 |
| 0.0765 | 0.1000 | 0.8034 |
| 0.1018 | 0.1500 | 0.8590 |
| 0.1210 | 0.2000 | 0.8866 |
| 0.1370 | 0.2500 | 0.9039 |
| 0.1505 | 0.3000 | 0.9159 |
| 0.1621 | 0.3500 | 0.9259 |
| 0.1723 | 0.4000 | 0.9323 |
| 0.1818 | 0.4500 | 0.9386 |
| 0.1906 | 0.5000 | 0.9442 |
| 0.1980 | 0.5500 | 0.9487 |
| 0.2038 | 0.6000 | 0.9523 |
| 0.2086 | 0.6500 | 0.9555 |
| 0.2131 | 0.7000 | 0.9585 |
| 0.2178 | 0.7500 | 0.9622 |
| 0.2233 | 0.8000 | 0.9667 |
| 0.2293 | 0.8500 | 0.9720 |
| 0.2352 | 0.9000 | 0.9783 |
| 0.2412 | 0.9500 | 0.9861 |

Nagai, J. - Isii, N., Volatility of fuels containing ethyl alcohol. I. Partial pressures of ethyl alcohol and ethyl ether in their mixtures and calculation of heat of mixture, J. Soc. Chem. Ind. Jpn. 1 (1935) 8B-12B.

**T / K = 283.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0796 | 0.0500 | 0.6116 |
| 0.1241 | 0.1000 | 0.7636 |
| 0.1619 | 0.1500 | 0.8269 |
| 0.1901 | 0.2000 | 0.8593 |
| 0.2149 | 0.2500 | 0.8801 |
| 0.2360 | 0.3000 | 0.8953 |
| 0.2539 | 0.3500 | 0.9068 |
| 0.2703 | 0.4000 | 0.9161 |
| 0.2864 | 0.4500 | 0.9245 |
| 0.2994 | 0.5000 | 0.9311 |
| 0.3093 | 0.5500 | 0.9362 |
| 0.3178 | 0.6000 | 0.9404 |
| 0.3267 | 0.6500 | 0.9457 |
| 0.3359 | 0.7000 | 0.9501 |
| 0.3453 | 0.7500 | 0.9556 |
| 0.3546 | 0.8000 | 0.9613 |
| 0.3631 | 0.8500 | 0.9675 |
| 0.3716 | 0.9000 | 0.9745 |
| 0.3801 | 0.9500 | 0.9841 |

Nagai, J. - Isii, N., Volatility of fuels containing ethyl alcohol. I. Partial pressures of ethyl alcohol and ethyl ether in their mixtures and calculation of heat of mixture, J. Soc. Chem. Ind. Jpn. 1 (1935) 8B-12B.

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1305 | 0.0500 | 0.5681 |
| 0.1934 | 0.1000 | 0.7224 |
| 0.2460 | 0.1500 | 0.7918 |
| 0.2908 | 0.2000 | 0.8317 |
| 0.3288 | 0.2500 | 0.8575 |
| 0.3613 | 0.3000 | 0.8760 |
| 0.3883 | 0.3500 | 0.8893 |
| 0.4109 | 0.4000 | 0.8995 |
| 0.4312 | 0.4500 | 0.9082 |
| 0.4499 | 0.5000 | 0.9159 |
| 0.4673 | 0.5500 | 0.9230 |
| 0.4831 | 0.6000 | 0.9294 |
| 0.4975 | 0.6500 | 0.9353 |
| 0.5094 | 0.7000 | 0.9405 |
| 0.5213 | 0.7500 | 0.9461 |
| 0.5339 | 0.8000 | 0.9529 |
| 0.5477 | 0.8500 | 0.9610 |
| 0.5614 | 0.9000 | 0.9704 |
| 0.5753 | 0.9500 | 0.9821 |

Gordon, A.R. - Hornibrook, E.J., Liquid-Vapor Equilibrium for the System Ethanol - Diethyl - Ether, Can. J. Res. Sect. B (1946) 263-267.

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0880 | 0.0050 | 0.1105 |
| 0.0975 | 0.0100 | 0.1985 |
| 0.1156 | 0.0200 | 0.3305 |
| 0.1504 | 0.0400 | 0.4950 |
| 0.1831 | 0.0600 | 0.5940 |
| 0.2135 | 0.0800 | 0.6600 |
| 0.2417 | 0.1000 | 0.7070 |
| 0.3046 | 0.1500 | 0.7815 |
| 0.3584 | 0.2000 | 0.8245 |
| 0.4029 | 0.2500 | 0.8520 |
| 0.4409 | 0.3000 | 0.8700 |
| 0.4738 | 0.3500 | 0.8830 |
| 0.5014 | 0.4000 | 0.8930 |

| | | |
|---|---|---|
| 0.5474 | 0.5000 | 0.9110 |
| 0.5852 | 0.6000 | 0.9250 |
| 0.6166 | 0.7000 | 0.9390 |
| 0.6469 | 0.8000 | 0.9560 |
| 0.6789 | 0.9000 | 0.9760 |
| 0.6962 | 0.9500 | 0.9880 |

Nagai, J. - Isii, N., Volatility of fuels containing ethyl alcohol. I. Partial pressures of ethyl alcohol and ethyl ether in their mixtures and calculation of heat of mixture, J. Soc. Chem. Ind. Jpn. 1 (1935) 8B-12B.

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2053 | 0.0500 | 0.5092 |
| 0.2973 | 0.1000 | 0.6771 |
| 0.3720 | 0.1500 | 0.7538 |
| 0.4332 | 0.2000 | 0.7977 |
| 0.4866 | 0.2500 | 0.8278 |
| 0.5193 | 0.3000 | 0.8455 |
| 0.5720 | 0.3500 | 0.8656 |
| 0.6060 | 0.4000 | 0.8785 |
| 0.6373 | 0.4500 | 0.8897 |
| 0.6649 | 0.5000 | 0.8993 |
| 0.6896 | 0.5500 | 0.9077 |
| 0.7114 | 0.6000 | 0.9153 |
| 0.7310 | 0.6500 | 0.9223 |
| 0.7626 | 0.7000 | 0.9305 |
| 0.7700 | 0.7500 | 0.9371 |
| 0.7879 | 0.8000 | 0.9451 |
| 0.8063 | 0.8500 | 0.9540 |
| 0.8247 | 0.9000 | 0.9651 |
| 0.8433 | 0.9500 | 0.9789 |

Nagai, J. - Isii, N., Volatility of fuels containing ethyl alcohol. I. Partial pressures of ethyl alcohol and ethyl ether in their mixtures and calculation of heat of mixture, J. Soc. Chem. Ind. Jpn. 1 (1935) 8B-12B.

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3173 | 0.0500 | 0.4618 |
| 0.4404 | 0.1000 | 0.6303 |
| 0.5446 | 0.1500 | 0.7150 |
| 0.6309 | 0.2000 | 0.7650 |
| 0.7059 | 0.2500 | 0.7992 |
| 0.7693 | 0.3000 | 0.8234 |
| 0.8234 | 0.3500 | 0.8420 |
| 0.8715 | 0.4000 | 0.8571 |
| 0.9167 | 0.4500 | 0.8706 |
| 0.9567 | 0.5000 | 0.8820 |
| 0.9893 | 0.5500 | 0.8912 |
| 1.019 | 0.6000 | 0.8998 |
| 1.047 | 0.6500 | 0.9083 |
| 1.074 | 0.7000 | 0.9167 |
| 1.102 | 0.7500 | 0.9257 |
| 1.129 | 0.8000 | 0.9357 |
| 1.155 | 0.8500 | 0.9466 |
| 1.180 | 0.9000 | 0.9598 |
| 1.204 | 0.9500 | 0.9762 |

Nagai, J. - Isii, N., Volatility of fuels containing ethyl alcohol. I. Partial pressures of ethyl alcohol and ethyl ether in their mixtures and calculation of heat of mixture, J. Soc. Chem. Ind. Jpn. 1 (1935) 8B-12B.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4853 | 0.0500 | 0.4203 |
| 0.6481 | 0.1000 | 0.5863 |
| 0.7794 | 0.1500 | 0.6723 |
| 0.8986 | 0.2000 | 0.7285 |
| 0.9983 | 0.2500 | 0.7666 |
| 1.084 | 0.3000 | 0.7946 |
| 1.158 | 0.3500 | 0.8161 |
| 1.226 | 0.4000 | 0.8341 |
| 1.290 | 0.4500 | 0.8496 |
| 1.342 | 0.5000 | 0.8621 |
| 1.388 | 0.5500 | 0.8732 |
| 1.428 | 0.6000 | 0.8835 |
| 1.468 | 0.6500 | 0.8939 |
| 1.504 | 0.7000 | 0.9040 |
| 1.543 | 0.7500 | 0.9148 |
| 1.578 | 0.8000 | 0.9268 |
| 1.612 | 0.8500 | 0.9396 |
| 1.644 | 0.9000 | 0.9543 |
| 1.674 | 0.9500 | 0.9727 |

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**Enthalpy of mixing**

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Villamañan, M.A. - Casanova, C. - Roux, A.H. - Grolier, J.-P.E., Calorimetric investigation of the interactions between oxygen and hydroxyl groups in (alcohol+ether) at 298.15 K, The Journal of Chemical Thermodynamics 3 (1982) 251-258. doi:10.1016/0021-9614(82)90015-5

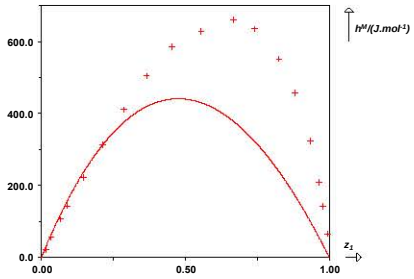
**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

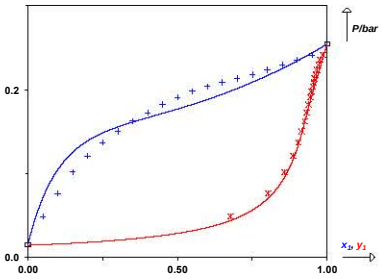
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 21.50 | 0.0146 |
| 55.70 | 0.0339 |
| 105.70 | 0.0673 |

| | |
|---|---|
| 143.10 | 0.0884 |
| 222.80 | 0.1479 |
| 313.60 | 0.2133 |
| 411.10 | 0.2853 |
| 503.80 | 0.3653 |
| 585.50 | 0.4545 |
| 627.90 | 0.5547 |
| 660.70 | 0.6678 |
| 635.20 | 0.7411 |
| 551.80 | 0.8258 |
| 456.80 | 0.8809 |
| 324.30 | 0.9330 |
| 209.10 | 0.9632 |
| 141.90 | 0.9786 |
| 65.90 | 0.9942 |

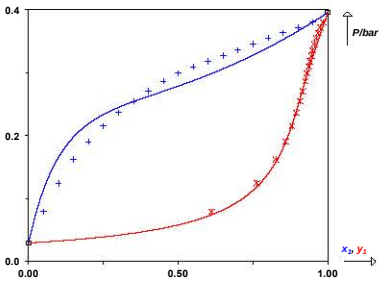
T/K = 298.15 - P/bar = 1.0132



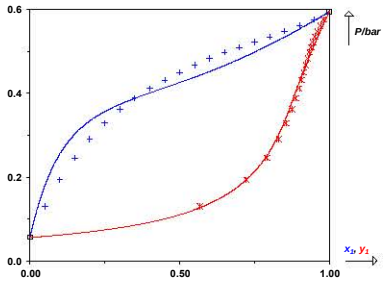

T/K = 273.15



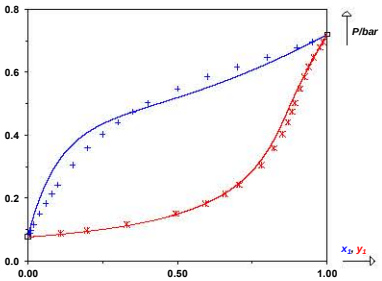

T/K = 283.15



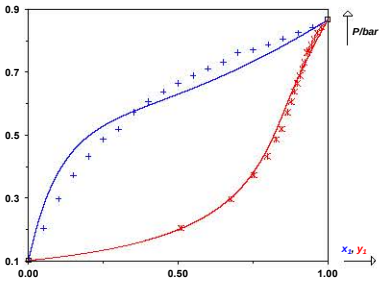

T/K = 293.15



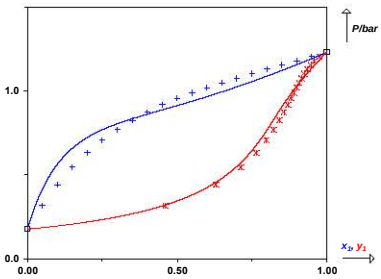

T/K = 298.15



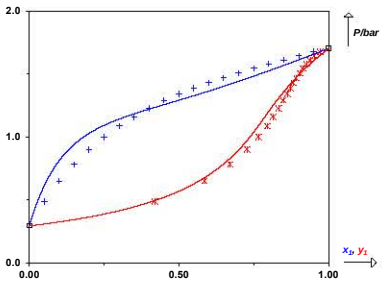

T/K = 303.15




T/K = 313.15




T/K = 323.15



## METHANOL (1) + 1,4-DIOXANE (2)

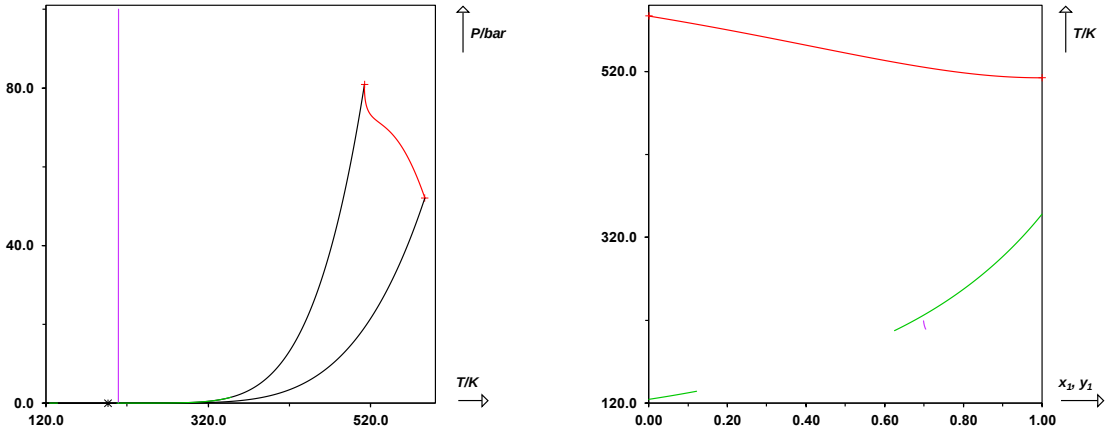
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 123-91-1 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | RYHBNJHYFVUHQT-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.50 | 587.00 |
| **$P_c$ / bar** | 80.84 | 52.08 |
| **ω** | 0.566 | 0.279 |

Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 313
B/MPa = 342

*Deviations*
MAPE on x = 5.5 %
MAPE on y = 2.3 %
MAPE on $h^M$ = 18 %



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**Isothermal phase equilibrium data**
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Kortüm, G. - Valent, V., Thermodynamische Mischungseffekte der Systeme Wasser(1)-1,4-Dioxan(2) und Methanol(1)-1,4-Dioxan(2); ein Vergleich, Berichte der Bunsengesellschaft für physikalische Chemie 8 (1977) 752-761. doi:10.1002/bbpc.19770810811

**T / K =** **308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1195 | 0.0700 | 0.3700 |
| 0.1301 | 0.0930 | 0.4270 |
| 0.1419 | 0.1140 | 0.4880 |
| 0.1571 | 0.1590 | 0.5540 |
| 0.1813 | 0.2290 | 0.6330 |
| 0.2030 | 0.3230 | 0.7030 |
| 0.2177 | 0.3860 | 0.7370 |
| 0.2283 | 0.4470 | 0.7660 |
| 0.2402 | 0.5410 | 0.7960 |
| 0.2507 | 0.6220 | 0.8250 |
| 0.2647 | 0.7680 | 0.8700 |
| 0.2708 | 0.8330 | 0.8980 |
| 0.2747 | 0.8940 | 0.9270 |
| 0.2776 | 0.9440 | 0.9560 |

Kortüm, G. - Valent, V., Thermodynamische Mischungseffekte der Systeme Wasser(1)-1,4-Dioxan(2) und Methanol(1)-1,4-Dioxan(2); ein Vergleich, Berichte der Bunsengesellschaft für physikalische Chemie 8 (1977) 752-761. doi:10.1002/bbpc.19770810811

**T / K =** **323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2371 | 0.0790 | 0.3720 |
| 0.2503 | 0.0930 | 0.4140 |
| 0.2739 | 0.1200 | 0.4780 |
| 0.3054 | 0.1650 | 0.5510 |
| 0.3449 | 0.2280 | 0.6250 |
| 0.3931 | 0.3240 | 0.6950 |
| 0.4208 | 0.3870 | 0.7350 |
| 0.4425 | 0.4570 | 0.7610 |
| 0.4675 | 0.5440 | 0.7960 |
| 0.4896 | 0.6370 | 0.8290 |
| 0.5150 | 0.7510 | 0.8650 |
| 0.5322 | 0.8420 | 0.9040 |
| 0.5421 | 0.8940 | 0.9320 |
| 0.5483 | 0.9430 | 0.9580 |

Kortüm, G. - Valent, V., Thermodynamische Mischungseffekte der Systeme Wasser(1)-1,4-Dioxan(2) und Methanol(1)-1,4-Dioxan(2); ein Vergleich, Berichte der Bunsengesellschaft für physikalische Chemie 8 (1977) 752-761. doi:10.1002/bbpc.19770810811

**T / K =** **333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3504 | 0.0810 | 0.3650 |
| 0.3638 | 0.0870 | 0.3860 |
| 0.4087 | 0.1280 | 0.4780 |
| 0.4533 | 0.1710 | 0.5520 |
| 0.5085 | 0.2310 | 0.6200 |
| 0.5756 | 0.3090 | 0.6870 |
| 0.6216 | 0.3830 | 0.7310 |
| 0.6552 | 0.4560 | 0.7610 |
| 0.7003 | 0.5680 | 0.8020 |
| 0.7315 | 0.6440 | 0.8270 |
| 0.7715 | 0.7620 | 0.8700 |
| 0.8025 | 0.8430 | 0.9060 |
| 0.8151 | 0.8940 | 0.9320 |
| 0.8288 | 0.9430 | 0.9600 |

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**Enthalpy of mixing**
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Ortega, J. - Chaar, M. - Placido, J., Excess enthalpies of 72 binary liquid mixtures of methyl n-alkanoates (C4 - C16) + alkan-1-ols (C2 - C10) at 298.15 K, ELDATA Int. Electron. J. Phys. Chem. Data 2 (1995) 139-166.

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 370.00 | 0.0810 |
| 560.20 | 0.1290 |
| 668.60 | 0.1590 |
| 795.70 | 0.1970 |
| 816.60 | 0.2020 |
| 948.00 | 0.2580 |
| 1018.9 | 0.3000 |
| 1061.5 | 0.3220 |
| 1107.7 | 0.3600 |
| 1130.7 | 0.4350 |
| 1039.5 | 0.5860 |
| 939.70 | 0.6710 |
| 904.00 | 0.6920 |
| 799.90 | 0.7480 |

| | |
|---|---|
| 549.90 | 0.8480 |
| 409.10 | 0.8890 |
| 292.80 | 0.9240 |
| 179.60 | 0.9500 |

Tamura, Kazuhiro - Bhuiyan, Mohammad Mainul Hossain, Excess molar enthalpies of (methanol+1-propanol)+oxane or 1,4-dioxane mixtures at the temperature 298.15 K, The Journal of Chemical Thermodynamics 10 (2003) 1657-1669. doi:10.1016/S0021-9614(03)00150-2

| **T / K =** | **298.15** |
|---|---|
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| 250.81 | 0.0500 |
| 475.42 | 0.1000 |
| 650.60 | 0.1500 |
| 796.29 | 0.2000 |
| 902.19 | 0.2500 |
| 988.17 | 0.3000 |
| 1050.2 | 0.3500 |
| 1086.7 | 0.4000 |
| 1102.0 | 0.4500 |
| 1096.0 | 0.5000 |
| 1079.9 | 0.5500 |
| 1040.9 | 0.6000 |
| 980.80 | 0.6500 |
| 902.79 | 0.7000 |
| 803.45 | 0.7500 |
| 687.83 | 0.8000 |
| 552.59 | 0.8500 |
| 394.89 | 0.9000 |
| 213.50 | 0.9500 |

Sitnyakovskii, I.B. - Gaile, A.A. - Semenov, L.V. - Koldobskaya, L.L. - Chupyra, O.S., Intermolecular interactions in dilute solutions of methanol in non-electrolytes, Zh. Obshch. Khim. 11 (1991) 2405-2410.

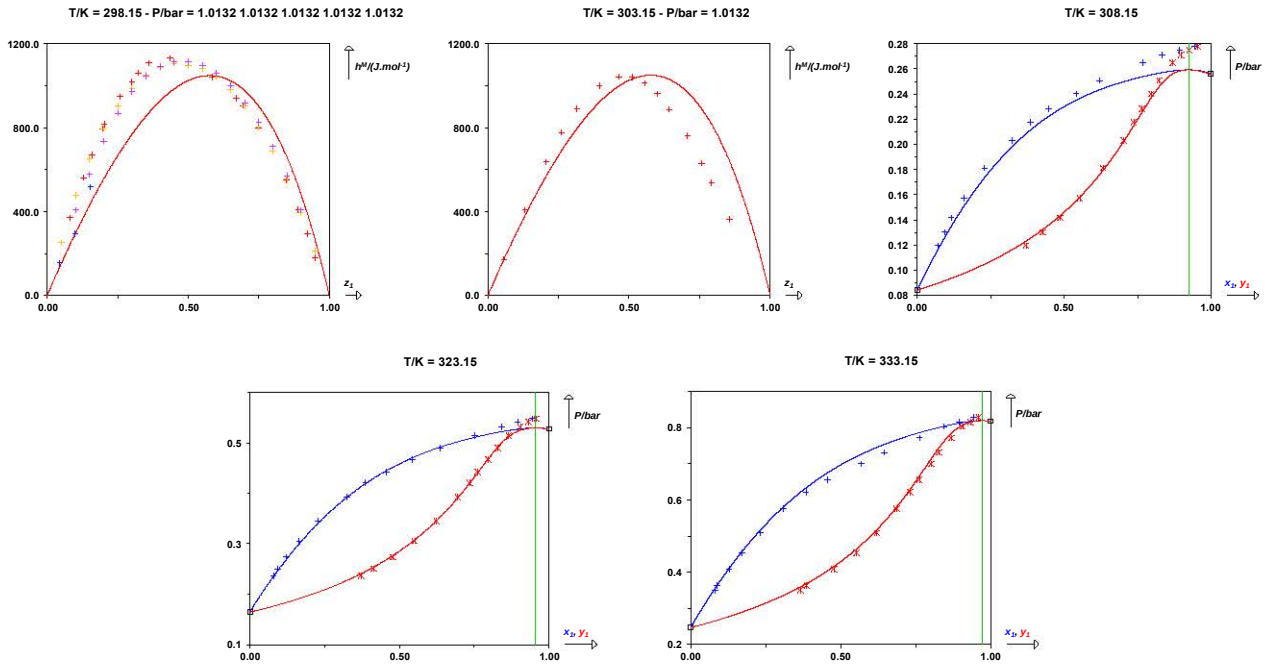
| **T / K =** | **298.15** |
|---|---|
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| 155.00 | 0.0450 |
| 293.00 | 0.0989 |
| 517.00 | 0.1539 |

Calvo, Encina - Brocos, Pilar - Piñeiro, Ángel - Pintos, Mercedes - Amigo, Alfredo - Bravo, Ramón - Roux, Alain H. - Roux-Desgranges, Geneviève, Heat Capacities, Excess Enthalpies, and Volumes of Mixtures Containing Cyclic Ethers. 4. Binary Systems 1,4-Dioxane + 1-Alkanols, Journal of Chemical & Engineering Data 5 (1999) 948-954. doi:10.1021/je990078z

| **T / K =** | **298.15** |
|---|---|
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| 406.10 | 0.9000 |
| 569.90 | 0.8500 |
| 708.70 | 0.8000 |
| 824.20 | 0.7500 |
| 919.30 | 0.7000 |
| 1001.2 | 0.6500 |
| 1059.4 | 0.6000 |
| 1097.5 | 0.5500 |
| 1115.0 | 0.5000 |
| 1113.7 | 0.4500 |
| 1090.6 | 0.4000 |
| 1045.7 | 0.3500 |
| 972.10 | 0.3000 |
| 869.30 | 0.2500 |
| 736.30 | 0.2000 |
| 575.80 | 0.1500 |
| 407.30 | 0.1000 |

Singh, P.P. - Verma, D.V. - Arora, P.S., Thermodynamics of binary methanol solutions, Thermochimica Acta 3 (1976) 267-280. doi:10.1016/0040-6031(76)85080-0

| **T / K =** | **303.15** |
|---|---|
| **P / bar =** | **UNKNOWN (1.0132)** |
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
| 172.60 | 0.0569 |
| 406.45 | 0.1308 |
| 635.14 | 0.2068 |
| 776.23 | 0.2612 |
| 890.32 | 0.3150 |
| 1000.0 | 0.3950 |
| 1040.7 | 0.4655 |
| 1039.0 | 0.5102 |
| 1010.0 | 0.5550 |
| 960.03 | 0.5998 |
| 885.67 | 0.6430 |
| 760.02 | 0.7080 |
| 630.57 | 0.7580 |
| 536.83 | 0.7930 |
| 362.78 | 0.8564 |


T/K = 298.15 - P/bar = 1.0132 1.0132 1.0132 1.0132 1.0132
T/K = 303.15 - P/bar = 1.0132
T/K = 308.15
T/K = 323.15
T/K = 333.15
P/bar
z1
x1, y1

## METHANOL (1) + THIOPHENE (2)

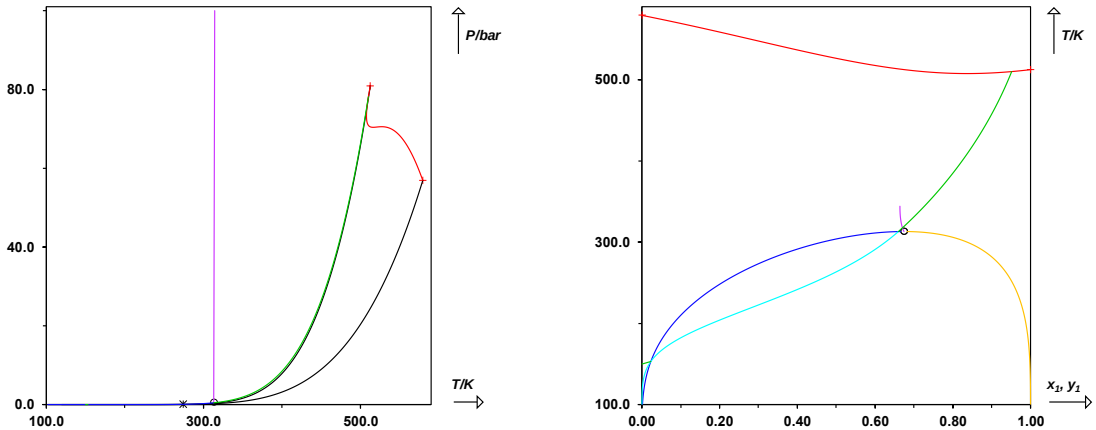
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 110-02-1 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | YTPLMLYBLZKORZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.50 | 579.35 |
| **$P_c$ / bar** | 80.84 | 56.90 |
| **ω** | 0.566 | 0.197 |

Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 551
B/MPa = 622

*Deviations*
MAPE on x = 26 %
MAPE on y = 15 %



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**Isothermal phase equilibrium data**

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Toghiani, Hossein - Toghiani, Rebecca K. - Viswanath, Dabir S., Vapor-liquid equilibria for the methanol-benzene and methanol-thiophene systems, Journal of Chemical & Engineering Data 1 (1994) 63-67. doi:10.1021/je00013a018

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2613 | 0.0008 | 0.0171 |
| 0.2676 | 0.0018 | 0.0407 |
| 0.2960 | 0.0067 | 0.1357 |
| 0.3268 | 0.0137 | 0.2259 |
| 0.3656 | 0.0238 | 0.3110 |
| 0.4102 | 0.0393 | 0.3907 |
| 0.4559 | 0.0668 | 0.4608 |
| 0.4934 | 0.1089 | 0.5111 |
| 0.5072 | 0.1362 | 0.5310 |
| 0.5266 | 0.1998 | 0.5575 |
| 0.5486 | 0.3682 | 0.5876 |
| 0.5536 | 0.4434 | 0.5999 |
| 0.5560 | 0.4841 | 0.6058 |
| 0.5580 | 0.5344 | 0.6144 |
| 0.5592 | 0.5739 | 0.6211 |
| 0.5600 | 0.6144 | 0.6298 |
| 0.5601 | 0.6503 | 0.6387 |
| 0.5595 | 0.6885 | 0.6494 |
| 0.5576 | 0.7293 | 0.6638 |
| 0.5538 | 0.7718 | 0.6824 |
| 0.5473 | 0.8146 | 0.7078 |
| 0.5392 | 0.8498 | 0.7343 |
| 0.5333 | 0.8698 | 0.7525 |
| 0.5222 | 0.8977 | 0.7852 |
| 0.5106 | 0.9213 | 0.8172 |
| 0.4973 | 0.9428 | 0.8544 |
| 0.4865 | 0.9578 | 0.8842 |
| 0.4769 | 0.9695 | 0.9114 |
| 0.4694 | 0.9776 | 0.9327 |
| 0.4653 | 0.9820 | 0.9442 |
| 0.4601 | 0.9870 | 0.9595 |
| 0.4565 | 0.9908 | 0.9706 |

Toghiani, Hossein - Toghiani, Rebecca K. - Viswanath, Dabir S., Vapor-liquid equilibria for the methanol-benzene and methanol-thiophene systems, Journal of Chemical & Engineering Data 1 (1994) 63-67. doi:10.1021/je00013a018

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3296 | 0.0022 | 0.0506 |
| 0.3474 | 0.0050 | 0.1026 |
| 0.3863 | 0.0129 | 0.2019 |
| 0.4459 | 0.0261 | 0.3154 |
| 0.5274 | 0.0526 | 0.4311 |
| 0.5844 | 0.0919 | 0.4972 |
| 0.6200 | 0.1357 | 0.5360 |
| 0.6418 | 0.1879 | 0.5570 |
| 0.6513 | 0.2179 | 0.5676 |
| 0.6653 | 0.2895 | 0.5830 |
| 0.6647 | 0.2901 | 0.5815 |
| 0.6757 | 0.3743 | 0.5948 |
| 0.6793 | 0.4185 | 0.6032 |
| 0.6828 | 0.4583 | 0.6086 |
| 0.6846 | 0.4948 | 0.6149 |
| 0.6866 | 0.5183 | 0.6175 |
| 0.6900 | 0.6050 | 0.6345 |
| 0.6898 | 0.6843 | 0.6550 |
| 0.6850 | 0.7578 | 0.6829 |
| 0.6782 | 0.8038 | 0.7075 |
| 0.6635 | 0.8587 | 0.7485 |
| 0.6431 | 0.9042 | 0.7988 |
| 0.6222 | 0.9362 | 0.8463 |
| 0.6094 | 0.9518 | 0.8758 |
| 0.5940 | 0.9681 | 0.9113 |
| 0.5809 | 0.9803 | 0.9420 |
| 0.5717 | 0.9880 | 0.9635 |

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**Isobaric phase equilibrium data**

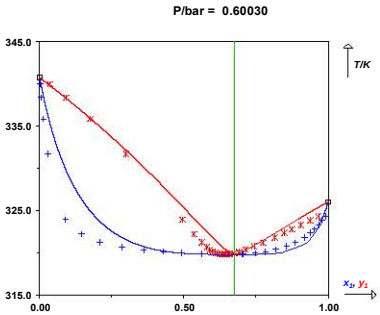
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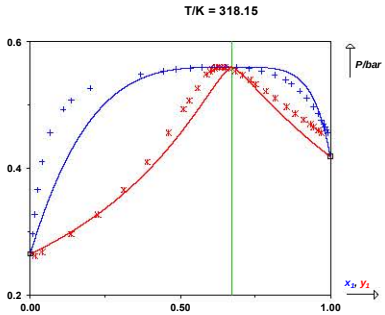
Toghiani, Hossein - Toghiani, Rebecca K. - Viswanath, Dabir S., Vapor-liquid equilibria for the methanol-benzene and methanol-thiophene systems, Journal of Chemical & Engineering Data 1 (1994) 63-67. doi:10.1021/je00013a018

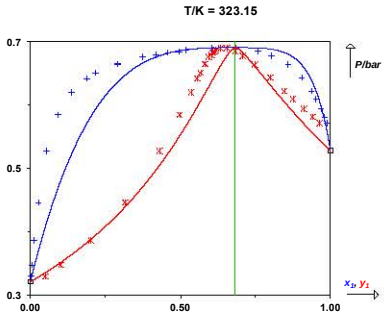
**P / bar = 0.6003**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 340.00 | 0.0034 | 0.0366 |
| 338.40 | 0.0067 | 0.0908 |
| 335.80 | 0.0139 | 0.1760 |
| 331.70 | 0.0279 | 0.3001 |
| 323.90 | 0.0901 | 0.4953 |
| 322.20 | 0.1448 | 0.5366 |
| 321.20 | 0.2089 | 0.5621 |
| 320.70 | 0.2856 | 0.5790 |
| 320.30 | 0.3609 | 0.5888 |
| 320.10 | 0.4289 | 0.5993 |
| 320.00 | 0.4924 | 0.6097 |
| 319.90 | 0.5610 | 0.6221 |
| 319.80 | 0.6153 | 0.6330 |
| 319.80 | 0.6310 | 0.6366 |

| | | |
|---|---|---|
| 319.80 | 0.6531 | 0.6424 |
| 319.80 | 0.6667 | 0.6458 |
| 319.90 | 0.7002 | 0.6563 |
| 319.80 | 0.7046 | 0.6573 |
| 319.90 | 0.7462 | 0.6738 |
| 320.10 | 0.7826 | 0.6918 |
| 320.40 | 0.8186 | 0.7136 |
| 320.70 | 0.8564 | 0.7441 |
| 321.20 | 0.8867 | 0.7748 |
| 321.80 | 0.9174 | 0.8154 |
| 322.30 | 0.9377 | 0.8482 |
| 322.80 | 0.9519 | 0.8751 |
| 323.30 | 0.9667 | 0.9068 |
| 323.80 | 0.9787 | 0.9378 |
| 324.30 | 0.9893 | 0.9663 |


P/bar = 0.60030
345.0
335.0
325.0
315.0
T/K
0.00
0.50
1.00
x1, y1


T/K = 318.15
0.6
0.4
0.2
P/bar
0.00
0.50
1.00
x1, y1


T/K = 323.15
0.7
0.5
0.3
P/bar
0.00
0.50
1.00
x1, y1

## ETHANOL (1) + DI-n-BUTYL ETHER (2)

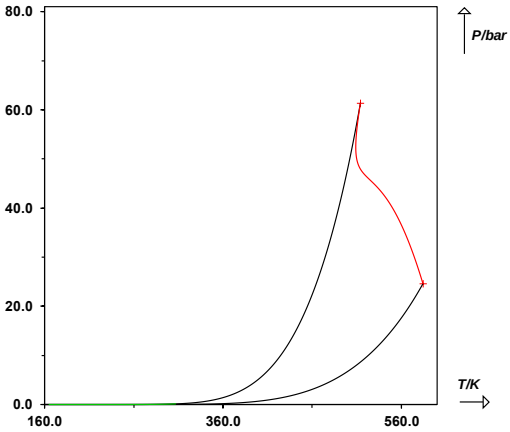
| | | |
|---|---|---|
| **CAS** | 64-17-5 | 142-96-1 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | DURPTKYDGMDSBL-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 584.10 |
| **$P_c$ / bar** | 61.37 | 24.60 |
| **ω** | 0.644 | 0.448 |

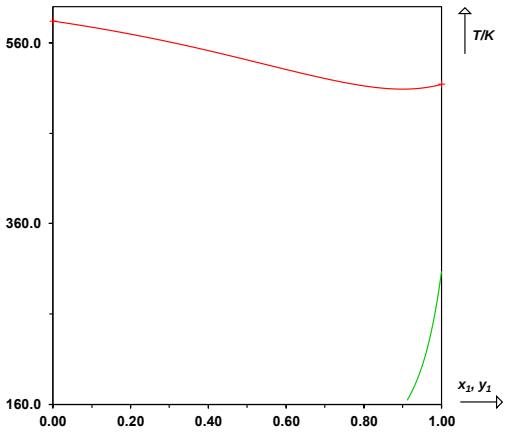
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 248
B/MPa = 72.6

*Deviations*
MAPE on x = 27 %
MAPE on y = 8.7 %
MAPE on $h^M$ = 38 %
MAPE on $c_P^M$ = 83 %



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**Isothermal phase equilibrium data**

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Gmehling, J., VLE data for the design of separation processes, AIChE Symp. Ser. 244 (1985) 121-129.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0658 | 0.0351 | 0.5026 |
| 0.0968 | 0.0704 | 0.6708 |
| 0.1261 | 0.1191 | 0.7631 |
| 0.1535 | 0.1655 | 0.8105 |
| 0.1784 | 0.2128 | 0.8404 |
| 0.1940 | 0.2478 | 0.8608 |
| 0.2100 | 0.3061 | 0.8687 |
| 0.2351 | 0.4634 | 0.8897 |
| 0.2481 | 0.5642 | 0.8992 |
| 0.2561 | 0.6034 | 0.9086 |
| 0.2634 | 0.7079 | 0.9161 |
| 0.2710 | 0.7834 | 0.9292 |
| 0.2751 | 0.8091 | 0.9380 |
| 0.2800 | 0.8650 | 0.9465 |
| 0.2876 | 0.9501 | 0.9782 |
| 0.2920 | 0.9927 | 0.9964 |

Gmehling, J., VLE data for the design of separation processes, AIChE Symp. Ser. 244 (1985) 121-129.

**T / K = 338.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1520 | 0.0416 | 0.5411 |
| 0.1787 | 0.0598 | 0.6228 |
| 0.2015 | 0.0722 | 0.6702 |
| 0.2361 | 0.0910 | 0.7223 |
| 0.2584 | 0.1074 | 0.7493 |
| 0.2773 | 0.1193 | 0.7701 |
| 0.3224 | 0.1503 | 0.8064 |
| 0.3666 | 0.1924 | 0.8413 |
| 0.4095 | 0.2518 | 0.8580 |
| 0.4346 | 0.3015 | 0.8670 |
| 0.4566 | 0.3553 | 0.8782 |
| 0.4788 | 0.4353 | 0.8876 |
| 0.4937 | 0.5205 | 0.8923 |
| 0.5147 | 0.6324 | 0.9065 |
| 0.5322 | 0.7386 | 0.9211 |
| 0.5560 | 0.8575 | 0.9401 |
| 0.5640 | 0.9026 | 0.9572 |
| 0.5706 | 0.9412 | 0.9702 |

Gmehling, J., VLE data for the design of separation processes, AIChE Symp. Ser. 244 (1985) 121-129.

**T / K = 352.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1654 | 0.0115 | 0.2473 |
| 0.2330 | 0.0325 | 0.4700 |
| 0.3198 | 0.0641 | 0.6310 |
| 0.4327 | 0.1121 | 0.7399 |
| 0.5091 | 0.1521 | 0.7822 |
| 0.6380 | 0.2314 | 0.8322 |
| 0.7672 | 0.3540 | 0.8694 |
| 0.8444 | 0.4822 | 0.8932 |
| 0.8865 | 0.5836 | 0.9045 |
| 0.9187 | 0.6672 | 0.9137 |
| 0.9472 | 0.7451 | 0.9247 |
| 0.9695 | 0.8031 | 0.9344 |
| 0.9808 | 0.8337 | 0.9403 |
| 1.002 | 0.8893 | 0.9532 |
| 1.015 | 0.9219 | 0.9640 |
| 1.031 | 0.9625 | 0.9806 |
| 1.036 | 0.9874 | 0.9928 |

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**Enthalpy of mixing**

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Villamañan, M.A. - Casanova, C. - Roux, A.H. - Grolier, J.-P.E., Calorimetric investigation of the interactions between oxygen and hydroxyl groups in (alcohol+ether) at 298.15 K, The Journal of Chemical Thermodynamics 3 (1982) 251-258. doi:10.1016/0021-9614(82)90015-5

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 98.00 | 0.0137 |
| 230.10 | 0.0405 |
| 385.00 | 0.0663 |
| 591.00 | 0.1153 |
| 720.70 | 0.1613 |
| 795.80 | 0.2043 |
| 845.30 | 0.2448 |
| 899.00 | 0.3361 |
| 899.10 | 0.4155 |
| 871.50 | 0.4851 |
| 827.60 | 0.5466 |
| 775.20 | 0.6015 |
| 716.50 | 0.6506 |
| 661.90 | 0.6949 |
| 602.50 | 0.7350 |
| 540.20 | 0.7716 |
| 478.30 | 0.8050 |

| | |
|---|---|
| 417.70 | 0.8356 |
| 356.70 | 0.8639 |
| 294.60 | 0.8899 |
| 236.40 | 0.9141 |
| 178.30 | 0.9366 |
| 121.00 | 0.9575 |
| 97.30 | 0.9655 |
| 75.40 | 0.9732 |
| 53.50 | 0.9808 |
| 45.20 | 0.9845 |
| 32.80 | 0.9881 |
| 24.10 | 0.9918 |
| 14.40 | 0.9953 |

Kim, Moon-Gab - Park, So-Jin - Hwang, In-Chan, Excess molar enthalpies for the binary and ternary mixtures of ether compounds (di-isopropyl ether, di-butyl ether, propyl vinyl ether) with ethanol and isooctane at 298.15 K, Korean Journal of Chemical Engineering 5 (2008) 1160-1164. doi:10.1007/s11814-008-0191-2

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 121.00 | 0.9540 |
| 248.50 | 0.9020 |
| 454.20 | 0.8030 |
| 619.70 | 0.7000 |
| 734.00 | 0.6070 |
| 816.70 | 0.5140 |
| 833.70 | 0.4610 |
| 846.50 | 0.4010 |
| 828.30 | 0.2970 |
| 753.40 | 0.2170 |
| 588.90 | 0.1240 |
| 417.70 | 0.1400 |
| 356.70 | 0.1900 |
| 294.60 | 0.2400 |
| 236.40 | 0.2900 |
| 178.30 | 0.3900 |
| 121.00 | 0.5600 |
| 97.30 | 0.7500 |
| 75.40 | 0.9600 |
| 53.50 | 1.280 |
| 45.20 | 1.660 |
| 32.80 | 1.900 |
| 24.10 | 2.290 |
| 14.40 | 2.700 |
| | 2.920 |
| | 3.440 |
| | 3.800 |
| | 4.740 |
| | 5.630 |
| | 6.380 |
| | 7.600 |
| | 8.310 |
| | 8.800 |
| | 9.330 |
| | 9.760 |
| | 9.820 |
| | 9.970 |
| | 9.460 |
| | 8.410 |
| | 6.890 |
| | 4.980 |
| | 2.620 |

| | |
|---|---|
| 0.0031 | |
| 0.0041 | |
| 0.0048 | |
| 0.0060 | |
| 0.0081 | |
| 0.0110 | |
| 0.0152 | |
| 0.0188 | |
| 0.0251 | |
| 0.0316 | |
| 0.0364 | |
| 0.0433 | |
| 0.0502 | |
| 0.0543 | |
| 0.0634 | |
| 0.0705 | |
| 0.0895 | |
| 0.1090 | |
| 0.1292 | |
| 0.1693 | |
| 0.1976 | |
| 0.2281 | |
| 0.2683 | |
| 0.3091 | |
| 0.3405 | |
| 0.4053 | |
| 0.5076 | |
| 0.6057 | |
| 0.7032 | |
| 0.8002 | |
| 0.9011 | |

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**Heat capacity of mixing**

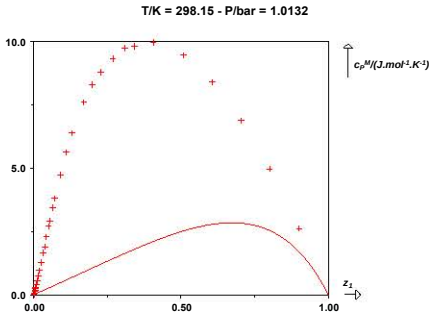
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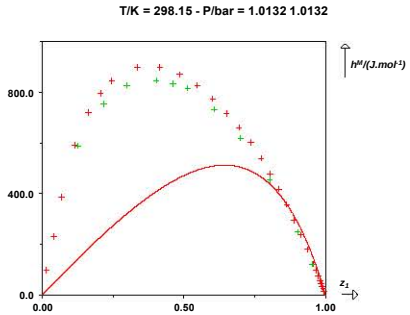
Tanaka, Reiji - Toyama, Satoru, Excess Molar Volumes and Excess Molar Heat Capacities for Binary Mixtures of Ethanol with Chlorocyclohexane, 1-Nitropropane, Dibutyl Ether, and Ethyl Acetate at the Temperature of 298.15 K, Journal of Chemical & Engineering Data 6 (1996) 1455-1458. doi:10.1021/je960179m

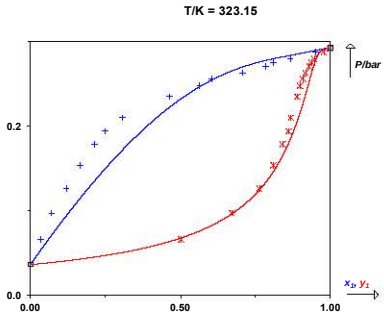
**T / K = 298.15**

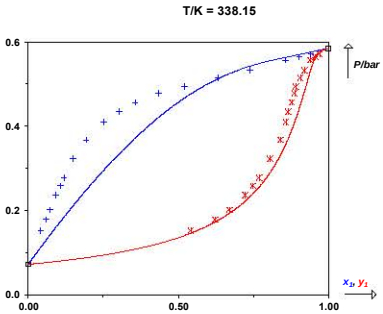
**P / bar = UNKNOWN (1.0132)**

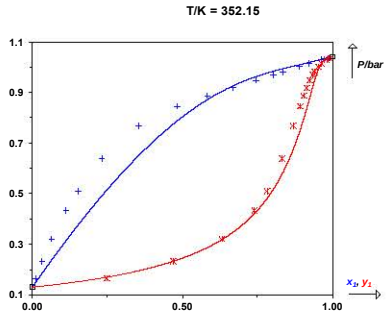
| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.0300 | 0.0009 |
| 0.0800 | 0.0019 |


T/K = 298.15 - P/bar = 1.0132
10.0
5.0
0.0
0.00
0.50
1.00
$c_p^M/(J.mol^{-1}.K^{-1})$
$z_1$


T/K = 298.15 - P/bar = 1.0132 1.0132
800.0
400.0
0.0
0.00
0.50
1.00
$h^M/(J.mol^{-1})$
$z_1$


T/K = 323.15
0.2
0.0
0.00
0.50
1.00
P/bar
$x_1, y_1$


T/K = 338.15
0.6
0.4
0.2
0.0
0.00
0.50
1.00
P/bar
$x_1, y_1$


T/K = 352.15
1.1
0.9
0.7
0.5
0.3
0.1
0.00
0.50
1.00
P/bar
$x_1, y_1$

## METHANOL (1) + METHYL tert-BUTYL ETHER (2)

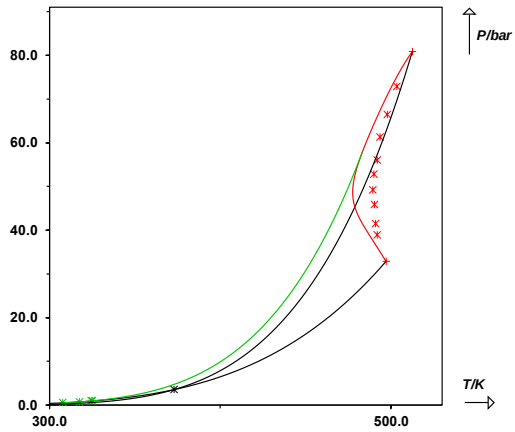
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 1634-04-4 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | BZLVMXJERCGZMT-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.50 | 497.10 |
| **$P_c$ / bar** | 80.84 | 32.86 |
| **ω** | 0.566 | 0.247 |

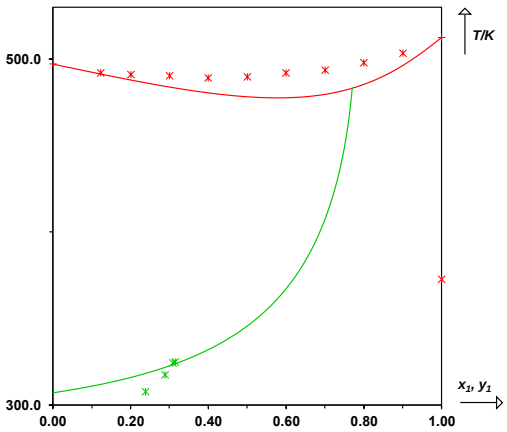
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 322
B/MPa = -94.6

*Deviations*
MAPE on x = 26 %
MAPE on y = 19 %
MAPE on $x_{az}$ = 20 %
MAPE on $P_{az}$ = 5.6 %
MAPE on $h^M$ = 73 %



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**Isothermal phase equilibrium data**

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Toghiani, Rebecca K - Toghiani, Hossein - Venkateswarlu, Gundapaneni, Vapor-liquid equilibria for methyl tert-butyl ether + methanol and tert-amyl methyl ether + methanol, Fluid Phase Equilibria 1-2 (1996) 157-168. doi:10.1016/0378-3812(96)03043-9

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3603 | 0.9972 | 0.9803 |
| 0.3659 | 0.9939 | 0.9613 |
| 0.3739 | 0.9887 | 0.9366 |
| 0.3927 | 0.9744 | 0.8860 |
| 0.4251 | 0.9488 | 0.8076 |
| 0.4410 | 0.9347 | 0.7603 |
| 0.4514 | 0.9259 | 0.7384 |
| 0.4659 | 0.9120 | 0.7031 |
| 0.4775 | 0.9005 | 0.6804 |
| 0.4936 | 0.8818 | 0.6503 |
| 0.5063 | 0.8654 | 0.6217 |
| 0.5141 | 0.8546 | 0.6085 |
| 0.5250 | 0.8398 | 0.5836 |
| 0.5356 | 0.8227 | 0.5681 |
| 0.5462 | 0.8063 | 0.5481 |
| 0.5546 | 0.7899 | 0.5340 |
| 0.5621 | 0.7752 | 0.5188 |
| 0.5717 | 0.7551 | 0.4990 |
| 0.5823 | 0.7343 | 0.4844 |
| 0.5932 | 0.7034 | 0.4592 |
| 0.5986 | 0.6876 | 0.4497 |
| 0.6069 | 0.6634 | 0.4402 |
| 0.6129 | 0.6396 | 0.4203 |
| 0.6225 | 0.6035 | 0.4028 |
| 0.6311 | 0.5658 | 0.3871 |
| 0.6378 | 0.5283 | 0.3692 |
| 0.6452 | 0.4809 | 0.3502 |
| 0.6501 | 0.4431 | 0.3358 |
| 0.6541 | 0.4060 | 0.3228 |
| 0.6577 | 0.3673 | 0.3034 |
| 0.6618 | 0.2884 | 0.2720 |
| 0.6622 | 0.2239 | 0.2370 |
| 0.6598 | 0.1766 | 0.2077 |
| 0.6584 | 0.1621 | 0.1991 |
| 0.6522 | 0.1194 | 0.1643 |
| 0.6347 | 0.0595 | 0.0991 |
| 0.6236 | 0.0360 | 0.0680 |

Lee, J.D. - Lee, T.J. - Park, S.J., Infinite dilution activity coefficients and vapor-liquid equilibria for the binary systems containing MTBE, Hwahak Konghak 5 (1995) 527-534.

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4489 | 0.9995 | 0.9970 |
| 0.4534 | 0.9972 | 0.9850 |
| 0.4721 | 0.9859 | 0.9358 |
| 0.4979 | 0.9701 | 0.8737 |
| 0.5415 | 0.9384 | 0.7801 |
| 0.5847 | 0.9040 | 0.6991 |
| 0.6246 | 0.8638 | 0.6322 |
| 0.6569 | 0.8240 | 0.5816 |
| 0.6891 | 0.7761 | 0.5332 |
| 0.7229 | 0.7032 | 0.4820 |
| 0.7482 | 0.6332 | 0.4409 |
| 0.7664 | 0.5512 | 0.4063 |
| 0.7834 | 0.4536 | 0.3621 |
| 0.7937 | 0.3335 | 0.3101 |
| 0.7894 | 0.1873 | 0.2261 |
| 0.7696 | 0.0970 | 0.1485 |
| 0.7515 | 0.0543 | 0.0936 |
| 0.7234 | 0.0079 | 0.0163 |

Fárková, Jana - Linek, Jan - Wichterle, Ivan, Isothermal vapour-liquid equilibria and excess volumes in the methanol-aliphatic ether systems, Fluid Phase Equilibria 1 (1995) 53-65. doi:10.1016/0378-3812(95)02710-V

**T / K = 325.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.6149 | 0.9957 | 0.9714 | |
| 0.6812 | 0.9619 | 0.8528 | |
| 0.7601 | 0.9158 | 0.7389 | |
| 0.7947 | 0.8911 | 0.6967 | |
| 0.8407 | 0.8506 | 0.6352 | |
| 0.8905 | 0.7918 | 0.5759 | |
| 0.9444 | 0.7111 | 0.5112 | |
| 0.9871 | 0.6062 | 0.4526 | |
| 0.9950 | 0.5772 | 0.4377 | |
| 1.011 | 0.5087 | 0.4064 | |
| 1.023 | 0.4471 | 0.3779 | |
| 1.030 | 0.3786 | 0.3466 | |
| 1.032 | 0.3140 | 0.3140 | AZEO |
| 1.032 | 0.3040 | 0.3097 | |
| 1.027 | 0.2397 | 0.2723 | |
| 1.021 | 0.1932 | 0.2420 | |
| 0.9967 | 0.1158 | 0.1772 | |
| 0.9502 | 0.0413 | 0.0790 | |

Toghiani, Rebecca K - Toghiani, Hossein - Venkateswarlu, Gundapaneni, Vapor-liquid equilibria for methyl tert-butyl ether + methanol and tert-amyl methyl ether + methanol, Fluid Phase Equilibria 1-2 (1996) 157-168. doi:10.1016/0378-3812(96)03043-9

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.8550 | 0.9978 | 0.9879 |
| 0.8696 | 0.9934 | 0.9660 |
| 0.8946 | 0.9844 | 0.9337 |
| 0.9213 | 0.9734 | 0.9000 |
| 0.9505 | 0.9607 | 0.8642 |
| 0.9715 | 0.9514 | 0.8359 |
| 1.005 | 0.9362 | 0.7986 |
| 1.043 | 0.9175 | 0.7543 |
| 1.078 | 0.8980 | 0.7183 |
| 1.107 | 0.8799 | 0.6907 |
| 1.114 | 0.8733 | 0.6775 |
| 1.134 | 0.8596 | 0.6589 |
| 1.157 | 0.8422 | 0.6362 |
| 1.178 | 0.8250 | 0.6184 |
| 1.199 | 0.8038 | 0.6005 |
| 1.216 | 0.7864 | 0.5755 |
| 1.250 | 0.7473 | 0.5512 |
| 1.266 | 0.7236 | 0.5278 |
| 1.287 | 0.6915 | 0.5050 |
| 1.302 | 0.6636 | 0.4916 |
| 1.317 | 0.6349 | 0.4758 |
| 1.334 | 0.5951 | 0.4537 |
| 1.343 | 0.5658 | 0.4395 |
| 1.358 | 0.5148 | 0.4226 |
| 1.369 | 0.4646 | 0.3978 |
| 1.377 | 0.4108 | 0.3744 |
| 1.379 | 0.3770 | 0.3609 |
| 1.381 | 0.3242 | 0.3323 |
| 1.375 | 0.2572 | 0.2958 |
| 1.356 | 0.1767 | 0.2424 |
| 1.217 | 0.0198 | 0.0420 |

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**Isobaric phase equilibrium data**

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Toghiani, Rebecca K - Toghiani, Hossein - Venkateswarlu, Gundapaneni, Vapor-liquid equilibria for methyl tert-butyl ether + methanol and tert-amyl methyl ether + methanol, Fluid Phase Equilibria 1-2 (1996) 157-168. doi:10.1016/0378-3812(96)03043-9

**P / bar = 0.5333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 321.97 | 0.9981 | 0.9881 |
| 321.61 | 0.9946 | 0.9689 |
| 320.94 | 0.9864 | 0.9299 |
| 320.50 | 0.9806 | 0.9117 |
| 319.82 | 0.9714 | 0.8768 |
| 319.37 | 0.9639 | 0.8544 |
| 318.75 | 0.9549 | 0.8254 |
| 318.14 | 0.9447 | 0.7946 |
| 317.52 | 0.9344 | 0.7654 |
| 316.66 | 0.9185 | 0.7273 |
| 315.94 | 0.9046 | 0.6949 |
| 315.26 | 0.8881 | 0.6640 |
| 314.42 | 0.8656 | 0.6264 |
| 313.95 | 0.8519 | 0.6059 |
| 313.40 | 0.8343 | 0.5827 |
| 313.05 | 0.8221 | 0.5632 |
| 313.01 | 0.8201 | 0.5623 |
| 312.73 | 0.8111 | 0.5539 |
| 311.96 | 0.7767 | 0.5182 |
| 311.98 | 0.7790 | 0.5170 |
| 311.54 | 0.7572 | 0.4977 |
| 311.21 | 0.7396 | 0.4854 |
| 310.90 | 0.7226 | 0.4701 |
| 310.52 | 0.6964 | 0.4530 |
| 310.14 | 0.6715 | 0.4362 |
| 309.75 | 0.6398 | 0.4182 |
| 309.47 | 0.6127 | 0.4011 |
| 309.20 | 0.5837 | 0.3875 |
| 308.90 | 0.5494 | 0.3712 |
| 308.58 | 0.5014 | 0.3556 |
| 308.26 | 0.4491 | 0.3297 |
| 308.04 | 0.4001 | 0.3101 |
| 307.87 | 0.3554 | 0.2918 |
| 307.71 | 0.2886 | 0.2627 |
| 307.66 | 0.2372 | 0.2379 |
| 307.82 | 0.1510 | 0.1868 |
| 308.02 | 0.1154 | 0.1570 |
| 308.45 | 0.0727 | 0.1112 |
| 308.97 | 0.0425 | 0.0748 |
| 309.67 | 0.0134 | 0.0253 |

Loras, Sonia - Aucejo, Antonio - Muñoz, Rosa - Wisniak, Jaime, Azeotropic Behavior in the System Methanol + Methyl 1,1-Dimethylethyl Ether, Journal of Chemical & Engineering Data 2 (1999) 203-208. doi:10.1021/je9801563

**P / bar = 0.7840**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 329.64 | 0.9853 | 0.9381 |

| | | |
|---|---|---|
| 328.10 | 0.9687 | 0.8695 |
| 325.49 | 0.9263 | 0.7475 |
| 323.21 | 0.8642 | 0.6367 |
| 321.86 | 0.8104 | 0.5732 |
| 320.95 | 0.7695 | 0.5362 |
| 320.22 | 0.7205 | 0.5011 |
| 319.26 | 0.6650 | 0.4583 |
| 318.53 | 0.5865 | 0.4255 |
| 318.24 | 0.5453 | 0.4055 |
| 318.02 | 0.5019 | 0.3864 |
| 317.87 | 0.4540 | 0.3677 |
| 317.71 | 0.4045 | 0.3483 |
| 317.63 | 0.3568 | 0.3249 |
| 317.62 | 0.3089 | 0.3017 |
| 317.59 | 0.2695 | 0.2801 |
| 317.61 | 0.2401 | 0.2627 |
| 317.74 | 0.1940 | 0.2377 |
| 317.93 | 0.1582 | 0.2083 |
| 318.33 | 0.1082 | 0.1673 |
| 318.97 | 0.0620 | 0.1129 |
| 319.67 | 0.0289 | 0.0607 |

Arce, Alberto - Martínez-Ageitos, José - Soto, Ana, VLE Measurements of Binary Mixtures of Methanol, Ethanol, 2-Methoxy-2-methylpropane, and 2-Methoxy-2-methylbutane at 101.32 kPa, Journal of Chemical & Engineering Data 4 (1996) 718-723. doi:10.1021/je950323o

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 337.05 | 0.9929 | 0.9690 |
| 336.48 | 0.9859 | 0.9413 |
| 335.58 | 0.9724 | 0.8959 |
| 334.85 | 0.9617 | 0.8614 |
| 334.33 | 0.9532 | 0.8382 |
| 333.39 | 0.9363 | 0.7914 |
| 332.82 | 0.9263 | 0.7620 |
| 332.42 | 0.9176 | 0.7430 |
| 331.96 | 0.9080 | 0.7235 |
| 331.52 | 0.8980 | 0.7024 |
| 331.07 | 0.8857 | 0.6833 |
| 330.58 | 0.8726 | 0.6611 |
| 330.07 | 0.8577 | 0.6391 |
| 329.62 | 0.8435 | 0.6204 |
| 328.87 | 0.8155 | 0.5903 |
| 328.43 | 0.7963 | 0.5714 |
| 327.94 | 0.7743 | 0.5501 |
| 327.54 | 0.7533 | 0.5323 |
| 327.18 | 0.7317 | 0.5149 |
| 326.77 | 0.7067 | 0.4965 |
| 326.39 | 0.6793 | 0.4783 |
| 326.05 | 0.6511 | 0.4608 |
| 325.72 | 0.6176 | 0.4437 |
| 325.45 | 0.5858 | 0.4295 |
| 325.26 | 0.5627 | 0.4185 |
| 325.08 | 0.5362 | 0.4064 |
| 324.94 | 0.5126 | 0.3962 |
| 324.79 | 0.4831 | 0.3834 |
| 324.61 | 0.4439 | 0.3673 |
| 324.51 | 0.4141 | 0.3547 |
| 324.45 | 0.3927 | 0.3450 |
| 324.40 | 0.3673 | 0.3343 |
| 324.37 | 0.3440 | 0.3237 |
| 324.33 | 0.3211 | 0.3131 |
| 324.33 | 0.2908 | 0.2984 |
| 324.34 | 0.2797 | 0.2930 |
| 324.35 | 0.2770 | 0.2919 |
| 324.37 | 0.2557 | 0.2806 |
| 324.41 | 0.2304 | 0.2659 |
| 324.50 | 0.2072 | 0.2516 |
| 324.61 | 0.1811 | 0.2348 |
| 324.82 | 0.1527 | 0.2138 |
| 325.54 | 0.0886 | 0.1528 |
| 326.15 | 0.0559 | 0.1109 |
| 326.83 | 0.0283 | 0.0678 |
| 327.57 | 0.0047 | 0.0243 |

Wang, Y. - Tong, A. - Su, Y. - Yang, Z., Isobaric Vapor-Liquid Equilibrium for the System MTBE-Methanol, Shiyou Huagong 7 (1989) 442-446.

**P / bar = 5.000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 383.36 | 0.9851 | 0.9555 |
| 381.91 | 0.9446 | 0.8694 |
| 381.33 | 0.9319 | 0.8441 |
| 380.16 | 0.9018 | 0.7998 |
| 378.56 | 0.8487 | 0.7376 |
| 377.88 | 0.8201 | 0.7045 |
| 376.94 | 0.7795 | 0.6702 |
| 376.57 | 0.7465 | 0.6481 |
| 376.10 | 0.7029 | 0.6151 |
| 375.63 | 0.6712 | 0.5890 |
| 375.02 | 0.5316 | 0.5215 |
| 374.94 | 0.4617 | 0.4849 |
| 375.33 | 0.3582 | 0.4224 |
| 375.70 | 0.3142 | 0.4059 |
| 376.24 | 0.2386 | 0.3494 |
| 377.05 | 0.1901 | 0.3136 |

| | | |
|---|---|---|
| 378.23 | 0.1365 | 0.2625 |
| 380.18 | 0.0859 | 0.1945 |
| 382.94 | 0.0398 | 0.1136 |

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**Enthalpy of mixing**

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Tusel-Langer, E. - Garcia Alonso, J. M. - Villamañan Olfos, M. A. - Lichtenthaler, R. N., Excess enthalpies of mixtures containing n-heptane, methanol and methyl tert-butyl ether (MTBE), Journal of Solution Chemistry 1 (1991) 153-163. doi:10.1007/BF00651647

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -7.300 | 0.9787 |
| -7.600 | 0.9636 |
| -5.800 | 0.9475 |
| 2.500 | 0.9216 |
| 14.90 | 0.8932 |
| 76.00 | 0.8022 |
| 159.20 | 0.6977 |
| 228.80 | 0.6021 |
| 283.60 | 0.5079 |
| 325.80 | 0.3920 |
| 328.20 | 0.2860 |
| 300.60 | 0.2035 |
| 217.70 | 0.1090 |
| 128.10 | 0.0566 |

Tusel-Langer, E. - Garcia Alonso, J. M. - Villamañan Olfos, M. A. - Lichtenthaler, R. N., Excess enthalpies of mixtures containing n-heptane, methanol and methyl tert-butyl ether (MTBE), Journal of Solution Chemistry 1 (1991) 153-163. doi:10.1007/BF00651647

**T / K = 313.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -7.500 | 0.9824 |
| 1.800 | 0.9635 |
| 4.900 | 0.9536 |
| 8.000 | 0.9433 |
| 12.70 | 0.9326 |
| 17.10 | 0.9216 |
| 28.60 | 0.8981 |
| 87.40 | 0.8150 |
| 145.50 | 0.7746 |
| 176.60 | 0.7062 |
| 253.70 | 0.6126 |
| 323.60 | 0.4947 |
| 360.00 | 0.4234 |
| 378.20 | 0.3414 |
| 366.70 | 0.2956 |
| 355.50 | 0.2461 |
| 323.60 | 0.1923 |
| 269.80 | 0.1339 |
| 205.50 | 0.0920 |
| 133.80 | 0.0566 |

Tusel-Langer, E. - Garcia Alonso, J. M. - Villamañan Olfos, M. A. - Lichtenthaler, R. N., Excess enthalpies of mixtures containing n-heptane, methanol and methyl tert-butyl ether (MTBE), Journal of Solution Chemistry 1 (1991) 153-163. doi:10.1007/BF00651647

**T / K = 323.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -1.700 | 0.9787 |
| 2.800 | 0.9636 |
| 9.400 | 0.9475 |
| 23.40 | 0.9216 |
| 46.10 | 0.8932 |
| 125.50 | 0.8022 |
| 225.50 | 0.6977 |
| 310.30 | 0.6021 |
| 379.30 | 0.5079 |
| 429.40 | 0.3920 |
| 432.10 | 0.2860 |
| 393.00 | 0.2035 |
| 274.20 | 0.1090 |
| 165.00 | 0.0566 |

Westerholt, A., Weiterentwicklung der Gruppenbeitragszustandsgleichung VTPR zur Beschreibung der TAME-Synthese und Spaltung durch systematische Messung fehlender Phasengleichgewichtsdaten und Anpassung der erforderlichen Parameter, Master's Thesis (2010) 1-113.

**T / K = 333.15**

**P / bar = 9.290**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 23.90 | 0.9448 |
| 67.90 | 0.8896 |
| 124.43 | 0.8344 |
| 185.28 | 0.7790 |
| 247.66 | 0.7236 |
| 306.01 | 0.6682 |
| 361.33 | 0.6129 |
| 417.69 | 0.5572 |

| | |
|---|---|
| 465.81 | 0.5018 |
| 495.37 | 0.4463 |
| 499.22 | 0.3905 |
| 498.64 | 0.3347 |
| 484.77 | 0.2791 |
| 448.00 | 0.2233 |
| 386.10 | 0.1675 |
| 285.91 | 0.1118 |
| 153.77 | 0.0560 |

Dahmani, Abdallah - Mokbel, Ilham - Jose, Jacques, Excess volume, excess enthalpy and vapour–liquid equilibria of N,N,N′,N′-tetramethyl-1,3-butanediamine + n-heptane or + cyclohexane mixtures, Fluid Phase Equilibria 1-2 (2002) 193-204. doi:10.1016/S0378-3812(02)00180-2

| **T / K =** | **363.15** |
|---|---|
| **P / bar =** | **6.000** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 42.47 | 0.9636 |
| 42.69 | 0.9632 |
| 101.86 | 0.9216 |
| 101.78 | 0.9208 |
| 174.41 | 0.8728 |
| 177.08 | 0.8714 |
| 269.71 | 0.8160 |
| 381.75 | 0.7462 |
| 384.94 | 0.7439 |
| 509.17 | 0.6622 |
| 509.99 | 0.6595 |
| 639.59 | 0.5575 |
| 741.11 | 0.4236 |
| 694.50 | 0.2462 |
| 696.03 | 0.2440 |
| 694.05 | 0.2440 |
| 563.34 | 0.1623 |
| 558.17 | 0.1623 |
| 299.33 | 0.0693 |
| 165.80 | 0.0355 |
| 164.88 | 0.0355 |
| 87.68 | 0.0179 |

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**Critical point**

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Han, Kewei - Xia, Shuqian - Ma, Peisheng - Yan, Fangyou - Liu, Tao, Measurement of critical temperatures and critical pressures for binary mixtures of methyl tert-butyl ether (MTBE)+alcohol and MTBE+alkane, The Journal of Chemical Thermodynamics (2013) 111-117. doi:10.1016/j.jct.2013.03.002

| T / K | P / bar | $x_1$ |
|---|---|---|
| 492.00 | 38.97 | 0.1231 |
| 491.00 | 41.52 | 0.2007 |
| 490.40 | 45.83 | 0.3001 |
| 489.20 | 49.26 | 0.3997 |
| 489.80 | 52.81 | 0.5003 |
| 491.90 | 56.05 | 0.6003 |
| 493.60 | 61.24 | 0.7002 |
| 497.70 | 66.48 | 0.8001 |
| 503.50 | 72.87 | 0.9000 |

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**Azeotropic point**

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Arce, Alberto - Martínez-Ageitos, José - Soto, Ana, VLE Measurements of Binary Mixtures of Methanol, Ethanol, 2-Methoxy-2-methylpropane, and 2-Methoxy-2-methylbutane at 101.32 kPa, Journal of Chemical & Engineering Data 4 (1996) 718-723. doi:10.1021/je950323o

| T / K | P / bar | $x_1$ |
|---|---|---|
| 324.32 | 1.013 | 0.3090 |

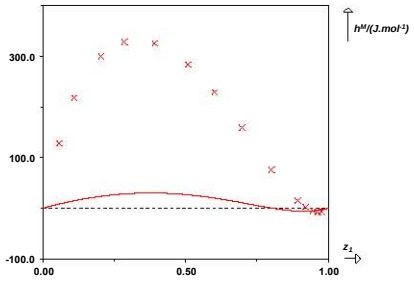
Toghiani, Rebecca K - Toghiani, Hossein - Venkateswarlu, Gundapaneni, Vapor-liquid equilibria for methyl tert-butyl ether + methanol and tert-amyl methyl ether + methanol, Fluid Phase Equilibria 1-2 (1996) 157-168. doi:10.1016/0378-3812(96)03043-9

| T / K | P / bar | $x_1$ |
|---|---|---|
| 307.65 | 0.5333 | 0.2380 |

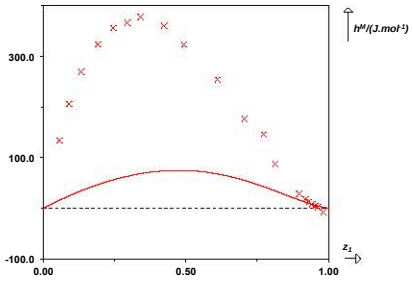
Loras, Sonia - Aucejo, Antonio - Muñoz, Rosa - Wisniak, Jaime, Azeotropic Behavior in the System Methanol + Methyl 1,1-Dimethylethyl Ether, Journal of Chemical & Engineering Data 2 (1999) 203-208. doi:10.1021/je9801563

| T / K | P / bar | $x_1$ |
|---|---|---|
| 317.58 | 0.7840 | 0.2890 |

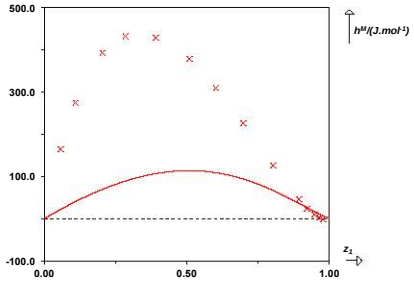
T/K = 298.15 - P/bar = 1.0100



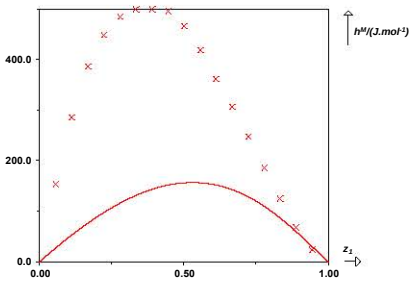

T/K = 313.15 - P/bar = 1.0100



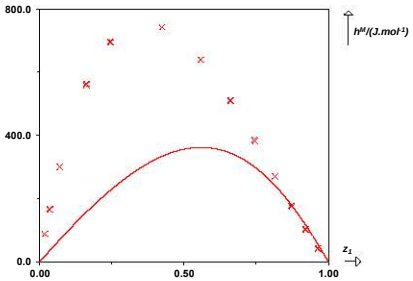

T/K = 323.15 - P/bar = 1.0100



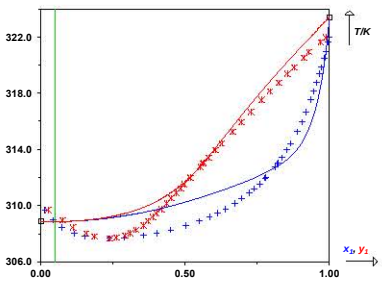

T/K = 333.15 - P/bar = 9.2900



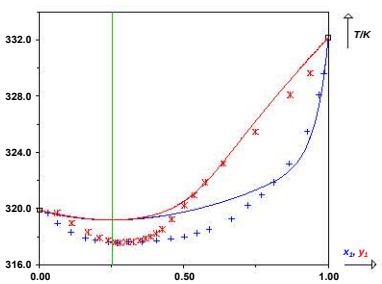

T/K = 363.15 - P/bar = 6.00



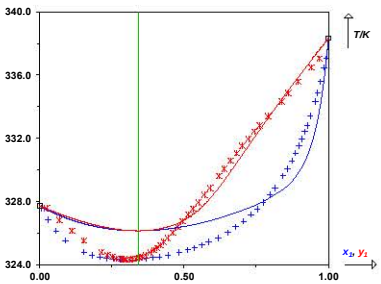

P/bar = 0.53330



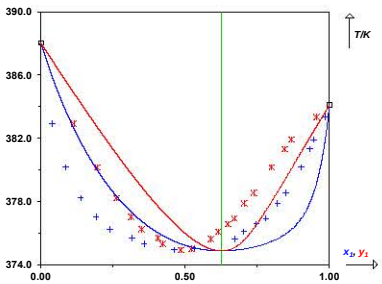

P/bar = 0.78400



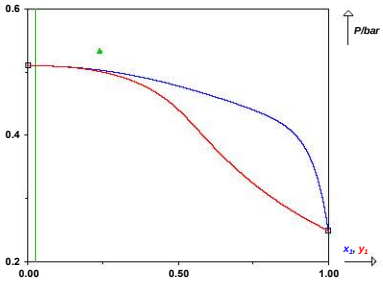

P/bar = 1.01320



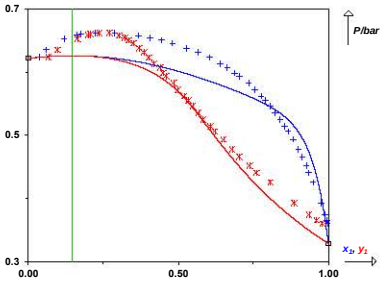

P/bar = 5.00000



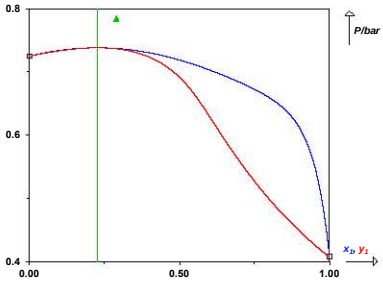

T/K = 307.65



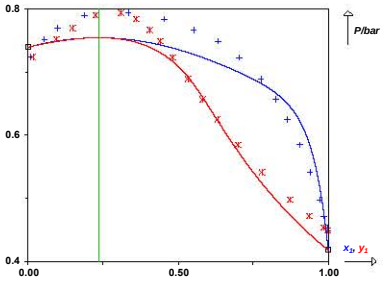

T/K = 313.15



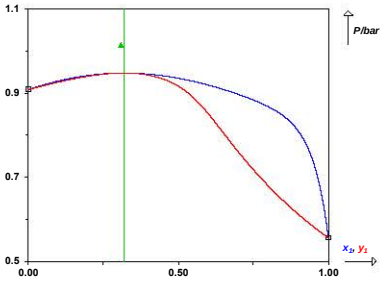

T/K = 317.58



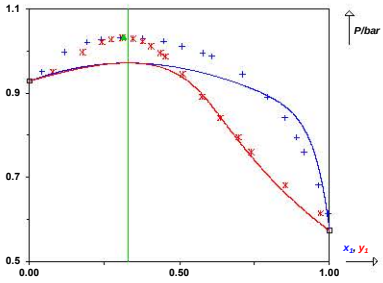

T/K = 318.15



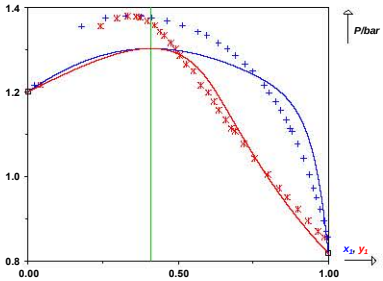

T/K = 324.32



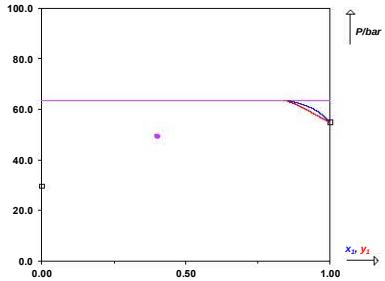

T/K = 325.00



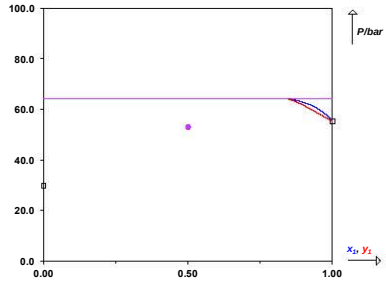
T/K = 333.15



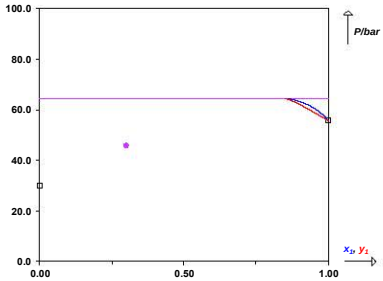

T/K = 489.20



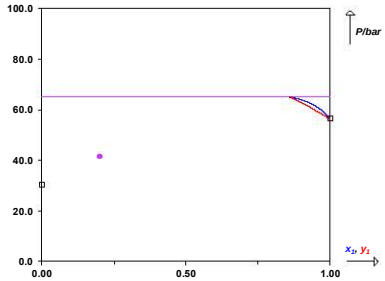

T/K = 489.80



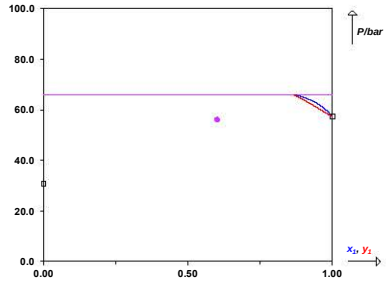

T/K = 490.40



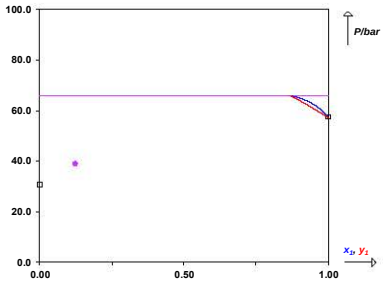

T/K = 491.00



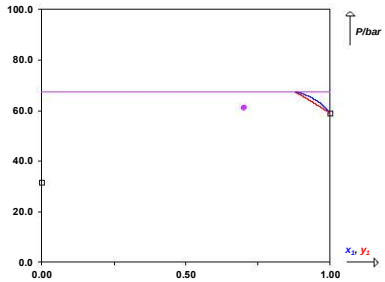

T/K = 491.90



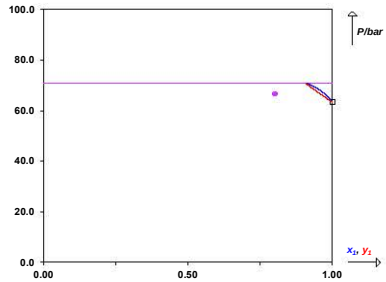

T/K = 492.00



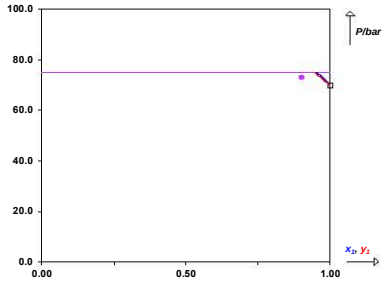

T/K = 493.60




T/K = 497.70




T/K = 503.50



## ETHANOL (1) + ETHYL ACETATE (2)

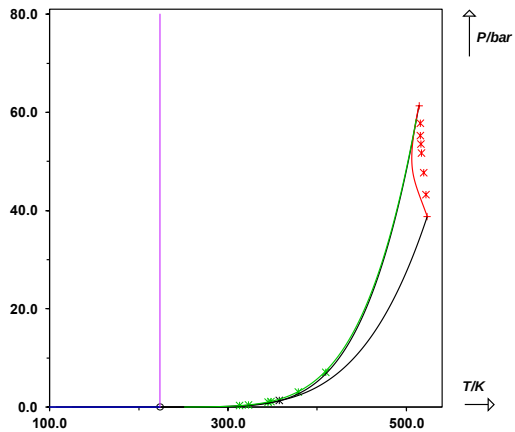
| | | |
|---|---|---|
| **CAS** | 64-17-5 | 141-78-6 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | XEKOWRVHYACXOJ-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 523.30 |
| **$P_c$ / bar** | 61.37 | 38.80 |
| **ω** | 0.644 | 0.366 |

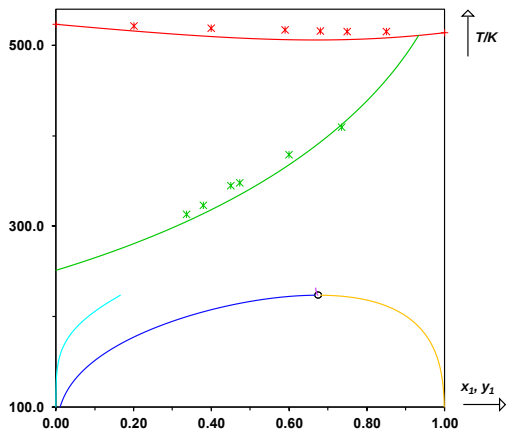
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 252
B/MPa = 322

*Deviations*
MAPE on x = 18 %
MAPE on y = 13 %
MAPE on $x_c$ = 120 %
MAPE on $P_c$ = 18 %
MAPE on $x_{az}$ = 9.7 %
MAPE on $P_{az}$ = 0.79 %
MAPE on $h^M$ = 16 %
MAPE on $c_P^M$ = 100 %



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**Isothermal phase equilibrium data**

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Mertl, I., Liquid-vapour equilibrium. IL. Phase equilibria in the ternary system ethyl acetate-ethanol-water, Collection of Czechoslovak Chemical Communications 2 (1972) 366-374. doi:10.1135/cccc19720366

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1821 | 0.9940 | 0.9780 | |
| 0.2012 | 0.9560 | 0.8560 | |
| 0.2175 | 0.9160 | 0.7730 | |
| 0.2440 | 0.8130 | 0.6300 | |
| 0.2559 | 0.7580 | 0.5720 | |
| 0.2662 | 0.6800 | 0.5160 | |
| 0.2777 | 0.5460 | 0.4400 | |
| 0.2802 | 0.5050 | 0.4260 | |
| 0.2824 | 0.4480 | 0.3930 | |
| 0.2842 | 0.3370 | 0.3360 | |
| 0.2842 | 0.3355 | 0.3355 | AZEO |
| 0.2828 | 0.2510 | 0.2840 | |
| 0.2728 | 0.1150 | 0.1710 | |
| 0.2674 | 0.0800 | 0.1290 | |
| 0.2604 | 0.0400 | 0.0720 | |

Pavlíček, Jan - Bogdanić, Grozdana - Wichterle, Ivan, Vapour–liquid and chemical equilibria in the ethyl ethanoate+ethanol+propyl ethanoate+propanol system accompanied with transesterification reaction, Fluid Phase Equilibria (2012) 61-68. doi:10.1016/j.fluid.2012.05.016

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.3022 | 0.9905 | 0.9667 | |
| 0.3170 | 0.9693 | 0.9037 | |
| 0.3428 | 0.9245 | 0.8027 | |
| 0.3591 | 0.8887 | 0.7440 | |
| 0.3737 | 0.8517 | 0.6926 | |
| 0.3917 | 0.7912 | 0.6287 | |
| 0.4113 | 0.6984 | 0.5569 | |
| 0.4214 | 0.6285 | 0.5111 | |
| 0.4289 | 0.5513 | 0.4682 | |
| 0.4340 | 0.4671 | 0.4241 | |
| 0.4360 | 0.3795 | 0.3795 | AZEO |
| 0.4360 | 0.3732 | 0.3733 | |
| 0.4327 | 0.2601 | 0.3059 | |
| 0.4242 | 0.1737 | 0.2362 | |
| 0.4148 | 0.1166 | 0.1788 | |
| 0.4012 | 0.0614 | 0.1069 | |
| 0.3868 | 0.0184 | 0.0360 | |

Mertl, I., Liquid-vapour equilibrium. IL. Phase equilibria in the ternary system ethyl acetate-ethanol-water, Collection of Czechoslovak Chemical Communications 2 (1972) 366-374. doi:10.1135/cccc19720366

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3790 | 0.9945 | 0.9815 |
| 0.4033 | 0.9630 | 0.8960 |
| 0.4336 | 0.9170 | 0.7990 |
| 0.4662 | 0.8490 | 0.7030 |
| 0.4804 | 0.8040 | 0.6520 |
| 0.4954 | 0.7570 | 0.6110 |
| 0.5152 | 0.6600 | 0.5470 |
| 0.5300 | 0.5360 | 0.4790 |
| 0.5360 | 0.4080 | 0.3990 |
| 0.5345 | 0.3180 | 0.3480 |
| 0.5326 | 0.2850 | 0.3260 |
| 0.5136 | 0.1470 | 0.2140 |
| 0.5020 | 0.1020 | 0.1610 |
| 0.4866 | 0.0560 | 0.0980 |

Nagata, Isamu - Yamada, Toshiro - Nakagawa, Shigeo, Excess Gibbs free energies and heats of mixing for binary systems ethyl acetate with methanol, ethanol, 1-propanol, and 2-propanol, Journal of Chemical & Engineering Data 3 (1975) 271-275. doi:10.1021/je60066a007

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4309 | 0.9190 | 0.8110 |
| 0.4517 | 0.8880 | 0.7600 |
| 0.4738 | 0.8350 | 0.6870 |
| 0.5062 | 0.7270 | 0.5940 |
| 0.5266 | 0.6150 | 0.5110 |
| 0.5318 | 0.5720 | 0.4890 |
| 0.5370 | 0.5050 | 0.4540 |
| 0.5389 | 0.4060 | 0.3960 |
| 0.5380 | 0.2920 | 0.3280 |
| 0.5250 | 0.1860 | 0.2510 |
| 0.5025 | 0.1100 | 0.1750 |

Mertl, I., Liquid-vapour equilibrium. IL. Phase equilibria in the ternary system ethyl acetate-ethanol-water, Collection of Czechoslovak Chemical Communications 2 (1972) 366-374. doi:10.1135/cccc19720366

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.7314 | 0.9935 | 0.9825 |
| 0.7458 | 0.9820 | 0.9540 |
| 0.8447 | 0.8690 | 0.7630 |

| | | |
|---|---|---|
| 0.8861 | 0.7900 | 0.6790 |
| 0.9071 | 0.7370 | 0.6330 |
| 0.9383 | 0.6130 | 0.5460 |
| 0.9466 | 0.5480 | 0.5070 |
| 0.9495 | 0.5120 | 0.4830 |
| 0.9482 | 0.3750 | 0.4030 |
| 0.9418 | 0.3090 | 0.3590 |
| 0.9303 | 0.2450 | 0.3190 |
| 0.9055 | 0.1780 | 0.2530 |
| 0.8687 | 0.0970 | 0.1610 |
| 0.8471 | 0.0680 | 0.1120 |
| 0.8207 | 0.0250 | 0.0520 |

Pavlíček, Jan - Bogdanić, Grozdana - Wichterle, Ivan, Vapour–liquid and chemical equilibria in the ethyl ethanoate+ethanol+propyl ethanoate+propanol system accompanied with transesterification reaction, Fluid Phase Equilibria (2012) 61-68. doi:10.1016/j.fluid.2012.05.016

**T / K = 348.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.9035 | 0.9890 | 0.9737 | |
| 0.9337 | 0.9646 | 0.9206 | |
| 0.9828 | 0.9171 | 0.8378 | |
| 1.014 | 0.8819 | 0.7863 | |
| 1.041 | 0.8447 | 0.7446 | |
| 1.072 | 0.7831 | 0.6830 | |
| 1.106 | 0.6898 | 0.6087 | |
| 1.122 | 0.6170 | 0.5607 | |
| 1.131 | 0.5411 | 0.5141 | |
| 1.134 | 0.4728 | 0.4728 | AZEO |
| 1.134 | 0.4582 | 0.4636 | |
| 1.127 | 0.3659 | 0.4045 | |
| 1.104 | 0.2525 | 0.3236 | |
| 1.071 | 0.1696 | 0.2465 | |
| 1.040 | 0.1139 | 0.1817 | |
| 1.003 | 0.0615 | 0.1092 | |
| 0.9651 | 0.0186 | 0.0359 | |

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**Isobaric phase equilibrium data**

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Li, Qunsheng - Zhang, Jiguo - Lei, Zhigang - Zhu, Jiujuan - Xing, Fengying, Isobaric Vapor-Liquid Equilibrium for Ethyl Acetate + Ethanol + 1-Ethyl-3-methylimidazolium Tetrafluoroborate, Journal of Chemical & Engineering Data 2 (2009) 193-197. doi:10.1021/je800175s

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 350.13 | 0.9510 | 0.8940 |
| 348.85 | 0.8930 | 0.8080 |
| 347.04 | 0.8050 | 0.7010 |
| 346.13 | 0.6770 | 0.6110 |
| 345.46 | 0.5820 | 0.5320 |
| 345.06 | 0.4830 | 0.4700 |
| 345.00 | 0.3900 | 0.4080 |
| 345.36 | 0.2910 | 0.3460 |
| 345.94 | 0.1950 | 0.2700 |
| 347.55 | 0.0870 | 0.1640 |
| 348.86 | 0.0380 | 0.0760 |

Susial, P. - Rodriguez-Henriquez, J.J. - Sosa-Rosario, A. - Rios-Santana, R., Vapor-Liquid Equilibrium of Ethyl Acetate + CnH2n+1OH (n= 1,2,3) Binary Systems at 0.3 MPa, Chinese Journal of Chemical Engineering 4 (2012) 723-730. doi:10.1016/S1004-9541(11)60241-3

**P / bar = 3.000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 386.65 | 0.0280 | 0.0560 |
| 386.15 | 0.0420 | 0.0830 |
| 385.75 | 0.0560 | 0.1090 |
| 384.45 | 0.0960 | 0.1730 |
| 383.45 | 0.1350 | 0.2220 |
| 382.45 | 0.1730 | 0.2690 |
| 381.65 | 0.2220 | 0.3260 |
| 381.35 | 0.2460 | 0.3480 |
| 380.95 | 0.2690 | 0.3700 |
| 380.55 | 0.3040 | 0.4020 |
| 380.25 | 0.3480 | 0.4340 |
| 379.35 | 0.4640 | 0.5230 |
| 379.25 | 0.4940 | 0.5420 |
| 379.15 | 0.5140 | 0.5520 |
| 379.05 | 0.6760 | 0.6420 |
| 379.15 | 0.7010 | 0.6590 |
| 379.25 | 0.7400 | 0.6920 |
| 380.25 | 0.8640 | 0.8080 |
| 381.15 | 0.9470 | 0.9100 |
| 381.85 | 0.9880 | 0.9710 |

Susial, Pedro - Sosa-Rosario, Aday - Rodríguez-Henríquez, Juan José - Rios-Santana, Raul, Vapor Pressure and VLE Data Measurements on Ethyl Acetate/Ethanol Binary System at 0.1, 0.5, and 0.7 MPa, JOURNAL OF CHEMICAL ENGINEERING OF JAPAN 3 (2011) 155-163. doi:10.1252/jcej.10we176

**P / bar = 7.000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 410.95 | 0.9940 | 0.9880 |

| | | |
|---|---|---|
| 410.65 | 0.9710 | 0.9590 |
| 410.15 | 0.9160 | 0.8970 |
| 409.95 | 0.8970 | 0.8770 |
| 409.85 | 0.8770 | 0.8570 |
| 409.65 | 0.6760 | 0.6920 |
| 409.75 | 0.6420 | 0.6670 |
| 409.95 | 0.6160 | 0.6510 |
| 410.05 | 0.5890 | 0.6420 |
| 410.25 | 0.5610 | 0.6250 |
| 410.45 | 0.5330 | 0.6070 |
| 410.65 | 0.5040 | 0.5890 |
| 411.05 | 0.4740 | 0.5710 |
| 411.85 | 0.4130 | 0.5230 |
| 412.35 | 0.3810 | 0.4940 |
| 412.95 | 0.3370 | 0.4540 |
| 413.85 | 0.2920 | 0.4140 |
| 414.35 | 0.2690 | 0.3920 |
| 415.05 | 0.2340 | 0.3590 |
| 416.65 | 0.1850 | 0.3040 |
| 417.65 | 0.1480 | 0.2570 |
| 418.45 | 0.1220 | 0.2220 |
| 419.25 | 0.0960 | 0.1850 |
| 422.05 | 0.0280 | 0.0700 |
| 422.65 | 0.0140 | 0.0420 |

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**Enthalpy of mixing**

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Ortega, J., Excess enthalpy. Ethanol-ethyl ethanoate system, Int. Data Ser. Sel. Data Mixtures Ser. A 3 (1995)

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 177.50 | 0.9651 |
| 363.70 | 0.9229 |
| 545.20 | 0.8787 |
| 712.30 | 0.8330 |
| 864.50 | 0.7862 |
| 997.10 | 0.7387 |
| 1109.3 | 0.6923 |
| 1199.0 | 0.6478 |
| 1277.3 | 0.6061 |
| 1284.8 | 0.6028 |
| 1328.0 | 0.5661 |
| 1345.0 | 0.5557 |
| 1379.7 | 0.4986 |
| 1378.1 | 0.4329 |
| 1315.6 | 0.3573 |
| 1161.9 | 0.2737 |
| 892.10 | 0.1848 |
| 539.20 | 0.0928 |

Zhang, Rui - Yan, Weidong - Wang, Xu - Lin, Ruisen, Molar excess enthalpies of ethyl acetate+alkanols at T=298.15K, p=10.0MPa, Thermochimica Acta 2 (2005) 155-161. doi:10.1016/j.tca.2005.03.009

**T / K = 298.15**

**P / bar = 100.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 141.00 | 0.9700 |
| 247.40 | 0.9460 |
| 365.90 | 0.9220 |
| 469.60 | 0.8960 |
| 566.00 | 0.8700 |
| 660.90 | 0.8430 |
| 755.10 | 0.8160 |
| 845.90 | 0.7870 |
| 931.10 | 0.7570 |
| 1007.3 | 0.7260 |
| 1082.3 | 0.6940 |
| 1148.0 | 0.6610 |
| 1204.2 | 0.6270 |
| 1250.7 | 0.5910 |
| 1297.6 | 0.5540 |
| 1328.2 | 0.5150 |
| 1337.5 | 0.4750 |
| 1330.4 | 0.4330 |
| 1309.3 | 0.3890 |
| 1259.2 | 0.3430 |
| 1192.7 | 0.2950 |
| 1087.9 | 0.2460 |
| 947.10 | 0.1930 |
| 763.20 | 0.1390 |
| 508.90 | 0.0810 |
| 399.50 | 0.0610 |
| 274.40 | 0.0400 |

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**Heat capacity of mixing**

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Tanaka, Reiji - Toyama, Satoru, Excess Molar Volumes and Excess Molar Heat Capacities for Binary Mixtures of Ethanol with Chlorocyclohexane, 1-Nitropropane, Dibutyl Ether, and Ethyl Acetate at the Temperature of 298.15 K, Journal of Chemical & Engineering Data 6 (1996) 1455-1458. doi:10.1021/je960179m

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 2.740 | 0.8926 |
| 4.700 | 0.7988 |
| 6.310 | 0.6959 |
| 7.250 | 0.5960 |
| 7.560 | 0.4972 |
| 7.170 | 0.3986 |
| 6.010 | 0.2981 |
| 5.280 | 0.2577 |
| 4.720 | 0.2287 |
| 4.120 | 0.1999 |
| 2.900 | 0.1493 |
| 2.430 | 0.1294 |
| 1.760 | 0.1007 |
| 1.518 | 0.0901 |
| 1.075 | 0.0696 |
| 0.9020 | 0.0603 |
| 0.7230 | 0.0505 |
| 0.5390 | 0.0403 |
| 0.3660 | 0.0291 |
| 0.2760 | 0.0233 |
| 0.2530 | 0.0209 |
| 0.1740 | 0.0160 |
| 0.1180 | 0.0120 |
| 0.1070 | 0.0097 |
| 0.0590 | 0.0071 |
| 0.0320 | 0.0050 |
| 0.0090 | 0.0031 |
| -0.0020 | 0.0014 |

Hu, Jianhua - Tamura, Katsutoshi - Murakami, Sachio, Excess thermodynamic properties of binary mixtures of ethyl acetate with benzene, ethanol, and 2,2,2-trifluoroethan-1-ol at 298.15 K, Fluid Phase Equilibria 1-2 (1997) 239-253. doi:10.1016/S0378-3812(97)00015-0

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.6300 | 0.9750 |
| 1.260 | 0.9500 |
| 2.490 | 0.9000 |
| 3.750 | 0.8500 |
| 4.540 | 0.8000 |
| 5.380 | 0.7500 |
| 6.100 | 0.7000 |
| 6.610 | 0.6500 |
| 6.960 | 0.6000 |
| 7.200 | 0.5500 |
| 7.270 | 0.5000 |
| 7.180 | 0.4500 |
| 6.990 | 0.4000 |
| 6.600 | 0.3500 |
| 5.990 | 0.3000 |
| 5.030 | 0.2506 |
| 4.100 | 0.2005 |
| 3.010 | 0.1504 |
| 1.890 | 0.1003 |
| 0.8200 | 0.0500 |
| 0.2300 | 0.0250 |

Wen-jun, Fang - Qing-sen, Yu - Rui-sen, Lin - Han-xing, Zong, Vapor heat capacity of binary and ternary systems, Thermochimica Acta 1-2 (1997) 43-47. doi:10.1016/S0040-6031(97)00135-4

**T / K = 404.60**

**P / bar = 1.013**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $z_1$ |
|---|---|
| 4.683 | 0.8082 |
| 6.018 | 0.6556 |
| 5.440 | 0.5154 |
| 2.369 | 0.3634 |
| 0.3300 | 0.2714 |
| 0.4537 | 0.1266 |

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**Critical point**

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Škerget, Mojca - Čretnik, Lucija - Knez, Željko - Škrinjar, Maja, Influence of the aromatic ring substituents on phase equilibria of vanillins in binary systems with CO2, Fluid Phase Equilibria 1 (2005) 11-19. doi:10.1016/j.fluid.2004.12.012

| T / K | P / bar | $x_1$ |
|---|---|---|
| 521.60 | 43.20 | 0.2000 |
| 519.20 | 47.70 | 0.4000 |
| 516.80 | 51.70 | 0.5900 |
| 515.90 | 53.50 | 0.6800 |
| 515.30 | 55.20 | 0.7500 |
| 515.40 | 57.80 | 0.8500 |

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**Azeotropic point**

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Susial, P. - Rodriguez-Henriquez, J.J. - Sosa-Rosario, A. - Rios-Santana, R., Vapor-Liquid Equilibrium of Ethyl Acetate + CnH2n+1OH (n= 1,2,3) Binary Systems at 0.3 MPa, Chinese Journal of Chemical Engineering 4

(2012) 723-730. doi:10.1016/S1004-9541(11)60241-3

| T / K | P / bar | $x_1$ |
|---|---|---|
| 378.95 | 3.000 | 0.5990 |

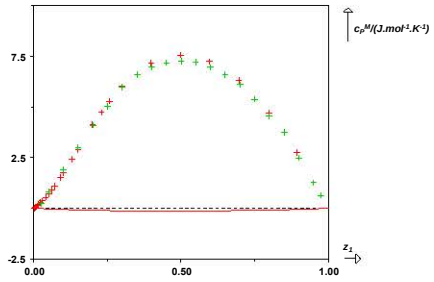
Susial, Pedro - Sosa-Rosario, Aday - Rodríguez-Henríquez, Juan José - Rios-Santana, Raul, Vapor Pressure and VLE Data Measurements on Ethyl Acetate/Ethanol Binary System at 0.1, 0.5, and 0.7 MPa, JOURNAL OF CHEMICAL ENGINEERING OF JAPAN 3 (2011) 155-163. doi:10.1252/jcej.10we176

| T / K | P / bar | $x_1$ |
|---|---|---|
| 409.50 | 7.000 | 0.7350 |

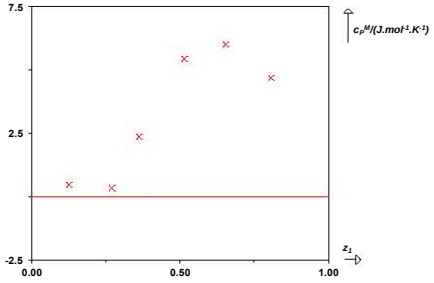
Li, Qunsheng - Zhang, Jiguo - Lei, Zhigang - Zhu, Jiujuan - Xing, Fengying, Isobaric Vapor-Liquid Equilibrium for Ethyl Acetate + Ethanol + 1-Ethyl-3-methylimidazolium Tetrafluoroborate, Journal of Chemical & Engineering Data 2 (2009) 193-197. doi:10.1021/je800175s

| T / K | P / bar | $x_1$ |
|---|---|---|
| 345.00 | 1.013 | 0.4500 |

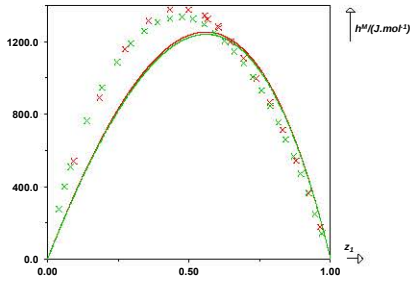
T/K = 298.15 - P/bar = 1.0132 1.0132



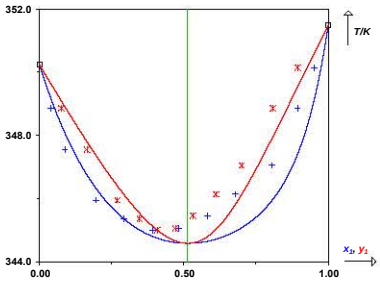

T/K = 404.60 - P/bar = 1.0132



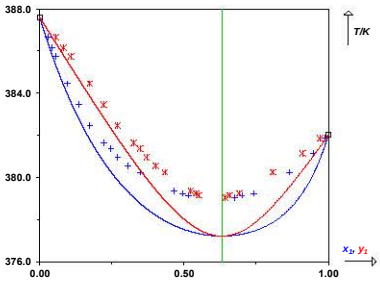

T/K = 298.15 - P/bar = 1.0100 100.00



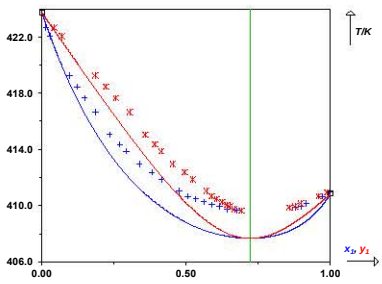

P/bar = 1.01320



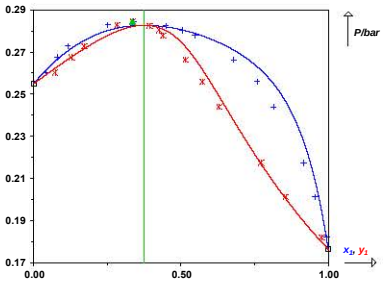

P/bar = 3.00000



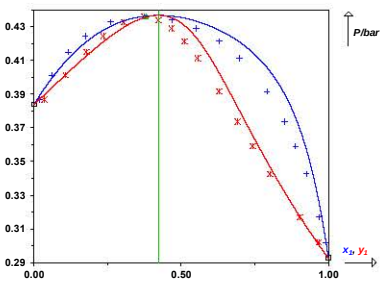

P/bar = 7.00000



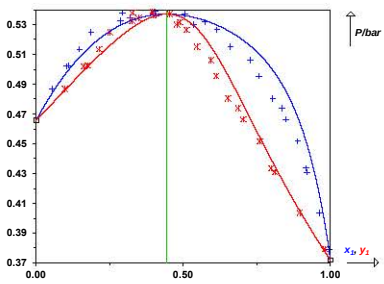

T/K = 313.15



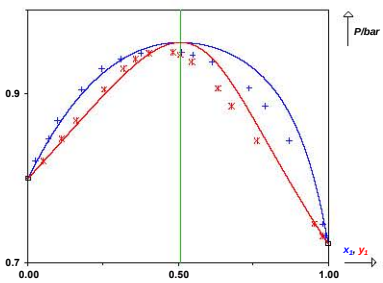

T/K = 323.15



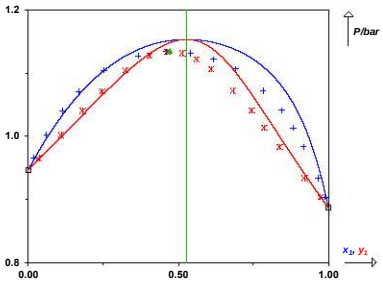

T/K = 328.15



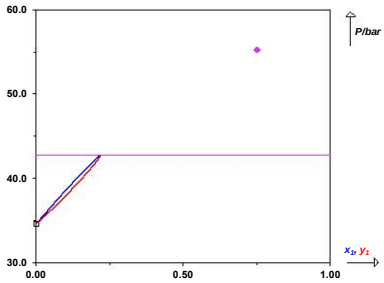

T/K = 343.15

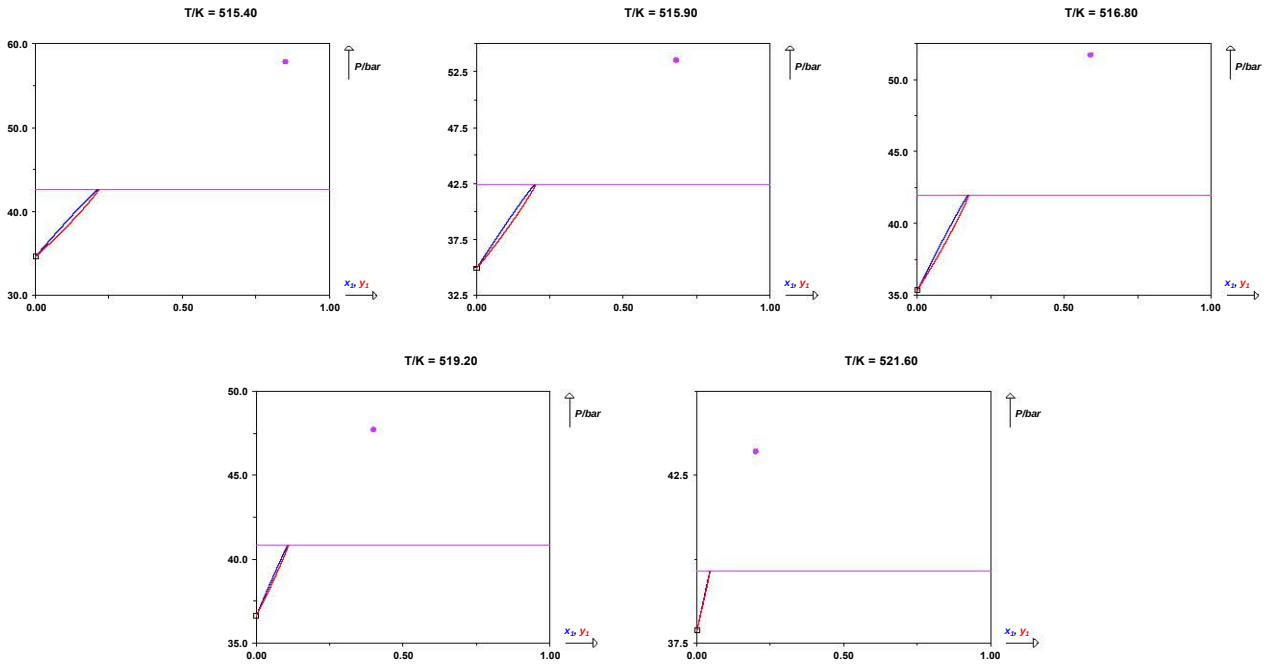



T/K = 348.15




T/K = 515.30




T/K = 515.40
P/bar
60.0
50.0
40.0
30.0
0.00
0.50
1.00
x1, y1
T/K = 515.90
P/bar
52.5
47.5
42.5
37.5
32.5
0.00
0.50
1.00
x1, y1
T/K = 516.80
P/bar
50.0
45.0
40.0
35.0
0.00
0.50
1.00
x1, y1
T/K = 519.20
P/bar
50.0
45.0
40.0
35.0
0.00
0.50
1.00
x1, y1
T/K = 521.60
P/bar
42.5
37.5
0.00
0.50
1.00
x1, y1

## ACETONE (1) + WATER (2)

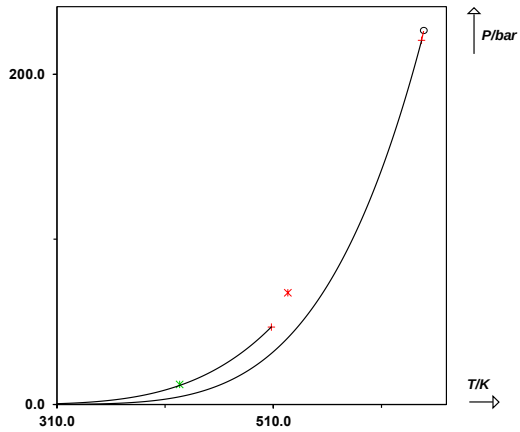
| | | |
|---|---|---|
| **CAS** | 67-64-1 | 7732-18-5 |
| **InChiKey** | CSCPPACGZOOCGX-UHFFFAOYSA-N | XLYOFNOQVPJJNP-UHFFFAOYSA-N |
| **$T_c$ / K** | 508.20 | 647.10 |
| **$P_c$ / bar** | 47.01 | 220.64 |
| **ω** | 0.307 | 0.345 |

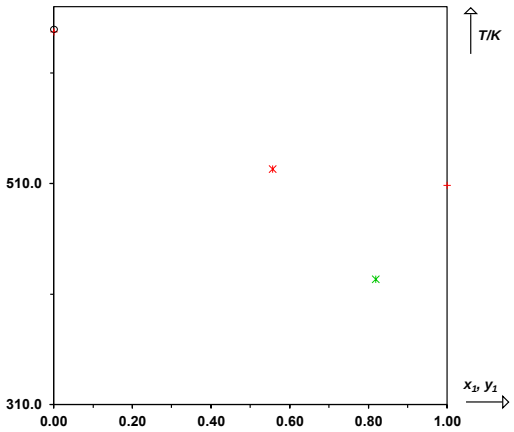
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 4050
B/MPa = -988

*Deviations*
MAPE on x = 180 %
MAPE on y = 21 %
MAPE on $h^M$ = 100 %
MAPE on $c_P^M$ = 93 %



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**Isothermal phase equilibrium data**

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Pierotti, G. J. - Deal, C. H. - Derr, E. L., Activity Coefficients and Molecular Structure, Industrial & Engineering Chemistry 1 (1959) 95-102. doi:10.1021/ie50589a048

**T / K = 288.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0280 | 0.0085 | 0.4040 |
| 0.0513 | 0.0284 | 0.6760 |
| 0.0793 | 0.0640 | 0.7670 |

Im, J.N. - Park, S.S. - Lee, H.O., Isothermal vapor-liquid equilibrium for the binary system acetone-water by the total pressure method, Korean Chemical Engineering Research 3 (1974) 179-187.

**T / K = 288.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0401 | 0.0201 | 0.5980 |
| 0.0961 | 0.0918 | 0.8481 |
| 0.1076 | 0.1135 | 0.8647 |
| 0.1388 | 0.2084 | 0.9056 |
| 0.1607 | 0.3260 | 0.9061 |
| 0.1677 | 0.4171 | 0.9188 |
| 0.1733 | 0.5314 | 0.9284 |
| 0.1771 | 0.6141 | 0.9290 |
| 0.1813 | 0.7273 | 0.9327 |
| 0.1843 | 0.8016 | 0.9390 |
| 0.1909 | 0.9452 | 0.9776 |

Treiner, Claude - Tzias, Pierre, Standard Gibbs Free Energy of Transfer of n-Bu4NBr from Water to Water-Organic Solvent Mixtures as Deduced from Precise Vapor Pressure Measurements at 298.15°K, Thermodynamic Behavior of Electrolytes in Mixed Solvents (1976) 303-317.

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0652 | 0.0158 | 0.5217 |
| 0.0837 | 0.0261 | 0.6133 |
| 0.1054 | 0.0404 | 0.6984 |
| 0.1378 | 0.0711 | 0.8060 |
| 0.1893 | 0.1172 | 0.8477 |
| 0.2145 | 0.1713 | 0.8688 |
| 0.2298 | 0.2372 | 0.8809 |
| 0.2441 | 0.3183 | 0.8901 |
| 0.2665 | 0.5572 | 0.9074 |

Im, J.N. - Park, S.S. - Lee, H.O., Isothermal vapor-liquid equilibrium for the binary system acetone-water by the total pressure method, Korean Chemical Engineering Research 3 (1974) 179-187.

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1127 | 0.0201 | 0.5148 |
| 0.2469 | 0.0918 | 0.7805 |
| 0.2694 | 0.1135 | 0.8103 |
| 0.3337 | 0.2084 | 0.8585 |
| 0.3717 | 0.3260 | 0.8691 |
| 0.3848 | 0.4171 | 0.8798 |
| 0.3990 | 0.5314 | 0.8870 |
| 0.4080 | 0.6141 | 0.8853 |
| 0.4229 | 0.7273 | 0.9074 |
| 0.4321 | 0.8016 | 0.9234 |
| 0.4517 | 0.9452 | 0.9770 |

Lieberwirth, I. - Schuberth, H., Das isotherme Dampf-Flüssigkeits-Phasengleichgewichtsverhalten des Systems Aceton/Wasser bei 35° C, Zeitschrift für Physikalische Chemie 1 (1979) doi:10.1515/zpch-1979-26090

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1833 | 0.0500 | 0.7060 |
| 0.2668 | 0.1000 | 0.8160 |
| 0.3102 | 0.1500 | 0.8440 |
| 0.3374 | 0.2000 | 0.8590 |
| 0.3541 | 0.2500 | 0.8710 |
| 0.3658 | 0.3000 | 0.8780 |
| 0.3738 | 0.3500 | 0.8820 |
| 0.3798 | 0.4000 | 0.8850 |
| 0.3853 | 0.4500 | 0.8880 |
| 0.3909 | 0.5000 | 0.8920 |
| 0.3973 | 0.5500 | 0.8970 |
| 0.4034 | 0.6000 | 0.9010 |
| 0.4098 | 0.6500 | 0.9070 |
| 0.4165 | 0.7000 | 0.9130 |
| 0.4233 | 0.7500 | 0.9200 |
| 0.4305 | 0.8000 | 0.9290 |
| 0.4382 | 0.8500 | 0.9390 |
| 0.4469 | 0.9000 | 0.9530 |
| 0.4561 | 0.9500 | 0.9720 |

Sokolova, E.P. - Morachevskii, A.G., Thermodynamic properties of the acetone-water system, Vestn Lenin U. Fiz. Kh 16 (1967) 110-115.

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1832 | 0.0490 | 0.7130 |
| 0.2893 | 0.1260 | 0.8230 |

| | | |
|---|---|---|
| 0.3349 | 0.1970 | 0.8530 |
| 0.3686 | 0.2980 | 0.8720 |
| 0.3921 | 0.4500 | 0.8810 |
| 0.4040 | 0.5720 | 0.8880 |
| 0.4320 | 0.7840 | 0.9160 |
| 0.4512 | 0.9010 | 0.9510 |

Im, J.N. - Park, S.S. - Lee, H.O., Isothermal vapor-liquid equilibrium for the binary system acetone-water by the total pressure method, Korean Chemical Engineering Research 3 (1974) 179-187.

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1909 | 0.0201 | 0.4716 |
| 0.3773 | 0.0918 | 0.7743 |
| 0.4197 | 0.1135 | 0.7844 |
| 0.5069 | 0.2084 | 0.8347 |
| 0.5537 | 0.3260 | 0.8492 |
| 0.5698 | 0.4171 | 0.8606 |
| 0.5922 | 0.5314 | 0.8657 |
| 0.6054 | 0.6141 | 0.8758 |
| 0.6237 | 0.7273 | 0.8967 |
| 0.6386 | 0.8016 | 0.9133 |
| 0.6698 | 0.9452 | 0.9669 |

Sokolova, E.P. - Morachevskii, A.G., Thermodynamic properties of the acetone-water system, Vestn Lenin U. Fiz. Kh 16 (1967) 110-115.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4038 | 0.0570 | 0.7100 |
| 0.4512 | 0.0760 | 0.7430 |
| 0.6072 | 0.1880 | 0.8210 |
| 0.6602 | 0.2980 | 0.8430 |
| 0.7018 | 0.4500 | 0.8540 |
| 0.7259 | 0.5720 | 0.8670 |
| 0.7679 | 0.7840 | 0.9000 |
| 0.7869 | 0.9010 | 0.9400 |

Griswold, J. - Wong, S.Y., Phase-equilibria in the acetone-methanol-water system from 100° into the critical region, Chemical Engineering Progress Symposium Series 3 (1952) 18-34.

**T / K = 423.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 6.722 | 0.0240 | 0.2950 | |
| 9.373 | 0.1630 | 0.5250 | |
| 11.68 | 0.5780 | 0.6770 | |
| 11.89 | 0.6860 | 0.7310 | |
| 11.95 | 0.7220 | 0.7500 | |
| 12.02 | 0.7630 | 0.7770 | |
| 12.00 | 0.8180 | 0.8180 | AZEO |
| 12.01 | 0.8180 | 0.8210 | |
| 11.99 | 0.8540 | 0.8450 | |
| 11.90 | 0.8870 | 0.8770 | |
| 11.82 | 0.9120 | 0.9020 | |
| 11.61 | 0.9600 | 0.9570 | |
| 11.56 | 0.9700 | 0.9680 | |

Griswold, J. - Wong, S.Y., Phase-equilibria in the acetone-methanol-water system from 100° into the critical region, Chemical Engineering Progress Symposium Series 3 (1952) 18-34.

**T / K = 523.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 40.40 | 0.0020 | 0.0150 |
| 40.96 | 0.0040 | 0.0250 |
| 41.78 | 0.0070 | 0.0390 |
| 46.61 | 0.0260 | 0.1380 |
| 55.43 | 0.1040 | 0.2920 |
| 60.40 | 0.2270 | 0.3630 |
| 63.02 | 0.2850 | 0.3920 |
| 63.36 | 0.2960 | 0.4000 |
| 65.43 | 0.4010 | 0.4620 |
| 65.78 | 0.4120 | 0.4660 |
| 66.88 | 0.4960 | 0.5210 |

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**Isobaric phase equilibrium data**

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Verhoeye, Lucien - De Schepper, Herman, The vapour-liquid equilibria of the binary, ternary and quaternary systems formed by acetone, methanol, propan-2-ol, and water, Journal of Applied Chemistry and Biotechnology 8 (2007) 607-619. doi:10.1002/jctb.5020230807

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 349.40 | 0.0490 | 0.6050 |
| 345.55 | 0.0690 | 0.6780 |
| 339.60 | 0.1270 | 0.7530 |
| 335.90 | 0.2000 | 0.7900 |
| 335.49 | 0.2760 | 0.8040 |
| 334.05 | 0.4000 | 0.8260 |
| 333.32 | 0.4950 | 0.8320 |
| 331.95 | 0.6500 | 0.8550 |
| 331.62 | 0.6940 | 0.8620 |
| 331.10 | 0.7500 | 0.8760 |
| 330.40 | 0.8290 | 0.9030 |
| 329.90 | 0.9000 | 0.9360 |

| | | |
|---|---|---|
| 329.60 | 0.9400 | 0.9590 |

Ochi, K. - Kojima, K., Vapor-liquid equilibriums for the system acetone + methanol + water, Kagaku Kogaku (1971) 583-586. doi:10.1252/kakoronbunshu1953.35.583

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 360.60 | 0.0164 | 0.3547 |
| 352.33 | 0.0346 | 0.5472 |
| 346.57 | 0.0573 | 0.6377 |
| 343.06 | 0.0826 | 0.7047 |
| 340.93 | 0.1044 | 0.7286 |
| 339.15 | 0.1337 | 0.7535 |
| 338.71 | 0.1446 | 0.7578 |
| 338.41 | 0.1511 | 0.7586 |
| 338.06 | 0.1576 | 0.7713 |
| 337.61 | 0.1708 | 0.7736 |
| 337.20 | 0.1851 | 0.7798 |
| 337.00 | 0.1923 | 0.7781 |
| 336.56 | 0.2122 | 0.7821 |
| 335.28 | 0.2836 | 0.7965 |
| 334.91 | 0.3115 | 0.8034 |
| 334.75 | 0.3264 | 0.8060 |
| 334.47 | 0.3495 | 0.8100 |
| 333.97 | 0.3989 | 0.8169 |
| 333.98 | 0.3998 | 0.8186 |
| 333.78 | 0.4212 | 0.8169 |
| 333.56 | 0.4473 | 0.8195 |
| 333.46 | 0.4510 | 0.8252 |
| 333.27 | 0.4806 | 0.8284 |
| 333.09 | 0.5060 | 0.8275 |
| 332.98 | 0.5184 | 0.8287 |
| 332.96 | 0.5212 | 0.8301 |
| 332.93 | 0.5244 | 0.8323 |
| 332.65 | 0.5574 | 0.8342 |
| 332.38 | 0.5911 | 0.8409 |
| 331.97 | 0.6409 | 0.8476 |
| 331.55 | 0.6932 | 0.8584 |
| 331.46 | 0.7207 | 0.8621 |
| 331.15 | 0.7417 | 0.8697 |
| 330.73 | 0.7856 | 0.8811 |
| 330.61 | 0.7996 | 0.8892 |
| 330.19 | 0.8469 | 0.9045 |
| 329.79 | 0.8956 | 0.9184 |
| 329.58 | 0.9307 | 0.9443 |
| 329.42 | 0.9472 | 0.9581 |
| 329.21 | 0.9867 | 0.9878 |

Kojima, K. - Tochigi, K. - Seki, H. - Watase, K., Determination of vapor-liquid equilibriums from boiling point curves, Kagaku Kogaku (1968) 149-153. doi:10.1252/kakoronbunshu1953.32.149

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 347.95 | 0.0500 | 0.6381 |
| 341.68 | 0.1000 | 0.7301 |
| 338.41 | 0.1500 | 0.7716 |
| 336.74 | 0.2000 | 0.7916 |
| 335.75 | 0.2500 | 0.8034 |
| 335.02 | 0.3000 | 0.8124 |
| 334.41 | 0.3500 | 0.8201 |
| 333.90 | 0.4000 | 0.8269 |
| 333.50 | 0.4500 | 0.8326 |
| 333.10 | 0.5000 | 0.8387 |
| 332.69 | 0.5500 | 0.8455 |
| 332.27 | 0.6000 | 0.8532 |
| 331.86 | 0.6500 | 0.8615 |
| 331.44 | 0.7000 | 0.8712 |
| 331.05 | 0.7500 | 0.8817 |
| 330.64 | 0.8000 | 0.8950 |
| 330.23 | 0.8500 | 0.9118 |
| 329.83 | 0.9000 | 0.9335 |
| 329.45 | 0.9500 | 0.9627 |

Othmer, Donald F. - Chudgar, Manu M. - Levy, Sherman L., Binary and Ternary Systems of Acetone, Methyl Ethyl Ketone, and Water, Industrial & Engineering Chemistry 8 (1952) 1872-1881. doi:10.1021/ie50512a042

**P / bar = 3.447**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 395.65 | 0.0170 | 0.3490 |
| 393.15 | 0.0240 | 0.3980 |
| 385.15 | 0.0550 | 0.5180 |
| 379.15 | 0.1070 | 0.6080 |
| 375.95 | 0.1940 | 0.6700 |
| 374.45 | 0.2730 | 0.6950 |
| 373.05 | 0.3880 | 0.7180 |
| 372.15 | 0.5450 | 0.7470 |
| 371.95 | 0.6330 | 0.7680 |
| 371.75 | 0.7780 | 0.8300 |
| 371.55 | 0.8900 | 0.9030 |
| 371.35 | 0.9500 | 0.9510 |

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**Enthalpy of mixing**

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French, H.T, Excess enthalpies of (acetone + water) at 278.15, 288.15, 298.15, 308.15, 318.15, and 323.15 K, The Journal of Chemical Thermodynamics 8 (1989) 801-809. doi:10.1016/0021-9614(89)90026-8

**T / K = 278.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -24.00 | 0.0019 |
| -73.00 | 0.0061 |
| -122.00 | 0.0104 |
| -168.00 | 0.0147 |
| -213.00 | 0.0190 |
| -276.00 | 0.0255 |
| -353.00 | 0.0342 |
| -424.00 | 0.0431 |
| -487.00 | 0.0522 |
| -544.00 | 0.0613 |
| -592.00 | 0.0704 |
| -636.00 | 0.0797 |
| -672.00 | 0.0887 |
| -715.00 | 0.1024 |
| -762.00 | 0.1215 |
| -792.00 | 0.1414 |
| -810.00 | 0.1618 |
| -817.00 | 0.1820 |
| -815.00 | 0.2025 |
| -805.00 | 0.2233 |
| -788.00 | 0.2440 |
| -771.00 | 0.2597 |
| -753.00 | 0.2654 |
| -758.00 | 0.2707 |
| -731.00 | 0.2817 |
| -705.00 | 0.2995 |
| -673.00 | 0.3192 |
| -638.00 | 0.3396 |
| -596.00 | 0.3620 |
| -547.00 | 0.3879 |
| -489.00 | 0.4167 |
| -421.00 | 0.4495 |
| -342.00 | 0.4868 |
| -251.00 | 0.5294 |
| -161.00 | 0.5715 |
| -77.00 | 0.6121 |
| -1.0000 | 0.6504 |
| 61.00 | 0.6844 |
| 122.00 | 0.7212 |
| 178.00 | 0.7627 |
| 221.00 | 0.8087 |
| 238.00 | 0.8486 |
| 230.00 | 0.8857 |
| 195.00 | 0.9225 |
| 140.00 | 0.9532 |
| 56.00 | 0.9841 |

Löwen, B. - Schulz, S., Excess molar enthalpies of acetone + water, cyclohexane, methanol, 1-propanol, 2-propanol, 1-butanol and 1-pentanol at 283.15, 298.15, 323.15, 343.15 and 363.15 K, Thermochimica Acta (1995) 69-82. doi:10.1016/0040-6031(95)02278-A

**T / K = 283.15**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -416.40 | 0.0460 |
| -661.00 | 0.0990 |
| -756.00 | 0.1510 |
| -772.90 | 0.1950 |
| -743.90 | 0.2480 |
| -672.60 | 0.3050 |
| -590.50 | 0.3490 |
| -601.40 | 0.3500 |
| -501.90 | 0.4040 |
| -416.60 | 0.4480 |
| -317.00 | 0.4970 |
| -211.90 | 0.5480 |
| -103.50 | 0.6020 |
| -12.30 | 0.6500 |
| 72.40 | 0.6990 |
| 147.10 | 0.7520 |
| 199.50 | 0.8010 |
| 228.80 | 0.8530 |
| 203.50 | 0.9010 |
| 144.20 | 0.9480 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 293.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -223.52 | 0.0264 |
| -453.88 | 0.0576 |
| -632.32 | 0.0948 |
| -732.67 | 0.1400 |
| -764.12 | 0.1963 |
| -687.30 | 0.2682 |
| -494.27 | 0.3631 |

| | |
|---|---|
| -185.10 | 0.4942 |
| 189.62 | 0.6874 |
| 248.83 | 0.7375 |
| 277.32 | 0.7928 |
| 255.16 | 0.8543 |
| 109.05 | 0.9229 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -209.00 | 0.0264 |
| -422.81 | 0.0576 |
| -590.23 | 0.0948 |
| -685.63 | 0.1400 |
| -708.45 | 0.1963 |
| -624.30 | 0.2682 |
| -422.46 | 0.3631 |
| -123.62 | 0.4942 |
| 244.75 | 0.6874 |
| 296.36 | 0.7375 |
| 306.64 | 0.7928 |
| 265.59 | 0.8543 |
| 104.09 | 0.9229 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 308.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -182.37 | 0.0264 |
| -384.16 | 0.0576 |
| -506.93 | 0.0948 |
| -591.39 | 0.1400 |
| -612.93 | 0.1963 |
| -514.77 | 0.2682 |
| -329.22 | 0.3631 |
| -7.000 | 0.4942 |
| 345.44 | 0.6874 |
| 376.48 | 0.7375 |
| 379.60 | 0.7928 |
| 314.29 | 0.8543 |
| 116.39 | 0.9229 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 323.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -138.31 | 0.0264 |
| -281.67 | 0.0577 |
| -381.66 | 0.0948 |
| -418.33 | 0.1400 |
| -365.36 | 0.1963 |
| -255.19 | 0.2682 |
| -83.37 | 0.3631 |
| 169.28 | 0.4942 |
| 438.53 | 0.6874 |
| 450.01 | 0.7375 |
| 401.52 | 0.7928 |
| 296.98 | 0.8543 |
| 48.05 | 0.9229 |

Löwen, B. - Schulz, S., Excess molar enthalpies of acetone + water, cyclohexane, methanol, 1-propanol, 2-propanol, 1-butanol and 1-pentanol at 283.15, 298.15, 323.15, 343.15 and 363.15 K, Thermochimica Acta (1995) 69-82. doi:10.1016/0040-6031(95)02278-A

**T / K = 343.15**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -173.10 | 0.0460 |
| -216.70 | 0.0990 |
| -207.90 | 0.1510 |
| -169.80 | 0.1950 |
| -103.90 | 0.2480 |
| -13.30 | 0.3050 |
| 65.10 | 0.3500 |
| 163.40 | 0.4040 |
| 247.30 | 0.4480 |
| 333.70 | 0.4970 |
| 413.50 | 0.5480 |
| 491.60 | 0.6020 |
| 542.20 | 0.6500 |
| 577.50 | 0.6990 |
| 586.60 | 0.7520 |
| 560.90 | 0.8010 |
| 502.00 | 0.8530 |
| 383.40 | 0.9010 |

227.50 0.9480

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**Heat capacity of mixing**

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Costas, Miguel - Patterson, Donald, Heat capacities of water + organic-solvent mixtures, Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases 10 (1985) doi:10.1039/f19858102381

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / $J.mol^{-1}.K^{-1}$ | $x_1$ |
|---|---|
| 8.711 | 0.6393 |
| 8.377 | 0.6443 |
| 7.100 | 0.7336 |
| 6.833 | 0.7407 |
| 6.007 | 0.7881 |
| 5.961 | 0.7912 |
| 4.662 | 0.8417 |
| 3.644 | 0.8775 |
| 1.910 | 0.9286 |
| 0.7597 | 0.9688 |
| 0.6918 | 0.9705 |

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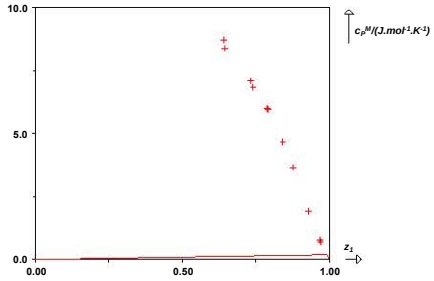
**Critical point**

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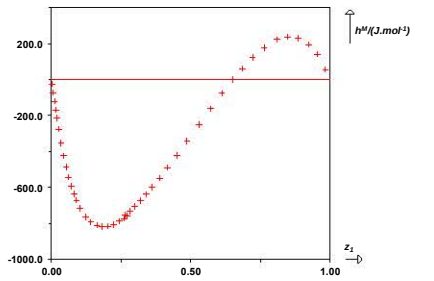
Musso, E. - Tesser, R. - Basile, G. - Di Serio, M. - Santacesaria, E., Description of the liquid–liquid equilibrium in binary and multicomponent CFC/lubricating oil mixtures by means of an extended Flory–Huggins model, Journal of Fluorine Chemistry 1 (2000) 41-51. doi:10.1016/S0022-1139(99)00255-9

| T / K | P / bar | $x_1$ |
|---|---|---|
| 523.15 | 67.57 | 0.5560 |

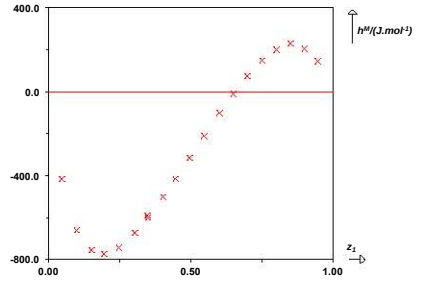
T/K = 298.15 - P/bar = 1.0132



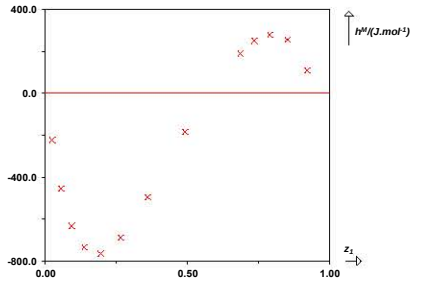

T/K = 278.15 - P/bar = 1.0132



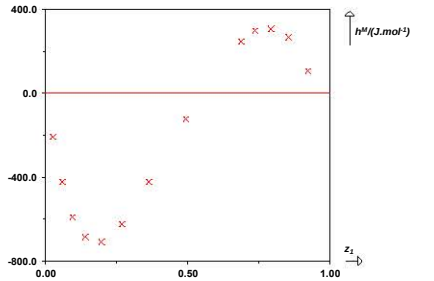

T/K = 283.15 - P/bar = 4.00



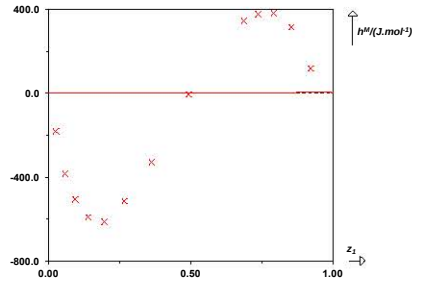

T/K = 293.15 - P/bar = 1.0100



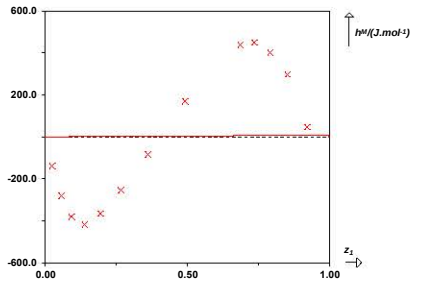

T/K = 298.15 - P/bar = 1.0100



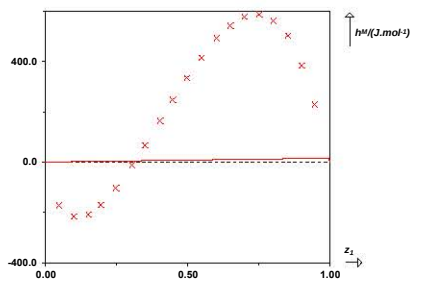

T/K = 308.15 - P/bar = 1.0100



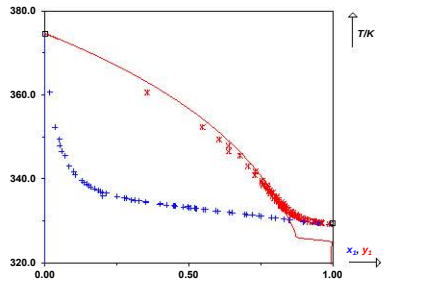

T/K = 323.15 - P/bar = 1.0100



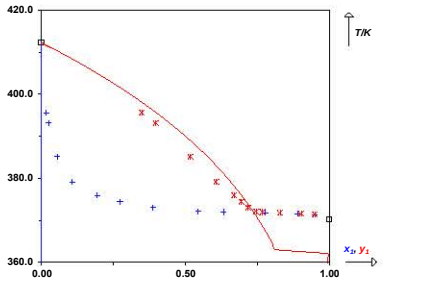

T/K = 343.15 - P/bar = 4.00



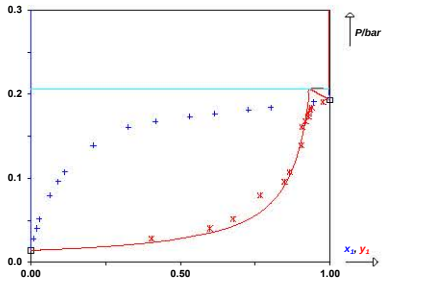

P/bar = 1.01330



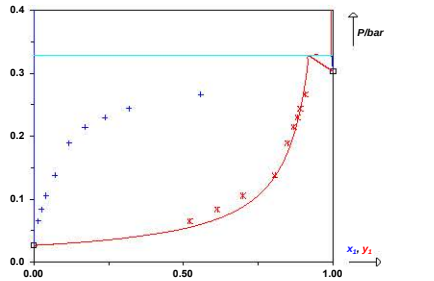

P/bar = 3.44730

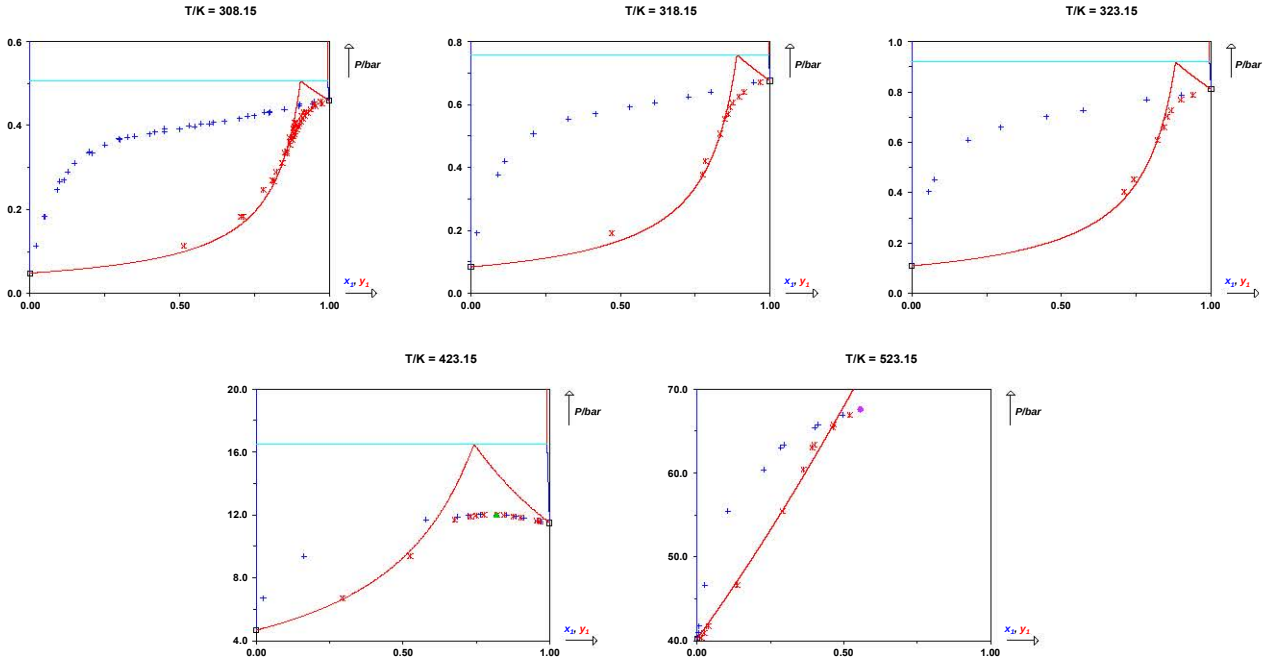



T/K = 288.15




T/K = 298.15




T/K = 308.15
P/bar
x1, y1
T/K = 318.15
P/bar
x1, y1
T/K = 323.15
P/bar
x1, y1
T/K = 423.15
P/bar
x1, y1
T/K = 523.15
P/bar
x1, y1

## ETHANOL (1) + METHYL ETHYL KETONE (2)

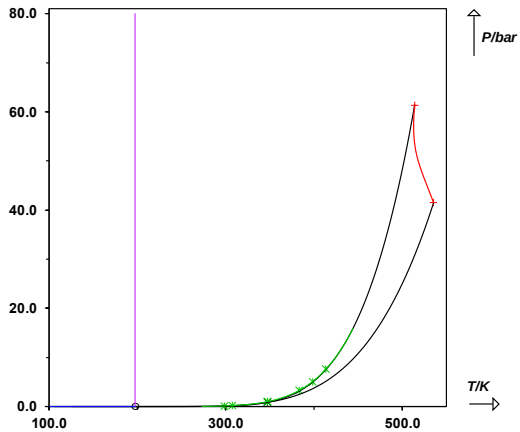
| | | |
|---|---|---|
| **CAS** | 64-17-5 | 78-93-3 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | ZWEHNKRNPOVVGH-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 535.50 |
| **$P_c$ / bar** | 61.37 | 41.50 |
| **ω** | 0.644 | 0.323 |

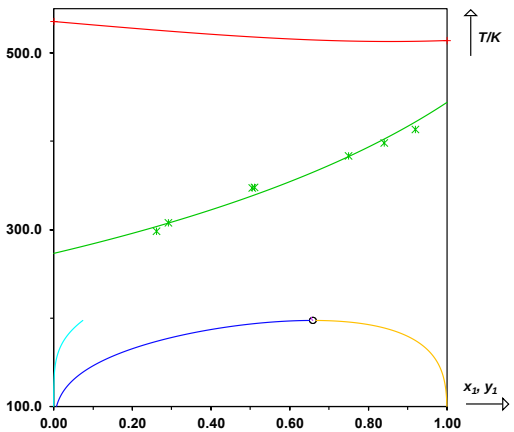
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 187
B/MPa = 304

*Deviations*
MAPE on x = 9.3 %
MAPE on y = 6.8 %
MAPE on $x_{az}$ = 9.0 %
MAPE on $P_{az}$ = 1.2 %
MAPE on $h^M$ = 13 %



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**Isothermal phase equilibrium data**

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Ohta, Tatsuhiko - Koyabu, Jitsuo - Nagata, Isamu, Vapor—liquid equilibria for the ternary Ethanol—2-butanone—benzene system at 298.15 K, Fluid Phase Equilibria 1 (1981) 65-73. doi:10.1016/0378-3812(81)87006-9

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.1263 | 0.0730 | 0.0970 | |
| 0.1280 | 0.1380 | 0.1650 | |
| 0.1304 | 0.2610 | 0.2610 | AZEO |
| 0.1305 | 0.2730 | 0.2680 | |
| 0.1285 | 0.3280 | 0.3020 | |
| 0.1268 | 0.4820 | 0.3800 | |
| 0.1257 | 0.5050 | 0.3980 | |
| 0.1240 | 0.5700 | 0.4320 | |
| 0.1188 | 0.6590 | 0.4860 | |
| 0.1100 | 0.7700 | 0.5830 | |
| 0.1047 | 0.8390 | 0.6580 | |
| 0.0960 | 0.9180 | 0.7780 | |
| 0.0924 | 0.9390 | 0.8140 | |

Narasigadu, Caleb - Naidoo, Paramespri - Coquelet, Christophe - Richon, Dominique - Ramjugernath, Deresh, Isothermal Vapor–Liquid Equilibrium Data for the Butan-2-one + Methanol or Ethanol Systems Using a Static-Analytic Microcell, Journal of Chemical & Engineering Data 5 (2013) 1280-1287. doi:10.1021/je400065j

**T / K = 383.30**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 2.716 | 0.1110 | 0.1870 | |
| 2.798 | 0.1600 | 0.2440 | |
| 2.903 | 0.2310 | 0.3280 | |
| 2.979 | 0.2900 | 0.3930 | |
| 3.045 | 0.3580 | 0.4500 | |
| 3.140 | 0.4650 | 0.5270 | |
| 3.218 | 0.6450 | 0.6700 | |
| 3.231 | 0.7500 | 0.7500 | AZEO |
| 3.231 | 0.7550 | 0.7520 | |
| 3.220 | 0.8580 | 0.8420 | |

Narasigadu, Caleb - Naidoo, Paramespri - Coquelet, Christophe - Richon, Dominique - Ramjugernath, Deresh, Isothermal Vapor–Liquid Equilibrium Data for the Butan-2-one + Methanol or Ethanol Systems Using a Static-Analytic Microcell, Journal of Chemical & Engineering Data 5 (2013) 1280-1287. doi:10.1021/je400065j

**T / K = 398.20**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 4.056 | 0.1350 | 0.2210 | |
| 4.235 | 0.2020 | 0.3040 | |
| 4.339 | 0.2440 | 0.3580 | |
| 4.574 | 0.3580 | 0.4700 | |
| 4.833 | 0.5370 | 0.6070 | |
| 4.884 | 0.5880 | 0.6510 | |
| 4.993 | 0.7490 | 0.7680 | |
| 5.014 | 0.8400 | 0.8400 | AZEO |
| 5.014 | 0.8420 | 0.8430 | |

Narasigadu, Caleb - Naidoo, Paramespri - Coquelet, Christophe - Richon, Dominique - Ramjugernath, Deresh, Isothermal Vapor–Liquid Equilibrium Data for the Butan-2-one + Methanol or Ethanol Systems Using a Static-Analytic Microcell, Journal of Chemical & Engineering Data 5 (2013) 1280-1287. doi:10.1021/je400065j

**T / K = 413.20**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.726 | 0.1220 | 0.2070 | |
| 6.077 | 0.2080 | 0.3200 | |
| 6.395 | 0.2950 | 0.4190 | |
| 6.627 | 0.3700 | 0.4910 | |
| 6.957 | 0.4920 | 0.5920 | |
| 7.102 | 0.5540 | 0.6400 | |
| 7.267 | 0.6410 | 0.7030 | |
| 7.407 | 0.7180 | 0.7590 | |
| 7.538 | 0.8350 | 0.8430 | |
| 7.569 | 0.9000 | 0.9030 | |
| 7.587 | 0.9160 | 0.9190 | |
| 7.587 | 0.9200 | 0.9200 | AZEO |

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**Isobaric phase equilibrium data**

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Martínez, Nelson F. - Lladosa, Estela - Burguet, MaCruz - Montón, Juan B., Isobaric vapour–liquid equilibria for binary systems of 2-butanone with ethanol, 1-propanol, and 2-propanol at 20 and 101.3 kPa, Fluid Phase Equilibria 1-2 (2008) 62-68. doi:10.1016/j.fluid.2008.06.004

**P / bar = 0.2000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 308.94 | 0.0360 | 0.0620 |
| 308.41 | 0.0920 | 0.1320 |
| 308.00 | 0.1470 | 0.1870 |
| 307.87 | 0.2070 | 0.2340 |
| 307.73 | 0.2630 | 0.2740 |
| 307.64 | 0.3220 | 0.3110 |
| 307.70 | 0.3720 | 0.3420 |

| | | |
|---|---|---|
| 307.82 | 0.4270 | 0.3760 |
| 308.12 | 0.4770 | 0.4050 |
| 308.29 | 0.5280 | 0.4360 |
| 308.50 | 0.5790 | 0.4670 |
| 308.82 | 0.6300 | 0.4990 |
| 309.23 | 0.6800 | 0.5380 |
| 309.69 | 0.7330 | 0.5800 |
| 310.30 | 0.7920 | 0.6340 |
| 311.00 | 0.8320 | 0.6870 |
| 311.87 | 0.8790 | 0.7440 |
| 312.87 | 0.9220 | 0.8090 |
| 313.91 | 0.9540 | 0.8820 |

Wen, Chao-Cheng - Tu, Chein-Hsiun, Vapor–liquid equilibria for binary and ternary mixtures of ethanol, 2-butanone, and 2,2,4-trimethylpentane at 101.3kPa, Fluid Phase Equilibria 2 (2007) 131-139. doi:10.1016/j.fluid.2007.06.005

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 351.69 | 0.0360 | 0.0600 |
| 351.00 | 0.0700 | 0.1120 |
| 350.36 | 0.1060 | 0.1610 |
| 349.71 | 0.1420 | 0.2050 |
| 348.90 | 0.1970 | 0.2700 |
| 348.32 | 0.2580 | 0.3320 |
| 347.95 | 0.3050 | 0.3680 |
| 347.69 | 0.3740 | 0.4200 |
| 347.55 | 0.4320 | 0.4540 |
| 347.48 | 0.4910 | 0.4950 |
| 347.50 | 0.5430 | 0.5340 |
| 347.56 | 0.5970 | 0.5650 |
| 347.70 | 0.6440 | 0.6040 |
| 347.91 | 0.6950 | 0.6420 |
| 348.21 | 0.7520 | 0.6920 |
| 348.58 | 0.7870 | 0.7290 |
| 349.06 | 0.8420 | 0.7810 |
| 349.70 | 0.8980 | 0.8410 |
| 350.45 | 0.9580 | 0.9140 |

Martínez, Nelson F. - Lladosa, Estela - Burguet, MaCruz - Montón, Juan B., Isobaric vapour–liquid equilibria for binary systems of 2-butanone with ethanol, 1-propanol, and 2-propanol at 20 and 101.3 kPa, Fluid Phase Equilibria 1-2 (2008) 62-68. doi:10.1016/j.fluid.2008.06.004

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 351.34 | 0.0400 | 0.0830 |
| 350.44 | 0.0870 | 0.1480 |
| 349.68 | 0.1400 | 0.2150 |
| 348.99 | 0.1990 | 0.2660 |
| 348.56 | 0.2450 | 0.3120 |
| 348.10 | 0.2960 | 0.3600 |
| 347.87 | 0.3450 | 0.3960 |
| 347.66 | 0.3920 | 0.4300 |
| 347.54 | 0.4460 | 0.4670 |
| 347.50 | 0.5010 | 0.5060 |
| 347.51 | 0.5590 | 0.5450 |
| 347.58 | 0.6080 | 0.5820 |
| 347.72 | 0.6570 | 0.6170 |
| 347.94 | 0.7090 | 0.6560 |
| 348.29 | 0.7640 | 0.7000 |
| 348.73 | 0.8210 | 0.7550 |
| 349.19 | 0.8660 | 0.8020 |
| 349.78 | 0.9120 | 0.8590 |
| 350.53 | 0.9570 | 0.9260 |

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**Enthalpy of mixing**

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Chao, Jian-Ping - Dai, Ming, Studies of thermodynamic properties of binary mixtures containing an alcohol, Thermochimica Acta (1991) 257-264. doi:10.1016/0040-6031(91)80355-M

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 133.90 | 0.0311 |
| 234.50 | 0.0564 |
| 321.20 | 0.0814 |
| 411.30 | 0.1058 |
| 493.20 | 0.1300 |
| 569.20 | 0.1525 |
| 711.20 | 0.1995 |
| 808.60 | 0.2440 |
| 894.20 | 0.2870 |
| 961.90 | 0.3286 |
| 1013.4 | 0.3689 |
| 1047.2 | 0.4079 |
| 1069.8 | 0.4457 |
| 1080.8 | 0.4823 |
| 1075.5 | 0.5178 |
| 1062.8 | 0.5523 |
| 1029.8 | 0.6021 |
| 980.50 | 0.6498 |
| 911.40 | 0.6955 |
| 830.10 | 0.7393 |
| 739.50 | 0.7812 |

| | |
|---|---|
| 630.20 | 0.8218 |
| 515.40 | 0.8607 |
| 391.90 | 0.8979 |
| 262.70 | 0.9341 |
| 127.10 | 0.9687 |

Iñarrea, J - Valero, J - Pérez, P - Gracia, M - Gutiérrez Losa, C, HmE and VmE of some (butanone or dipropylether + an alkanol) mixtures, The Journal of Chemical Thermodynamics 2 (1988) 193-199. doi:10.1016/0021-9614(88)90154-1

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 357.00 | 0.0826 |
| 451.00 | 0.1096 |
| 610.00 | 0.1630 |
| 782.00 | 0.2340 |
| 892.00 | 0.2987 |
| 910.00 | 0.3141 |
| 955.00 | 0.3350 |
| 989.00 | 0.3766 |
| 1032.0 | 0.4509 |
| 1012.0 | 0.5429 |
| 985.00 | 0.5852 |
| 893.00 | 0.6808 |
| 734.00 | 0.7672 |
| 569.00 | 0.8363 |
| 420.00 | 0.8871 |
| 342.00 | 0.9057 |

Nagata, Isamu - Ohta, Tatsuhiko - Nakagawa, Shigeo, Excess Gibbs Free Energies And Heats Of Mixing For Binary Alcoholic Liquid Mixtures, Journal of Chemical Engineering of Japan 4 (1976) 276-281. doi:10.1252/jcej.9.276

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 465.99 | 0.0966 |
| 479.39 | 0.1005 |
| 504.51 | 0.1074 |
| 646.86 | 0.1541 |
| 776.65 | 0.2049 |
| 787.12 | 0.2083 |
| 960.87 | 0.2918 |
| 973.01 | 0.2999 |
| 1083.1 | 0.4112 |
| 1078.5 | 0.4956 |
| 1075.6 | 0.4989 |
| 999.81 | 0.5994 |
| 860.39 | 0.6963 |
| 866.67 | 0.7011 |
| 859.13 | 0.7033 |
| 655.65 | 0.8009 |
| 391.88 | 0.8965 |

Nagata, Isamu - Tago, Osamu - Takahashi, Takeshi, Heats of Mixing for Binary Methyl Ethyl Ketone, Methyl Acetate-Alcohol Systems, Chemical engineering 10 (1970) 1107-1112,a1. doi:10.1252/kakoronbunshu1953.34.1107

**T / K =** **308.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 539.50 | 0.1173 |
| 820.90 | 0.2171 |
| 1029.0 | 0.3145 |
| 1105.0 | 0.4056 |
| 1112.0 | 0.4558 |
| 1125.0 | 0.5049 |
| 1105.0 | 0.5528 |
| 1048.0 | 0.6127 |
| 909.60 | 0.7080 |
| 683.50 | 0.8076 |
| 392.00 | 0.9047 |

Iñarrea, J - Valero, J - Pérez, P - Gracia, M - Gutiérrez Losa, C, HmE and VmE of some (butanone or dipropylether + an alkanol) mixtures, The Journal of Chemical Thermodynamics 2 (1988) 193-199. doi:10.1016/0021-9614(88)90154-1

**T / K =** **308.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 378.00 | 0.0825 |
| 528.00 | 0.1232 |
| 741.00 | 0.1912 |
| 887.00 | 0.2604 |
| 1076.0 | 0.4637 |
| 1068.0 | 0.5260 |
| 1070.0 | 0.5318 |
| 1056.0 | 0.5567 |
| 1041.0 | 0.5830 |
| 892.00 | 0.7089 |
| 661.00 | 0.8065 |
| 261.00 | 0.9381 |

Pikkarainen, Liisa, Excess enthalpies of binary solvent mixtures of 2-butanone with aliphatic alcohols,

Thermochimica Acta 2 (1987) 239-244. doi:10.1016/0040-6031(87)80044-8

**T / K = 313.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 489.00 | 0.1030 |
| 589.00 | 0.1333 |
| 877.00 | 0.2372 |
| 975.00 | 0.2762 |
| 1155.0 | 0.3833 |
| 1139.0 | 0.4356 |
| 1120.0 | 0.5316 |
| 1076.0 | 0.6064 |
| 976.00 | 0.6768 |
| 849.00 | 0.7548 |
| 758.00 | 0.7935 |
| 535.00 | 0.8618 |
| 362.00 | 0.9125 |
| 268.00 | 0.9395 |

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**Azeotropic point**

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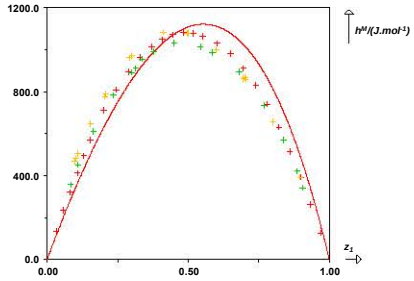
Wen, Chao-Cheng - Tu, Chein-Hsiun, Vapor–liquid equilibria for binary and ternary mixtures of ethanol, 2-butanone, and 2,2,4-trimethylpentane at 101.3kPa, Fluid Phase Equilibria 2 (2007) 131-139. doi:10.1016/j.fluid.2007.06.005

| T / K | P / bar | $x_1$ |
|---|---|---|
| 347.46 | 1.013 | 0.5040 |

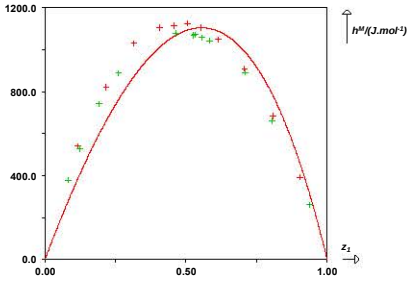
Martínez, Nelson F. - Lladosa, Estela - Burguet, MaCruz - Montón, Juan B., Isobaric vapour–liquid equilibria for binary systems of 2-butanone with ethanol, 1-propanol, and 2-propanol at 20 and 101.3 kPa, Fluid Phase Equilibria 1-2 (2008) 62-68. doi:10.1016/j.fluid.2008.06.004

| T / K | P / bar | $x_1$ |
|---|---|---|
| 307.60 | 0.2000 | 0.2920 |
| 347.50 | 1.013 | 0.5100 |

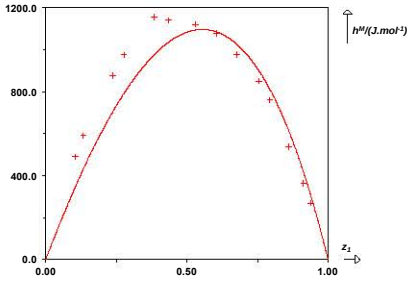
T/K = 298.15 - P/bar = 1.0132 1.0132 1.0132



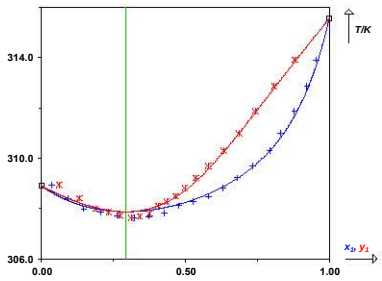

T/K = 308.15 - P/bar = 1.0132 1.0132



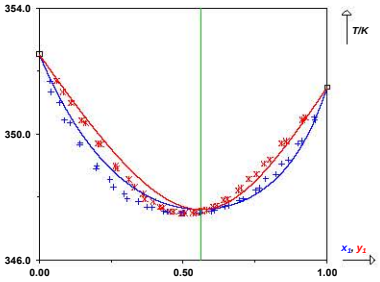

T/K = 313.15 - P/bar = 1.0132



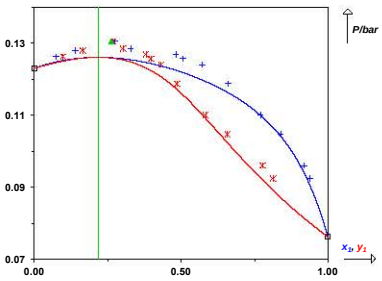

P/bar = 0.20000



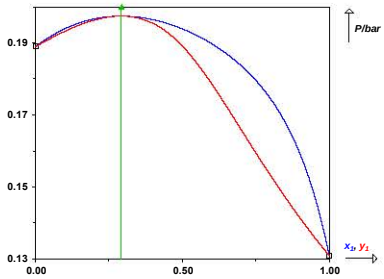

P/bar = 1.01300



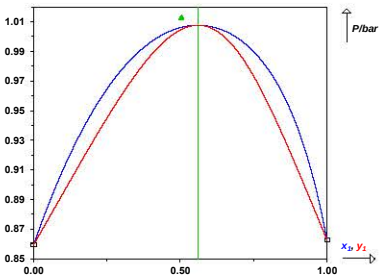

T/K = 298.15



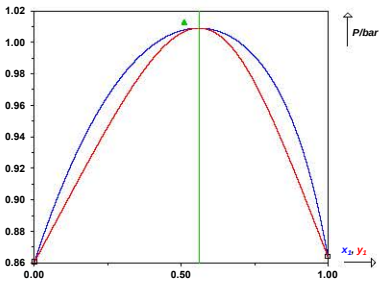

T/K = 307.60



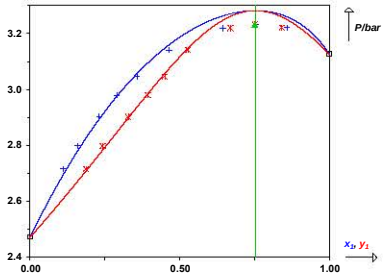

T/K = 347.46



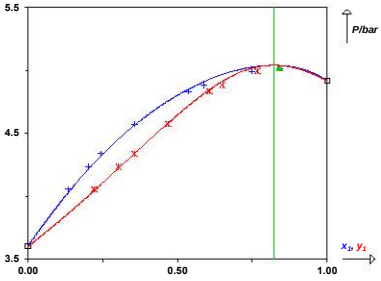

T/K = 347.50



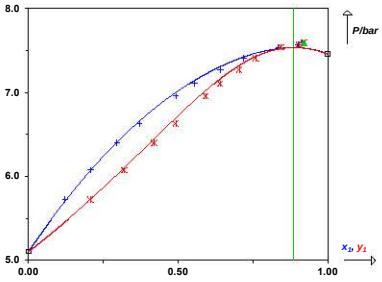

T/K = 383.30




T/K = 398.20




T/K = 413.20



## ETHANOL (1) + ACETONE (2)

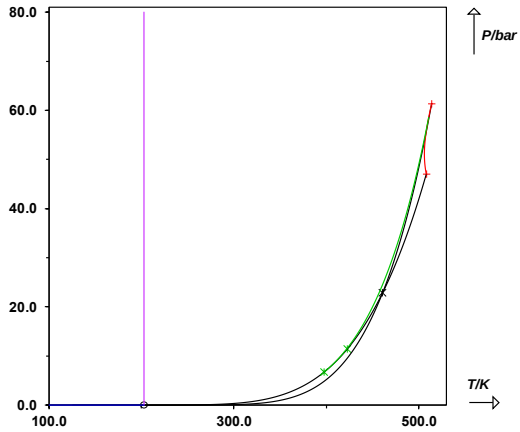
| | | |
|---|---|---|
| **CAS** | 64-17-5 | 67-64-1 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | CSCPPACGZOOCGX-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 508.20 |
| **$P_c$ / bar** | 61.37 | 47.01 |
| **ω** | 0.644 | 0.307 |

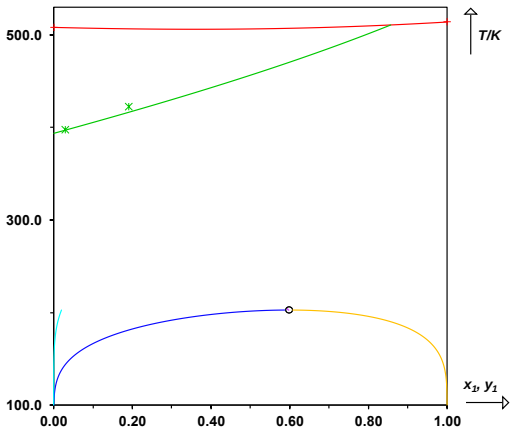
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 174
B/MPa = 369

Deviations
MAPE on x = 11 %
MAPE on y = 9.5 %
MAPE on $x_{az}$ = 11 %
MAPE on $P_{az}$ = 1.1 %
MAPE on $h^M$ = 14 %



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**Isothermal phase equilibrium data**

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Vinichenko, I.G. - Susarev, M.P., Study and calculation of the liquid-vapor equilibrium in the acetone-ethanol-hexane system, J. Appl. Chem. USSR 7 (1966) 1475-1478.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4602 | 0.9380 | 0.7830 |
| 0.5249 | 0.8750 | 0.6610 |
| 0.6236 | 0.7500 | 0.4960 |
| 0.7173 | 0.6250 | 0.3810 |
| 0.7746 | 0.5000 | 0.2880 |
| 0.8418 | 0.3750 | 0.2090 |
| 0.8921 | 0.2500 | 0.1470 |
| 0.9369 | 0.1250 | 0.0720 |

Lee, M.-J - Hu, C.-H, Isothermal vapor-liquid equilibria for mixtures of ethanol, acetone, and diisopropyl ether, Fluid Phase Equilibria 1 (1995) 83-98. doi:10.1016/0378-3812(95)02705-J

**T / K = 344.19**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.9460 | 0.9050 | 0.7440 |
| 1.063 | 0.8090 | 0.5890 |
| 1.188 | 0.7070 | 0.4760 |
| 1.300 | 0.6120 | 0.3970 |
| 1.381 | 0.5110 | 0.3270 |
| 1.441 | 0.4080 | 0.2630 |
| 1.504 | 0.3050 | 0.2030 |
| 1.570 | 0.2050 | 0.1460 |
| 1.614 | 0.1100 | 0.0830 |

Lee, M.-J - Hu, C.-H, Isothermal vapor-liquid equilibria for mixtures of ethanol, acetone, and diisopropyl ether, Fluid Phase Equilibria 1 (1995) 83-98. doi:10.1016/0378-3812(95)02705-J

**T / K = 353.18**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.312 | 0.9056 | 0.7650 |
| 1.475 | 0.8100 | 0.6160 |
| 1.614 | 0.7080 | 0.5030 |
| 1.750 | 0.6130 | 0.4230 |
| 1.847 | 0.5110 | 0.3490 |
| 1.909 | 0.4090 | 0.2850 |
| 2.006 | 0.3050 | 0.2180 |
| 2.063 | 0.2040 | 0.1550 |
| 2.118 | 0.1100 | 0.0870 |

Lee, M.-J - Hu, C.-H, Isothermal vapor-liquid equilibria for mixtures of ethanol, acetone, and diisopropyl ether, Fluid Phase Equilibria 1 (1995) 83-98. doi:10.1016/0378-3812(95)02705-J

**T / K = 363.19**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.943 | 0.9058 | 0.7540 |
| 2.179 | 0.8100 | 0.6260 |
| 2.329 | 0.7080 | 0.5340 |
| 2.446 | 0.6130 | 0.4630 |
| 2.550 | 0.5110 | 0.3910 |
| 2.652 | 0.4090 | 0.3200 |
| 2.728 | 0.3050 | 0.2470 |
| 2.785 | 0.2050 | 0.1720 |
| 2.829 | 0.1110 | 0.0980 |

Campbell, Scott W. - Wilsak, Richard A. - Thodos, George, Vapor-liquid equilibrium measurements for the ethanol-acetone system at 372.7, 397.7, and 422.6 K, Journal of Chemical & Engineering Data 3 (1987) 357-362. doi:10.1021/je00049a021

**T / K = 372.70**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.586 | 0.8840 | 0.7730 |
| 2.772 | 0.7960 | 0.6690 |
| 2.975 | 0.6990 | 0.5640 |
| 3.158 | 0.5850 | 0.4650 |
| 3.327 | 0.4700 | 0.3770 |
| 3.451 | 0.3550 | 0.2820 |
| 3.547 | 0.2390 | 0.1980 |
| 3.613 | 0.1290 | 0.1150 |
| 3.640 | 0.0760 | 0.0660 |

Campbell, Scott W. - Wilsak, Richard A. - Thodos, George, Vapor-liquid equilibrium measurements for the ethanol-acetone system at 372.7, 397.7, and 422.6 K, Journal of Chemical & Engineering Data 3 (1987) 357-362. doi:10.1021/je00049a021

**T / K = 397.70**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.219 | 0.9220 | 0.8770 | |
| 5.574 | 0.8300 | 0.7440 | |
| 5.898 | 0.7180 | 0.6160 | |
| 6.123 | 0.6000 | 0.5360 | |
| 6.302 | 0.5090 | 0.4540 | |
| 6.405 | 0.4530 | 0.3950 | |
| 6.529 | 0.3420 | 0.3050 | |
| 6.615 | 0.2330 | 0.2110 | |
| 6.664 | 0.1440 | 0.1300 | |
| 6.681 | 0.0760 | 0.0690 | |
| 6.688 | 0.0300 | 0.0300 | AZEO |

| | | |
|---|---|---|
| 6.660 | 0.0210 | 0.0230 |

Campbell, Scott W. - Wilsak, Richard A. - Thodos, George, Vapor-liquid equilibrium measurements for the ethanol-acetone system at 372.7, 397.7, and 422.6 K, Journal of Chemical & Engineering Data 3 (1987) 357-362. doi:10.1021/je00049a021

**T / K = 422.60**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 10.01 | 0.9240 | 0.8910 | |
| 10.47 | 0.8010 | 0.7580 | |
| 10.75 | 0.6960 | 0.6590 | |
| 11.02 | 0.5870 | 0.5530 | |
| 11.19 | 0.4760 | 0.4490 | |
| 11.30 | 0.3760 | 0.3610 | |
| 11.34 | 0.2710 | 0.2640 | |
| 11.36 | 0.1900 | 0.1900 | AZEO |
| 11.35 | 0.1760 | 0.1770 | |
| 11.32 | 0.1090 | 0.1160 | |

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**Isobaric phase equilibrium data**

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Ku, Hsu-Chen - Tu, Chein-Hsiun, Isobaric vapor–liquid equilibria for mixtures of acetone, ethanol, and 2,2,4-trimethylpentane at 101.3kPa, Fluid Phase Equilibria 1 (2005) 99-108. doi:10.1016/j.fluid.2005.01.007

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 348.91 | 0.9560 | 0.8710 |
| 346.65 | 0.9150 | 0.7680 |
| 344.53 | 0.8680 | 0.6750 |
| 342.69 | 0.8250 | 0.5970 |
| 341.17 | 0.7730 | 0.5370 |
| 339.81 | 0.7240 | 0.4830 |
| 338.39 | 0.6720 | 0.4290 |
| 337.32 | 0.6200 | 0.3910 |
| 336.24 | 0.5670 | 0.3490 |
| 335.37 | 0.5190 | 0.3150 |
| 334.51 | 0.4620 | 0.2810 |
| 333.78 | 0.4140 | 0.2510 |
| 333.06 | 0.3610 | 0.2230 |
| 332.43 | 0.3120 | 0.1970 |
| 331.81 | 0.2550 | 0.1650 |
| 331.20 | 0.2040 | 0.1330 |
| 330.66 | 0.1510 | 0.1020 |
| 330.17 | 0.0990 | 0.0710 |
| 329.69 | 0.0490 | 0.0350 |

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**Enthalpy of mixing**

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Lietzmann, Andreas - Loewen, Burkhard - Schulz, Siegfried, Excess Molar Enthalpies of Propanone + Heptane, Propanone + Ethanol, Ethanol + Heptane, and 2-Propanol + Water at 283.15, 298.15, 323.15, 343.15, and 363.15 K, Journal of Chemical & Engineering Data 4 (1994) 785-788. doi:10.1021/je00016a033

**T / K = 283.15**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 198.10 | 0.9500 |
| 376.30 | 0.8980 |
| 525.40 | 0.8500 |
| 667.00 | 0.7970 |
| 782.50 | 0.7460 |
| 872.70 | 0.6940 |
| 938.20 | 0.6470 |
| 999.00 | 0.5920 |
| 1038.7 | 0.5410 |
| 1043.7 | 0.4900 |
| 1040.7 | 0.4430 |
| 1019.6 | 0.3970 |
| 975.70 | 0.3440 |
| 910.40 | 0.2950 |
| 835.40 | 0.2530 |
| 702.20 | 0.1950 |
| 586.60 | 0.1520 |
| 401.20 | 0.0950 |
| 225.30 | 0.0500 |

Lietzmann, Andreas - Loewen, Burkhard - Schulz, Siegfried, Excess Molar Enthalpies of Propanone + Heptane, Propanone + Ethanol, Ethanol + Heptane, and 2-Propanol + Water at 283.15, 298.15, 323.15, 343.15, and 363.15 K, Journal of Chemical & Engineering Data 4 (1994) 785-788. doi:10.1021/je00016a033

**T / K = 298.15**

**P / bar = 4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 210.30 | 0.9500 |
| 396.40 | 0.8980 |
| 561.10 | 0.8500 |
| 712.00 | 0.7970 |
| 826.90 | 0.7460 |
| 926.00 | 0.6940 |
| 995.70 | 0.6470 |
| 1052.2 | 0.5920 |
| 1096.8 | 0.5410 |

| | |
|---|---|
| 1101.3 | 0.4900 |
| 1095.5 | 0.4430 |
| 1069.5 | 0.3970 |
| 1020.3 | 0.3440 |
| 945.30 | 0.2950 |
| 860.20 | 0.2530 |
| 712.70 | 0.1950 |
| 582.90 | 0.1520 |
| 385.00 | 0.0950 |
| 213.20 | 0.0500 |

Shen, S. - Wang, Y. - Shi, J., Determination of Excess Enthalpies and the Prediction of Vapor - Liquid Equilibria for Some Ketone Alcohol Systems, Gaoxiao Huaxue Gongcheng Xuebao 1 (1990) 1-7.

**T / K =** **308.16**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 313.70 | 0.9303 |
| 625.60 | 0.8525 |
| 772.30 | 0.8085 |
| 991.40 | 0.7249 |
| 1114.2 | 0.6426 |
| 1151.2 | 0.5994 |
| 1181.6 | 0.5418 |
| 1173.1 | 0.4361 |
| 1068.0 | 0.3296 |
| 827.00 | 0.2067 |
| 450.10 | 0.0983 |
| 346.50 | 0.0743 |

Lietzmann, Andreas - Loewen, Burkhard - Schulz, Siegfried, Excess Molar Enthalpies of Propanone + Heptane, Propanone + Ethanol, Ethanol + Heptane, and 2-Propanol + Water at 283.15, 298.15, 323.15, 343.15, and 363.15 K, Journal of Chemical & Engineering Data 4 (1994) 785-788. doi:10.1021/je00016a033

**T / K =** **323.15**

**P / bar =** **4.000**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 479.10 | 0.8980 |
| 666.40 | 0.8500 |
| 834.50 | 0.7970 |
| 976.60 | 0.7460 |
| 1076.7 | 0.6940 |
| 1160.3 | 0.6470 |
| 1223.4 | 0.5920 |
| 1269.2 | 0.5410 |
| 1269.1 | 0.4900 |
| 1256.0 | 0.4430 |
| 1219.0 | 0.3970 |
| 1161.2 | 0.3440 |
| 1069.7 | 0.2950 |
| 972.70 | 0.2530 |
| 806.00 | 0.1950 |
| 662.60 | 0.1520 |
| 439.20 | 0.0950 |

Lien, Pei-Jung - Lin, Ho-mu - Lee, Ming-Jer, Excess Molar Enthalpies for Binary Mixtures of Ethanol + Acetone, + Octane, + Cyclohexane and 1-Propanol + Acetone, + Octane, + Heptane at 323.15 K, Journal of Chemical & Engineering Data 2 (2003) 359-361. doi:10.1021/je020149l

**T / K =** **323.15**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 255.00 | 0.0500 |
| 483.00 | 0.1020 |
| 652.00 | 0.1500 |
| 805.00 | 0.2000 |
| 928.00 | 0.2520 |
| 1018.0 | 0.3000 |
| 1085.0 | 0.3520 |
| 1124.0 | 0.4000 |
| 1144.0 | 0.4520 |
| 1139.0 | 0.5010 |
| 1109.0 | 0.5510 |
| 1066.0 | 0.6000 |
| 1005.0 | 0.6500 |
| 919.00 | 0.7020 |
| 818.00 | 0.7520 |
| 701.00 | 0.8000 |
| 560.00 | 0.8500 |
| 392.00 | 0.9010 |
| 211.00 | 0.9500 |

Lietzmann, Andreas - Loewen, Burkhard - Schulz, Siegfried, Excess Molar Enthalpies of Propanone + Heptane, Propanone + Ethanol, Ethanol + Heptane, and 2-Propanol + Water at 283.15, 298.15, 323.15, 343.15, and 363.15 K, Journal of Chemical & Engineering Data 4 (1994) 785-788. doi:10.1021/je00016a033

**T / K =** **343.15**

**P / bar =** **4.000**

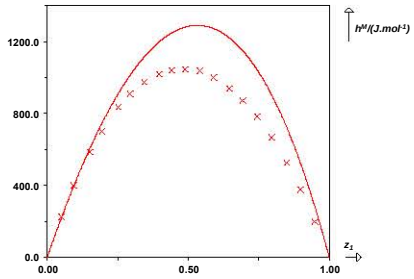
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 496.40 | 0.8980 |
| 686.10 | 0.8500 |
| 862.00 | 0.7970 |

| | |
|---|---|
| 1010.5 | 0.7460 |
| 1114.1 | 0.6940 |
| 1199.5 | 0.6470 |
| 1262.5 | 0.5920 |
| 1309.3 | 0.5410 |
| 1309.4 | 0.4900 |
| 1283.6 | 0.4430 |
| 1242.6 | 0.3970 |
| 1172.7 | 0.3440 |
| 1073.9 | 0.2950 |
| 964.10 | 0.2530 |
| 791.20 | 0.1950 |
| 653.20 | 0.1520 |
| 426.20 | 0.0950 |

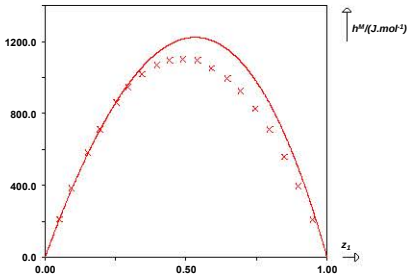
Lietzmann, Andreas - Loewen, Burkhard - Schulz, Siegfried, Excess Molar Enthalpies of Propanone + Heptane, Propanone + Ethanol, Ethanol + Heptane, and 2-Propanol + Water at 283.15, 298.15, 323.15, 343.15, and 363.15 K, Journal of Chemical & Engineering Data 4 (1994) 785-788. doi:10.1021/je00016a033

| **T / K =** | **363.15** |
|---|---|
| **P / bar =** | **4.000** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 241.20 | 0.9540 |
| 491.30 | 0.9000 |
| 693.40 | 0.8490 |
| 859.90 | 0.7950 |
| 978.20 | 0.7510 |
| 1089.7 | 0.6980 |
| 1160.9 | 0.6500 |
| 1209.0 | 0.5980 |
| 1226.2 | 0.5490 |
| 1222.3 | 0.5050 |
| 1193.1 | 0.4520 |
| 1144.8 | 0.4050 |
| 1063.5 | 0.3480 |
| 973.10 | 0.3000 |
| 841.60 | 0.2430 |
| 724.10 | 0.2010 |
| 568.90 | 0.1500 |
| 364.40 | 0.0910 |
| 280.10 | 0.0700 |

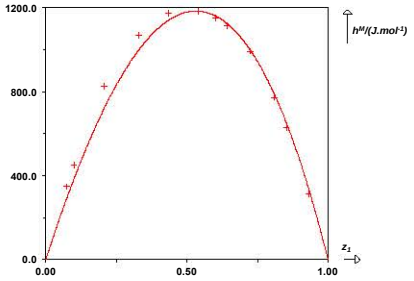
T/K = 283.15 - P/bar = 4.00



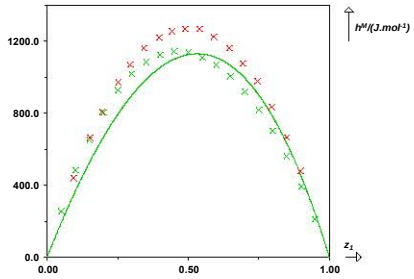

T/K = 298.15 - P/bar = 4.00



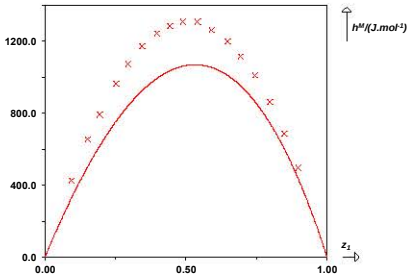

T/K = 308.16 - P/bar = 1.0132



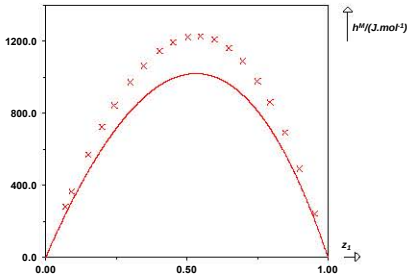

T/K = 323.15 - P/bar = 4.00 1.0132



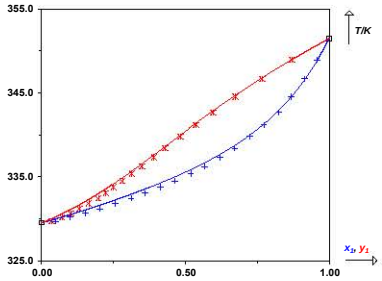

T/K = 343.15 - P/bar = 4.00



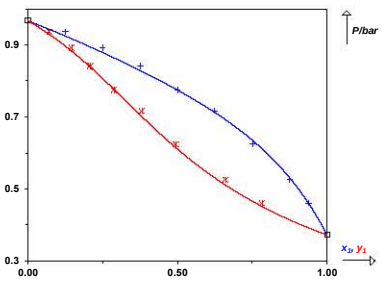

T/K = 363.15 - P/bar = 4.00



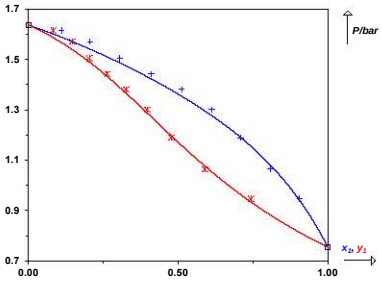

P/bar = 1.01300



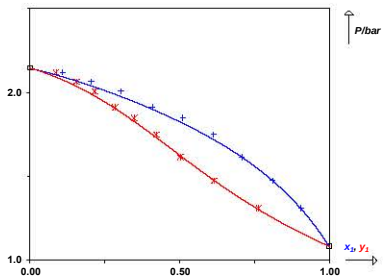

T/K = 328.15



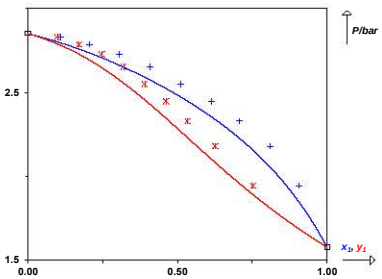

T/K = 344.19



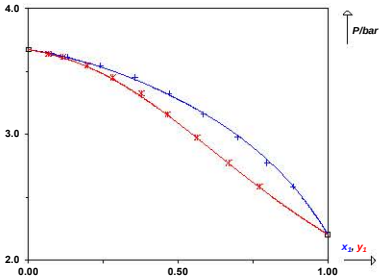

T/K = 353.18



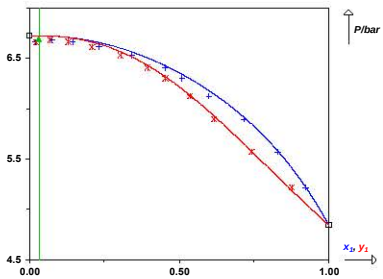

T/K = 363.19



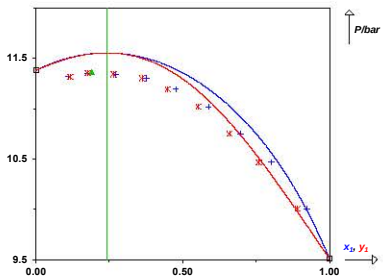

T/K = 372.70




T/K = 397.70




T/K = 422.60



## METHANOL (1) + DIISOPROPYL ETHER (2)

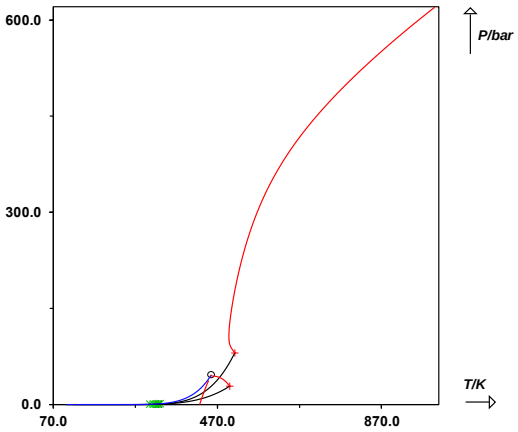
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 108-20-3 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | ZAFNJMIOTHYJRJ-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.5 | 500.05 |
| **$P_c$ / bar** | 80.84 | 28.8 |
| **ω** | 0.566 | 0.339 |

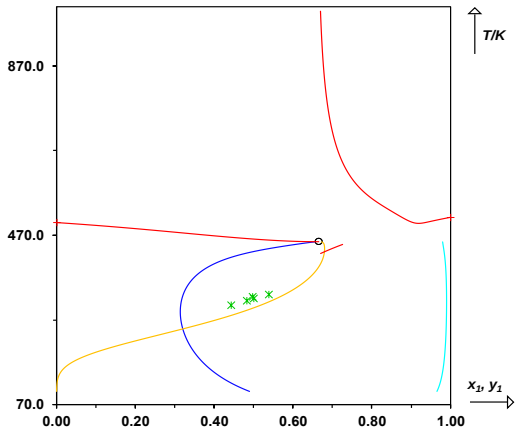
Non ideal with entropic causes

**PPR78 results**

*Parameters*
A/MPa = 611
B/MPa = -178

*Deviations*
MAPE on x = 48 %
MAPE on y = 15 %
MAPE on $h^M$ = 81 %
MAPE on $c_P^M$ = 27 %



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**Isothermal phase equilibrium data**

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Reddy, Prashant - Benecke, Travis P. - Ramjugernath, Deresh, Isothermal (vapour+liquid) equilibria for binary mixtures of diisopropyl ether with (methanol, or ethanol, or 1-butanol): Experimental data, correlations, and predictions, The Journal of Chemical Thermodynamics (2013) 330-339. doi:10.1016/j.jct.2012.11.005

**T / K = 305.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.3291 | 0.9490 | 0.6980 | |
| 0.3739 | 0.8930 | 0.5900 | |
| 0.3956 | 0.8420 | 0.5410 | |
| 0.4119 | 0.7810 | 0.5050 | |
| 0.4229 | 0.6900 | 0.4630 | |
| 0.4236 | 0.6040 | 0.4550 | |
| 0.4243 | 0.5320 | 0.4500 | |
| 0.4245 | 0.4730 | 0.4470 | |
| 0.4247 | 0.4610 | 0.4440 | |
| 0.4249 | 0.4540 | 0.4390 | |
| 0.4252 | 0.4430 | 0.4430 | AZEO |
| 0.4253 | 0.4290 | 0.4350 | |
| 0.4233 | 0.3680 | 0.4520 | |
| 0.4195 | 0.2410 | 0.4330 | |
| 0.4115 | 0.1710 | 0.4130 | |
| 0.3975 | 0.1190 | 0.3810 | |
| 0.3551 | 0.0540 | 0.2770 | |

Reddy, Prashant - Benecke, Travis P. - Ramjugernath, Deresh, Isothermal (vapour+liquid) equilibria for binary mixtures of diisopropyl ether with (methanol, or ethanol, or 1-butanol): Experimental data, correlations, and predictions, The Journal of Chemical Thermodynamics (2013) 330-339. doi:10.1016/j.jct.2012.11.005

**T / K = 315.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.4391 | 0.9890 | 0.8780 | |
| 0.4939 | 0.9630 | 0.7600 | |
| 0.5456 | 0.9290 | 0.6640 | |
| 0.5819 | 0.8910 | 0.6090 | |
| 0.6206 | 0.8000 | 0.5470 | |
| 0.6453 | 0.6740 | 0.5110 | |
| 0.6562 | 0.5420 | 0.4900 | |
| 0.6537 | 0.4930 | 0.4870 | |
| 0.6555 | 0.4820 | 0.4820 | AZEO |
| 0.6557 | 0.4810 | 0.4840 | |
| 0.6568 | 0.4740 | 0.4820 | |
| 0.6486 | 0.4130 | 0.4750 | |
| 0.6452 | 0.2940 | 0.4590 | |
| 0.6396 | 0.2210 | 0.4420 | |
| 0.6145 | 0.1410 | 0.4030 | |
| 0.5876 | 0.1020 | 0.3710 | |
| 0.5251 | 0.0550 | 0.2780 | |

Fárková, Jana - Linek, Jan - Wichterle, Ivan, Isothermal vapour-liquid equilibria and excess volumes in the methanol-aliphatic ether systems, Fluid Phase Equilibria 1 (1995) 53-65. doi:10.1016/0378-3812(95)02710-V

**T / K = 320.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.5202 | 0.0318 | 0.1012 | |
| 0.5424 | 0.0514 | 0.1530 | |
| 0.6017 | 0.1212 | 0.2737 | |
| 0.6250 | 0.1628 | 0.3206 | |
| 0.6609 | 0.2692 | 0.3979 | |
| 0.6750 | 0.3503 | 0.4390 | |
| 0.6843 | 0.4789 | 0.4914 | |
| 0.6847 | 0.5000 | 0.5000 | AZEO |
| 0.6828 | 0.5847 | 0.5273 | |
| 0.6737 | 0.6842 | 0.5753 | |
| 0.6534 | 0.7789 | 0.6348 | |
| 0.6240 | 0.8533 | 0.6996 | |
| 0.5880 | 0.9094 | 0.7697 | |
| 0.5487 | 0.9535 | 0.8489 | |
| 0.5182 | 0.9764 | 0.9153 | |
| 0.4998 | 0.9899 | 0.9588 | |

Reddy, Prashant - Benecke, Travis P. - Ramjugernath, Deresh, Isothermal (vapour+liquid) equilibria for binary mixtures of diisopropyl ether with (methanol, or ethanol, or 1-butanol): Experimental data, correlations, and predictions, The Journal of Chemical Thermodynamics (2013) 330-339. doi:10.1016/j.jct.2012.11.005

**T / K = 325.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.6886 | 0.9790 | 0.8740 | |
| 0.7589 | 0.9550 | 0.7710 | |
| 0.8285 | 0.9210 | 0.6800 | |
| 0.9096 | 0.8410 | 0.5910 | |
| 0.9647 | 0.7000 | 0.5290 | |
| 0.9687 | 0.5410 | 0.5100 | |
| 0.9683 | 0.5120 | 0.5050 | |
| 0.9684 | 0.4990 | 0.5000 | |
| 0.9684 | 0.4980 | 0.4980 | AZEO |
| 0.9685 | 0.4960 | 0.4910 | |
| 0.9694 | 0.4510 | 0.4870 | |

| | | |
|---|---|---|
| 0.9684 | 0.3730 | 0.4850 |
| 0.9676 | 0.3110 | 0.4840 |
| 0.9575 | 0.2580 | 0.4640 |
| 0.9367 | 0.1910 | 0.4400 |
| 0.8687 | 0.0990 | 0.3730 |
| 0.7695 | 0.0430 | 0.2720 |

Fárková, Jana - Linek, Jan - Wichterle, Ivan, Isothermal vapour-liquid equilibria and excess volumes in the methanol-aliphatic ether systems, Fluid Phase Equilibria 1 (1995) 53-65. doi:10.1016/0378-3812(95)02710-V

**T / K = 330.00**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.7321 | 0.0247 | 0.0824 | |
| 0.7917 | 0.0619 | 0.1761 | |
| 0.8441 | 0.0975 | 0.2484 | |
| 0.9251 | 0.1858 | 0.3480 | |
| 0.9992 | 0.3681 | 0.4631 | |
| 1.015 | 0.5187 | 0.5248 | |
| 1.016 | 0.5307 | 0.5295 | |
| 1.016 | 0.5390 | 0.5390 | AZEO |
| 1.011 | 0.6314 | 0.5691 | |
| 0.9950 | 0.7310 | 0.6158 | |
| 0.9836 | 0.7680 | 0.6428 | |
| 0.9410 | 0.8481 | 0.7122 | |
| 0.9151 | 0.8805 | 0.7472 | |
| 0.8811 | 0.9139 | 0.7920 | |
| 0.8360 | 0.9494 | 0.8531 | |
| 0.7979 | 0.9729 | 0.9085 | |
| 0.7780 | 0.9835 | 0.9409 | |
| 0.7570 | 0.9939 | 0.9742 | |

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**Enthalpy of mixing**

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Letcher, Trevor M. - Govender, Penny U., Excess Molar Enthalpies of an Alkanol + a Branched Chain Ether at the Temperature 298.15 K, Journal of Chemical & Engineering Data 4 (1995) 997-1000. doi:10.1021/je00020a060

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 150.40 | 0.0880 |
| 189.60 | 0.1320 |
| 218.60 | 0.2270 |
| 215.60 | 0.2760 |
| 202.00 | 0.3400 |
| 179.40 | 0.4040 |
| 142.60 | 0.5320 |
| 103.30 | 0.6050 |
| 101.40 | 0.6060 |
| 53.20 | 0.7020 |
| 43.30 | 0.7080 |
| 39.20 | 0.7160 |
| 20.00 | 0.7560 |
| 6.400 | 0.7750 |
| -25.50 | 0.8460 |
| -34.80 | 0.8740 |
| -37.90 | 0.9280 |
| -35.50 | 0.9630 |
| -26.10 | 0.9760 |
| -12.70 | 0.9860 |
| -6.100 | 0.9930 |

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**Heat capacity of mixing**

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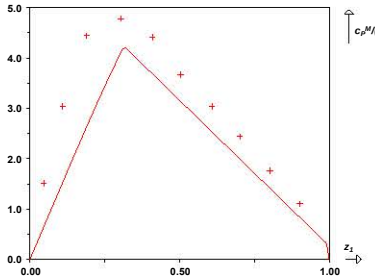
Piñeiro, Ángel, Excess volumes and isobaric heat capacities of diisopropyl ether with several alkanols at 298.15K, Fluid Phase Equilibria 2 (2004) 245-256. doi:10.1016/j.fluid.2003.11.003

**T / K = 298.15**

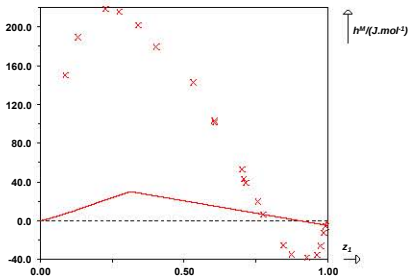
**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 1.510 | 0.0458 |
| 3.040 | 0.1096 |
| 4.440 | 0.1903 |
| 4.780 | 0.3043 |
| 4.410 | 0.4080 |
| 3.670 | 0.5023 |
| 3.030 | 0.6080 |
| 2.440 | 0.7011 |
| 1.760 | 0.8023 |
| 1.100 | 0.9011 |

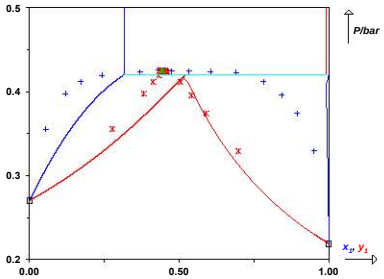
T/K = 298.15 - P/bar = 1.0132



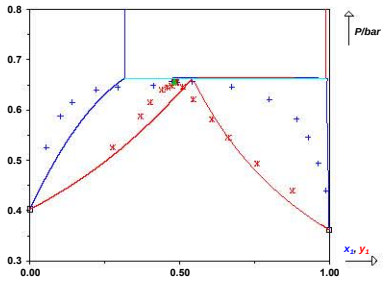

T/K = 298.15 - P/bar = 1.0100



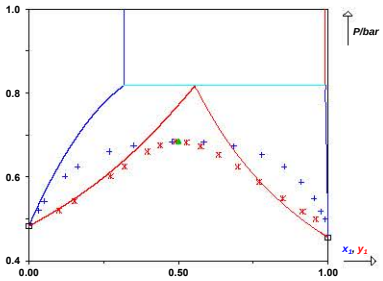

T/K = 305.15



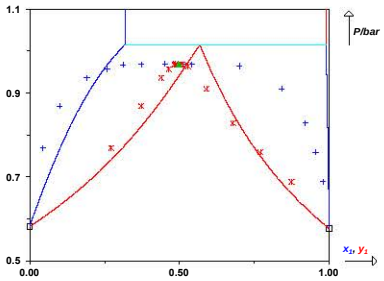

T/K = 315.15



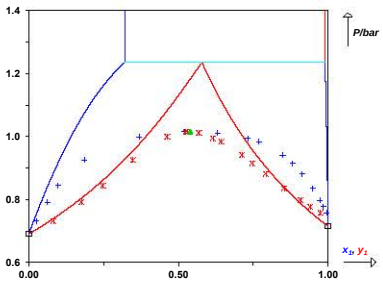

T/K = 320.00




T/K = 325.15




T/K = 330.00



# SA-SA systems (AC = 9)

## WATER (1) + ETHYLENEDIAMINE (2)

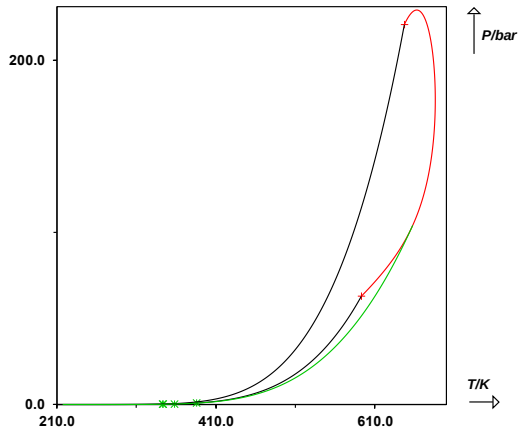
| | | |
|---|---|---|
| **CAS** | 7732-18-5 | 107-15-3 |
| **InChiKey** | XLYOFNOQVPJJNP-UHFFFAOYSA-N | PIICEJLVQHRZGT-UHFFFAOYSA-N |
| **$T_c$ / K** | 647.10 | 593.00 |
| **$P_c$ / bar** | 220.64 | 62.90 |
| **ω** | 0.345 | 0.472 |

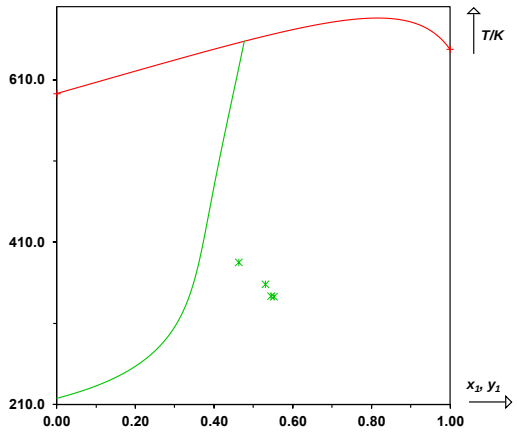
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = -224
B/MPa = 322

*Deviations*
MAPE on x = 19 %
MAPE on y = 40 %
MAPE on $x_{az}$ = 36 %
MAPE on $P_{az}$ = 11 %



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**Isobaric phase equilibrium data**

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Schmelzer, J. - Quitzsdi, K., Isobare Flüssigkeit-Dampfgleichgewichte der binären Systeme Benzol-Äthylendiamin und Wasser-Äthylendiamin, Zeitschrift für Physikalische Chemie 1 (1973) doi:10.1515/zpch-1973-25231

**P / bar = 0.1333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 338.99 | 0.1440 | 0.0850 |
| 340.04 | 0.2290 | 0.1380 |
| 340.82 | 0.3010 | 0.2020 |
| 341.88 | 0.3670 | 0.2790 |
| 342.04 | 0.3830 | 0.2950 |
| 342.46 | 0.4200 | 0.3300 |
| 343.05 | 0.4780 | 0.4050 |
| 343.43 | 0.5030 | 0.4620 |
| 343.55 | 0.5390 | 0.5410 |
| 343.45 | 0.5580 | 0.5750 |
| 342.91 | 0.5900 | 0.6450 |
| 342.32 | 0.6300 | 0.7420 |
| 341.50 | 0.6660 | 0.8040 |
| 339.72 | 0.7150 | 0.8800 |
| 338.42 | 0.7480 | 0.9180 |
| 332.19 | 0.8340 | 0.9850 |
| 328.08 | 0.9070 | 0.9960 |

Rivenq, F., Ebulliometry of water-ethylenediamine mixtures, Bull. Soc. Chim. Fr. (1963) 1606-1608.

**P / bar = 0.1333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 337.65 | 0.0788 | 0.0483 |
| 339.15 | 0.1907 | 0.1022 |
| 340.75 | 0.2855 | 0.1806 |
| 342.25 | 0.3778 | 0.2834 |
| 342.65 | 0.4437 | 0.3687 |
| 342.85 | 0.5102 | 0.4744 |
| 342.95 | 0.5472 | 0.5396 |
| 342.85 | 0.5573 | 0.5647 |
| 342.65 | 0.6227 | 0.7020 |
| 341.95 | 0.6582 | 0.7743 |
| 341.55 | 0.6706 | 0.8017 |
| 340.65 | 0.6986 | 0.8562 |
| 339.65 | 0.7131 | 0.8778 |
| 338.95 | 0.7270 | 0.9020 |
| 336.15 | 0.7643 | 0.9437 |
| 335.15 | 0.7791 | 0.9586 |
| 333.95 | 0.7952 | 0.9660 |
| 331.95 | 0.8276 | 0.9835 |
| 330.35 | 0.8546 | 0.9896 |
| 329.25 | 0.8763 | 0.9930 |
| 328.05 | 0.9011 | 0.9961 |
| 327.15 | 0.9216 | 0.9970 |
| 326.35 | 0.9418 | 0.9988 |
| 325.75 | 0.9604 | 0.9991 |

Rivenq, F., Ebulliometry of water-ethylenediamine mixtures, Bull. Soc. Chim. Fr. (1963) 1606-1608.

**P / bar = 0.2666**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 353.75 | 0.0698 | 0.0514 |
| 355.05 | 0.1882 | 0.1220 |
| 356.15 | 0.2877 | 0.2031 |
| 357.05 | 0.3849 | 0.3147 |
| 357.65 | 0.4624 | 0.4177 |
| 357.85 | 0.5170 | 0.5074 |
| 357.85 | 0.5434 | 0.5535 |
| 357.75 | 0.5707 | 0.6064 |
| 357.55 | 0.5975 | 0.6591 |
| 356.45 | 0.6668 | 0.7893 |
| 354.85 | 0.6977 | 0.8459 |
| 353.55 | 0.7270 | 0.8932 |
| 353.35 | 0.7334 | 0.8960 |
| 351.35 | 0.7658 | 0.9382 |
| 350.05 | 0.7873 | 0.9520 |
| 349.25 | 0.7979 | 0.9625 |
| 347.25 | 0.8311 | 0.9796 |
| 345.65 | 0.8541 | 0.9861 |
| 344.15 | 0.8773 | 0.9908 |
| 341.95 | 0.9224 | 0.9970 |
| 341.15 | 0.9429 | 0.9982 |
| 340.55 | 0.9607 | 0.9988 |

Rivenq, F., Ebulliometry of water-ethylenediamine mixtures, Bull. Soc. Chim. Fr. (1963) 1606-1608.

**P / bar = 0.7999**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 383.15 | 0.0728 | 0.0545 |
| 383.95 | 0.1957 | 0.1599 |
| 384.45 | 0.2834 | 0.2435 |
| 384.95 | 0.3723 | 0.3443 |
| 385.15 | 0.4373 | 0.4210 |
| 385.25 | 0.4654 | 0.4684 |
| 385.15 | 0.4876 | 0.4991 |
| 384.95 | 0.5383 | 0.5802 |
| 384.75 | 0.5585 | 0.6053 |
| 384.25 | 0.5941 | 0.6620 |

| | | |
|---|---|---|
| 383.45 | 0.6300 | 0.7318 |
| 381.85 | 0.6942 | 0.8323 |
| 380.45 | 0.7278 | 0.8754 |
| 378.65 | 0.7629 | 0.9135 |
| 376.65 | 0.7991 | 0.9509 |
| 375.95 | 0.8131 | 0.9553 |
| 374.55 | 0.8287 | 0.9681 |
| 373.15 | 0.8551 | 0.9806 |
| 371.65 | 0.8793 | 0.9867 |
| 370.55 | 0.9015 | 0.9924 |
| 369.55 | 0.9224 | 0.9948 |
| 368.65 | 0.9433 | 0.9970 |
| 367.95 | 0.9621 | 0.9985 |

Ragaini, V. - Zanderighi, L. - Santi, R., The liquid-vapor equilibrium of the ethylenediamine-water system, Atti Soc. Peloritana Sci. Fis. Mat. Nat. (1968) 537-548.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 389.96 | 0.0876 | 0.0576 |
| 390.96 | 0.1957 | 0.1599 |
| 391.46 | 0.2769 | 0.2457 |
| 391.76 | 0.3705 | 0.3556 |
| 391.76 | 0.4876 | 0.5004 |
| 391.56 | 0.5238 | 0.5535 |
| 390.86 | 0.6008 | 0.6649 |
| 389.56 | 0.6493 | 0.7621 |
| 388.86 | 0.6789 | 0.8030 |
| 388.26 | 0.6915 | 0.8210 |
| 386.96 | 0.7286 | 0.8718 |
| 386.56 | 0.7365 | 0.8818 |
| 385.56 | 0.7570 | 0.8997 |
| 385.06 | 0.7636 | 0.9109 |
| 382.66 | 0.8017 | 0.9475 |
| 381.16 | 0.8287 | 0.9667 |
| 379.36 | 0.8551 | 0.9783 |
| 378.16 | 0.8803 | 0.9857 |
| 376.96 | 0.9029 | 0.9914 |
| 376.06 | 0.9229 | 0.9945 |
| 374.46 | 0.9614 | 0.9982 |

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**Azeotropic point**

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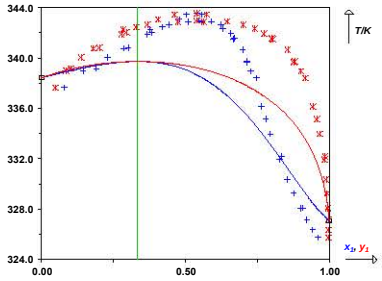
Schmelzer, J. - Quitzsdi, K., Isobare Flüssigkeit-Dampfgleichgewichte der binären Systeme Benzol-Äthylendiamin und Wasser-Äthylendiamin, Zeitschrift für Physikalische Chemie 1 (1973) doi:10.1515/zpch-1973-25231

| T / K | P / bar | $x_1$ |
|---|---|---|
| 343.57 | 0.1333 | 0.5450 |

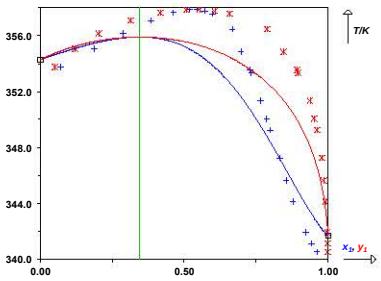
Rivenq, F., Ebulliometry of water-ethylenediamine mixtures, Bull. Soc. Chim. Fr. (1963) 1606-1608.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 385.25 | 0.7999 | 0.4624 |
| 357.95 | 0.2666 | 0.5304 |
| 343.05 | 0.1333 | 0.5523 |

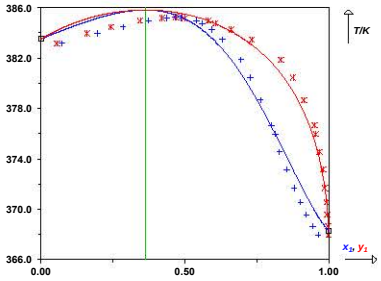
P/bar = 0.13332



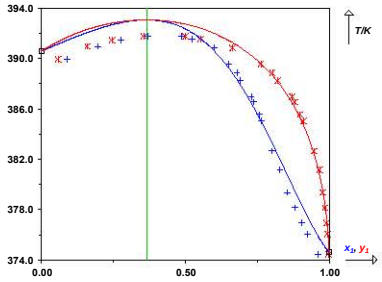

P/bar = 0.26664



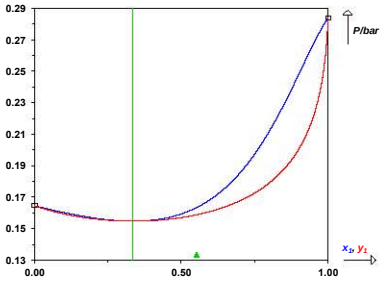

P/bar = 0.79993



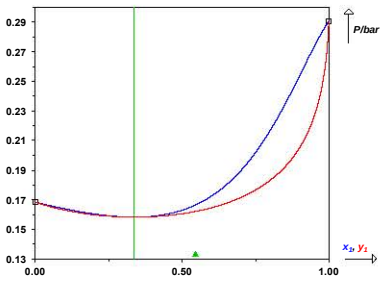

P/bar = 1.01330



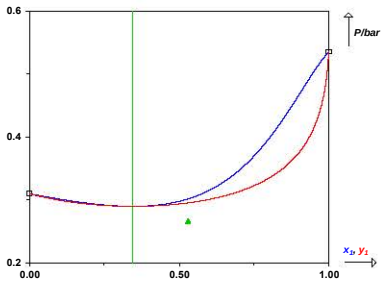

T/K = 343.05



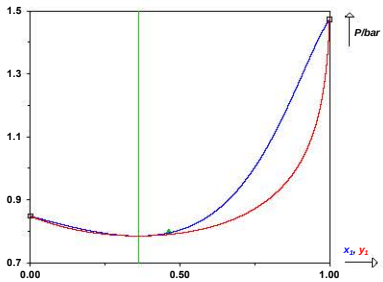

T/K = 343.57




T/K = 357.95




T/K = 385.25



## WATER (1) + 1-PENTANOL (2)

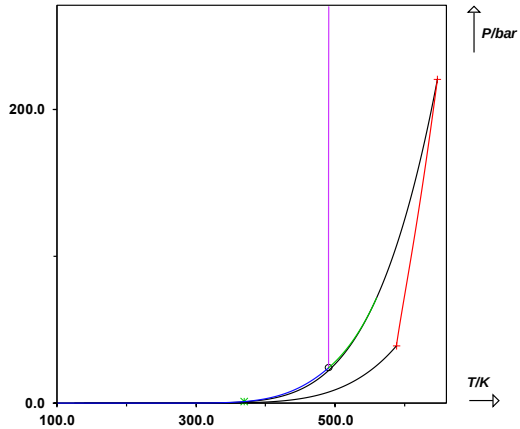
| | | |
|---|---|---|
| **CAS** | 7732-18-5 | 71-41-0 |
| **InChiKey** | XLYOFNOQVPJJNP-UHFFFAOYSA-N | AMQJEAYHLZJPGS-UHFFFAOYSA-N |
| **$T_c$ / K** | 647.096 | 588.1 |
| **$P_c$ / bar** | 220.64 | 38.97 |
| **ω** | 0.345 | 0.575 |

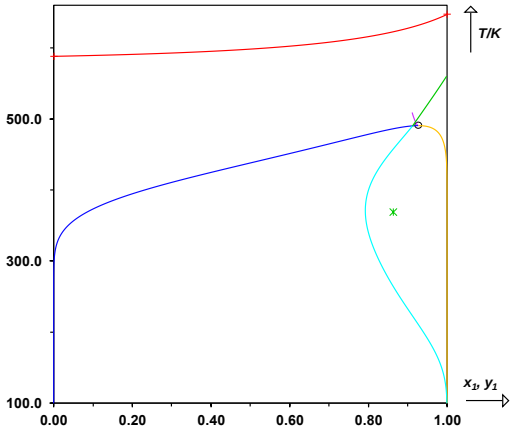
Unknown ideality

**PPR78 results**

*Parameters*
A/MPa = 5300
B/MPa = 20000

*Deviations*
MAPE on x = 41 %
MAPE on y = 18 %
MAPE on $h^M$ = 81 %



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**Isobaric phase equilibrium data**

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Cho, T.H. - Ochi, K. - Kojima, K., Isobaric vapor-liquid equilibria for binary systems with limited miscibility, water-n-amyl alcohol and water-isoamyl alcohol, Kagaku Kogaku Ronbunshu 2 (1984) 181-183.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 410.65 | 0.0012 | 0.0170 |
| 409.19 | 0.0050 | 0.0655 |
| 407.11 | 0.0109 | 0.1319 |
| 406.37 | 0.0131 | 0.1543 |
| 404.67 | 0.0185 | 0.2052 |
| 402.96 | 0.0247 | 0.2531 |
| 401.75 | 0.0290 | 0.2860 |
| 399.84 | 0.0367 | 0.3365 |
| 398.51 | 0.0425 | 0.3704 |
| 396.82 | 0.0499 | 0.4099 |
| 395.14 | 0.0583 | 0.4486 |
| 393.43 | 0.0674 | 0.4865 |
| 392.93 | 0.0707 | 0.4973 |
| 389.91 | 0.0895 | 0.5574 |
| 388.66 | 0.0981 | 0.5809 |
| 385.91 | 0.1194 | 0.6300 |
| 383.81 | 0.1383 | 0.6646 |
| 381.11 | 0.1662 | 0.7072 |
| 379.76 | 0.1836 | 0.7271 |
| 377.61 | 0.2121 | 0.7568 |
| 375.95 | 0.2410 | 0.7797 |
| 375.20 | 0.2543 | 0.7896 |
| 373.65 | 0.2868 | 0.8092 |
| 373.09 | 0.3007 | 0.8163 |
| 370.61 | 0.3781 | 0.8460 |
| 369.90 | 0.4117 | 0.8541 |
| 369.21 | 0.9950 | 0.8681 |
| 369.32 | 0.9952 | 0.8708 |
| 369.77 | 0.9958 | 0.8854 |
| 370.70 | 0.9972 | 0.9157 |
| 371.73 | 0.9985 | 0.9507 |
| 372.21 | 0.9991 | 0.9672 |

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**Enthalpy of mixing**

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Marongiu, Bruno - Ferino, Italo - Monaci, Roberto - Solinas, Vincenzo - Torrazza, Sergio, Thermodynamic properties of aqueous non-electrolyte mixtures. Alkanols + water systems., Journal of Molecular Liquids 4 (1984) 229-247. doi:10.1016/0167-7322(84)80027-6

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -15.00 | 0.9980 |
| -42.00 | 0.9941 |
| 3.000 | 0.9429 |
| 110.00 | 0.8571 |
| 351.00 | 0.6807 |
| 486.00 | 0.5715 |
| 600.00 | 0.4754 |
| 707.00 | 0.3930 |
| 812.00 | 0.2962 |
| 850.00 | 0.2286 |
| 728.00 | 0.1477 |
| 564.00 | 0.0995 |
| 400.00 | 0.0604 |

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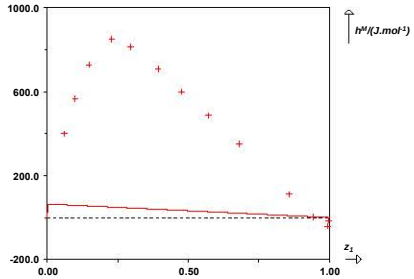
**Three-phase line**

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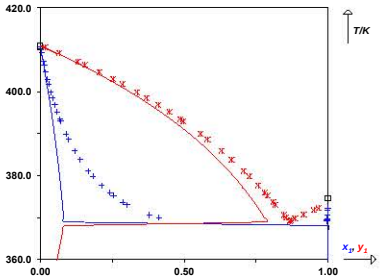
M.-J. Lee - L.-H. Tsai - G.-B. Hong - H. Lin, Multiphase Coexistence for Aqueous Systems with Amyl Alcohol and Amyl Acetate, Industrial & Engineering Chemistry Research. 41 (2002) 3247–3252. doi:10.1021/ie0105371.

| T / K | P / bar | $x_{1a}$ | $x_{1b}$ | $y_1$ |
|---|---|---|---|---|
| 343.20 | 0.35 | 0.3982 | 0.9959 | 0.8887 |
| 353.20 | 0.53 | 0.4305 | 0.9958 | 0.8493 |
| 363.20 | 0.81 | 0.4547 | 0.9953 | 0.8454 |
| 369.20 | 1.02 | 0.4735 | 0.9950 | 0.8418 |
| 373.20 | 1.17 | 0.4815 | 0.9943 | 0.8394 |
| 378.20 | 1.45 | 0.4944 | 0.9942 | 0.8360 |
| 383.20 | 1.70 | 0.5087 | 0.9938 | 0.8319 |
| 388.20 | 2.05 | 0.5196 | 0.9937 | 0.8259 |
| 393.20 | 2.40 | 0.5275 | 0.9936 | 0.8229 |

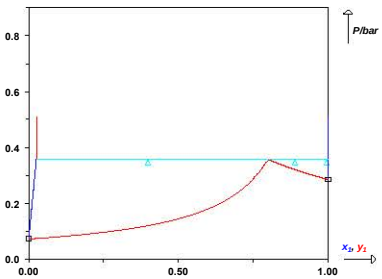
T/K = 298.15 - P/bar = 1.0132



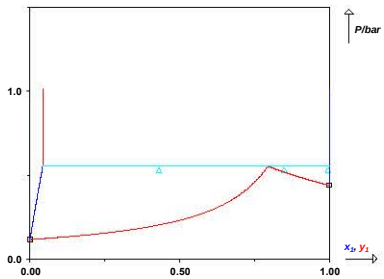

P/bar = 1.01330



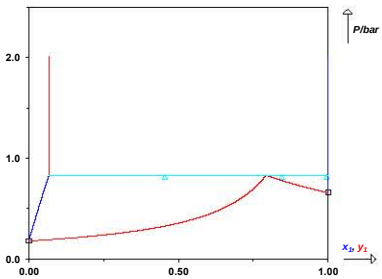

T/K = 343.20



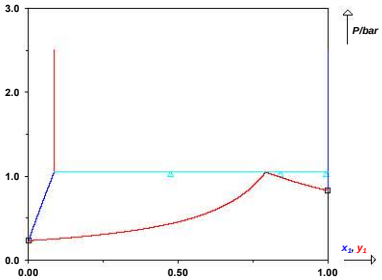

T/K = 353.20



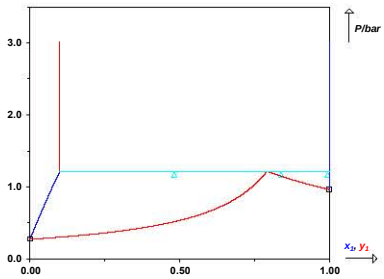

T/K = 363.20



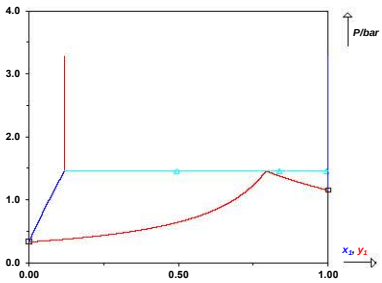

T/K = 369.20



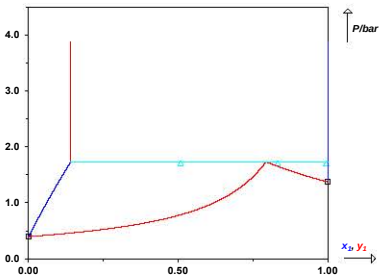

T/K = 373.20



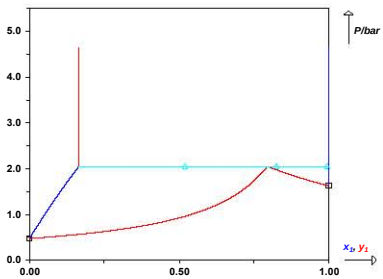

T/K = 378.20



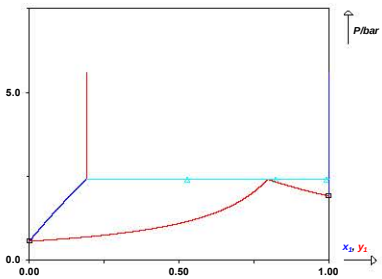

T/K = 383.20




T/K = 388.20




T/K = 393.20



## METHANOL (1) + 1-BUTANOL (2)

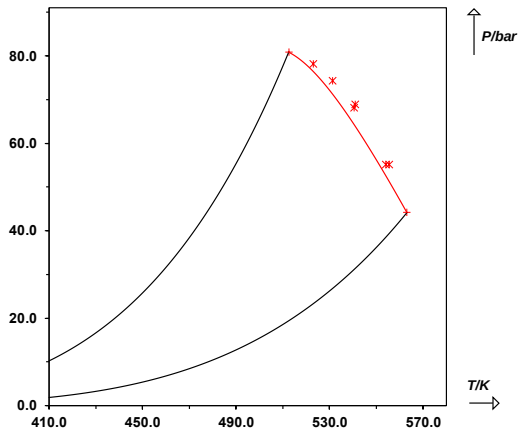
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 71-36-3 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | LRHPLDYGYMQRHN-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.50 | 563.10 |
| **$P_c$ / bar** | 80.84 | 44.14 |
| **ω** | 0.566 | 0.588 |

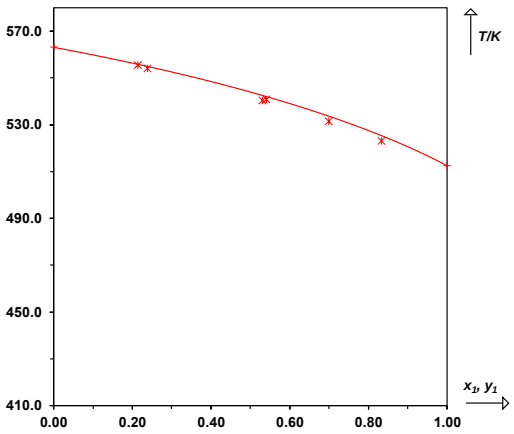
Ideal

**PPR78 results**

*Parameters*
A/MPa = 15.5
B/MPa = 50.6

*Deviations*
MAPE on x = 17 %
MAPE on y = 13 %
MAPE on $x_c$ = 7.4 %
MAPE on $P_c$ = 5.1 %
MAPE on $h^M$ = 30 %
MAPE on $c_P^M$ = 33 %



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**Isothermal phase equilibrium data**

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Polák, Jiří - Murakami, Sachio - Lam, V. T. - Pflug, H. D. - Benson, G. C., Molar excess enthalpies, volumes, and Gibbs free energies of methanol – isomeric butanol systems at 25 °C, Canadian Journal of Chemistry 16 (1970) 2457-2465. doi:10.1139/v70-417

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0245 | 0.0871 | 0.6569 |
| 0.0261 | 0.0953 | 0.6800 |
| 0.0299 | 0.1200 | 0.7302 |
| 0.0320 | 0.1295 | 0.7482 |
| 0.0384 | 0.1690 | 0.8010 |
| 0.0495 | 0.2340 | 0.8564 |
| 0.0549 | 0.2654 | 0.8751 |
| 0.0619 | 0.3072 | 0.8946 |
| 0.0637 | 0.3173 | 0.8993 |
| 0.0700 | 0.3557 | 0.9128 |
| 0.0714 | 0.3628 | 0.9150 |
| 0.0802 | 0.4172 | 0.9310 |
| 0.0817 | 0.4258 | 0.9329 |
| 0.0868 | 0.4569 | 0.9396 |
| 0.0943 | 0.5048 | 0.9487 |
| 0.1068 | 0.5845 | 0.9612 |
| 0.1175 | 0.6544 | 0.9702 |
| 0.1277 | 0.7237 | 0.9772 |
| 0.1416 | 0.8164 | 0.9855 |
| 0.1489 | 0.8660 | 0.9894 |
| 0.1584 | 0.9290 | 0.9943 |

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**Isobaric phase equilibrium data**

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Arce, Alberto - Martinez-Ageitos, José - Rodil, Eva - Soto, Ana, Phase equilibria involved in extractive distillation of 2-methoxy-2-methylpropane+methanol using 1-butanol as entrainer, Fluid Phase Equilibria 1-2 (2000) 207-218. doi:10.1016/S0378-3812(00)00364-2

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 386.44 | 0.0271 | 0.1480 |
| 384.73 | 0.0419 | 0.2139 |
| 367.00 | 0.2298 | 0.6604 |
| 363.33 | 0.2785 | 0.7297 |
| 361.05 | 0.3227 | 0.7771 |
| 357.91 | 0.3729 | 0.8199 |
| 355.76 | 0.4282 | 0.8526 |
| 353.06 | 0.4912 | 0.8873 |
| 349.94 | 0.5650 | 0.9173 |
| 347.06 | 0.6422 | 0.9397 |
| 345.09 | 0.7086 | 0.9553 |
| 342.96 | 0.7819 | 0.9705 |
| 341.42 | 0.8418 | 0.9795 |
| 340.23 | 0.8907 | 0.9854 |
| 339.23 | 0.9333 | 0.9913 |
| 338.26 | 0.9736 | 0.9971 |

Kay, W.B. - Donham, W.E., Liquid-vapour equilibria in the iso-butanol—n-butanol, methanol—n-butanol and diethyl ether—n-butanol systems, Chemical Engineering Science 1 (1955) 1-16. doi:10.1016/0009-2509(55)85001-4

**P / bar = 55.16**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 553.15 | 0.2290 | 0.2510 |
| 543.15 | 0.3140 | 0.4010 |
| 533.15 | 0.4090 | 0.5370 |
| 523.15 | 0.5130 | 0.6530 |
| 513.15 | 0.6370 | 0.7630 |
| 503.15 | 0.7800 | 0.8700 |
| 493.15 | 0.9490 | 0.9730 |

Kay, W.B. - Donham, W.E., Liquid-vapour equilibria in the iso-butanol—n-butanol, methanol—n-butanol and diethyl ether—n-butanol systems, Chemical Engineering Science 1 (1955) 1-16. doi:10.1016/0009-2509(55)85001-4

**P / bar = 68.95**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 533.15 | 0.5980 | 0.6570 |
| 523.15 | 0.7100 | 0.7790 |
| 513.15 | 0.8430 | 0.8910 |

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**Enthalpy of mixing**

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Stokes, R.H, Excess enthalpies of (butan-1-ol + methanol) at 278.15, 298.15, and 318.15 K, The Journal of Chemical Thermodynamics 11 (1988) 1349-1352. doi:10.1016/0021-9614(88)90172-3

**T / K = 278.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 7.400 | 0.0154 |
| 22.70 | 0.0480 |
| 46.10 | 0.0997 |
| 72.60 | 0.1625 |
| 94.00 | 0.2180 |

| | |
|---|---|
| 111.60 | 0.2681 |
| 125.70 | 0.3133 |
| 137.20 | 0.3543 |
| 146.40 | 0.3921 |
| 156.70 | 0.4433 |
| 165.30 | 0.5027 |
| 169.40 | 0.5540 |
| 170.30 | 0.5976 |
| 168.70 | 0.6314 |
| 168.90 | 0.6354 |
| 166.40 | 0.6593 |
| 165.70 | 0.6691 |
| 162.80 | 0.6876 |
| 161.30 | 0.6988 |
| 157.60 | 0.7165 |
| 150.80 | 0.7457 |
| 142.30 | 0.7749 |
| 131.60 | 0.8049 |
| 118.60 | 0.8350 |
| 103.30 | 0.8652 |
| 85.10 | 0.8957 |
| 69.80 | 0.9184 |
| 58.80 | 0.9334 |
| 46.70 | 0.9486 |
| 34.00 | 0.9638 |
| 20.40 | 0.9789 |
| 6.700 | 0.9933 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 293.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 3.720 | 0.0441 |
| 19.04 | 0.0860 |
| 33.55 | 0.1260 |
| 45.66 | 0.1641 |
| 58.52 | 0.2006 |
| 106.10 | 0.3608 |
| 135.47 | 0.4918 |
| 152.40 | 0.6009 |
| 147.37 | 0.6931 |
| 131.11 | 0.7721 |
| 105.99 | 0.8405 |
| 73.28 | 0.9003 |
| 36.03 | 0.9531 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 298.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 3.690 | 0.0441 |
| 18.42 | 0.0860 |
| 31.77 | 0.1260 |
| 43.85 | 0.1641 |
| 56.74 | 0.2006 |
| 95.76 | 0.3608 |
| 127.83 | 0.4918 |
| 138.29 | 0.6009 |
| 146.86 | 0.6931 |
| 122.61 | 0.7721 |
| 99.61 | 0.8405 |
| 69.69 | 0.9003 |
| 34.51 | 0.9531 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 303.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 3.390 | 0.0441 |
| 15.21 | 0.0860 |
| 27.05 | 0.1260 |
| 38.83 | 0.1641 |
| 48.65 | 0.2006 |
| 90.82 | 0.3608 |
| 117.23 | 0.4918 |
| 130.22 | 0.6009 |
| 129.69 | 0.6931 |
| 117.17 | 0.7721 |
| 95.06 | 0.8405 |
| 66.57 | 0.9003 |
| 32.68 | 0.9531 |

Stokes, R.H, Excess enthalpies of (butan-1-ol + methanol) at 278.15, 298.15, and 318.15 K, The Journal of Chemical Thermodynamics 11 (1988) 1349-1352. doi:10.1016/0021-9614(88)90172-3

**T / K = 318.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 4.700 | 0.0206 |
| 13.70 | 0.0586 |
| 22.00 | 0.0930 |
| 34.10 | 0.1425 |
| 49.10 | 0.2027 |
| 62.20 | 0.2556 |
| 76.30 | 0.3148 |
| 90.10 | 0.3774 |
| 102.50 | 0.4410 |
| 112.30 | 0.5032 |
| 118.10 | 0.5557 |
| 121.00 | 0.6010 |
| 121.60 | 0.6401 |
| 122.90 | 0.6457 |
| 120.60 | 0.6741 |
| 122.10 | 0.6756 |
| 120.20 | 0.7055 |
| 116.80 | 0.7359 |
| 111.90 | 0.7665 |
| 105.10 | 0.7972 |
| 96.20 | 0.8286 |
| 85.20 | 0.8593 |
| 73.70 | 0.8859 |
| 61.80 | 0.9096 |
| 50.60 | 0.9294 |
| 40.70 | 0.9453 |
| 30.00 | 0.9611 |
| 18.60 | 0.9768 |
| 6.300 | 0.9924 |

Benson, George C. - Benson, George C. - Anand, Subhash C. - Kiyohara, Osamu, Thermodynamic properties of some cycloalkane-cycloalkanol systems at 298. 15.deg.K. II, Journal of Chemical & Engineering Data 3 (1974) 258-261. doi:10.1021/je60062a027

**T / K = 323.15**

**P / bar = 1.010**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 2.370 | 0.0441 |
| 8.230 | 0.0860 |
| 15.38 | 0.1260 |
| 22.17 | 0.1641 |
| 29.50 | 0.2006 |
| 61.26 | 0.3608 |
| 88.70 | 0.4918 |
| 104.11 | 0.6009 |
| 108.37 | 0.6931 |
| 99.49 | 0.7721 |
| 82.39 | 0.8405 |
| 58.45 | 0.9003 |
| 28.75 | 0.9531 |

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**Heat capacity of mixing**

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Ogawa, Hideo - Murakami, Sachio, Excess volumes, isentropic compressions, and isobaric heat capacities for methanol mixed with other alkanols at 25°C, Journal of Solution Chemistry 4 (1987) 315-326. doi:10.1007/BF00646123

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.6040 | 0.1000 |
| -1.040 | 0.2001 |
| -1.319 | 0.3001 |
| -1.428 | 0.4001 |
| -1.409 | 0.5001 |
| -1.276 | 0.6001 |
| -1.039 | 0.7001 |
| -0.8890 | 0.7501 |
| -0.7280 | 0.8001 |
| -0.5590 | 0.8500 |
| -0.3770 | 0.9000 |
| -0.1910 | 0.9500 |

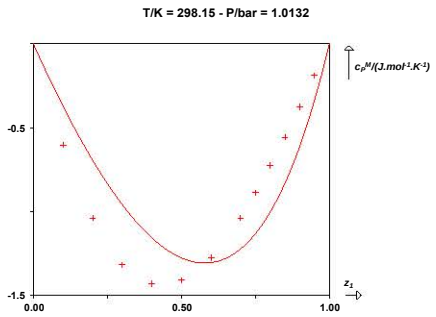
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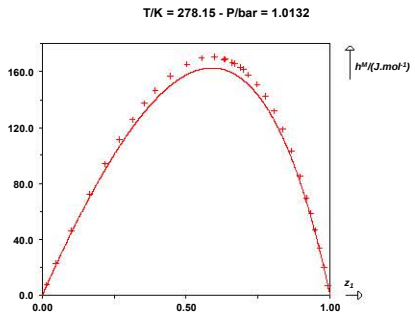
**Critical point**

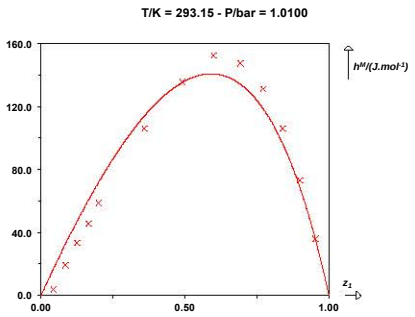
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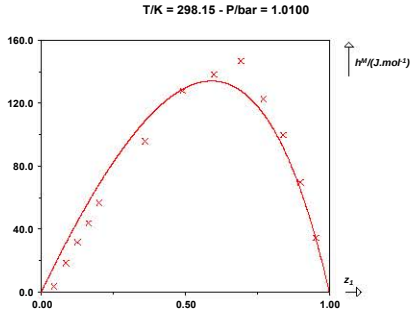
Kay, W.B. - Donham, W.E., Liquid-vapour equilibria in the iso-butanol—n-butanol, methanol—n-butanol and diethyl ether—n-butanol systems, Chemical Engineering Science 1 (1955) 1-16. doi:10.1016/0009-2509(55)85001-4

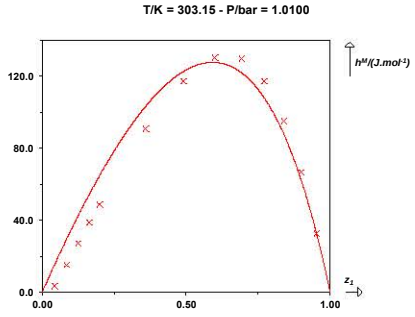
| T / K | P / bar | $x_1$ |
|---|---|---|
| 522.99 | 78.12 | 0.8334 |
| 531.37 | 74.29 | 0.6993 |
| 540.42 | 68.13 | 0.5307 |
| 554.11 | 55.08 | 0.2381 |
| 555.45 | 55.16 | 0.2140 |
| 540.85 | 68.95 | 0.5400 |

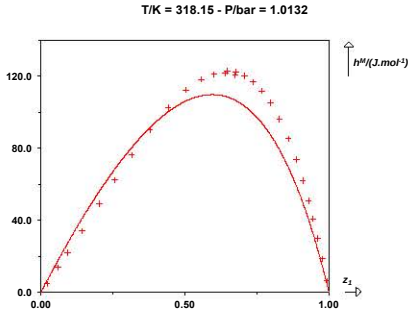

T/K = 298.15 - P/bar = 1.0132
$c_p^M$/(J.mol$^{-1}$.K$^{-1}$)
$z_1$

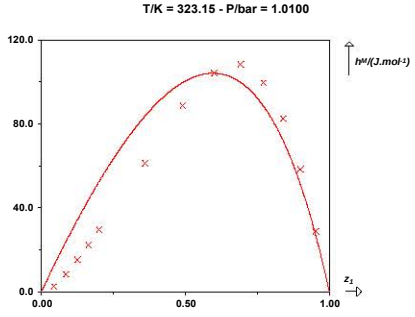

T/K = 278.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
$z_1$

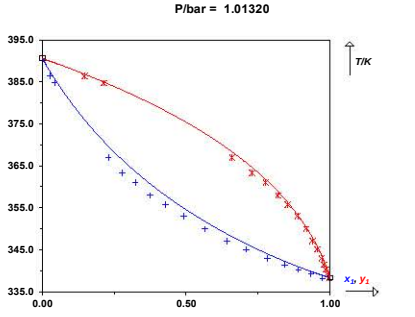

T/K = 293.15 - P/bar = 1.0100
$h^M$/(J.mol$^{-1}$)
$z_1$

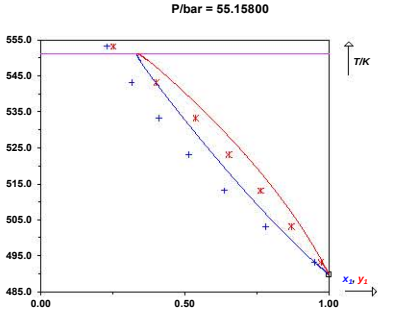

T/K = 298.15 - P/bar = 1.0100
$h^M$/(J.mol$^{-1}$)
$z_1$

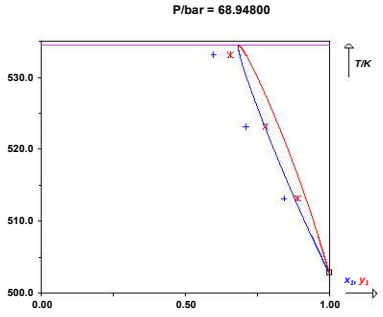

T/K = 303.15 - P/bar = 1.0100
$h^M$/(J.mol$^{-1}$)
$z_1$

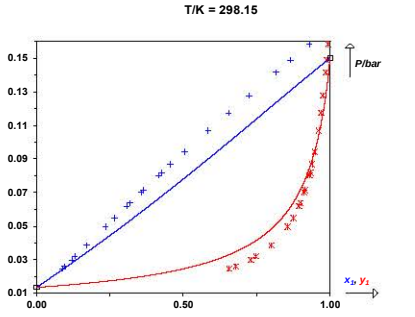

T/K = 318.15 - P/bar = 1.0132
$h^M$/(J.mol$^{-1}$)
$z_1$

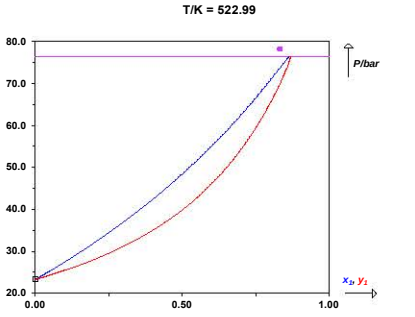

T/K = 323.15 - P/bar = 1.0100
$h^M$/(J.mol$^{-1}$)
$z_1$

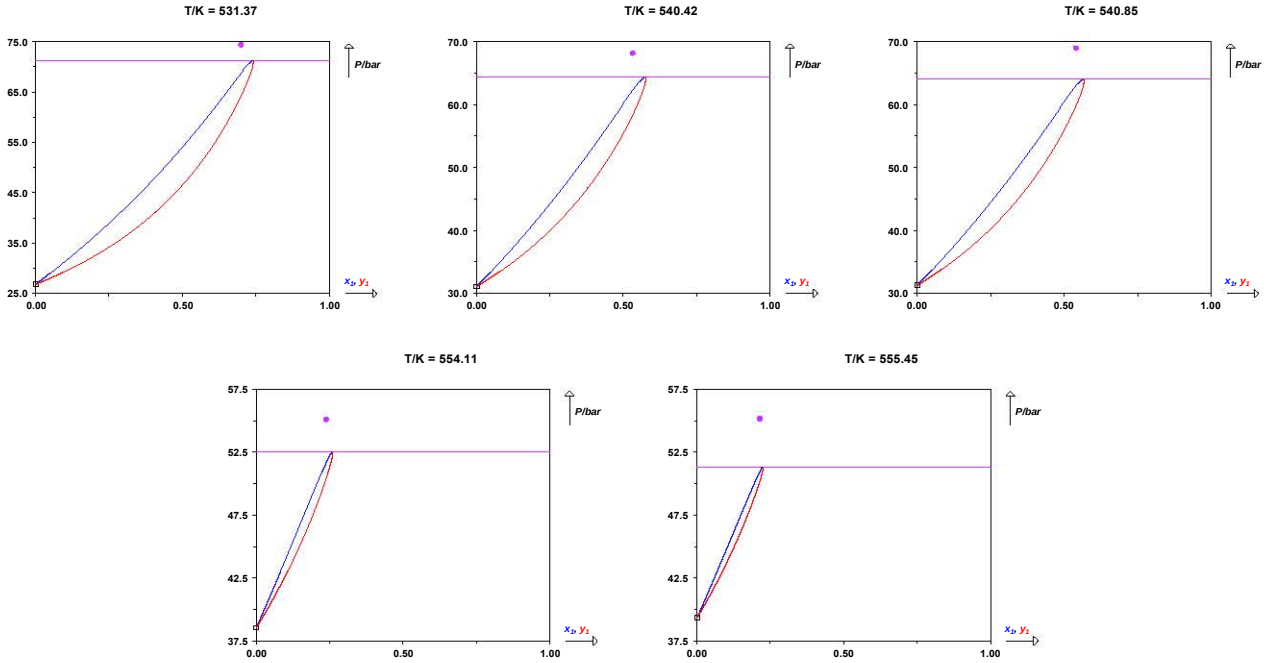

P/bar = 1.01320
T/K
$x_1$, $y_1$


P/bar = 55.15800
T/K
$x_1$, $y_1$


P/bar = 68.94800
T/K
$x_1$, $y_1$


T/K = 298.15
P/bar
$x_1$, $y_1$


T/K = 522.99
P/bar
$x_1$, $y_1$


T/K = 531.37
P/bar
x1, y1
T/K = 540.42
P/bar
x1, y1
T/K = 540.85
P/bar
x1, y1
T/K = 554.11
P/bar
x1, y1
T/K = 555.45
P/bar
x1, y1

## ETHANOL (1) + ACETIC ACID (2)

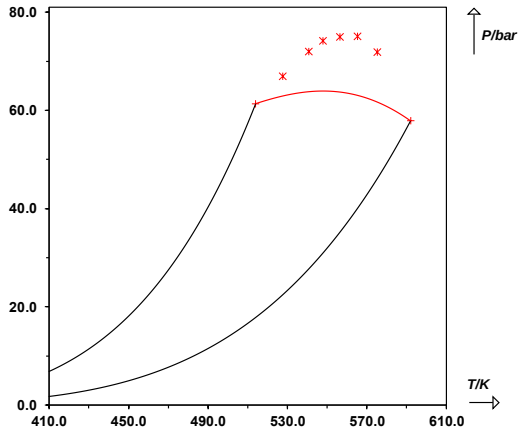
| | | |
|---|---|---|
| **CAS** | 64-17-5 | 64-19-7 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | QTBSBXVTEAMEQO-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 591.95 |
| **$P_c$ / bar** | 61.37 | 57.86 |
| **ω** | 0.644 | 0.467 |

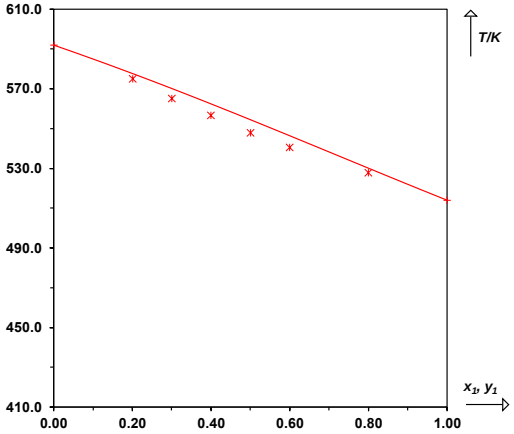
Ideal

**PPR78 results**

*Parameters*
A/MPa = 37.4
B/MPa = 23.7

*Deviations*
MAPE on x = 16 %
MAPE on y = 35 %
MAPE on $x_c$ = 14 %
MAPE on $P_c$ = 13 %
MAPE on $h^M$ = 68 %



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**Isothermal phase equilibrium data**

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Wright, E. H. M. - Akhtar, B. A., Soluble surface films of short-chain monocarboxylic acids on organic and aqueous substrates, Journal of the Chemical Society B: Physical Organic (1970) doi:10.1039/j29700000151

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0333 | 0.1000 | 0.2800 |
| 0.0400 | 0.2200 | 0.5000 |
| 0.0533 | 0.3600 | 0.6750 |
| 0.0600 | 0.4400 | 0.7667 |
| 0.0660 | 0.5100 | 0.8182 |
| 0.0747 | 0.6200 | 0.8839 |
| 0.0800 | 0.7000 | 0.9083 |
| 0.0880 | 0.8000 | 0.9470 |

Miyamoto, Shinji - Nakamura, Shinichi - Iwai, Yoshio - Arai, Yasuhiko, Measurement of Isothermal Vapor−Liquid Equilibria for Binary and Ternary Systems Containing Monocarboxylic Acid, Journal of Chemical & Engineering Data 5 (2001) 1225-1230. doi:10.1021/je0003849

**T / K = 323.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0820 | 0.0290 | 0.0550 |
| 0.0840 | 0.0580 | 0.1100 |
| 0.0900 | 0.0960 | 0.1800 |
| 0.1210 | 0.2900 | 0.5030 |
| 0.1600 | 0.4880 | 0.7630 |
| 0.2100 | 0.6860 | 0.9190 |
| 0.2720 | 0.8940 | 0.9860 |
| 0.2870 | 0.9470 | 0.9950 |
| 0.2960 | 0.9780 | 0.9980 |

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**Isobaric phase equilibrium data**

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Reichl, Albert - Daiminger, Ulrich - Schmidt, Adolf - Davies, Michael - Hoffmann, Ulrich - Brinkmeier, Clemens - Reder, Christoph - Marquardt, Wolfgang, A non-recycle flow still for the experimental determination of vapor–liquid equilibria in reactive systems, Fluid Phase Equilibria 1 (1998) 113-134. doi:10.1016/S0378-3812(98)00409-9

**P / bar = 1.014**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 388.85 | 0.0311 | 0.0686 |
| 387.20 | 0.0586 | 0.1117 |
| 383.35 | 0.1288 | 0.2561 |
| 380.05 | 0.2003 | 0.3893 |
| 376.35 | 0.2808 | 0.5245 |
| 371.80 | 0.3991 | 0.6634 |
| 369.90 | 0.4408 | 0.7222 |
| 366.90 | 0.5129 | 0.8064 |
| 362.30 | 0.6396 | 0.8941 |
| 359.25 | 0.7162 | 0.9343 |
| 355.70 | 0.8432 | 0.9714 |
| 353.75 | 0.9110 | 0.9923 |

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**Enthalpy of mixing**

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Zhao, Junyang - Bao, Jingdan - Hu, Ying, Excess molar enthalpies of (an alkanol + a carboxylic acid) at 298.15 K measured with a Picker calorimeter, The Journal of Chemical Thermodynamics 8 (1989) 811-818. doi:10.1016/0021-9614(89)90027-X

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 99.86 | 0.0288 |
| 186.27 | 0.0655 |
| 244.02 | 0.1042 |
| 308.25 | 0.1426 |
| 336.55 | 0.1844 |
| 352.95 | 0.2381 |
| 350.73 | 0.3042 |
| 302.90 | 0.4103 |
| 239.78 | 0.5085 |
| 156.21 | 0.6080 |
| 80.96 | 0.7123 |
| 44.62 | 0.8120 |
| 23.02 | 0.8864 |
| 10.84 | 0.9423 |

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**Critical point**

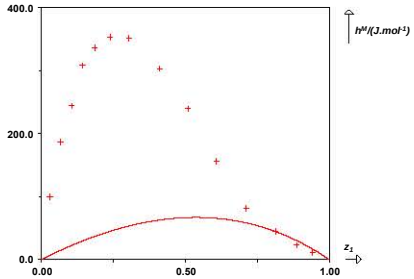
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Škerget, Mojca - Čretnik, Lucija - Knez, Željko - Škrinjar, Maja, Influence of the aromatic ring substituents on phase equilibria of vanillins in binary systems with CO2, Fluid Phase Equilibria 1 (2005) 11-19. doi:10.1016/j.fluid.2004.12.012

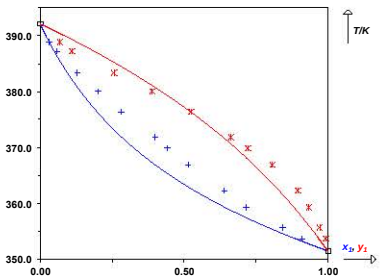
| T / K | P / bar | $x_1$ |
|---|---|---|
| 575.10 | 71.90 | 0.2000 |
| 565.10 | 75.10 | 0.3000 |
| 556.50 | 74.90 | 0.4000 |
| 547.70 | 74.10 | 0.5000 |
| 540.60 | 72.00 | 0.6000 |

| | | |
|---|---|---|
| 527.70 | 66.90 | 0.8000 |

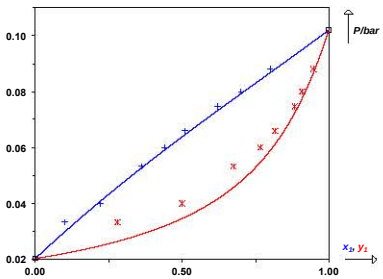
T/K = 298.15 - P/bar = 1.0132



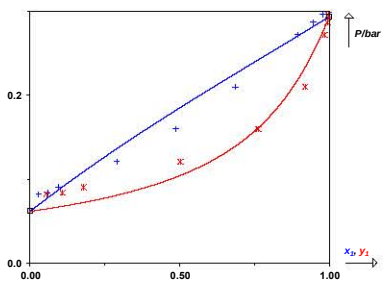

P/bar = 1.01400



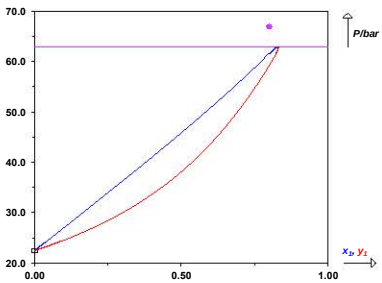

T/K = 303.15



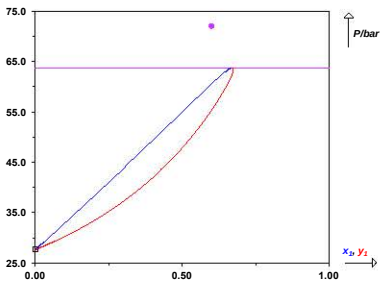

T/K = 323.20



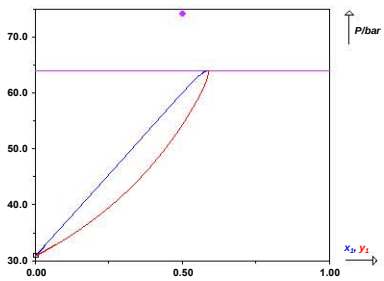

T/K = 527.70



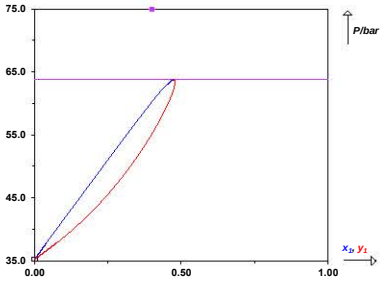

T/K = 540.60



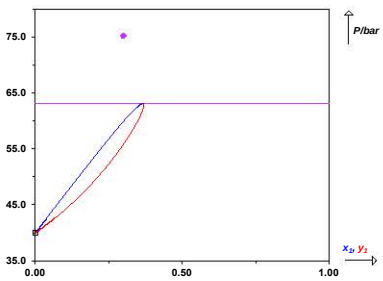

T/K = 547.70



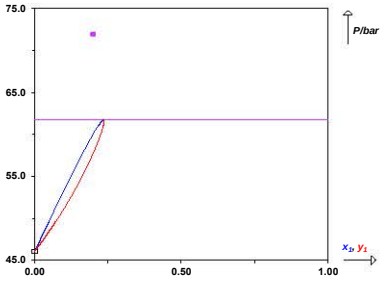

T/K = 556.50




T/K = 565.10




T/K = 575.10



## METHANOL (1) + ETHANOL (2)

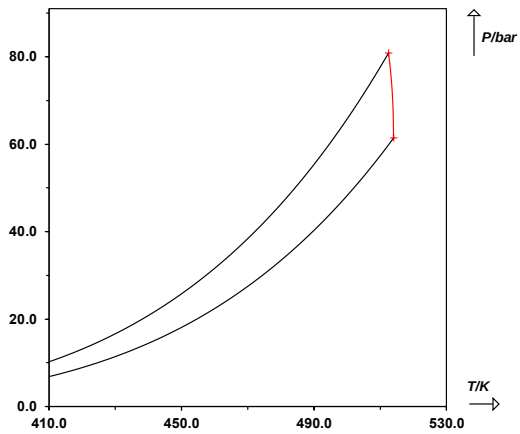
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 64-17-5 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | LFQSCWFLJHTTHZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.50 | 514.00 |
| **$P_c$ / bar** | 80.84 | 61.37 |
| **ω** | 0.566 | 0.644 |

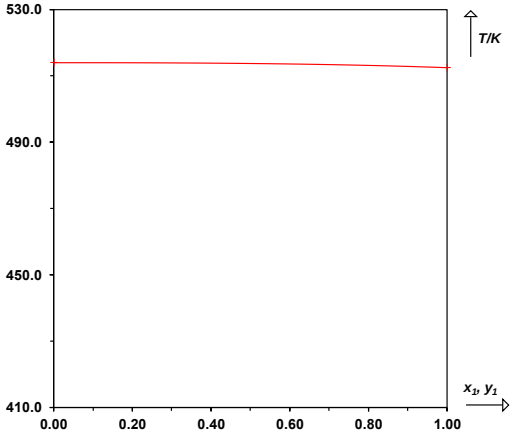
Ideal

**PPR78 results**

*Parameters*
A/MPa = -1.93
B/MPa = 2.23

*Deviations*
MAPE on x = 17 %
MAPE on y = 15 %
MAPE on $h^M$ = 17 %
MAPE on $c_P^M$ = 100 %



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**Isothermal phase equilibrium data**

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Kooner, Zs - Fenby, Dv, Vapour pressure study of the deuterium exchange reaction in methanol-ethanol systems: equilibrium constant determination, Australian Journal of Chemistry 9 (1980) doi:10.1071/CH9801943

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0823 | 0.0431 | 0.0860 |
| 0.0884 | 0.1129 | 0.2112 |
| 0.1013 | 0.2564 | 0.4230 |
| 0.1063 | 0.3110 | 0.4903 |
| 0.1132 | 0.3879 | 0.5752 |
| 0.1156 | 0.4135 | 0.6011 |
| 0.1220 | 0.4843 | 0.6678 |
| 0.1286 | 0.5563 | 0.7288 |
| 0.1294 | 0.5654 | 0.7360 |
| 0.1345 | 0.6206 | 0.7782 |
| 0.1366 | 0.6437 | 0.7949 |
| 0.1444 | 0.7296 | 0.8528 |
| 0.1537 | 0.8303 | 0.9131 |
| 0.1660 | 0.9656 | 0.9836 |

Hall, D.J. - Mash, C.J. - Pemberton, R.C., Vapor liquid equilibriums for the systems water-methanol, water-ethanol, methanol-ethanol, and water-methanol-ethanol at 298.15 K determined by a rapid transpiration method (1979) 1-13.

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0856 | 0.0841 | 0.1610 |
| 0.0905 | 0.1353 | 0.2470 |
| 0.0956 | 0.1902 | 0.3310 |
| 0.1042 | 0.2919 | 0.4670 |
| 0.1104 | 0.3585 | 0.5430 |
| 0.1176 | 0.4414 | 0.6280 |
| 0.1264 | 0.5372 | 0.7150 |
| 0.1356 | 0.6392 | 0.7920 |
| 0.1458 | 0.7489 | 0.8650 |
| 0.1548 | 0.8535 | 0.9280 |
| 0.1612 | 0.9165 | 0.9610 |

Oh, Seung-Kyo - Campbell, Scott W., Total Pressure Measurements for Copper(II) Chloride + Methanol + Ethanol at 303.15 K, Journal of Chemical & Engineering Data 2 (1995) 504-508. doi:10.1021/je00018a033

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.465 | 0.1610 | 0.2250 |
| 2.782 | 0.4280 | 0.5290 |
| 3.016 | 0.5910 | 0.6910 |
| 3.318 | 0.8280 | 0.8780 |
| 3.469 | 0.9480 | 0.9670 |

Butcher, K. L. - Robinson, W. I., An apparatus for determining high-pressure liquid-vapour equilibrium data. I. The methanol-ethanol system, Journal of Applied Chemistry 10 (2007) 289-292. doi:10.1002/jctb.5010161003

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.330 | 0.0620 | 0.0890 |
| 2.448 | 0.1500 | 0.2130 |
| 2.510 | 0.2130 | 0.2880 |
| 2.592 | 0.2820 | 0.3700 |
| 2.717 | 0.3860 | 0.4860 |
| 2.875 | 0.4920 | 0.5970 |
| 2.999 | 0.5880 | 0.6860 |
| 3.103 | 0.6780 | 0.7640 |
| 3.330 | 0.8380 | 0.8890 |
| 3.447 | 0.9410 | 0.9610 |

Butcher, K. L. - Robinson, W. I., An apparatus for determining high-pressure liquid-vapour equilibrium data. I. The methanol-ethanol system, Journal of Applied Chemistry 10 (2007) 289-292. doi:10.1002/jctb.5010161003

**T / K = 393.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 4.385 | 0.0610 | 0.0820 |
| 4.557 | 0.1500 | 0.2000 |
| 4.661 | 0.2120 | 0.2770 |
| 4.806 | 0.2820 | 0.3600 |
| 4.999 | 0.3860 | 0.4730 |
| 5.226 | 0.4910 | 0.5820 |
| 5.440 | 0.5890 | 0.6750 |
| 5.619 | 0.6780 | 0.7530 |
| 5.971 | 0.8380 | 0.8820 |
| 6.205 | 0.9420 | 0.9590 |

Butcher, K. L. - Robinson, W. I., An apparatus for determining high-pressure liquid-vapour equilibrium data. I. The methanol-ethanol system, Journal of Applied Chemistry 10 (2007) 289-292. doi:10.1002/jctb.5010161003

**T / K = 433.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 12.76 | 0.0600 | 0.0750 |
| 13.14 | 0.1490 | 0.1850 |
| 13.38 | 0.2080 | 0.2530 |

| | | |
|---|---|---|
| 13.69 | 0.2810 | 0.3390 |
| 14.17 | 0.3750 | 0.4410 |
| 14.72 | 0.4870 | 0.5560 |
| 15.24 | 0.5880 | 0.6520 |
| 15.69 | 0.6730 | 0.7280 |
| 16.51 | 0.8360 | 0.8670 |
| 17.06 | 0.9400 | 0.9510 |

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**Isobaric phase equilibrium data**

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Arce, Alberto - Martinez-Ageitos, José - Rodil, Eva - Soto, Ana, Measurement and prediction of isobaric vapour–liquid equilibrium data of the system ethanol+methanol+2-methoxy-2-methylpropane, Fluid Phase Equilibria 1-2 (1998) 139-153. doi:10.1016/S0378-3812(98)00227-1

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 350.71 | 0.0418 | 0.0673 |
| 349.88 | 0.0923 | 0.1446 |
| 348.98 | 0.1564 | 0.2326 |
| 348.21 | 0.2026 | 0.2911 |
| 347.57 | 0.2510 | 0.3544 |
| 346.78 | 0.2981 | 0.4089 |
| 346.09 | 0.3440 | 0.4617 |
| 345.40 | 0.3920 | 0.5160 |
| 344.65 | 0.4453 | 0.5716 |
| 343.96 | 0.4938 | 0.6193 |
| 343.21 | 0.5501 | 0.6767 |
| 342.43 | 0.6075 | 0.7288 |
| 341.86 | 0.6512 | 0.7683 |
| 341.19 | 0.7072 | 0.8089 |
| 340.66 | 0.7420 | 0.8358 |
| 340.05 | 0.7964 | 0.8735 |
| 339.27 | 0.8619 | 0.9162 |
| 338.78 | 0.9007 | 0.9378 |
| 338.22 | 0.9421 | 0.9650 |
| 337.83 | 0.9793 | 0.9832 |

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**Enthalpy of mixing**

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Wóycicki, W., Enthalpies of mixing of some binary mixtures of benzene, cyclohexane, and pyridine, and their methyl and ethyl derivatives, The Journal of Chemical Thermodynamics 1 (1972) 1-8. doi:10.1016/S0021-9614(72)80002-8

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 0.9000 | 0.0734 |
| 1.700 | 0.1460 |
| 2.500 | 0.2348 |
| 3.200 | 0.3167 |
| 3.900 | 0.3974 |
| 4.400 | 0.4712 |
| 4.600 | 0.5394 |
| 4.700 | 0.6002 |
| 4.600 | 0.6519 |
| 4.400 | 0.6965 |
| 3.500 | 0.7998 |
| 2.700 | 0.8535 |
| 1.900 | 0.9049 |
| 1.200 | 0.9465 |
| 0.6000 | 0.9756 |

Trampe, D. Mark - Eckert, Charles A., Calorimetric measurement of partial molar excess enthalpies at infinite dilution, Journal of Chemical & Engineering Data 1 (1991) 112-118. doi:10.1021/je00001a033

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 2.699 | 0.8933 |
| 2.427 | 0.9057 |
| 2.158 | 0.9180 |
| 1.892 | 0.9301 |
| 1.565 | 0.9421 |
| 1.257 | 0.9539 |
| 0.9510 | 0.9656 |
| 0.6320 | 0.9772 |
| 0.3020 | 0.9887 |

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**Heat capacity of mixing**

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Ogawa, Hideo - Murakami, Sachio, Excess volumes, isentropic compressions, and isobaric heat capacities for methanol mixed with other alkanols at 25°C, Journal of Solution Chemistry 4 (1987) 315-326. doi:10.1007/BF00646123

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.1400 | 0.1000 |
| -0.2610 | 0.2000 |
| -0.3160 | 0.3000 |
| -0.3460 | 0.4000 |

| | |
|---|---|
| -0.3430 | 0.5000 |
| -0.3120 | 0.6000 |
| -0.2530 | 0.7000 |
| -0.1950 | 0.7995 |
| -0.1550 | 0.8500 |
| -0.1130 | 0.9000 |
| -0.0680 | 0.9500 |

Fang, Wen-jun - Yu, Qing-sen - Lin, Rui-sen - Zong, Han-xing, Vapor heat capacities of some polar–polar binary systems, Thermochimica Acta (2000) 19-23. doi:10.1016/S0040-6031(99)00431-1

**T / K = 402.20**

**P / bar = 1.013**

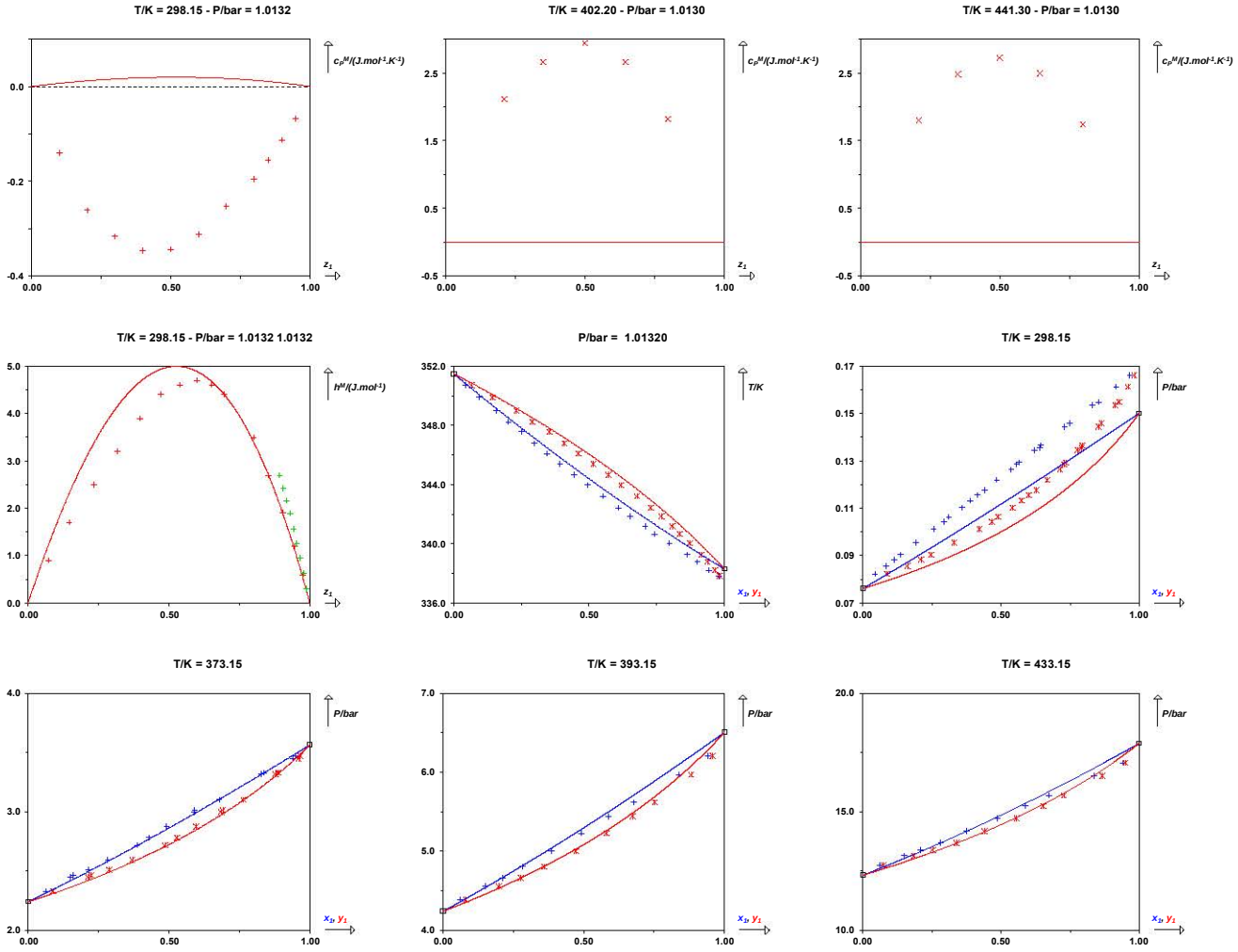
| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $z_1$ |
|---|---|
| 2.110 | 0.2103 |
| 2.660 | 0.3502 |
| 2.940 | 0.4993 |
| 2.660 | 0.6444 |
| 1.820 | 0.7980 |

Fang, Wen-jun - Yu, Qing-sen - Lin, Rui-sen - Zong, Han-xing, Vapor heat capacities of some polar–polar binary systems, Thermochimica Acta (2000) 19-23. doi:10.1016/S0040-6031(99)00431-1

**T / K = 441.30**

**P / bar = 1.013**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $z_1$ |
|---|---|
| 1.800 | 0.2103 |
| 2.480 | 0.3502 |
| 2.720 | 0.4993 |
| 2.490 | 0.6444 |
| 1.740 | 0.7980 |


T/K = 298.15 - P/bar = 1.0132
T/K = 402.20 - P/bar = 1.0130
T/K = 441.30 - P/bar = 1.0130
T/K = 298.15 - P/bar = 1.0132 1.0132
P/bar = 1.01320
T/K = 298.15
T/K = 373.15
T/K = 393.15
T/K = 433.15

## 2-METHYL-2-PROPANOL (1) + 1-BUTANOL (2)

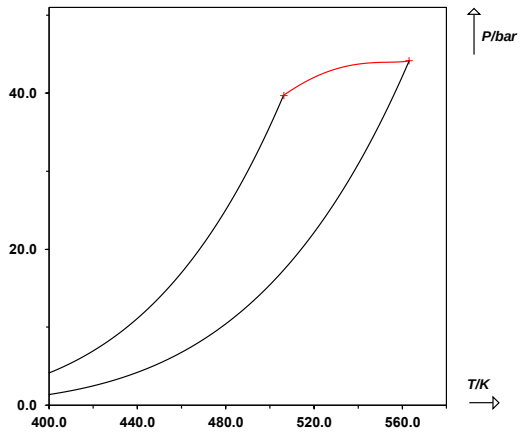
| | | |
|---|---|---|
| **CAS** | 75-65-0 | 71-36-3 |
| **InChiKey** | DKGAVHZHDRPRBM-UHFFFAOYSA-N | LRHPLDYGYMQRHN-UHFFFAOYSA-N |
| **$T_c$ / K** | 506.20 | 563.10 |
| **$P_c$ / bar** | 39.72 | 44.14 |
| **ω** | 0.615 | 0.588 |

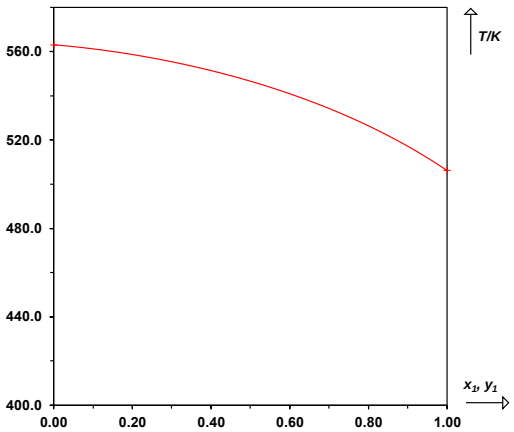
Ideal

**PPR78 results**

*Parameters*
A/MPa = -124
B/MPa = -82.7

*Deviations*
MAPE on x = 20 %
MAPE on y = 19 %
MAPE on $h^M$ = 9.7 %



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**Isothermal phase equilibrium data**

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Geiseler, G. - Sühnel, K. - Quitzsch, K., Exzeßeigenschaften der binären Mischsysteme aus den isomeren Butanolen, Zeitschrift für Physikalische Chemie 1 (1973) doi:10.1515/zpch-1973-25425

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0273 | 0.0240 | 0.0900 |
| 0.0307 | 0.0620 | 0.2130 |
| 0.0381 | 0.1420 | 0.4210 |
| 0.0448 | 0.2140 | 0.5550 |
| 0.0530 | 0.2950 | 0.6650 |
| 0.0582 | 0.3470 | 0.7200 |
| 0.0705 | 0.4500 | 0.8070 |
| 0.0786 | 0.5260 | 0.8550 |
| 0.0854 | 0.5810 | 0.8860 |
| 0.0889 | 0.6110 | 0.8980 |
| 0.0952 | 0.6600 | 0.9220 |
| 0.0983 | 0.6880 | 0.9280 |
| 0.1111 | 0.7870 | 0.9590 |
| 0.1158 | 0.8170 | 0.9690 |
| 0.1273 | 0.9030 | 0.9860 |
| 0.1317 | 0.9400 | 0.9910 |

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**Isobaric phase equilibrium data**

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Quitzsch, K. - Köhler, S. - Taubert, K. - Geiseler, G., Isobare Flüssigkeit-Dampf-Gleichgewichte der „quasi-idealen" binären Systeme n-Butanol/sek.-Butanol und n-Butanol/tert.-Butanol, Journal für Praktische Chemie 3 (1969) 429-437. doi:10.1002/prac.19693110312

**P / bar = 0.1333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 337.91 | 0.1000 | 0.3080 |
| 333.37 | 0.2000 | 0.5230 |
| 329.66 | 0.3000 | 0.6650 |
| 326.24 | 0.4000 | 0.7660 |
| 323.08 | 0.5000 | 0.8410 |
| 320.41 | 0.6000 | 0.8930 |
| 318.12 | 0.7000 | 0.9310 |
| 316.06 | 0.8000 | 0.9620 |
| 314.18 | 0.9000 | 0.9850 |

Quitzsch, K. - Köhler, S. - Taubert, K. - Geiseler, G., Isobare Flüssigkeit-Dampf-Gleichgewichte der „quasi-idealen" binären Systeme n-Butanol/sek.-Butanol und n-Butanol/tert.-Butanol, Journal für Praktische Chemie 3 (1969) 429-437. doi:10.1002/prac.19693110312

**P / bar = 0.4000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 361.65 | 0.1000 | 0.2840 |
| 356.90 | 0.2000 | 0.4920 |
| 352.78 | 0.3000 | 0.6310 |
| 349.21 | 0.4000 | 0.7310 |
| 346.04 | 0.5000 | 0.8100 |
| 342.95 | 0.6000 | 0.8730 |
| 340.35 | 0.7000 | 0.9200 |
| 338.02 | 0.8000 | 0.9550 |
| 335.88 | 0.9000 | 0.9820 |

Quitzsch, K. - Köhler, S. - Taubert, K. - Geiseler, G., Isobare Flüssigkeit-Dampf-Gleichgewichte der „quasi-idealen" binären Systeme n-Butanol/sek.-Butanol und n-Butanol/tert.-Butanol, Journal für Praktische Chemie 3 (1969) 429-437. doi:10.1002/prac.19693110312

**P / bar = 0.6666**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 374.23 | 0.1000 | 0.2770 |
| 369.57 | 0.2000 | 0.4730 |
| 365.30 | 0.3000 | 0.6170 |
| 361.43 | 0.4000 | 0.7240 |
| 357.99 | 0.5000 | 0.8050 |
| 354.91 | 0.6000 | 0.8670 |
| 352.12 | 0.7000 | 0.9160 |
| 349.61 | 0.8000 | 0.9520 |
| 347.42 | 0.9000 | 0.9790 |

Quitzsch, K. - Köhler, S. - Taubert, K. - Geiseler, G., Isobare Flüssigkeit-Dampf-Gleichgewichte der „quasi-idealen" binären Systeme n-Butanol/sek.-Butanol und n-Butanol/tert.-Butanol, Journal für Praktische Chemie 3 (1969) 429-437. doi:10.1002/prac.19693110312

**P / bar = 0.9333**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 383.21 | 0.1000 | 0.2690 |
| 378.25 | 0.2000 | 0.4680 |
| 373.96 | 0.3000 | 0.6110 |
| 370.20 | 0.4000 | 0.7180 |
| 366.57 | 0.5000 | 0.8010 |
| 363.25 | 0.6000 | 0.8630 |
| 360.32 | 0.7000 | 0.9110 |
| 357.84 | 0.8000 | 0.9490 |
| 355.65 | 0.9000 | 0.9780 |

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**Enthalpy of mixing**

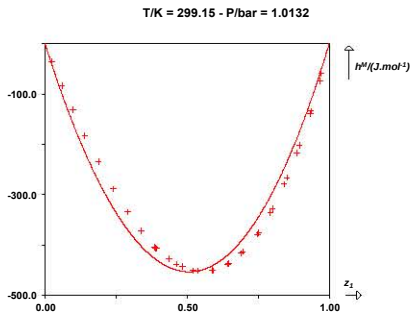
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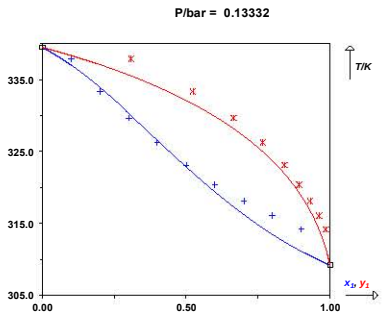
Murakami, Sachio - Benson, G. C., Thermodynamic Properties of Some Isomeric Butyl Alcohol Mixtures, Bulletin of the Chemical Society of Japan 1 (1973) 74-79. doi:10.1246/bcsj.46.74

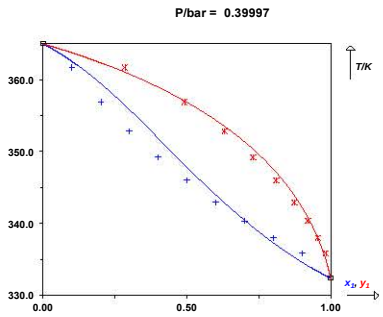
**T / K =** **299.15**

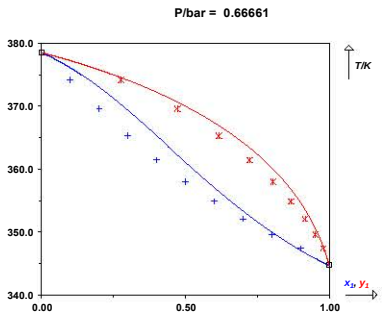
**P / bar =** **UNKNOWN (1.0132)**

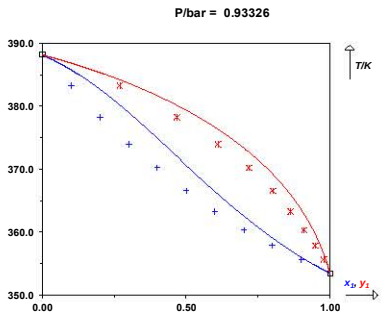
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -35.80 | 0.0253 |
| -83.50 | 0.0604 |
| -131.60 | 0.0978 |
| -182.70 | 0.1397 |
| -233.90 | 0.1875 |
| -288.80 | 0.2410 |
| -334.10 | 0.2905 |
| -372.10 | 0.3381 |
| -403.80 | 0.3863 |
| -405.60 | 0.3892 |
| -406.50 | 0.3923 |
| -427.20 | 0.4369 |
| -437.50 | 0.4625 |
| -442.70 | 0.4841 |
| -450.80 | 0.5216 |
| -451.40 | 0.5364 |
| -449.90 | 0.5891 |
| -450.50 | 0.5896 |
| -437.40 | 0.6430 |
| -437.00 | 0.6450 |
| -416.10 | 0.6915 |
| -413.20 | 0.6957 |
| -378.10 | 0.7473 |
| -375.00 | 0.7515 |
| -335.30 | 0.7935 |
| -328.00 | 0.8007 |
| -279.10 | 0.8415 |
| -266.50 | 0.8518 |
| -217.20 | 0.8856 |
| -202.30 | 0.8954 |
| -138.80 | 0.9323 |
| -133.90 | 0.9351 |
| -74.00 | 0.9657 |
| -59.90 | 0.9728 |

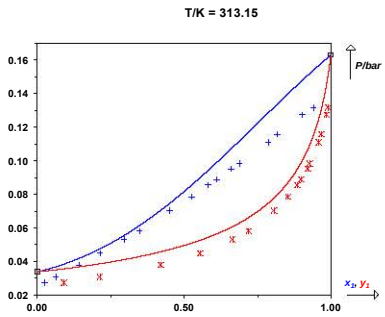

T/K = 299.15 - P/bar = 1.0132
hᴹ/(J.mol⁻¹)
-100.0
-300.0
-500.0
0.00
0.50
1.00
z₁


P/bar = 0.13332
T/K
335.0
325.0
315.0
305.0
0.00
0.50
1.00
x₁, y₁


P/bar = 0.39997
T/K
360.0
350.0
340.0
330.0
0.00
0.50
1.00
x₁, y₁


P/bar = 0.66661
T/K
380.0
370.0
360.0
350.0
340.0
0.00
0.50
1.00
x₁, y₁


P/bar = 0.93326
T/K
390.0
380.0
370.0
360.0
350.0
0.00
0.50
1.00
x₁, y₁


T/K = 313.15
P/bar
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
0.50
1.00
x₁, y₁

## ETHANOL (1) + 3-METHYL-1-BUTANOL (2)

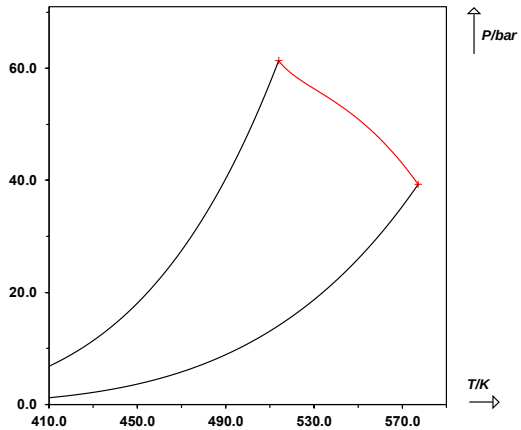
| | | |
|---|---|---|
| **CAS** | 64-17-5 | 123-51-3 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | PHTQWCKDNZKARW-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 577.20 |
| **$P_c$ / bar** | 61.37 | 39.30 |
| **ω** | 0.644 | 0.590 |

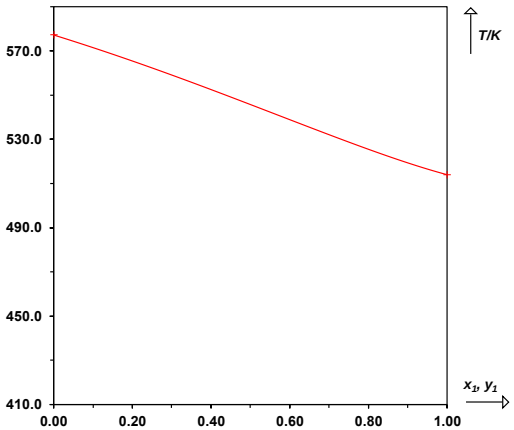
Ideal

**PPR78 results**

*Parameters*
A/MPa = 22.6
B/MPa = -43.8

*Deviations*
MAPE on x = 5.8 %
MAPE on y = 8.7 %



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**Isothermal phase equilibrium data**

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Udovenko, V.V. - Frid, Ts.B., Heats of vaporization of binary mixtures. II, Zh. Fiz. Khim. (1948) 1135-1145.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0567 | 0.1000 | 0.6280 |
| 0.0872 | 0.2000 | 0.7840 |
| 0.1171 | 0.3000 | 0.8580 |
| 0.1457 | 0.4000 | 0.9000 |
| 0.1732 | 0.5000 | 0.9290 |
| 0.1983 | 0.6000 | 0.9500 |
| 0.2241 | 0.7000 | 0.9660 |
| 0.2491 | 0.8000 | 0.9790 |
| 0.2722 | 0.9000 | 0.9900 |

Udovenko, V.V. - Frid, Ts.B., Heats of vaporization of binary mixtures. II, Zh. Fiz. Khim. (1948) 1135-1145.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0949 | 0.1000 | 0.5940 |
| 0.1437 | 0.2000 | 0.7610 |
| 0.1905 | 0.3000 | 0.8400 |
| 0.2357 | 0.4000 | 0.8870 |
| 0.2774 | 0.5000 | 0.9200 |
| 0.3189 | 0.6000 | 0.9430 |
| 0.3588 | 0.7000 | 0.9700 |
| 0.3965 | 0.8000 | 0.9760 |
| 0.4348 | 0.9000 | 0.9890 |

Udovenko, V.V. - Frid, Ts.B., Heats of vaporization of binary mixtures. II, Zh. Fiz. Khim. (1948) 1135-1145.

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1572 | 0.1000 | 0.5600 |
| 0.2304 | 0.2000 | 0.7320 |
| 0.3020 | 0.3000 | 0.8180 |
| 0.3713 | 0.4000 | 0.8720 |
| 0.4366 | 0.5000 | 0.9080 |
| 0.4988 | 0.6000 | 0.9340 |
| 0.5600 | 0.7000 | 0.9550 |
| 0.6180 | 0.8000 | 0.9720 |
| 0.6755 | 0.9000 | 0.9870 |

Udovenko, V.V. - Frid, Ts.B., Heats of vaporization of binary mixtures. II, Zh. Fiz. Khim. (1948) 1135-1145.

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2467 | 0.1000 | 0.5260 |
| 0.3564 | 0.2000 | 0.7070 |
| 0.4614 | 0.3000 | 0.7990 |
| 0.5614 | 0.4000 | 0.8560 |
| 0.6514 | 0.5000 | 0.9060 |
| 0.7434 | 0.6000 | 0.9260 |
| 0.8335 | 0.7000 | 0.9490 |
| 0.9194 | 0.8000 | 0.9690 |
| 1.002 | 0.9000 | 0.9850 |

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**Isobaric phase equilibrium data**

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Duran, Jairo A. - Córdoba, Fernando P. - Gil, Iván D. - Rodríguez, Gerardo - Orjuela, Alvaro, Vapor–liquid equilibrium of the ethanol+3-methyl-1-butanol system at 50.66, 101.33 and 151.99kPa, Fluid Phase Equilibria (2013) 128-134. doi:10.1016/j.fluid.2012.11.004

**P / bar = 0.5066**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 374.70 | 0.0697 | 0.3849 |
| 360.32 | 0.2336 | 0.7298 |
| 356.55 | 0.2951 | 0.7901 |
| 348.21 | 0.4911 | 0.8990 |
| 340.95 | 0.7153 | 0.9606 |
| 338.27 | 0.8182 | 0.9772 |

Gay, L., Distillation and rectification of complex mixtures. II, Chim. Ind. Genie Chim. 2 (1927) 187-203.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 403.15 | 0.0047 | 0.0265 |
| 400.65 | 0.0235 | 0.1240 |
| 398.15 | 0.0435 | 0.2125 |
| 395.65 | 0.0650 | 0.2980 |
| 393.15 | 0.0885 | 0.3735 |
| 388.15 | 0.1405 | 0.5100 |
| 383.15 | 0.2010 | 0.6230 |
| 378.15 | 0.2725 | 0.7185 |
| 373.15 | 0.3570 | 0.7980 |
| 368.15 | 0.4590 | 0.8620 |
| 363.15 | 0.5810 | 0.9193 |
| 360.65 | 0.6520 | 0.9353 |
| 358.15 | 0.7310 | 0.9552 |
| 355.65 | 0.8185 | 0.9729 |
| 353.15 | 0.9165 | 0.9889 |

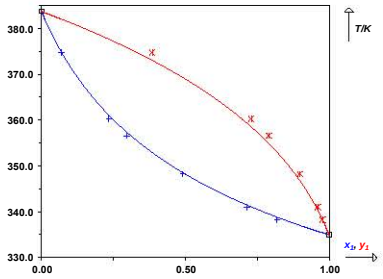
Duran, Jairo A. - Córdoba, Fernando P. - Gil, Iván D. - Rodríguez, Gerardo - Orjuela, Alvaro, Vapor–liquid equilibrium of the ethanol+3-methyl-1-butanol system

at 50.66, 101.33 and 151.99kPa, Fluid Phase Equilibria (2013) 128-134. doi:10.1016/j.fluid.2012.11.004

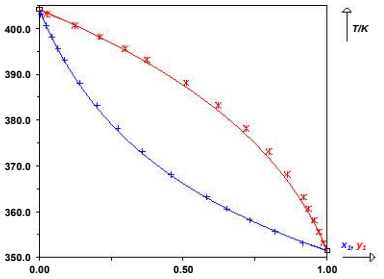
**P / bar =** **1.520**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 394.42 | 0.1887 | 0.6189 |
| 382.29 | 0.3729 | 0.8074 |
| 379.83 | 0.4265 | 0.8385 |
| 372.50 | 0.6166 | 0.9192 |
| 371.19 | 0.6578 | 0.9311 |
| 369.33 | 0.7068 | 0.9433 |
| 361.72 | 0.9940 | 0.9990 |

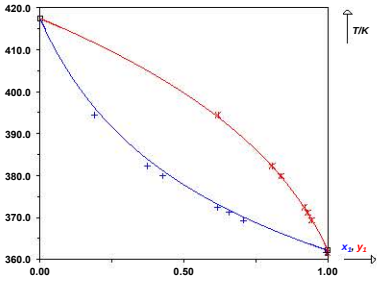
P/bar = 0.50660



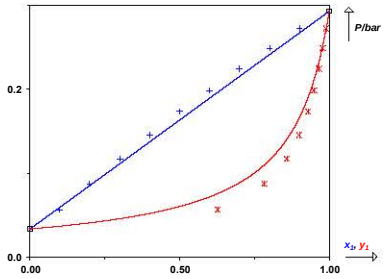

P/bar = 1.01330



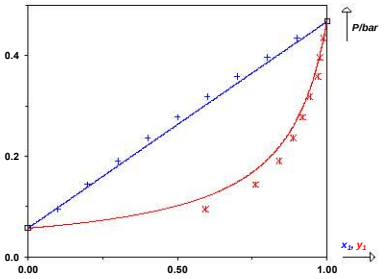

P/bar = 1.51990



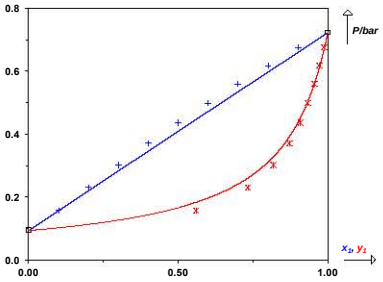

T/K = 323.15



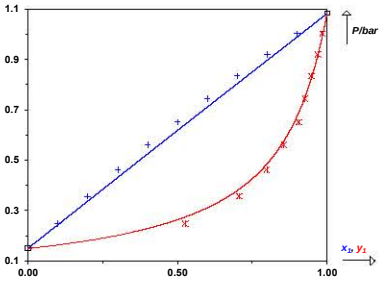

T/K = 333.15




T/K = 343.15




T/K = 353.15



## METHANOL (1) + 3-METHYL-1-BUTANOL (2)

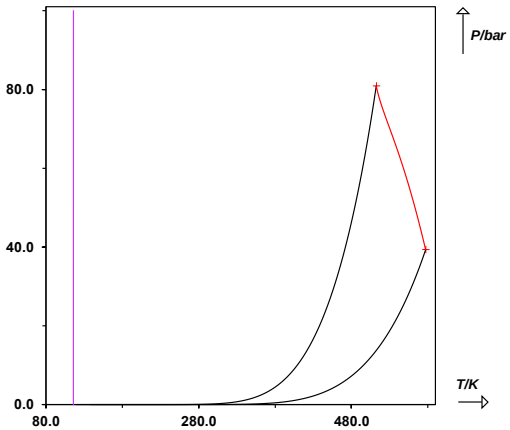
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 123-51-3 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | PHTQWCKDNZKARW-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.50 | 577.20 |
| **$P_c$ / bar** | 80.84 | 39.30 |
| **ω** | 0.566 | 0.590 |

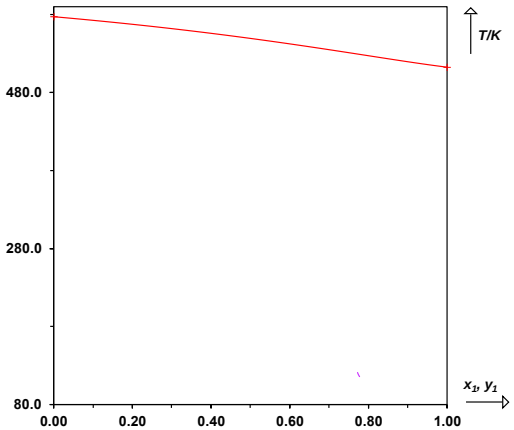
Ideal

**PPR78 results**

*Parameters*
A/MPa = 142
B/MPa = 154

*Deviations*
MAPE on x = 6.2 %
MAPE on y = 13 %



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**Isothermal phase equilibrium data**

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Kim, J.S. - Lee, J.M., The prediction of vapor-liquid equilibrium data for methanol/3-methyl-1-butanol system at constant temperature, Kongop Hwahak 6 (2005) 749-754.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1020 | 0.1180 | 0.7990 |
| 0.1332 | 0.1640 | 0.8520 |
| 0.1472 | 0.1860 | 0.8680 |
| 0.1697 | 0.2240 | 0.8910 |
| 0.1868 | 0.2530 | 0.9050 |
| 0.2100 | 0.2920 | 0.9210 |
| 0.2396 | 0.3420 | 0.9340 |
| 0.2540 | 0.3660 | 0.9400 |
| 0.2810 | 0.4140 | 0.9500 |
| 0.3158 | 0.4840 | 0.9610 |
| 0.3322 | 0.5130 | 0.9640 |
| 0.3704 | 0.5900 | 0.9720 |
| 0.3985 | 0.6430 | 0.9770 |
| 0.4054 | 0.6570 | 0.9780 |
| 0.4341 | 0.7150 | 0.9830 |
| 0.4569 | 0.7650 | 0.9860 |
| 0.4901 | 0.8380 | 0.9910 |
| 0.5278 | 0.8920 | 0.9940 |

Kim, J.S. - Lee, J.M., The prediction of vapor-liquid equilibrium data for methanol/3-methyl-1-butanol system at constant temperature, Kongop Hwahak 6 (2005) 749-754.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1220 | 0.1060 | 0.7600 |
| 0.1537 | 0.1480 | 0.8200 |
| 0.2263 | 0.2450 | 0.8910 |
| 0.2475 | 0.2740 | 0.9040 |
| 0.2729 | 0.3080 | 0.9170 |
| 0.3321 | 0.3910 | 0.9390 |
| 0.3530 | 0.4230 | 0.9440 |
| 0.3721 | 0.4520 | 0.9500 |
| 0.4057 | 0.5040 | 0.9580 |
| 0.4245 | 0.5340 | 0.9620 |
| 0.4566 | 0.5810 | 0.9670 |
| 0.4750 | 0.6120 | 0.9710 |
| 0.4885 | 0.6340 | 0.9730 |
| 0.5194 | 0.6870 | 0.9780 |
| 0.5462 | 0.7320 | 0.9820 |
| 0.5713 | 0.7750 | 0.9850 |
| 0.6089 | 0.8400 | 0.9900 |
| 0.6324 | 0.8850 | 0.9930 |
| 0.6582 | 0.9320 | 0.9960 |

Udovenko, V.V. - Frid, Ts.B., Heats of vaporization of binary mixtures. II, Zh. Fiz. Khim. (1948) 1135-1145.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1420 | 0.1000 | 0.7290 |
| 0.2360 | 0.2000 | 0.8540 |
| 0.3245 | 0.3000 | 0.9050 |
| 0.4068 | 0.4000 | 0.9350 |
| 0.5585 | 0.6000 | 0.9670 |
| 0.6290 | 0.7000 | 0.9780 |
| 0.7011 | 0.8000 | 0.9860 |
| 0.7653 | 0.9000 | 0.9940 |

Kim, J.S. - Lee, J.M., The prediction of vapor-liquid equilibrium data for methanol/3-methyl-1-butanol system at constant temperature, Kongop Hwahak 6 (2005) 749-754.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1668 | 0.1270 | 0.7750 |
| 0.2101 | 0.1740 | 0.8330 |
| 0.2269 | 0.1930 | 0.8490 |
| 0.2469 | 0.2150 | 0.8640 |
| 0.3020 | 0.2770 | 0.8970 |
| 0.3513 | 0.3340 | 0.9160 |
| 0.3641 | 0.3500 | 0.9210 |
| 0.3848 | 0.3750 | 0.9280 |
| 0.4246 | 0.4240 | 0.9390 |
| 0.4654 | 0.4740 | 0.9490 |
| 0.4937 | 0.5120 | 0.9550 |
| 0.5277 | 0.5580 | 0.9610 |
| 0.5444 | 0.5830 | 0.9640 |
| 0.5876 | 0.6420 | 0.9720 |
| 0.6100 | 0.6740 | 0.9750 |
| 0.6512 | 0.7310 | 0.9800 |
| 0.6782 | 0.7680 | 0.9830 |
| 0.7271 | 0.8180 | 0.9870 |
| 0.7378 | 0.8580 | 0.9900 |
| 0.7798 | 0.9250 | 0.9950 |

Kim, J.S. - Lee, J.M., The prediction of vapor-liquid equilibrium data for methanol/3-methyl-1-butanol system at constant temperature, Kongop Hwahak 6 (2005) 749-754.

**T / K = 338.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|

| | | |
|---|---|---|
| 0.1913 | 0.1070 | 0.7250 |
| 0.2189 | 0.1320 | 0.7650 |
| 0.2790 | 0.1860 | 0.8280 |
| 0.3220 | 0.2240 | 0.8590 |
| 0.3648 | 0.2610 | 0.8800 |
| 0.4504 | 0.3420 | 0.9110 |
| 0.4817 | 0.3740 | 0.9200 |
| 0.5312 | 0.4250 | 0.9330 |
| 0.5564 | 0.4500 | 0.9390 |
| 0.6169 | 0.5130 | 0.9510 |
| 0.6819 | 0.5860 | 0.9610 |
| 0.7217 | 0.6310 | 0.9670 |
| 0.7529 | 0.6670 | 0.9710 |
| 0.7761 | 0.6930 | 0.9740 |
| 0.8099 | 0.7320 | 0.9780 |
| 0.8274 | 0.7530 | 0.9800 |
| 0.8897 | 0.8300 | 0.9870 |
| 0.9394 | 0.8770 | 0.9910 |
| 0.9715 | 0.9300 | 0.9950 |

Udovenko, V.V. - Frid, Ts.B., Heats of vaporization of binary mixtures. II, Zh. Fiz. Khim. (1948) 1135-1145.

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2207 | 0.1000 | 0.6810 |
| 0.3606 | 0.2000 | 0.8280 |
| 0.4918 | 0.3000 | 0.8880 |
| 0.6145 | 0.4000 | 0.9220 |
| 0.7283 | 0.5000 | 0.9440 |
| 0.8294 | 0.6000 | 0.9600 |
| 0.9351 | 0.7000 | 0.9730 |
| 1.039 | 0.8000 | 0.9840 |
| 1.135 | 0.9000 | 0.9920 |

Kim, J.S. - Lee, J.M., The prediction of vapor-liquid equilibrium data for methanol/3-methyl-1-butanol system at constant temperature, Kongop Hwahak 6 (2005) 749-754.

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2260 | 0.1040 | 0.7010 |
| 0.2870 | 0.1470 | 0.7670 |
| 0.3296 | 0.1790 | 0.8080 |
| 0.4050 | 0.2350 | 0.8550 |
| 0.4616 | 0.2770 | 0.8780 |
| 0.4678 | 0.2920 | 0.8840 |
| 0.5182 | 0.3210 | 0.8960 |
| 0.5404 | 0.3400 | 0.9030 |
| 0.5993 | 0.3780 | 0.9150 |
| 0.6501 | 0.4330 | 0.9300 |
| 0.6883 | 0.4650 | 0.9370 |
| 0.7415 | 0.5130 | 0.9470 |
| 0.7686 | 0.5410 | 0.9510 |
| 0.8045 | 0.5750 | 0.9560 |
| 0.8527 | 0.6220 | 0.9630 |
| 0.9287 | 0.6950 | 0.9730 |
| 0.9590 | 0.7250 | 0.9760 |
| 1.016 | 0.7800 | 0.9810 |
| 1.073 | 0.8370 | 0.9860 |
| 1.148 | 0.9140 | 0.9930 |

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**Isobaric phase equilibrium data**

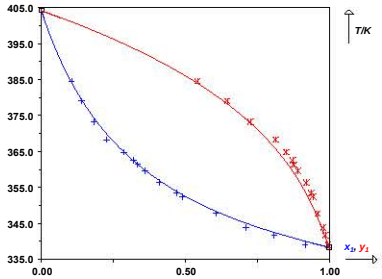
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Resa, JoséM - González, Cristina - Moradillo, Blanca - Ruiz, Aitor, Isobaric vapor-liquid equilibria of 3-methyl-1-butanol with methanol and vinyl acetate at 101.3 kPa, Fluid Phase Equilibria 1-2 (1997) 205-213. doi:10.1016/S0378-3812(97)00027-7

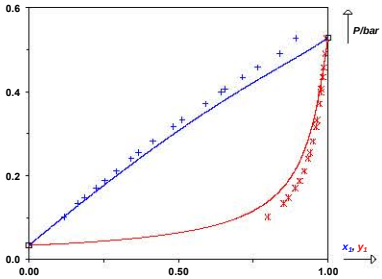
**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 384.50 | 0.1040 | 0.5420 |
| 379.00 | 0.1380 | 0.6460 |
| 373.20 | 0.1840 | 0.7260 |
| 368.30 | 0.2270 | 0.8140 |
| 364.80 | 0.2850 | 0.8510 |
| 362.50 | 0.3200 | 0.8730 |
| 361.40 | 0.3350 | 0.8770 |
| 359.60 | 0.3610 | 0.8920 |
| 356.40 | 0.4090 | 0.9200 |
| 353.50 | 0.4700 | 0.9380 |
| 352.50 | 0.4900 | 0.9440 |
| 347.80 | 0.6060 | 0.9600 |
| 343.80 | 0.7100 | 0.9800 |
| 341.70 | 0.8080 | 0.9870 |
| 339.10 | 0.9170 | 0.9960 |

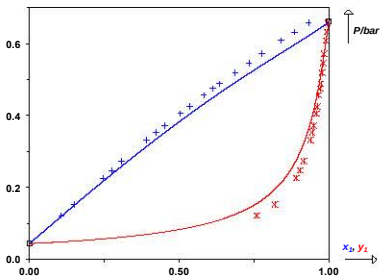
P/bar = 1.01300



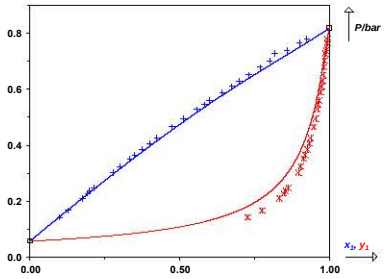

T/K = 323.15



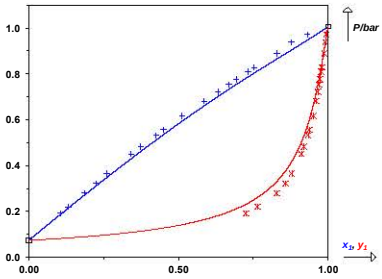

T/K = 328.15



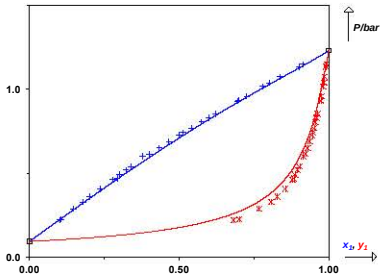

T/K = 333.15




T/K = 338.15




T/K = 343.15



## METHANOL (1) + 1-PROPANOL (2)

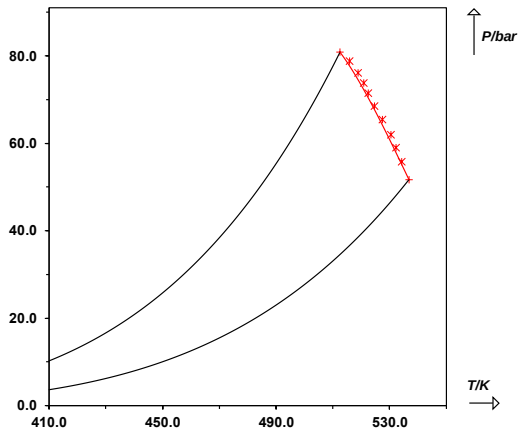
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 71-23-8 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | BDERNNFJNOPAEC-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.50 | 536.80 |
| **$P_c$ / bar** | 80.84 | 51.69 |
| **ω** | 0.566 | 0.621 |

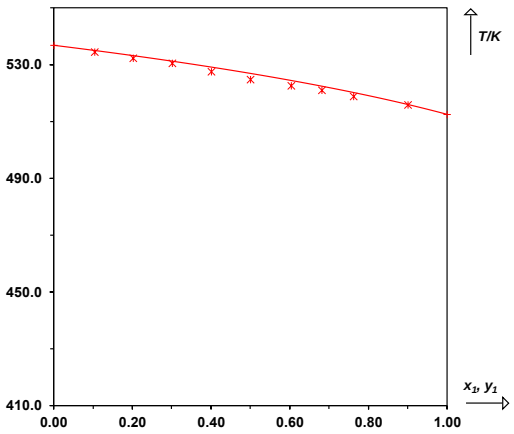
Ideal

**PPR78 results**

*Parameters*
A/MPa = 10.7
B/MPa = 33.2

*Deviations*
MAPE on x = 11 %
MAPE on y = 9.1 %
MAPE on $x_c$ = 14 %
MAPE on $P_c$ = 1.8 %
MAPE on $h^M$ = 4.4 %
MAPE on $c_P{}^M$ = 25 %



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**Isothermal phase equilibrium data**

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Yamamoto, Hideki - Fukase, Koji - Shibata, Junji, Vapor−Liquid Equilibria for Alcohol + Alcohol + Sodium Iodide at 298.15 K, Journal of Chemical & Engineering Data 5 (1996) 1066-1070. doi:10.1021/je9600966

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0341 | 0.0420 | 0.1960 |
| 0.0510 | 0.1530 | 0.5350 |
| 0.0725 | 0.3040 | 0.7310 |
| 0.0787 | 0.3510 | 0.7780 |
| 0.0916 | 0.4340 | 0.8240 |
| 0.1065 | 0.5410 | 0.8860 |
| 0.1162 | 0.6050 | 0.9080 |
| 0.1321 | 0.7230 | 0.9470 |
| 0.1542 | 0.8780 | 0.9800 |

Gregorowicz, J., Adsorption of eicosane and 1,2-hexanediol from supercritical carbon dioxide on activated carbon and chromosorb, Fluid Phase Equilibria 2 (2005) 142-148. doi:10.1016/j.fluid.2005.09.020

**T / K = 333.17**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2266 | 0.0368 | 0.1391 |
| 0.2373 | 0.0528 | 0.1916 |
| 0.2429 | 0.0611 | 0.2172 |
| 0.2462 | 0.0649 | 0.2308 |
| 0.2553 | 0.0764 | 0.2620 |
| 0.2691 | 0.1007 | 0.3223 |
| 0.2950 | 0.1393 | 0.4077 |
| 0.3239 | 0.1842 | 0.4857 |
| 0.3442 | 0.2151 | 0.5337 |
| 0.3752 | 0.2625 | 0.5977 |
| 0.4127 | 0.3206 | 0.6609 |
| 0.4526 | 0.3806 | 0.7180 |
| 0.4939 | 0.4459 | 0.7664 |
| 0.5325 | 0.5022 | 0.8063 |
| 0.5639 | 0.5520 | 0.8342 |
| 0.5915 | 0.5970 | 0.8562 |
| 0.6156 | 0.6338 | 0.8744 |
| 0.6596 | 0.7034 | 0.9037 |
| 0.6799 | 0.7370 | 0.9154 |
| 0.7084 | 0.7830 | 0.9332 |
| 0.7370 | 0.8275 | 0.9485 |
| 0.7698 | 0.8804 | 0.9661 |
| 0.7973 | 0.9238 | 0.9785 |
| 0.8268 | 0.9707 | 0.9923 |

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**Isobaric phase equilibrium data**

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Gultekin, Nurbay, Vapor-liquid equilibria at 1 atm for ternary and quaternary systems composed of acetone, methanol, 2-propanol, and 1-propanol, Journal of Chemical & Engineering Data 2 (1990) 132-136. doi:10.1021/je00060a010

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 365.45 | 0.0920 | 0.2350 |
| 362.03 | 0.1800 | 0.4120 |
| 357.05 | 0.2800 | 0.5620 |
| 355.68 | 0.3200 | 0.6100 |
| 353.40 | 0.3800 | 0.6750 |
| 351.30 | 0.4590 | 0.7530 |
| 347.61 | 0.5810 | 0.8320 |
| 347.42 | 0.5830 | 0.8350 |
| 344.43 | 0.6800 | 0.8880 |
| 342.55 | 0.7640 | 0.9280 |
| 341.45 | 0.8220 | 0.9400 |
| 340.23 | 0.8620 | 0.9550 |

Kojima, K. - Tochigi, K. - Seki, H. - Watase, K., Determination of vapor-liquid equilibriums from boiling point curves, Kagaku Kogaku (1968) 149-153. doi:10.1252/kakoronbunshu1953.32.149

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 367.41 | 0.0500 | 0.1487 |
| 364.61 | 0.1000 | 0.2785 |
| 362.16 | 0.1500 | 0.3809 |
| 359.93 | 0.2000 | 0.4664 |
| 357.82 | 0.2500 | 0.5408 |
| 355.87 | 0.3000 | 0.6043 |
| 354.01 | 0.3500 | 0.6602 |
| 352.34 | 0.4000 | 0.7069 |
| 350.71 | 0.4500 | 0.7494 |
| 349.16 | 0.5000 | 0.7871 |
| 347.73 | 0.5500 | 0.8196 |
| 346.39 | 0.6000 | 0.8483 |
| 345.08 | 0.6500 | 0.8747 |
| 343.88 | 0.7000 | 0.8975 |
| 342.78 | 0.7500 | 0.9176 |
| 341.70 | 0.8000 | 0.9366 |
| 340.64 | 0.8500 | 0.9545 |
| 339.57 | 0.9000 | 0.9715 |
| 338.60 | 0.9500 | 0.9861 |

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**Enthalpy of mixing**

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Wóycicki, W., Enthalpies of mixing of some binary mixtures of benzene, cyclohexane, and pyridine, and their methyl and ethyl derivatives, The Journal of Chemical Thermodynamics 1 (1972) 1-8. doi:10.1016/S0021-9614(72)80002-8

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 7.500 | 0.0319 |
| 21.40 | 0.0916 |
| 39.80 | 0.1794 |
| 56.20 | 0.2693 |
| 69.80 | 0.3577 |
| 78.30 | 0.4427 |
| 83.10 | 0.5226 |
| 83.80 | 0.5816 |
| 84.10 | 0.5894 |
| 82.70 | 0.6347 |
| 82.20 | 0.6488 |
| 78.90 | 0.6916 |
| 78.50 | 0.6981 |
| 73.60 | 0.7403 |
| 72.50 | 0.7475 |
| 63.00 | 0.8030 |
| 51.80 | 0.8525 |
| 39.20 | 0.8970 |
| 27.40 | 0.9319 |
| 15.00 | 0.9646 |
| 5.500 | 0.9875 |

Trampe, D. Mark - Eckert, Charles A., Calorimetric measurement of partial molar excess enthalpies at infinite dilution, Journal of Chemical & Engineering Data 1 (1991) 112-118. doi:10.1021/je00001a033

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 5.820 | 0.9869 |
| 5.530 | 0.9874 |
| 5.070 | 0.9886 |
| 4.520 | 0.9897 |
| 4.090 | 0.9909 |
| 3.540 | 0.9920 |
| 3.050 | 0.9932 |
| 2.540 | 0.9943 |
| 2.010 | 0.9955 |
| 1.510 | 0.9966 |

Barès, D. - Metzger, J., Modèles d'autoassociations de bases aza-aromatiques par étude calorimétrique comparative de solutions binaires interprétation structurale, Journal de Chimie Physique et de Physico-Chimie Biologique 10 (1973) 1540-1545. doi:10.1051/jcp/1973701540

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 45.00 | 0.1899 |
| 69.70 | 0.3341 |
| 81.80 | 0.4396 |
| 87.30 | 0.5660 |
| 84.70 | 0.6507 |
| 71.80 | 0.7788 |
| 50.40 | 0.8632 |
| 29.70 | 0.9282 |

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**Heat capacity of mixing**

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Ogawa, Hideo - Murakami, Sachio, Excess volumes, isentropic compressions, and isobaric heat capacities for methanol mixed with other alkanols at 25°C, Journal of Solution Chemistry 4 (1987) 315-326. doi:10.1007/BF00646123

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| -0.4110 | 0.0979 |
| -0.7180 | 0.1963 |
| -0.9080 | 0.2952 |
| -0.9810 | 0.3945 |
| -0.9670 | 0.4942 |
| -0.9790 | 0.5944 |
| -0.7110 | 0.6951 |
| -0.6090 | 0.7456 |
| -0.5020 | 0.7963 |
| -0.3840 | 0.8470 |
| -0.2630 | 0.8979 |
| -0.1350 | 0.9489 |

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**Critical point**

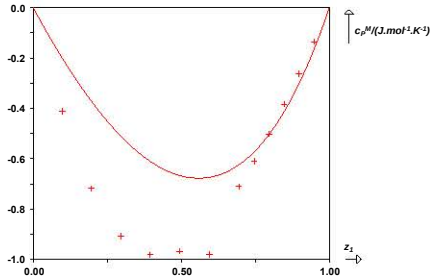
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Wang, Lipu - Han, Kewei - Xia, Shuqian - Ma, Peisheng - Yan, Fangyou, Measurement and correlation of critical properties for binary mixtures and ternary mixtures containing gasoline additives, The Journal of

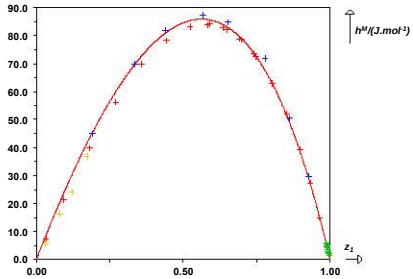
Chemical Thermodynamics (2014) 161-168.
doi:10.1016/j.jct.2014.01.025

| T / K | P / bar | $x_1$ |
|---|---|---|
| 515.80 | 78.85 | 0.9002 |
| 518.80 | 76.13 | 0.7626 |
| 520.90 | 73.79 | 0.6822 |
| 522.50 | 71.41 | 0.6039 |
| 524.70 | 68.45 | 0.5009 |
| 527.50 | 65.42 | 0.4005 |
| 530.40 | 61.98 | 0.3015 |
| 532.20 | 58.93 | 0.2016 |
| 534.30 | 55.73 | 0.1045 |

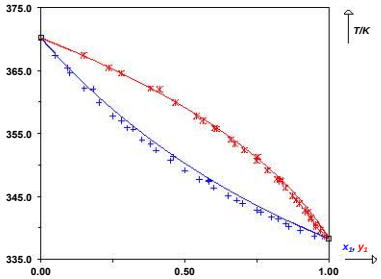
T/K = 298.15 - P/bar = 1.0132



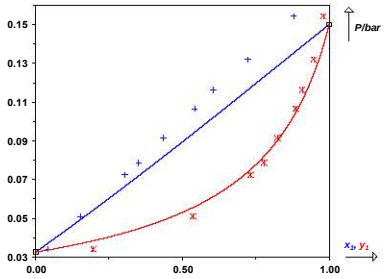

T/K = 298.15 - P/bar = 1.0132 1.0132 1.0132 1.0132



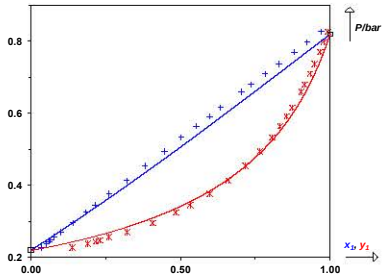

P/bar = 1.01330



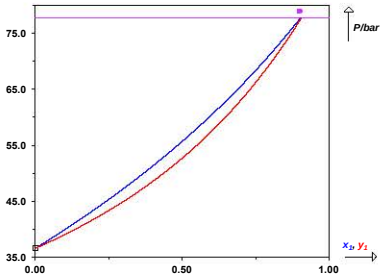

T/K = 298.15



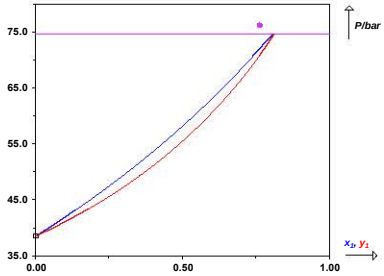

T/K = 333.17



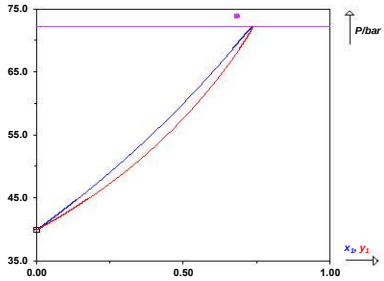

T/K = 515.80



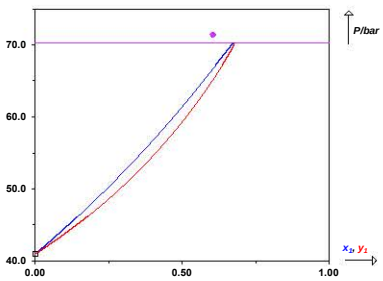

T/K = 518.80



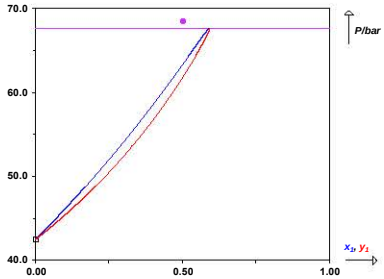

T/K = 520.90



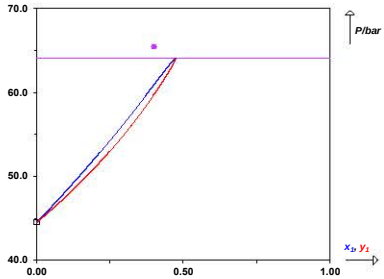

T/K = 522.50



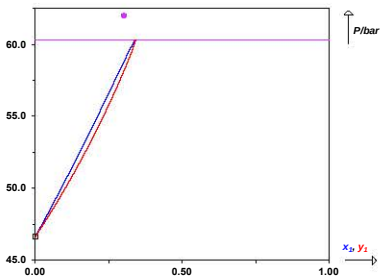

T/K = 524.70



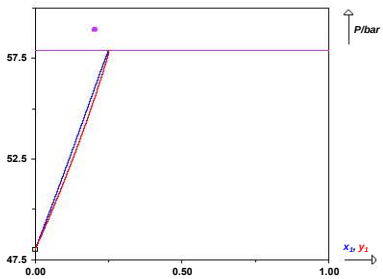

T/K = 527.50



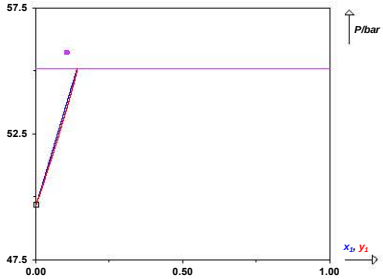

T/K = 530.40




T/K = 532.20




T/K = 534.30



## AMMONIA (1) + WATER (2)

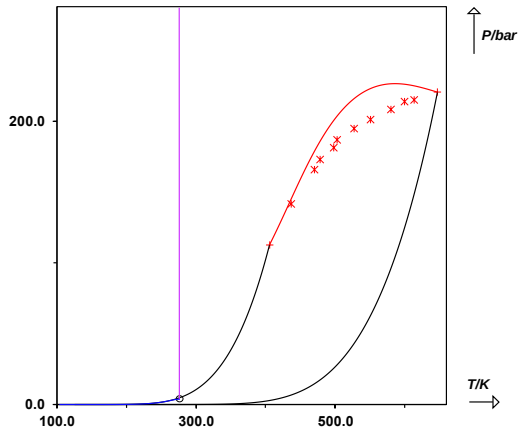
| | | |
|---|---|---|
| **CAS** | 7664-41-7 | 7732-18-5 |
| **InChiKey** | QGZKDVFQNNGYKY-UHFFFAOYSA-N | XLYOFNOQVPJJNP-UHFFFAOYSA-N |
| **$T_c$ / K** | 405.65 | 647.096 |
| **$P_c$ / bar** | 112.80 | 220.64 |
| **ω** | 0.253 | 0.345 |

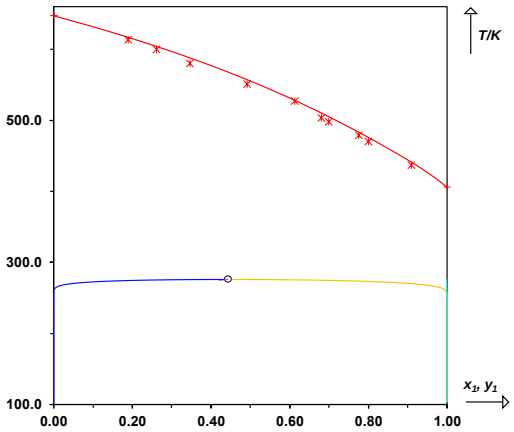
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 178
B/MPa = 4040

*Deviations*
MAPE on x = 40 %
MAPE on y = 13 %
MAPE on $x_c$ = 5.8 %
MAPE on $P_c$ = 7.8 %



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**Isothermal phase equilibrium data**

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Wilson, T.A., The total and partial vapor pressures of aqueous ammonia solutions, Univ. Illinois Eng. Exp. Stand. Bull. (1925)

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0240 | 0.0500 | 0.7570 |
| 0.0410 | 0.1000 | 0.8680 |
| 0.1090 | 0.2000 | 0.9557 |
| 0.2900 | 0.3000 | 0.9857 |
| 0.6860 | 0.4000 | 0.9949 |
| 1.340 | 0.5000 | 0.9978 |
| 2.152 | 0.6000 | 0.9989 |
| 2.950 | 0.7000 | 0.9994 |
| 3.403 | 0.8000 | 0.9997 |
| 3.792 | 0.9000 | 0.9999 |
| 3.685 | 0.8500 | 0.9998 |
| 2.818 | 0.7020 | 0.9994 |
| 2.424 | 0.6500 | 0.9991 |
| 1.604 | 0.5330 | 0.9980 |
| 0.3430 | 0.3210 | 0.9883 |
| 0.2930 | 0.3050 | 0.9858 |
| 0.1711 | 0.2540 | 0.9742 |
| 0.0277 | 0.1080 | 0.8160 |

Wilson, T.A., The total and partial vapor pressures of aqueous ammonia solutions, Univ. Illinois Eng. Exp. Stand. Bull. (1925)

**T / K = 273.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0235 | 0.0500 | 0.7570 |
| 0.0414 | 0.1000 | 0.8680 |
| 0.1091 | 0.2000 | 0.9557 |
| 0.2901 | 0.3000 | 0.9857 |
| 0.6858 | 0.4000 | 0.9949 |
| 1.340 | 0.5000 | 0.9978 |
| 2.152 | 0.6000 | 0.9989 |
| 2.950 | 0.7000 | 0.9994 |
| 3.403 | 0.8000 | 0.9997 |
| 3.792 | 0.9000 | 0.9999 |

Wilson, T.A., The total and partial vapor pressures of aqueous ammonia solutions, Univ. Illinois Eng. Exp. Stand. Bull. (1925)

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.46 | 0.7370 | 0.9984 |
| 9.723 | 0.6640 | 0.9976 |
| 8.631 | 0.6200 | 0.9970 |
| 6.921 | 0.5520 | 0.9955 |
| 2.667 | 0.3640 | 0.9840 |
| 1.804 | 0.3105 | 0.9729 |
| 1.783 | 0.3080 | 0.9716 |
| 1.488 | 0.2850 | 0.9659 |
| 0.9445 | 0.2310 | 0.9416 |
| 0.2990 | 0.1127 | 0.7850 |

Gillespie, P.C. - Wilding, W.V. - Wilson, G.M., Vapor-liquid equilibrium measurements on the ammonia-water system from 313 K to 589 K, AIChE Symp. Ser. 256 (1987) 97-127.

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.538 | 0.2930 | 0.9667 |
| 5.447 | 0.5118 | 0.9945 |
| 9.928 | 0.6892 | 0.9982 |
| 11.03 | 0.7350 | 0.9986 |
| 12.27 | 0.7900 | 0.9990 |
| 14.06 | 0.8850 | 0.9994 |

Gillespie, P.C. - Wilding, W.V. - Wilson, G.M., Vapor-liquid equilibrium measurements on the ammonia-water system from 313 K to 589 K, AIChE Symp. Ser. 256 (1987) 97-127.

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.538 | 0.2930 | 0.9667 |
| 5.447 | 0.5118 | 0.9945 |
| 9.928 | 0.6892 | 0.9982 |
| 11.03 | 0.7350 | 0.9986 |
| 12.27 | 0.7900 | 0.9990 |
| 14.06 | 0.8850 | 0.9994 |

Inomata, Hiroshi - Ikawa, Noboru - Arai, Kunio - Saito, Shozaburo, Vapor-liquid equilibria for the ammonia-methanol-water system, Journal of Chemical & Engineering Data 1 (1988) 26-29. doi:10.1021/je00051a010

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.600 | 0.1970 | 0.9280 |
| 3.400 | 0.3180 | 0.9750 |
| 6.500 | 0.4400 | 0.9910 |
| 10.60 | 0.5540 | 0.9960 |
| 15.50 | 0.6830 | 0.9980 |
| 20.70 | 0.8320 | 0.9990 |

Huang, Weijia - Sun, Guangming - Zheng, Danxing - Dong, Li - Wu, Xianghong - Chen, Juan, Vapor–Liquid

Equilibrium Measurements of NH3 + H2O + Ionic Liquid ([Dmim]Cl, [Dmim]BF4, and [Dmim]DMP) Systems, Journal of Chemical & Engineering Data 5 (2013) 1354-1360. doi:10.1021/je400109a

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.040 | 0.3030 | 0.9810 |
| 3.980 | 0.3520 | 0.9840 |
| 4.850 | 0.3920 | 0.9850 |

Wilson, T.A., The total and partial vapor pressures of aqueous ammonia solutions, Univ. Illinois Eng. Exp. Stand. Bull. (1925)

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.40 | 0.5400 | 0.9924 |
| 7.429 | 0.4440 | 0.9858 |
| 5.087 | 0.3740 | 0.9765 |
| 4.150 | 0.3400 | 0.9694 |
| 3.208 | 0.2990 | 0.9571 |
| 2.934 | 0.2860 | 0.9533 |
| 2.068 | 0.2380 | 0.9284 |
| 1.456 | 0.1920 | 0.8920 |
| 0.9087 | 0.1360 | 0.8140 |
| 0.7319 | 0.1139 | 0.7620 |

Gillespie, P.C. - Wilding, W.V. - Wilson, G.M., Vapor-liquid equilibrium measurements on the ammonia-water system from 313 K to 589 K, AIChE Symp. Ser. 256 (1987) 97-127.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.054 | 0.2945 | 0.9551 |
| 9.584 | 0.5110 | 0.9904 |
| 17.10 | 0.6965 | 0.9965 |
| 18.89 | 0.7638 | 0.9974 |
| 20.41 | 0.8033 | 0.9979 |
| 23.79 | 0.9063 | 0.9988 |

Gillespie, P.C. - Wilding, W.V. - Wilson, G.M., Vapor-liquid equilibrium measurements on the ammonia-water system from 313 K to 589 K, AIChE Symp. Ser. 256 (1987) 97-127.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.054 | 0.2945 | 0.9551 |
| 9.584 | 0.5110 | 0.9904 |
| 17.10 | 0.6965 | 0.9965 |
| 18.89 | 0.7638 | 0.9974 |
| 20.41 | 0.8033 | 0.9979 |
| 23.79 | 0.9063 | 0.9988 |

Clifford, I. I. - Hunter, E., The System Ammonia–Water at Temperatures up to 150°C. and at Pressures up to Twenty Atmospheres., The Journal of Physical Chemistry 1 (1932) 101-118. doi:10.1021/j150343a014

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2434 | 0.0101 | 0.1801 |
| 0.2896 | 0.0208 | 0.2997 |
| 0.3709 | 0.0386 | 0.4448 |
| 0.4358 | 0.0521 | 0.5698 |
| 0.4937 | 0.0637 | 0.6154 |
| 0.5916 | 0.0832 | 0.7078 |
| 0.6385 | 0.0911 | 0.7341 |
| 1.118 | 0.1613 | 0.8493 |
| 1.470 | 0.1979 | 0.9049 |

Clifford, I. I. - Hunter, E., The System Ammonia–Water at Temperatures up to 150°C. and at Pressures up to Twenty Atmospheres., The Journal of Physical Chemistry 1 (1932) 101-118. doi:10.1021/j150343a014

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2434 | 0.0096 | 0.1720 |
| 0.2896 | 0.0197 | 0.2880 |
| 0.3709 | 0.0366 | 0.4310 |
| 0.4358 | 0.0494 | 0.5560 |
| 0.4937 | 0.0604 | 0.6020 |
| 0.5916 | 0.0790 | 0.6960 |
| 0.6385 | 0.0866 | 0.7230 |
| 1.118 | 0.1538 | 0.8420 |
| 1.470 | 0.1891 | 0.9000 |

Wilson, T.A., The total and partial vapor pressures of aqueous ammonia solutions, Univ. Illinois Eng. Exp. Stand. Bull. (1925)

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 8.551 | 0.3680 | 0.9664 |
| 4.534 | 0.2650 | 0.9261 |
| 1.979 | 0.1490 | 0.7990 |
| 1.496 | 0.1150 | 0.7240 |

Gillespie, P.C. - Wilding, W.V. - Wilson, G.M., Vapor-liquid equilibrium measurements on the ammonia-water system from 313 K to 589 K, AIChE Symp. Ser. 256 (1987) 97-127.

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|

| | | |
|---|---|---|
| 5.757 | 0.3098 | 0.9445 |
| 15.51 | 0.5107 | 0.9836 |
| 27.51 | 0.7141 | 0.9933 |
| 28.75 | 0.7436 | 0.9940 |
| 29.65 | 0.7674 | 0.9945 |
| 32.27 | 0.8131 | 0.9954 |
| 32.54 | 0.8246 | 0.9957 |
| 36.40 | 0.8956 | 0.9970 |
| 38.13 | 0.9293 | 0.9978 |

Gillespie, P.C. - Wilding, W.V. - Wilson, G.M., Vapor-liquid equilibrium measurements on the ammonia-water system from 313 K to 589 K, AIChE Symp. Ser. 256 (1987) 97-127.

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.757 | 0.3098 | 0.9445 |
| 15.51 | 0.5107 | 0.9836 |
| 27.51 | 0.7141 | 0.9933 |
| 28.75 | 0.7436 | 0.9940 |
| 29.65 | 0.7674 | 0.9945 |
| 32.27 | 0.8131 | 0.9954 |
| 32.54 | 0.8246 | 0.9957 |
| 36.40 | 0.8956 | 0.9970 |
| 38.13 | 0.9293 | 0.9978 |

Clifford, I. I. - Hunter, E., The System Ammonia–Water at Temperatures up to 150°C. and at Pressures up to Twenty Atmospheres., The Journal of Physical Chemistry 1 (1932) 101-118. doi:10.1021/j150343a014

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5530 | 0.0101 | 0.1500 |
| 0.6426 | 0.0208 | 0.2935 |
| 0.7708 | 0.0359 | 0.3943 |
| 0.7964 | 0.0386 | 0.4247 |
| 1.044 | 0.0637 | 0.5450 |
| 1.240 | 0.0832 | 0.6440 |

Clifford, I. I. - Hunter, E., The System Ammonia–Water at Temperatures up to 150°C. and at Pressures up to Twenty Atmospheres., The Journal of Physical Chemistry 1 (1932) 101-118. doi:10.1021/j150343a014

**T / K = 353.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.5530 | 0.0096 | 0.1430 |
| 0.6426 | 0.0197 | 0.2820 |
| 0.7708 | 0.0340 | 0.3810 |
| 0.7963 | 0.0366 | 0.4110 |
| 1.044 | 0.0604 | 0.5310 |
| 1.240 | 0.0790 | 0.6310 |

Rizvi, Syed S. H. - Heidemann, Robert A., Vapor-liquid equilibria in the ammonia-water system, Journal of Chemical & Engineering Data 2 (1987) 183-191. doi:10.1021/je00048a017

**T / K = 359.70**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.160 | 0.0368 | 0.2025 |
| 1.210 | 0.0428 | 0.2352 |
| 1.530 | 0.0777 | 0.4114 |
| 1.920 | 0.1064 | 0.5534 |
| 2.530 | 0.1399 | 0.6826 |
| 3.860 | 0.2054 | 0.8150 |
| 6.230 | 0.2837 | 0.8948 |
| 6.440 | 0.2935 | 0.9053 |
| 7.670 | 0.3261 | 0.9154 |
| 11.89 | 0.4173 | 0.9517 |
| 15.10 | 0.4724 | 0.9635 |
| 15.16 | 0.4805 | 0.9655 |
| 19.17 | 0.5442 | 0.9750 |
| 24.15 | 0.6162 | 0.9831 |
| 30.93 | 0.7257 | 0.9890 |
| 31.47 | 0.7337 | 0.9898 |
| 35.23 | 0.7997 | 0.9918 |
| 40.62 | 0.8934 | 0.9957 |
| 45.24 | 0.9711 | 0.9980 |

Clifford, I. I. - Hunter, E., The System Ammonia–Water at Temperatures up to 150°C. and at Pressures up to Twenty Atmospheres., The Journal of Physical Chemistry 1 (1932) 101-118. doi:10.1021/j150343a014

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 1.078 | 0.0053 | 0.0647 |
| 1.221 | 0.0155 | 0.1884 |
| 1.452 | 0.0315 | 0.3283 |

Gillespie, P.C. - Wilding, W.V. - Wilson, G.M., Vapor-liquid equilibrium measurements on the ammonia-water system from 313 K to 589 K, AIChE Symp. Ser. 256 (1987) 97-127.

**T / K = 394.25**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.103 | 0.0439 | 0.3727 |
| 4.344 | 0.0849 | 0.5651 |
| 11.72 | 0.2548 | 0.8659 |
| 34.82 | 0.5070 | 0.9584 |
| 54.49 | 0.6830 | 0.9752 |

Rizvi, Syed S. H. - Heidemann, Robert A., Vapor-liquid equilibria in the ammonia-water system, Journal of Chemical & Engineering Data 2 (1987) 183-191. doi:10.1021/je00048a017

**T / K = 405.50**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.580 | 0.0111 | 0.1111 |
| 4.520 | 0.0350 | 0.3077 |
| 6.650 | 0.0942 | 0.5691 |
| 11.58 | 0.1848 | 0.7839 |
| 20.85 | 0.3085 | 0.8780 |
| 31.28 | 0.4113 | 0.9169 |
| 42.26 | 0.5063 | 0.9348 |
| 50.66 | 0.5790 | 0.9557 |
| 59.09 | 0.6375 | 0.9680 |
| 100.66 | 0.9318 | 0.9897 |
| 111.93 | 0.9931 | 0.9932 |

Rizvi, Syed S. H. - Heidemann, Robert A., Vapor-liquid equilibria in the ammonia-water system, Journal of Chemical & Engineering Data 2 (1987) 183-191. doi:10.1021/je00048a017

**T / K = 422.50**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.630 | 0.0192 | 0.1303 |
| 6.250 | 0.0348 | 0.2240 |
| 6.420 | 0.0374 | 0.2429 |
| 7.080 | 0.0512 | 0.3216 |
| 8.810 | 0.0848 | 0.4727 |
| 11.05 | 0.1297 | 0.5913 |
| 18.32 | 0.2220 | 0.7620 |
| 26.69 | 0.3078 | 0.8279 |
| 36.71 | 0.3934 | 0.8701 |
| 49.89 | 0.4876 | 0.8951 |
| 70.10 | 0.6098 | 0.9140 |
| 82.23 | 0.6780 | 0.9169 |
| 102.14 | 0.7852 | 0.9163 |
| 113.96 | 0.8588 | 0.9429 |
| 114.73 | 0.8714 | 0.9140 |
| 117.63 | 0.8740 | 0.9153 |

Rizvi, Syed S. H. - Heidemann, Robert A., Vapor-liquid equilibria in the ammonia-water system, Journal of Chemical & Engineering Data 2 (1987) 183-191. doi:10.1021/je00048a017

**T / K = 451.50**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 11.06 | 0.0174 | 0.1302 |
| 11.94 | 0.0352 | 0.2518 |
| 14.16 | 0.0571 | 0.3695 |
| 17.09 | 0.0859 | 0.4659 |
| 23.64 | 0.1720 | 0.6829 |
| 33.53 | 0.2391 | 0.7524 |
| 51.72 | 0.3354 | 0.8326 |
| 70.72 | 0.4668 | 0.8834 |
| 88.51 | 0.5480 | 0.9013 |
| 100.45 | 0.5857 | 0.8995 |
| 116.77 | 0.6817 | 0.9023 |
| 130.57 | 0.7335 | 0.8927 |
| 139.39 | 0.7764 | 0.8879 |
| 147.23 | 0.8167 | 0.8863 |
| 151.64 | 0.8602 | 0.8695 |
| 151.14 | 0.8717 | 0.8854 |

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**Isobaric phase equilibrium data**

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Clifford, I. I. - Hunter, E., The System Ammonia–Water at Temperatures up to 150°C. and at Pressures up to Twenty Atmospheres., The Journal of Physical Chemistry 1 (1932) 101-118. doi:10.1021/j150343a014

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 363.15 | 0.0290 | 0.3180 |
| 353.15 | 0.0610 | 0.5260 |
| 343.15 | 0.1000 | 0.7000 |
| 333.15 | 0.1440 | 0.8250 |
| 323.15 | 0.1900 | 0.9020 |
| 313.15 | 0.2400 | 0.9450 |
| 303.15 | 0.2910 | 0.9700 |
| 293.15 | 0.3460 | 0.9850 |
| 283.15 | 0.4060 | 0.9920 |

Chu, J.C. - Getty, R.J. - Brennecke, L.F. - Paul, R., Distillation Equilibrium Data (1950)

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 364.65 | 0.0210 | 0.2320 |
| 357.95 | 0.0410 | 0.4210 |
| 352.15 | 0.0610 | 0.5550 |
| 346.65 | 0.0820 | 0.6700 |
| 341.55 | 0.1020 | 0.7390 |
| 330.25 | 0.1600 | 0.8510 |
| 319.35 | 0.2100 | 0.9210 |
| 309.75 | 0.2600 | 0.9580 |
| 291.35 | 0.3620 | 0.9910 |
| 283.15 | 0.4160 | 0.9960 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 2.533**

| T / K | $x_1$ |
|---|---|
| 383.25 | 0.0500 |
| 369.45 | 0.1000 |
| 357.15 | 0.1500 |
| 345.95 | 0.2000 |
| 335.55 | 0.2500 |
| 325.75 | 0.3000 |
| 307.15 | 0.4000 |
| 290.55 | 0.5000 |
| 278.05 | 0.6000 |
| 270.05 | 0.7000 |
| 264.95 | 0.8000 |
| 261.35 | 0.9000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 2.533**

| T / K | $y_1$ |
|---|---|
| 394.85 | 0.1500 |
| 388.95 | 0.3000 |
| 382.05 | 0.4500 |
| 373.75 | 0.6000 |
| 366.45 | 0.7000 |
| 357.15 | 0.8000 |
| 350.75 | 0.8500 |
| 342.55 | 0.9000 |
| 330.05 | 0.9500 |
| 316.35 | 0.9800 |
| 307.85 | 0.9900 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 4.560**

| T / K | $x_1$ |
|---|---|
| 403.85 | 0.0500 |
| 389.75 | 0.1000 |
| 377.05 | 0.1500 |
| 365.25 | 0.2000 |
| 354.65 | 0.2500 |
| 344.25 | 0.3000 |
| 324.85 | 0.4000 |
| 307.75 | 0.5000 |
| 294.85 | 0.6000 |
| 286.25 | 0.7000 |
| 280.55 | 0.8000 |
| 276.45 | 0.9000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 4.560**

| T / K | $y_1$ |
|---|---|
| 400.05 | 0.4500 |
| 390.85 | 0.6000 |
| 382.85 | 0.7000 |
| 372.65 | 0.8000 |
| 366.05 | 0.8500 |
| 357.15 | 0.9000 |
| 343.55 | 0.9500 |
| 327.65 | 0.9800 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 4.560**

| T / K | $y_1$ |
|---|---|
| 414.55 | 0.1500 |
| 407.65 | 0.3000 |

Clifford, I. I. - Hunter, E., The System Ammonia–Water at Temperatures up to 150°C. and at Pressures up to Twenty Atmospheres., The Journal of Physical Chemistry 1 (1932) 101-118. doi:10.1021/j150343a014

**P / bar = 6.080**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 403.15 | 0.0960 | 0.5710 |
| 393.15 | 0.1350 | 0.6990 |
| 383.15 | 0.1760 | 0.7840 |
| 373.15 | 0.2200 | 0.8480 |
| 363.15 | 0.2660 | 0.9000 |
| 353.15 | 0.3140 | 0.9420 |
| 343.15 | 0.3660 | 0.9700 |

Clifford, I. I. - Hunter, E., The System Ammonia–Water at Temperatures up to 150°C. and at Pressures up to Twenty Atmospheres., The Journal of Physical Chemistry 1 (1932) 101-118. doi:10.1021/j150343a014

**P / bar = 6.080**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 423.15 | 0.0260 | 0.1950 |
| 413.15 | 0.0590 | 0.4000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 6.080**

| T / K | $x_1$ |
|---|---|
| 400.95 | 0.1000 |
| 388.05 | 0.1500 |
| 376.05 | 0.2000 |
| 365.15 | 0.2500 |
| 354.35 | 0.3000 |
| 334.65 | 0.4000 |
| 317.35 | 0.5000 |
| 303.65 | 0.6000 |
| 295.05 | 0.7000 |
| 289.15 | 0.8000 |
| 284.65 | 0.9000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 6.080**

| T / K | $x_1$ |
|---|---|
| 415.05 | 0.0500 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 6.080**

| T / K | $y_1$ |
|---|---|
| 399.85 | 0.6000 |
| 391.45 | 0.7000 |
| 380.75 | 0.8000 |
| 373.85 | 0.8500 |
| 364.45 | 0.9000 |
| 349.75 | 0.9500 |
| 332.95 | 0.9800 |
| 322.45 | 0.9900 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 6.080**

| T / K | $y_1$ |
|---|---|
| 425.05 | 0.1500 |
| 417.85 | 0.3000 |
| 409.65 | 0.4500 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 9.119**

| T / K | $x_1$ |
|---|---|
| 404.45 | 0.1500 |
| 392.25 | 0.2000 |
| 380.75 | 0.2500 |
| 369.75 | 0.3000 |
| 349.45 | 0.4000 |
| 331.35 | 0.5000 |
| 317.45 | 0.6000 |
| 308.35 | 0.7000 |
| 301.95 | 0.8000 |
| 297.25 | 0.9000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 9.119**

| T / K | $x_1$ |
|---|---|
| 432.15 | 0.0500 |
| 417.85 | 0.1000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 9.119**

| T / K | $y_1$ |
|---|---|
| 404.55 | 0.7000 |
| 393.15 | 0.8000 |
| 385.55 | 0.8500 |
| 375.65 | 0.9000 |
| 359.65 | 0.9500 |
| 340.75 | 0.9800 |
| 328.85 | 0.9900 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 9.119**

| T / K | $y_1$ |
|---|---|
| 440.75 | 0.1500 |

| | |
|---|---|
| 432.95 | 0.3000 |
| 424.15 | 0.4500 |
| 413.45 | 0.6000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 11.15**

| T / K | $x_1$ |
|---|---|
| 401.05 | 0.2000 |
| 389.25 | 0.2500 |
| 378.05 | 0.3000 |
| 357.45 | 0.4000 |
| 338.85 | 0.5000 |
| 324.65 | 0.6000 |
| 315.55 | 0.7000 |
| 308.95 | 0.8000 |
| 304.05 | 0.9000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 11.15**

| T / K | $x_1$ |
|---|---|
| 441.05 | 0.0500 |
| 426.65 | 0.1000 |
| 413.15 | 0.1500 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 11.15**

| T / K | $y_1$ |
|---|---|
| 399.45 | 0.8000 |
| 391.65 | 0.8500 |
| 381.35 | 0.9000 |
| 364.75 | 0.9500 |
| 344.95 | 0.9800 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 11.15**

| T / K | $y_1$ |
|---|---|
| 449.05 | 0.1500 |
| 440.85 | 0.3000 |
| 431.65 | 0.4500 |
| 420.35 | 0.6000 |
| 411.25 | 0.7000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 15.20**

| T / K | $x_1$ |
|---|---|
| 402.85 | 0.2500 |
| 391.45 | 0.3000 |
| 370.25 | 0.4000 |
| 351.15 | 0.5000 |
| 336.95 | 0.6000 |
| 327.25 | 0.7000 |
| 320.15 | 0.8000 |
| 315.05 | 0.9000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 15.20**

| T / K | $x_1$ |
|---|---|
| 455.15 | 0.0500 |
| 441.05 | 0.1000 |
| 427.55 | 0.1500 |
| 414.85 | 0.2000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 15.20**

| T / K | $y_1$ |
|---|---|
| 401.15 | 0.8500 |
| 390.15 | 0.9000 |
| 372.65 | 0.9500 |
| 352.55 | 0.9800 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 15.20**

| T / K | $y_1$ |
|---|---|
| 462.45 | 0.1500 |
| 453.65 | 0.3000 |
| 443.85 | 0.4500 |
| 431.45 | 0.6000 |
| 421.95 | 0.7000 |

| | |
|---|---|
| 409.65 | 0.8000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 19.25**

| T / K | $x_1$ |
|---|---|
| 402.85 | 0.3000 |
| 380.65 | 0.4000 |
| 361.35 | 0.5000 |
| 346.65 | 0.6000 |
| 336.85 | 0.7000 |
| 329.55 | 0.8000 |
| 324.05 | 0.9000 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 19.25**

| T / K | $x_1$ |
|---|---|
| 467.15 | 0.0500 |
| 452.85 | 0.1000 |
| 439.35 | 0.1500 |
| 426.25 | 0.2000 |
| 414.05 | 0.2500 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 19.25**

| T / K | $y_1$ |
|---|---|
| 397.05 | 0.9000 |
| 378.35 | 0.9500 |
| 358.65 | 0.9800 |

Wucherer, J., Measurement of the pressure, temperature and composition of the liquid and vapor phases of ammonia-water mixtures in the saturated state, Z. gesamte Kaelte-Ind. (1932) 136-140.

**P / bar = 19.25**

| T / K | $y_1$ |
|---|---|
| 473.45 | 0.1500 |
| 464.15 | 0.3000 |
| 453.65 | 0.4500 |
| 440.55 | 0.6000 |
| 430.65 | 0.7000 |
| 417.75 | 0.8000 |
| 408.95 | 0.8500 |

---

**Critical point**

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Sakabe, A. - Arai, D. - Miyamoto, H. - Uematsu, M., Measurements of the critical parameters for {xNH3+(1−x)H2O} with x=(0.9098,0.7757,0.6808), The Journal of Chemical Thermodynamics 10 (2008) 1527-1530. doi:10.1016/j.jct.2008.05.017

| T / K | P / bar | $x_1$ |
|---|---|---|
| 436.56 | 141.82 | 0.9098 |
| 478.58 | 173.07 | 0.7757 |
| 503.06 | 186.93 | 0.6808 |

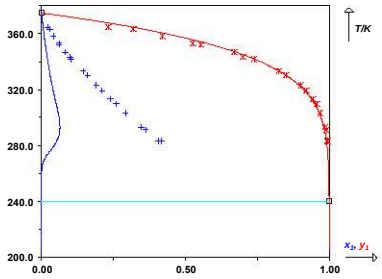
Polikhronidi, N.G. - Abdulagatov, I.M. - Batyrova, R.G. - Stepanov, G.V., PVT measurements of water-ammonia refrigerant mixture in the critical and supercritical regions, International Journal of Refrigeration 8 (2009) 1897-1913. doi:10.1016/j.ijrefrig.2009.07.008

| T / K | P / bar | $x_1$ |
|---|---|---|
| 599.67 | 214.08 | 0.2607 |

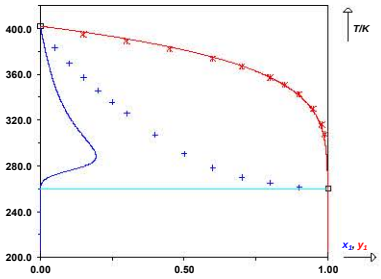
Sassen, C. L. - Van Kwartel, R. A. C. - Van der Kooi, H. J. - De Swaan Arons, J., Vapor-liquid equilibria for the system ammonia + water up to the critical region, Journal of Chemical & Engineering Data 2 (1990) 140-144. doi:10.1021/je00060a013

| T / K | P / bar | $x_1$ |
|---|---|---|
| 613.50 | 215.20 | 0.1890 |
| 580.10 | 208.30 | 0.3460 |
| 551.10 | 201.30 | 0.4910 |
| 527.30 | 194.90 | 0.6130 |
| 498.10 | 181.30 | 0.6990 |
| 470.00 | 165.70 | 0.8000 |

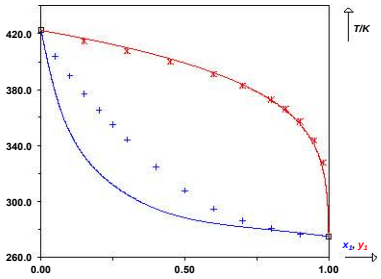
P/bar = 1.01320



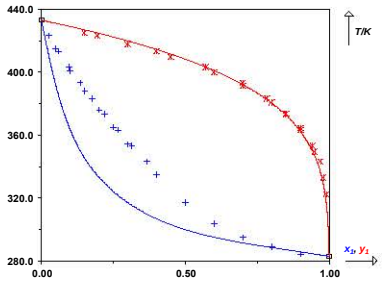

P/bar = 2.53310



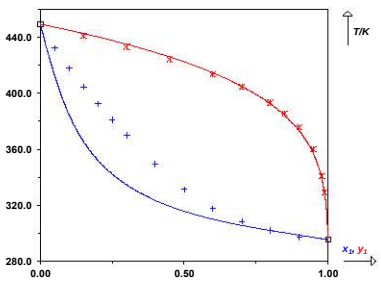

P/bar = 4.55960



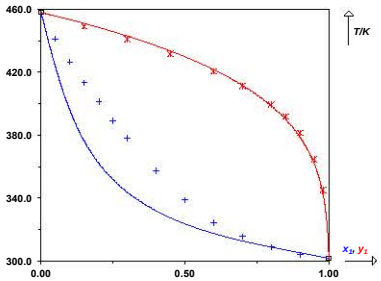

P/bar = 6.07950



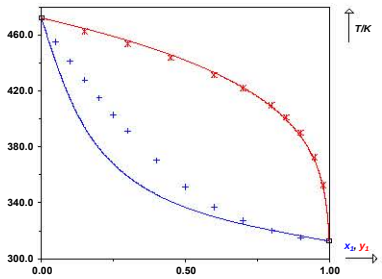

P/bar = 9.11920



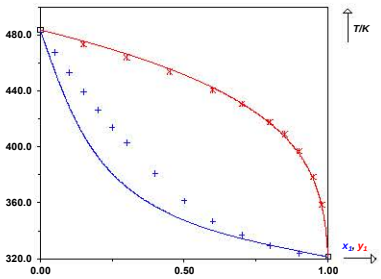

P/bar = 11.14600



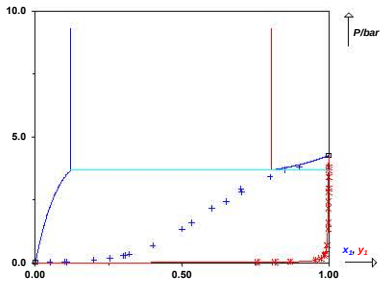

P/bar = 15.19900



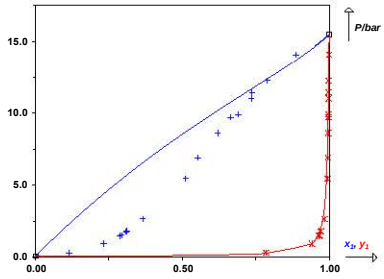

P/bar = 19.25200



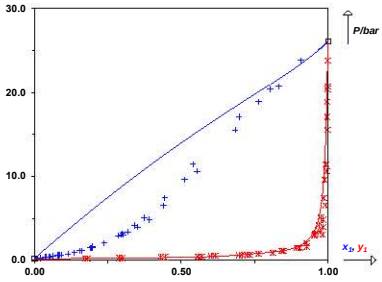

T/K = 273.15



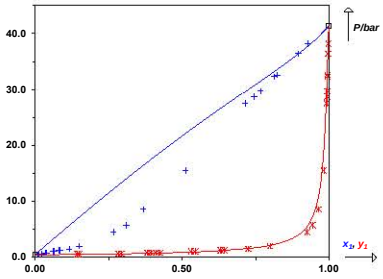

T/K = 313.15



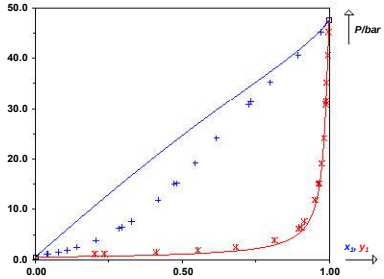

T/K = 333.15



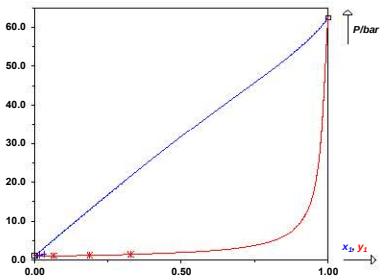

T/K = 353.15



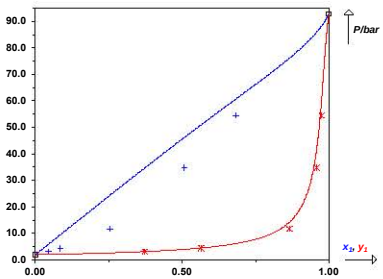

T/K = 359.70



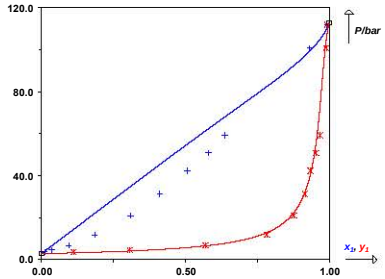

T/K = 373.15



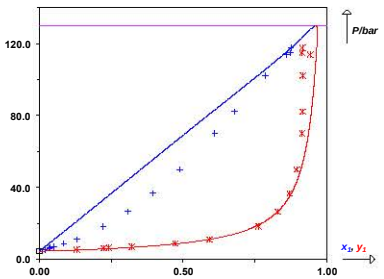

T/K = 394.25



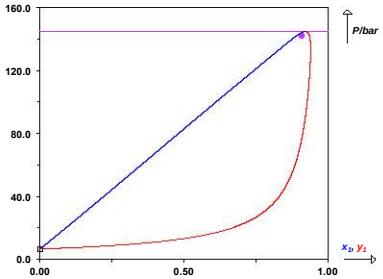
T/K = 405.50



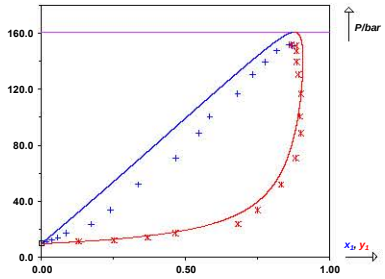

T/K = 422.50



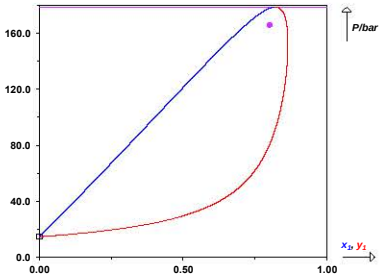

T/K = 436.56



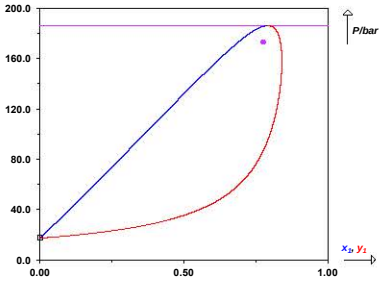

T/K = 451.50



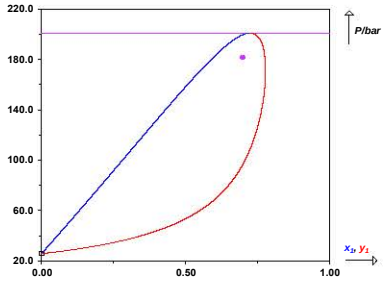

T/K = 470.00



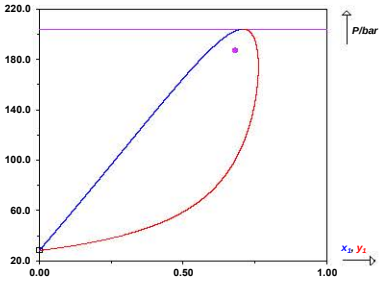

T/K = 478.58



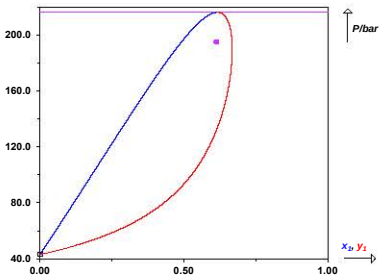

T/K = 498.10



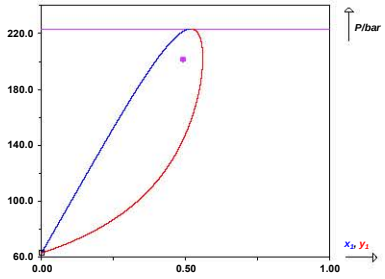

T/K = 503.06



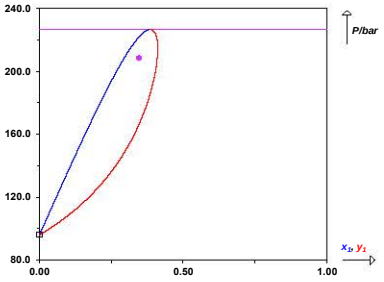

T/K = 527.30



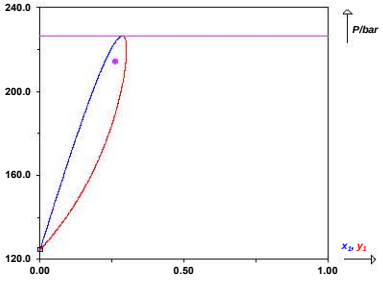

T/K = 551.10



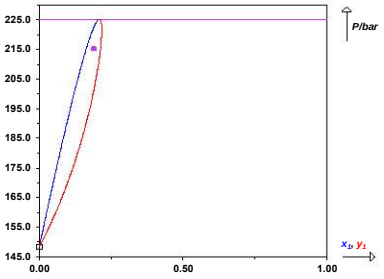

T/K = 580.10




T/K = 599.67




T/K = 613.50



## AMMONIA (1) + ACETONITRILE (2)

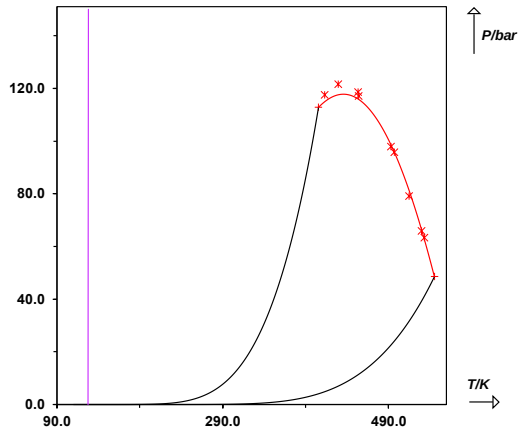
| | | |
|---|---|---|
| **CAS** | 7664-41-7 | 75-05-8 |
| **InChiKey** | QGZKDVFQNNGYKY-UHFFFAOYSA-N | WEVYAHXRMPXWCK-UHFFFAOYSA-N |
| **$T_c$ / K** | 405.65 | 545.50 |
| **$P_c$ / bar** | 112.80 | 48.50 |
| **ω** | 0.253 | 0.342 |

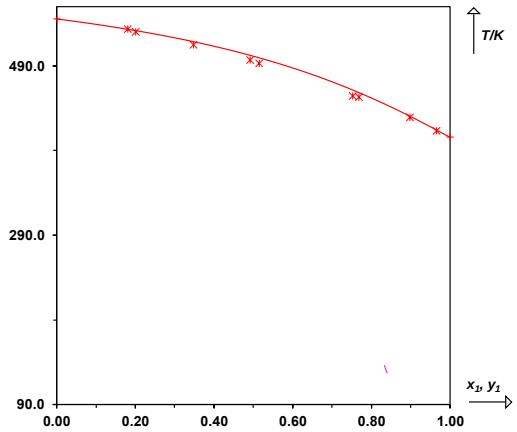
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 224
B/MPa = 270

*Deviations*
MAPE on x = 4.4 %
MAPE on y = 11 %
MAPE on $x_c$ = 6.8 %
MAPE on $P_c$ = 1.4 %



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**Isothermal phase equilibrium data**

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Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 2.026 | 0.2250 | 0.9000 |
| 4.053 | 0.4500 | 0.9630 |
| 6.080 | 0.6950 | 0.9850 |
| 8.106 | 0.9250 | 0.9970 |

Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.066 | 0.2000 | 0.8500 |
| 10.13 | 0.4080 | 0.9500 |
| 15.20 | 0.6000 | 0.9800 |
| 20.27 | 0.7800 | 0.9930 |

Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.066 | 0.0730 | 0.5700 |
| 10.13 | 0.1700 | 0.7900 |
| 15.20 | 0.2900 | 0.8800 |
| 20.27 | 0.3950 | 0.9200 |
| 30.40 | 0.5900 | 0.9500 |
| 40.53 | 0.7450 | 0.9700 |

Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

**T / K = 373.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 50.66 | 0.8700 | 0.9850 |

Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

**T / K = 413.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 10.13 | 0.0700 | 0.5150 | |
| 20.27 | 0.2030 | 0.7500 | |
| 30.40 | 0.3400 | 0.8230 | |
| 40.53 | 0.4700 | 0.8600 | |
| 60.80 | 0.6500 | 0.9090 | |
| 81.06 | 0.7870 | 0.9430 | |
| 101.30 | 0.8900 | 0.9670 | |
| 117.50 | 0.9650 | 0.9650 | CRIT |

Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

**T / K = 453.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 20.27 | 0.0920 | 0.4700 | |
| 40.53 | 0.2800 | 0.6730 | |
| 60.80 | 0.4380 | 0.7370 | |
| 81.06 | 0.5500 | 0.7680 | |
| 101.30 | 0.6480 | 0.7750 | |
| 118.50 | 0.7680 | 0.7680 | CRIT |

Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

**T / K = 493.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 40.53 | 0.1380 | 0.3930 | |
| 60.80 | 0.2700 | 0.4830 | |
| 81.06 | 0.3780 | 0.5100 | |
| 97.98 | 0.5150 | 0.5150 | CRIT |

Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

**T / K = 533.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 50.66 | 0.0750 | 0.1270 | |
| 60.80 | 0.1300 | 0.1730 | |
| 63.33 | 0.1800 | 0.1800 | CRIT |

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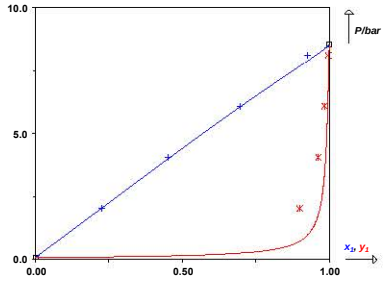
**Critical point**

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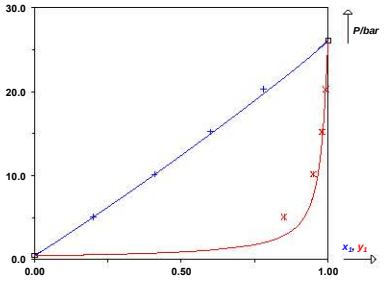
Tyvina, T.N. - Naumova, A.A. - Fokina, V.V., Liquid-gas equilibrium in an acetonitrile-ammonia system, J. Appl. Chem. USSR 11 (1979) 2458-2460.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 530.15 | 65.86 | 0.2010 |
| 515.15 | 79.03 | 0.3480 |
| 497.15 | 95.75 | 0.4920 |
| 454.15 | 117.00 | 0.7520 |
| 429.15 | 121.60 | 0.8970 |

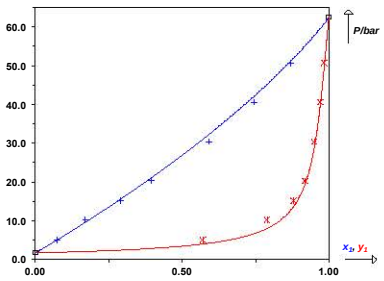
T/K = 293.15



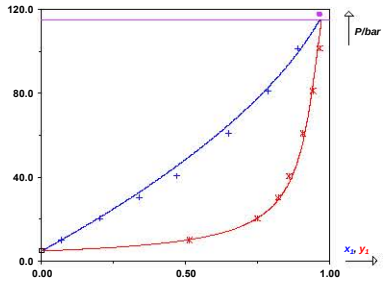

T/K = 333.15



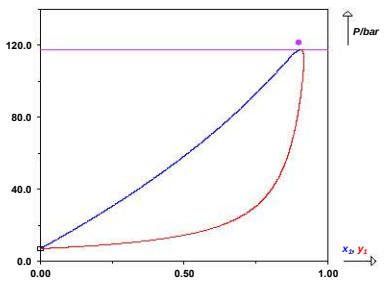

T/K = 373.15



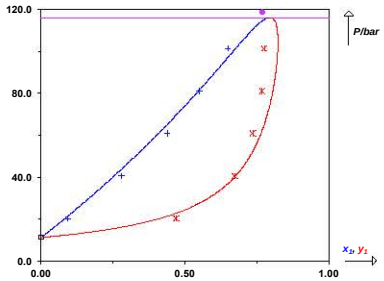

T/K = 413.15



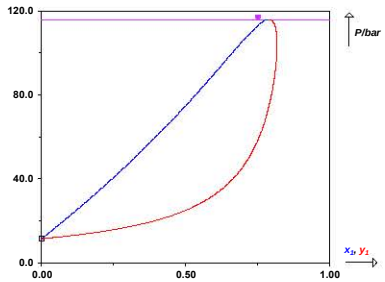

T/K = 429.15



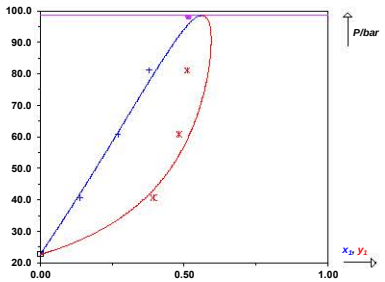

T/K = 453.15



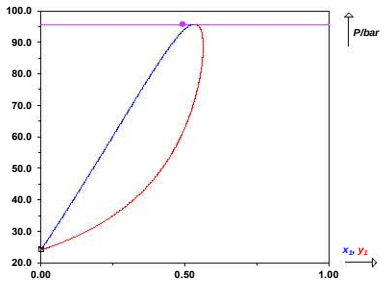

T/K = 454.15



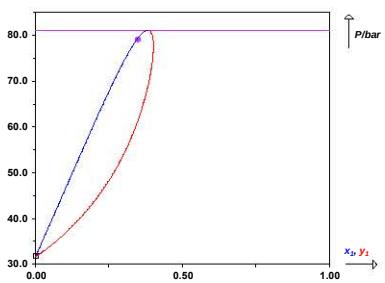

T/K = 493.15



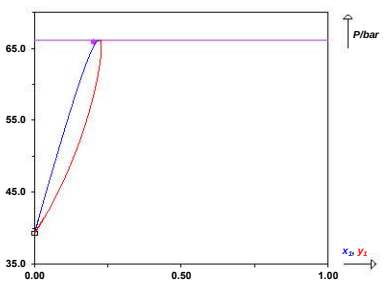

T/K = 497.15



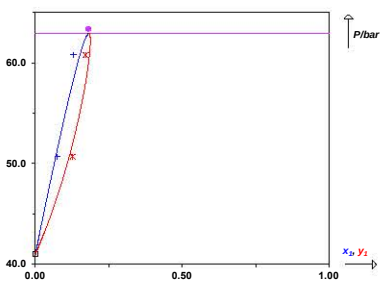

T/K = 515.15




T/K = 530.15




T/K = 533.15



## WATER (1) + ALLYL ALCOHOL (2)

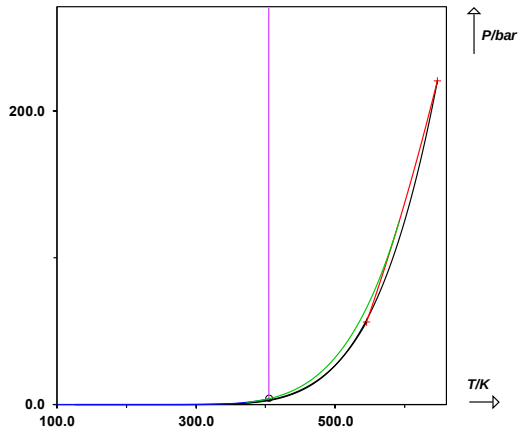
| | | |
|---|---|---|
| **CAS** | 7732-18-5 | 107-18-6 |
| **InChiKey** | XLYOFNOQVPJJNP-UHFFFAOYSA-N | XXROGKLTLUQVRX-UHFFFAOYSA-N |
| **$T_c$ / K** | 647.10 | 545.10 |
| **$P_c$ / bar** | 220.64 | 56.20 |
| **ω** | 0.345 | 0.570 |

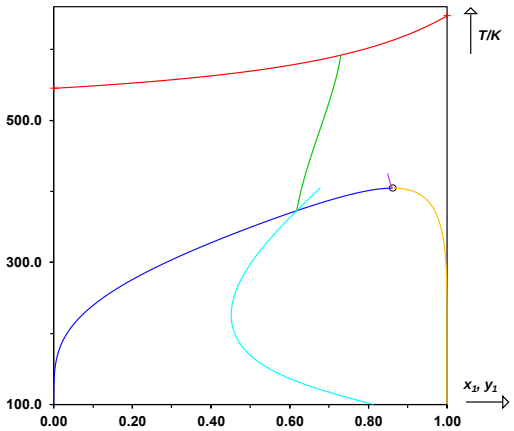
Non ideal with unknown causes

**PPR78 results**

*Parameters*
A/MPa = 1370
B/MPa = 2120

*Deviations*
MAPE on x = 37 %
MAPE on y = 8.4 %



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**Isothermal phase equilibrium data**

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Ewert, M., Theory of concentrated solutions. XIII. Aqueous solutions of organic compounds, Bull. Soc. Chim. Belg. (1936) 493-515.

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1051 | 0.9000 | 0.6459 |
| 0.1104 | 0.8000 | 0.5676 |
| 0.1121 | 0.7000 | 0.5196 |
| 0.1132 | 0.6000 | 0.4865 |
| 0.1133 | 0.5000 | 0.4553 |
| 0.1127 | 0.4000 | 0.4284 |
| 0.1100 | 0.3000 | 0.3867 |
| 0.1049 | 0.2000 | 0.3240 |
| 0.0964 | 0.1000 | 0.2144 |

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**Isobaric phase equilibrium data**

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Aucejo, A. - Loras, S. - Monton, J.B., Isobaric vapor-liquid equilibria of prop-2-en-1-ol (allyl alcohol) + water system at 30, 60, and 100 kPa, ELDATA: The International Electronic Journal of Physico-Chemical Data 1 (1996) 1-4.

**P / bar = 0.3000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 340.33 | 0.9949 | 0.9276 |
| 339.41 | 0.9903 | 0.8951 |
| 338.22 | 0.9833 | 0.8414 |
| 336.85 | 0.9728 | 0.7827 |
| 335.58 | 0.9564 | 0.7226 |
| 334.38 | 0.9355 | 0.6738 |
| 333.90 | 0.9293 | 0.6574 |
| 333.56 | 0.9136 | 0.6466 |
| 333.25 | 0.9051 | 0.6349 |
| 332.82 | 0.8754 | 0.6190 |
| 332.55 | 0.8445 | 0.6105 |
| 332.39 | 0.8024 | 0.6046 |
| 332.17 | 0.7527 | 0.5926 |
| 332.04 | 0.7064 | 0.6043 |
| 332.03 | 0.6461 | 0.5776 |
| 331.98 | 0.5817 | 0.5638 |
| 331.96 | 0.5108 | 0.5449 |
| 332.01 | 0.4555 | 0.5254 |
| 332.23 | 0.3911 | 0.4981 |
| 332.51 | 0.3318 | 0.4678 |
| 333.03 | 0.2680 | 0.4279 |
| 333.72 | 0.2198 | 0.3844 |
| 334.55 | 0.1710 | 0.3301 |
| 335.73 | 0.1144 | 0.2495 |
| 336.62 | 0.0820 | 0.1947 |
| 337.54 | 0.0499 | 0.1361 |

Aucejo, A. - Loras, S. - Monton, J.B., Isobaric vapor-liquid equilibria of prop-2-en-1-ol (allyl alcohol) + water system at 30, 60, and 100 kPa, ELDATA: The International Electronic Journal of Physico-Chemical Data 1 (1996) 1-4.

**P / bar = 0.6000**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 357.05 | 0.9923 | 0.9207 |
| 356.22 | 0.9885 | 0.8948 |
| 355.00 | 0.9805 | 0.8359 |
| 353.63 | 0.9682 | 0.7883 |
| 352.34 | 0.9596 | 0.7335 |
| 351.22 | 0.9422 | 0.6946 |
| 350.44 | 0.9262 | 0.6686 |
| 349.83 | 0.9023 | 0.6467 |
| 349.37 | 0.8762 | 0.6317 |
| 348.96 | 0.8449 | 0.6204 |
| 348.88 | 0.8078 | 0.6081 |
| 348.67 | 0.7643 | 0.5987 |
| 348.49 | 0.6888 | 0.5922 |
| 348.34 | 0.6534 | 0.5802 |
| 348.20 | 0.5920 | 0.5648 |
| 348.19 | 0.5283 | 0.5453 |
| 348.37 | 0.4642 | 0.5233 |
| 348.53 | 0.4027 | 0.4961 |
| 348.85 | 0.3448 | 0.4669 |
| 349.33 | 0.2830 | 0.4258 |
| 350.18 | 0.2121 | 0.3645 |
| 351.39 | 0.1617 | 0.3050 |
| 352.70 | 0.1070 | 0.2289 |
| 353.47 | 0.0765 | 0.1737 |
| 354.61 | 0.0452 | 0.1092 |

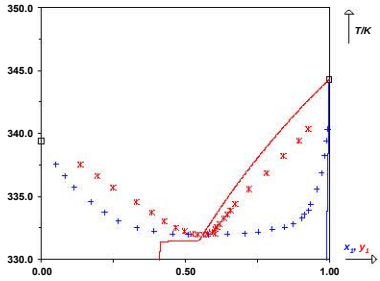
Aucejo, A. - Loras, S. - Monton, J.B., Isobaric vapor-liquid equilibria of prop-2-en-1-ol (allyl alcohol) + water system at 30, 60, and 100 kPa, ELDATA: The International Electronic Journal of Physico-Chemical Data 1 (1996) 1-4.

**P / bar = 1.000**

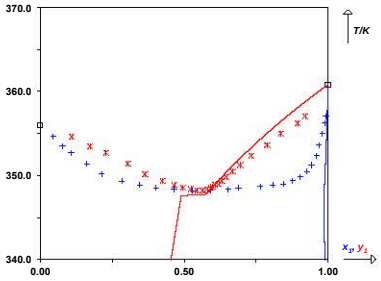
| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 370.39 | 0.9916 | 0.9134 |
| 369.31 | 0.9863 | 0.8737 |
| 368.10 | 0.9813 | 0.8243 |
| 366.95 | 0.9729 | 0.7842 |
| 366.04 | 0.9615 | 0.7455 |

| | | |
|---|---|---|
| 364.96 | 0.9506 | 0.7128 |
| 364.02 | 0.9354 | 0.6831 |
| 363.17 | 0.9116 | 0.6582 |
| 362.69 | 0.8943 | 0.6453 |
| 362.12 | 0.8605 | 0.6261 |
| 361.97 | 0.8248 | 0.6186 |
| 361.68 | 0.7797 | 0.6062 |
| 361.46 | 0.7245 | 0.5953 |
| 361.35 | 0.6631 | 0.5803 |
| 361.32 | 0.5888 | 0.5643 |
| 361.30 | 0.5176 | 0.5407 |
| 361.33 | 0.4633 | 0.5185 |
| 361.45 | 0.3960 | 0.4887 |
| 361.86 | 0.3355 | 0.4529 |
| 362.77 | 0.2695 | 0.4036 |
| 363.53 | 0.2136 | 0.3541 |
| 364.56 | 0.1585 | 0.2885 |
| 366.09 | 0.0965 | 0.1979 |
| 367.18 | 0.0599 | 0.1384 |
| 368.33 | 0.0288 | 0.0653 |

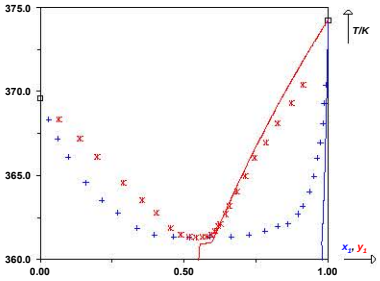
P/bar = 0.30001



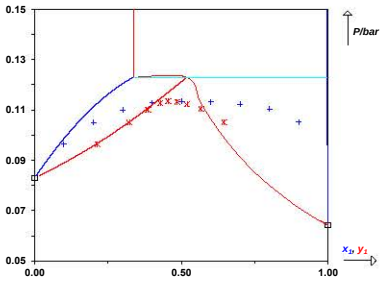

P/bar = 0.60003




P/bar = 1.00010




T/K = 313.15



## WATER (1) + PHENOL (2)

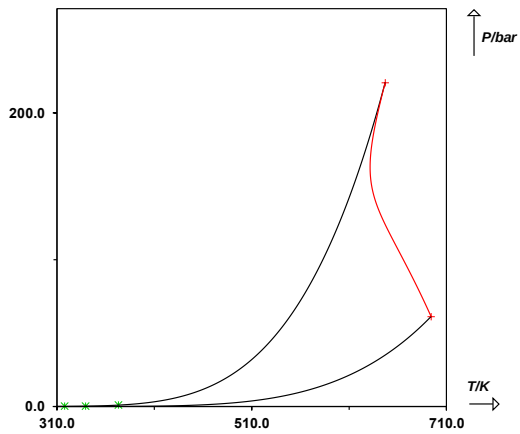
| | | |
|---|---|---|
| **CAS** | 7732-18-5 | 108-95-2 |
| **InChiKey** | XLYOFNOQVPJJNP-UHFFFAOYSA-N | ISWSIDIOOBJBQZ-UHFFFAOYSA-N |
| **$T_c$ / K** | 647.10 | 694.25 |
| **$P_c$ / bar** | 220.64 | 61.30 |
| **ω** | 0.345 | 0.443 |

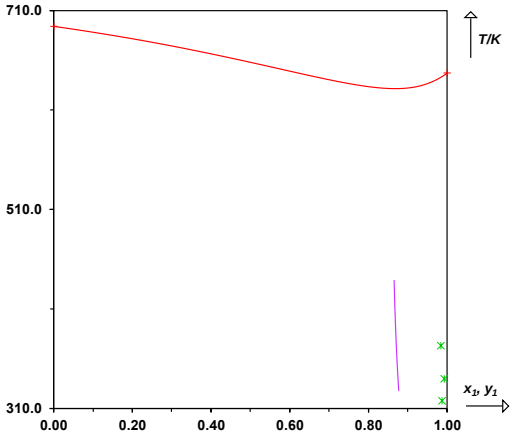
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 762
B/MPa = 303

*Deviations*
MAPE on x = 80 %
MAPE on y = 11 %
MAPE on $h^M$ = 14 %
MAPE on $c_P^M$ = 41 %



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**Isothermal phase equilibrium data**

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Weller, Rolf - Schuberth, Horst - Leibnitz, Eberhard, Phasengleichgewichtsmessungen. IV. Die Phasengleichgewichte dampfförmig/flüssig des Systems Phenol/n-Butylacetat/Wasser bei 44,4°C, Journal für Praktische Chemie 5-6 (1963) 234-249. doi:10.1002/prac.19630210502

**T / K = 317.55**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.0120 | 0.0501 | 0.8248 | |
| 0.0195 | 0.0963 | 0.8977 | |
| 0.0280 | 0.1391 | 0.9329 | |
| 0.0381 | 0.1787 | 0.9559 | |
| 0.0453 | 0.2156 | 0.9656 | |
| 0.0544 | 0.2500 | 0.9727 | |
| 0.0640 | 0.2975 | 0.9769 | |
| 0.0741 | 0.3672 | 0.9801 | |
| 0.0800 | 0.4273 | 0.9821 | |
| 0.0837 | 0.4796 | 0.9830 | |
| 0.0867 | 0.5256 | 0.9836 | |
| 0.0883 | 0.5663 | 0.9843 | |
| 0.0895 | 0.5998 | 0.9849 | |
| 0.0927 | 0.7002 | 0.9864 | |
| 0.0935 | 0.9871 | 0.9871 | AZEO |
| 0.0935 | 0.9953 | 0.9939 | |

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**Isobaric phase equilibrium data**

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Kliment, V. - Fried, V. - Pick, J., Liquid-vapor equilibrium. XXXIII. The systems butyl acetate-phenol and water-phenol, Collect. Czech. Chem. Commun. (1964) 2008-2015.

**P / bar = 0.2666**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 399.65 | 0.0040 | 0.3740 |
| 385.35 | 0.0290 | 0.6530 |
| 353.45 | 0.2910 | 0.9460 |
| 351.90 | 0.3180 | 0.9520 |
| 344.40 | 0.5000 | 0.9740 |
| 341.45 | 0.5780 | 0.9770 |
| 340.75 | 0.6130 | 0.9790 |
| 340.20 | 0.6600 | 0.9810 |
| 340.00 | 0.6880 | 0.9830 |
| 339.65 | 0.9430 | 0.9920 |
| 339.60 | 0.9950 | 0.9940 |
| 339.65 | 0.9975 | 0.9960 |

Chou, C.H. - Perng, J.L. - Lee, M.D. - Chen, Y.P., Vapor-liquid equilibrium measurements of the ternary system of ethanol, water and phenol at 760mmHg, J. Chin. Inst. Chem. Eng. 6 (1987) 393-399.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 454.55 | 0.0001 | 0.0075 |
| 447.51 | 0.0154 | 0.2940 |
| 413.05 | 0.1019 | 0.7827 |
| 385.97 | 0.3087 | 0.9397 |
| 380.83 | 0.3838 | 0.9509 |
| 374.41 | 0.5679 | 0.9736 |
| 373.17 | 0.7215 | 0.9778 |
| 373.00 | 0.8088 | 0.9786 |
| 372.92 | 0.9847 | 0.9839 |
| 372.97 | 0.9938 | 0.9907 |

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**Enthalpy of mixing**

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Schuermann, E. - Diederichs, R., Heats of mixing of phenol-water systems, Ber. Bunsen-Ges. Phys. Chem. 5 (1964) 429-434.

**T / K = 323.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / $J.mol^{-1}$ | $x_1$ |
|---|---|
| 467.67 | 0.2174 |
| 714.12 | 0.3680 |
| 814.61 | 0.4825 |
| 826.13 | 0.5667 |
| 790.69 | 0.6344 |
| 739.58 | 0.6906 |
| 667.07 | 0.7359 |
| 602.10 | 0.7759 |
| 451.44 | 0.8399 |
| 333.61 | 0.8878 |
| 250.74 | 0.9245 |
| 178.86 | 0.9547 |
| 148.05 | 0.9682 |
| 56.63 | 0.9899 |

Schuermann, E. - Diederichs, R., Heats of mixing of phenol-water systems, Ber. Bunsen-Ges. Phys. Chem. 5 (1964) 429-434.

**T / K = 333.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / $J.mol^{-1}$ | $x_1$ |
|---|---|
| 432.45 | 0.2084 |
| 696.90 | 0.3687 |

| | |
|---|---|
| 794.88 | 0.4784 |
| 848.45 | 0.5643 |
| 769.13 | 0.6881 |
| 720.34 | 0.7377 |
| 649.74 | 0.7764 |
| 503.59 | 0.8386 |
| 386.71 | 0.8870 |
| 296.65 | 0.9233 |
| 213.24 | 0.9544 |
| 128.78 | 0.9793 |
| 61.25 | 0.9903 |

Schuermann, E. - Diederichs, R., Heats of mixing of phenol-water systems, Ber. Bunsen-Ges. Phys. Chem. 5 (1964) 429-434.

**T / K = 343.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 396.42 | 0.2084 |
| 673.97 | 0.3698 |
| 811.58 | 0.4786 |
| 846.31 | 0.5660 |
| 869.83 | 0.6004 |
| 856.47 | 0.6340 |
| 796.97 | 0.6918 |
| 785.69 | 0.7007 |
| 778.68 | 0.7168 |
| 693.79 | 0.7774 |
| 558.29 | 0.8385 |
| 420.82 | 0.8998 |
| 266.79 | 0.9500 |
| 192.98 | 0.9700 |
| 101.73 | 0.9854 |

Schuermann, E. - Diederichs, R., Heats of mixing of phenol-water systems, Ber. Bunsen-Ges. Phys. Chem. 5 (1964) 429-434.

**T / K = 358.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 380.64 | 0.2156 |
| 664.50 | 0.3677 |
| 818.87 | 0.4741 |
| 873.16 | 0.5650 |
| 896.09 | 0.6319 |
| 854.60 | 0.6905 |
| 827.12 | 0.7366 |
| 764.86 | 0.7760 |
| 705.16 | 0.8079 |
| 632.51 | 0.8405 |
| 510.21 | 0.8864 |
| 402.10 | 0.9236 |
| 293.04 | 0.9538 |
| 169.28 | 0.9789 |
| 84.09 | 0.9901 |

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**Heat capacity of mixing**

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Ferguson, J. B., The System Water-Phenol, The Journal of Physical Chemistry 5 (1926) 757-763. doi:10.1021/j150275a013

**T / K = 345.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 3.173 | 0.5678 |
| 4.686 | 0.7767 |
| 5.027 | 0.8862 |
| 2.426 | 0.9542 |

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**Azeotropic point**

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Chou, C.H. - Perng, J.L. - Lee, M.D. - Chen, Y.P., Vapor-liquid equilibrium measurements of the ternary system of ethanol, water and phenol at 760mmHg, J. Chin. Inst. Chem. Eng. 6 (1987) 393-399.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 372.92 | 1.013 | 0.9835 |

Kliment, V. - Fried, V. - Pick, J., Liquid-vapor equilibrium. XXXIII. The systems butyl acetate-phenol and water-phenol, Collect. Czech. Chem. Commun. (1964) 2008-2015.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 339.55 | 0.2666 | 0.9930 |

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**Three-phase line**

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A.N. Campbell - A.J.R. Campbell, Concentrations, Total and Partial Vapor Pressures, Surface Tensions and Viscosities, in the Systems Phenol—Water and Phenol—Water—4% Succinic Acid, Journal of the American Chemical Society. 59 (1937) 2481–2488. doi:10.1021/ja01291a001.

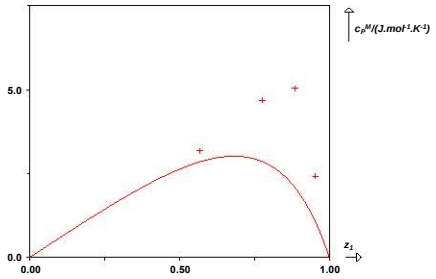
| T / K | P / bar | $x_{1a}$ | $x_{1b}$ | $y_1$ |
|---|---|---|---|---|
| 299.35 | 0.0323 | 0.6830 | 0.9847 | 0.9915 |

| | | | | |
|---|---|---|---|---|
| 333.05 | 0.1935 | 0.8041 | 0.9698 | 0.9839 |

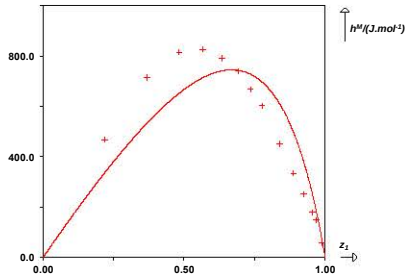
F.A.H. Schreinemakers, On the composition of the vapour-phase in the system Water-Phenol, with one and with two liquid-phases, Proc. K. Ned. Akad. Wet. Nat. Sci. 3 (1901) 1–11.

| T / K | P / bar | $x_{1a}$ | $x_{1b}$ | $y_1$ |
|---|---|---|---|---|
| 302.95 | 0.0387 | 0.6913 | 0.9836 | 0.9880 |
| 311.35 | 0.0640 | 0.7201 | 0.9803 | 0.9858 |
| 315.55 | 0.0827 | 0.7291 | 0.9792 | 0.9860 |
| 329.45 | 0.1253 | 0.7542 | 0.9746 | 0.9852 |
| 329.65 | 0.1680 | 0.7769 | 0.9686 | 0.9840 |
| 333.25 | 0.2000 | 0.7976 | 0.9623 | 0.9835 |
| 337.55 | 0.2426 | 0.8498 | 0.9474 | 0.9822 |

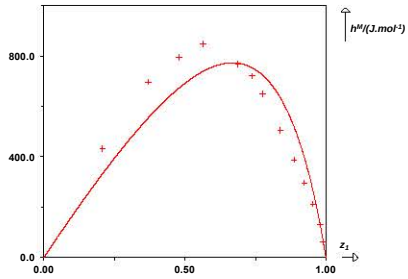
T/K = 345.15 - P/bar = 1.0132



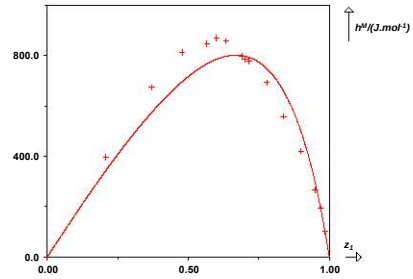

T/K = 323.15 - P/bar = 1.0132



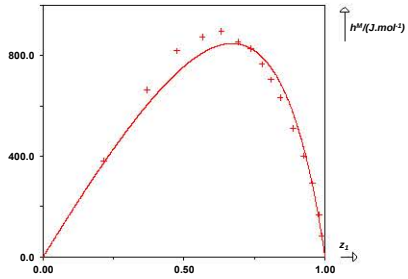

T/K = 333.15 - P/bar = 1.0132



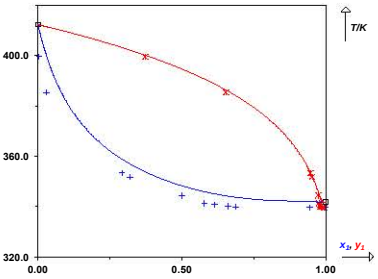

T/K = 343.15 - P/bar = 1.0132



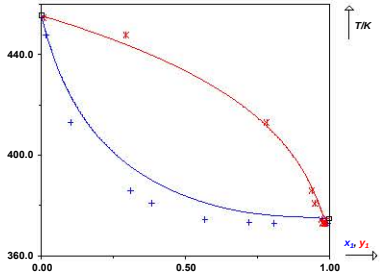

T/K = 358.15 - P/bar = 1.0132



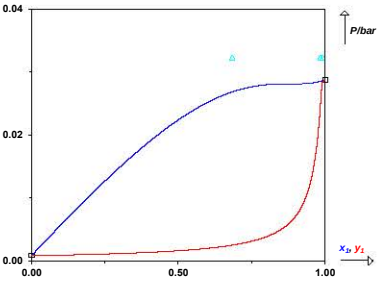

P/bar = 0.26660



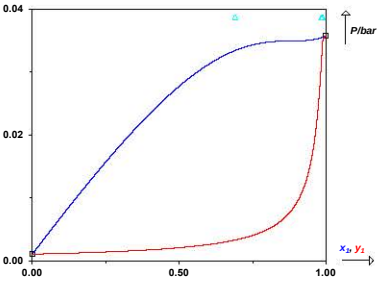

P/bar = 1.01330



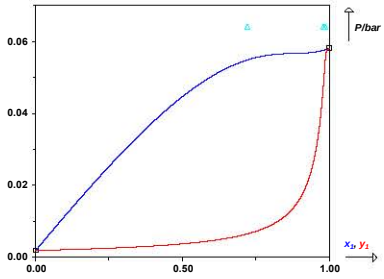

T/K = 299.35



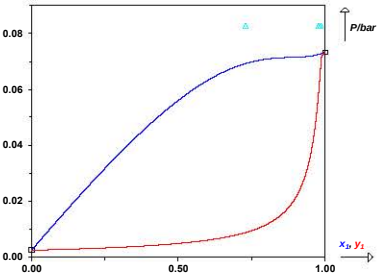

T/K = 302.95



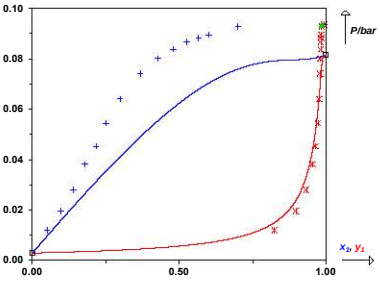

T/K = 311.35



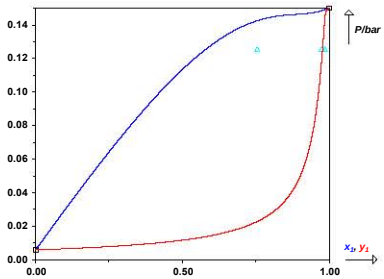

T/K = 315.55



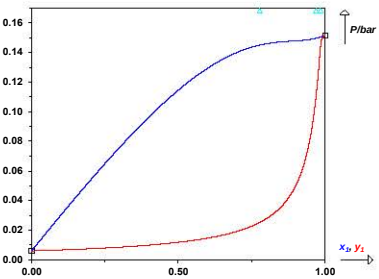

T/K = 317.55



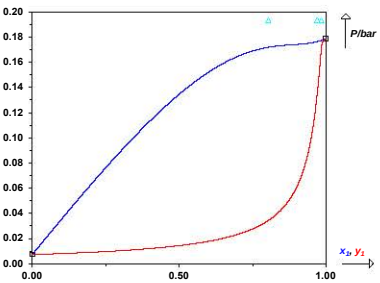

T/K = 329.45



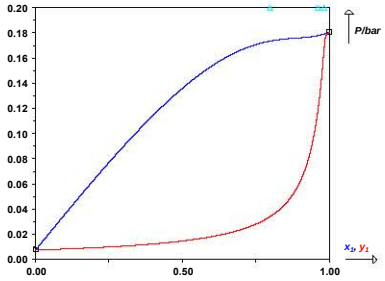

T/K = 329.65



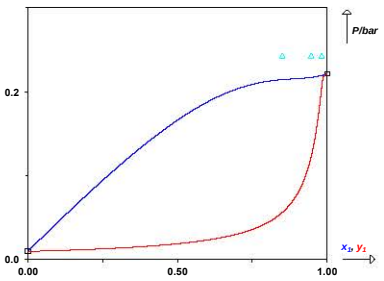

T/K = 333.05



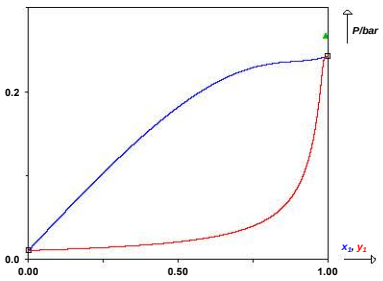
T/K = 333.25



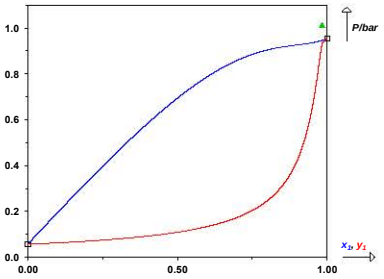

T/K = 337.55




T/K = 339.55




T/K = 372.92



# METHYL FORMATE (1) + METHANOL (2)

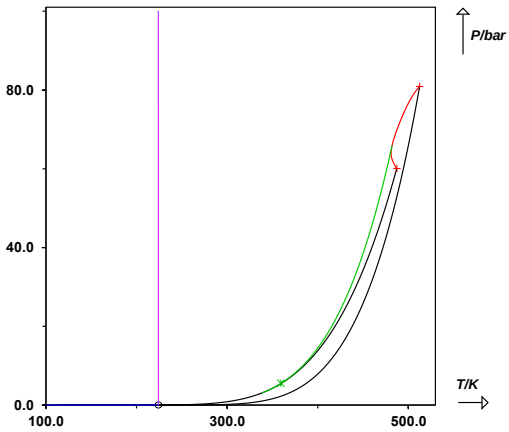
| | | |
|---|---|---|
| **CAS** | 107-31-3 | 67-56-1 |
| **InChiKey** | TZIHFWKZFHZASV-UHFFFAOYSA-N | OKKJLVBELUTLKV-UHFFFAOYSA-N |
| **$T_c$ / K** | 487.20 | 512.50 |
| **$P_c$ / bar** | 60.00 | 80.84 |
| **ω** | 0.256 | 0.566 |

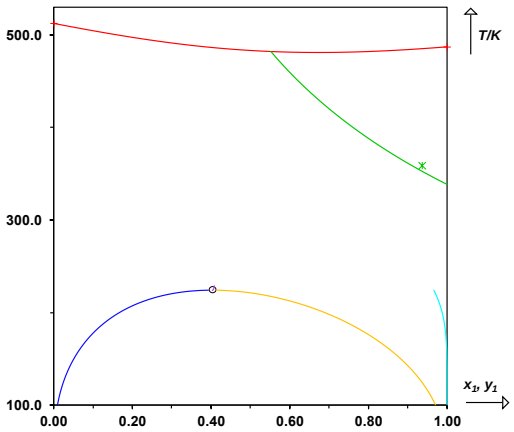
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 414
B/MPa = 356

*Deviations*
MAPE on x = 13 %
MAPE on y = 7.3 %
MAPE on $x_{az}$ = 23 %
MAPE on $P_{az}$ = 1.7 %
MAPE on $h^M$ = 17 %



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**Isothermal phase equilibrium data**

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Polak, Jiri - Lu, B.C.-Y, Excess Gibbs free energies and excess volumes of methyl formate + methanol and methyl formate + ethanol at 298.15 K, The Journal of Chemical Thermodynamics 3 (1972) 469-476. doi:10.1016/0021-9614(72)90031-6

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2868 | 0.0509 | 0.4291 |
| 0.3650 | 0.0916 | 0.5641 |
| 0.4711 | 0.1707 | 0.6847 |
| 0.5174 | 0.2183 | 0.7216 |
| 0.5658 | 0.2808 | 0.7551 |
| 0.5975 | 0.3330 | 0.7718 |
| 0.6392 | 0.4191 | 0.7911 |
| 0.6713 | 0.5029 | 0.8092 |
| 0.6953 | 0.5788 | 0.8278 |
| 0.7080 | 0.6226 | 0.8397 |
| 0.7234 | 0.6785 | 0.8549 |
| 0.7349 | 0.7221 | 0.8658 |
| 0.7490 | 0.7788 | 0.8827 |
| 0.7656 | 0.8523 | 0.9038 |
| 0.7805 | 0.9260 | 0.9387 |

Arce, Alberto - Rodríguez, Héctor - Soto, Ana, Use of a green and cheap ionic liquid to purify gasoline octane boosters, Green Chem. 3 (2007) 247-253. doi:10.1039/B611139D

**T / K = 303.20**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3933 | 0.0700 | 0.4790 |
| 0.4266 | 0.0830 | 0.5330 |
| 0.4533 | 0.1000 | 0.5600 |
| 0.4933 | 0.1220 | 0.6020 |
| 0.5000 | 0.1260 | 0.6000 |
| 0.5200 | 0.1390 | 0.6250 |
| 0.5226 | 0.1410 | 0.6270 |
| 0.5480 | 0.1620 | 0.6520 |
| 0.5720 | 0.1800 | 0.6730 |
| 0.6013 | 0.2070 | 0.6880 |
| 0.6120 | 0.2130 | 0.7110 |
| 0.6400 | 0.2450 | 0.7300 |
| 0.6813 | 0.2900 | 0.7570 |
| 0.7133 | 0.3300 | 0.7710 |
| 0.7399 | 0.3800 | 0.7920 |
| 0.7773 | 0.4400 | 0.8030 |
| 0.8173 | 0.5220 | 0.8200 |
| 0.8453 | 0.6250 | 0.8450 |
| 0.8839 | 0.7380 | 0.8770 |
| 0.8933 | 0.7880 | 0.8920 |
| 0.8999 | 0.8320 | 0.9100 |

Sundberg, Aarne T. - Uusi-Kyyny, Petri - Pakkanen, Minna - Alopaeus, Ville, Vapor−Liquid Equilibrium for Methoxymethane + Methyl Formate, Methoxymethane + Hexane, and Methyl Formate + Methanol, Journal of Chemical & Engineering Data 5 (2011) 2634-2640. doi:10.1021/je200140m

**T / K = 358.94**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 2.359 | 0.0108 | 0.0667 | |
| 2.579 | 0.0300 | 0.1608 | |
| 2.777 | 0.0488 | 0.2325 | |
| 5.519 | 0.9370 | 0.9370 | AZEO |

Sundberg, Aarne T. - Uusi-Kyyny, Petri - Pakkanen, Minna - Alopaeus, Ville, Vapor−Liquid Equilibrium for Methoxymethane + Methyl Formate, Methoxymethane + Hexane, and Methyl Formate + Methanol, Journal of Chemical & Engineering Data 5 (2011) 2634-2640. doi:10.1021/je200140m

**T / K = 358.94**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 3.565 | 0.1459 | 0.4437 | |
| 3.869 | 0.1962 | 0.5055 | |
| 5.519 | 0.9370 | 0.9370 | AZEO |

Sundberg, Aarne T. - Uusi-Kyyny, Petri - Pakkanen, Minna - Alopaeus, Ville, Vapor−Liquid Equilibrium for Methoxymethane + Methyl Formate, Methoxymethane + Hexane, and Methyl Formate + Methanol, Journal of Chemical & Engineering Data 5 (2011) 2634-2640. doi:10.1021/je200140m

**T / K = 358.94**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 5.147 | 0.5983 | 0.7429 | |
| 5.234 | 0.6483 | 0.7645 | |
| 5.311 | 0.6982 | 0.7870 | |
| 5.379 | 0.7484 | 0.8115 | |
| 5.438 | 0.7976 | 0.8382 | |
| 5.483 | 0.8486 | 0.8698 | |
| 5.512 | 0.8988 | 0.9059 | |
| 5.519 | 0.9370 | 0.9370 | AZEO |

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**Isobaric phase equilibrium data**

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Zeng, J. - Fu, C. - Hu, W.L., Study on the VLE for methyl formate-methanol system, Tianranqi Huagong 5 (2000) 54-56.

**P / bar =** **1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 334.63 | 0.0192 | 0.1325 |
| 330.27 | 0.0472 | 0.2823 |
| 323.00 | 0.1120 | 0.4962 |
| 316.61 | 0.2090 | 0.6450 |
| 313.05 | 0.3009 | 0.7168 |
| 310.83 | 0.3891 | 0.7599 |
| 309.72 | 0.4472 | 0.7816 |
| 308.21 | 0.5502 | 0.8132 |
| 307.21 | 0.6384 | 0.8376 |
| 306.55 | 0.7077 | 0.8565 |
| 305.98 | 0.7720 | 0.8764 |
| 305.44 | 0.8404 | 0.9008 |
| 305.05 | 0.9026 | 0.9296 |
| 304.80 | 0.9589 | 0.9653 |

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**Enthalpy of mixing**

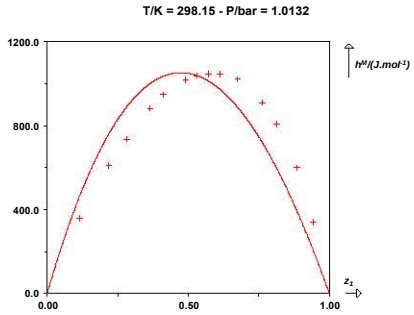
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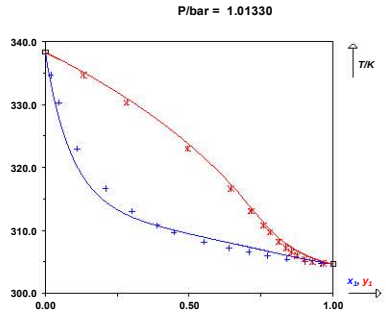
Kasprzycka-Guttman, T. - Wilczura, H., Thermodynamic properties of solutions: enthalpy of mixing of 2,4-lutidine + n-alkanes, Thermochimica Acta (1992) 25-30. doi:10.1016/0040-6031(92)80181-U

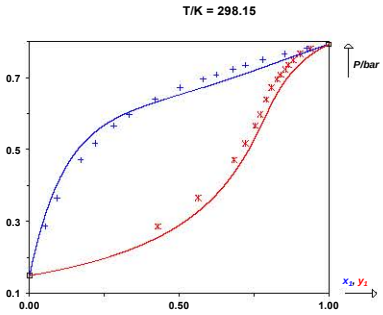
**T / K =** **298.15**

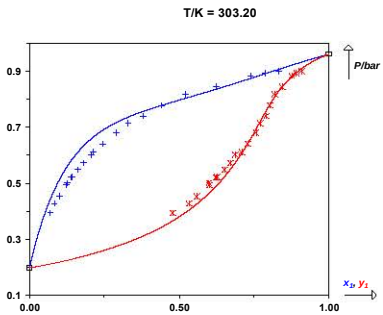
**P / bar =** **UNKNOWN (1.0132)**

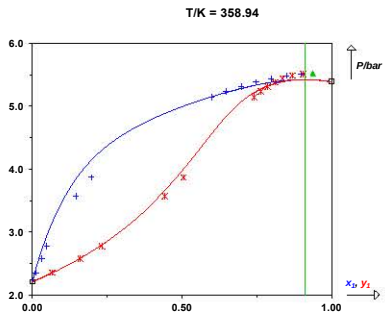
| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 358.00 | 0.1135 |
| 608.00 | 0.2174 |
| 736.00 | 0.2815 |
| 882.00 | 0.3651 |
| 948.00 | 0.4122 |
| 1019.0 | 0.4914 |
| 1038.0 | 0.5311 |
| 1045.0 | 0.5724 |
| 1046.0 | 0.6134 |
| 1021.0 | 0.6749 |
| 909.00 | 0.7613 |
| 807.00 | 0.8135 |
| 600.00 | 0.8848 |
| 340.00 | 0.9432 |


T/K = 298.15 - P/bar = 1.0132
1200.0
800.0
400.0
0.0
0.00
0.50
1.00
$h^{M}$/(J.mol$^{-1}$)
$z_1$


P/bar = 1.01330
340.0
330.0
320.0
310.0
300.0
0.00
0.50
1.00
T/K
$x_1$, $y_1$


T/K = 298.15
0.7
0.5
0.3
0.1
0.00
0.50
1.00
P/bar
$x_1$, $y_1$


T/K = 303.20
0.9
0.7
0.5
0.3
0.1
0.00
0.50
1.00
P/bar
$x_1$, $y_1$


T/K = 358.94
6.0
5.0
4.0
3.0
2.0
0.00
0.50
1.00
P/bar
$x_1$, $y_1$

## ETHYL FORMATE (1) + WATER (2)

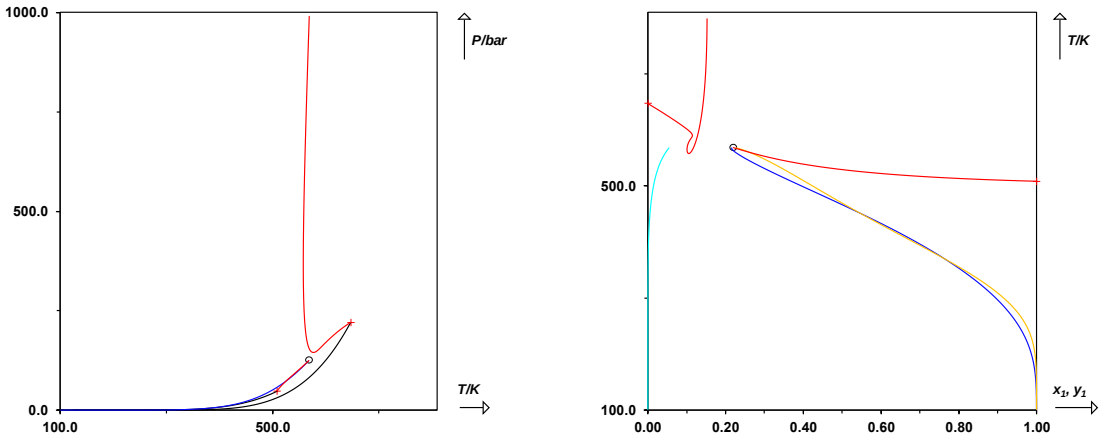
| | | |
|---|---|---|
| **CAS** | 109-94-4 | 7732-18-5 |
| **InChiKey** | WBJINCZRORDGAQ-UHFFFAOYSA-N | XLYOFNOQVPJJNP-UHFFFAOYSA-N |
| **$T_c$ / K** | 508.40 | 647.10 |
| **$P_c$ / bar** | 47.40 | 220.64 |
| **ω** | 0.285 | 0.345 |

Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 2010
B/MPa = 2290

*Deviations*
MAPE on x = 51 %
MAPE on y = 12 %
MAPE on $h^M$ = 17 %



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**Isothermal phase equilibrium data**

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Linek, Jan - Wichterle, Ivan - Marsh, Kenneth N., Vapor−Liquid Equilibria for Water + Diacetone Alcohol, Ethyl Methanoate + Water, and Ethyl Methanoate + Phenol, Journal of Chemical & Engineering Data 6 (1996) 1219-1222. doi:10.1021/je960183y

**T / K = 300.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0789 | 0.0034 | 0.4824 |
| 0.1547 | 0.0075 | 0.7114 |
| 0.2064 | 0.0110 | 0.7947 |
| 0.2366 | 0.0143 | 0.8126 |
| 0.3183 | 0.0209 | 0.8909 |
| 0.3545 | 0.0230 | 0.9157 |
| 0.3659 | 0.0245 | 0.9273 |

Linek, Jan - Wichterle, Ivan - Marsh, Kenneth N., Vapor−Liquid Equilibria for Water + Diacetone Alcohol, Ethyl Methanoate + Water, and Ethyl Methanoate + Phenol, Journal of Chemical & Engineering Data 6 (1996) 1219-1222. doi:10.1021/je960183y

**T / K = 320.00**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2776 | 0.0048 | 0.6965 |
| 0.3700 | 0.0082 | 0.7897 |
| 0.4704 | 0.0113 | 0.8271 |
| 0.5816 | 0.0147 | 0.8538 |
| 0.6912 | 0.0200 | 0.8705 |
| 0.6953 | 0.0205 | 0.8759 |
| 0.8102 | 0.0260 | 0.8926 |

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**Enthalpy of mixing**

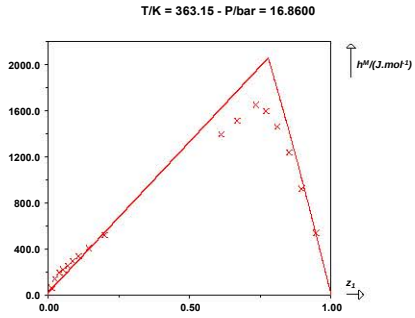
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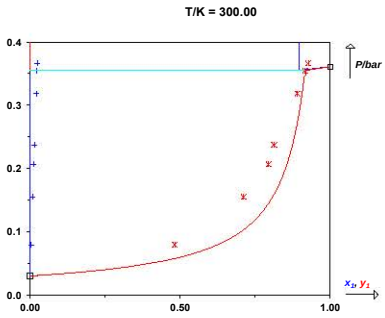
Krummen, M., Experimentelle Untersuchung des Aktivitätskoeffizienten bei unendlicher Verdünnung in ausgewählten Lösungsmitteln und Lösungsmittelgemischen als Grundlage für die Synthese thermischer Trennprozesse, Thesis (2002) 1-198.

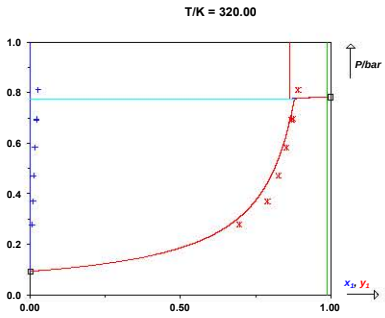
**T / K = 363.15**

**P / bar = 16.86**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 61.00 | 0.0117 |
| 137.00 | 0.0244 |
| 191.00 | 0.0382 |
| 221.00 | 0.0532 |
| 254.00 | 0.0697 |
| 291.00 | 0.0879 |
| 332.00 | 0.1080 |
| 404.00 | 0.1425 |
| 519.00 | 0.1990 |
| 1396.0 | 0.6115 |
| 1514.0 | 0.6692 |
| 1651.0 | 0.7349 |
| 1595.0 | 0.7713 |
| 1460.0 | 0.8103 |
| 1235.0 | 0.8523 |
| 924.00 | 0.8976 |
| 539.00 | 0.9467 |


T/K = 363.15 - P/bar = 16.8600
2000.0
1600.0
1200.0
800.0
400.0
0.0
0.00
0.50
1.00
$h^{M}$/(J.mol$^{-1}$)
$z_1$


T/K = 300.00
0.4
0.3
0.2
0.1
0.0
0.00
0.50
1.00
P/bar
$x_1$, $y_1$


T/K = 320.00
1.0
0.8
0.6
0.4
0.2
0.0
0.00
0.50
1.00
P/bar
$x_1$, $y_1$

## ETHANOL (1) + ETHYL FORMATE (2)

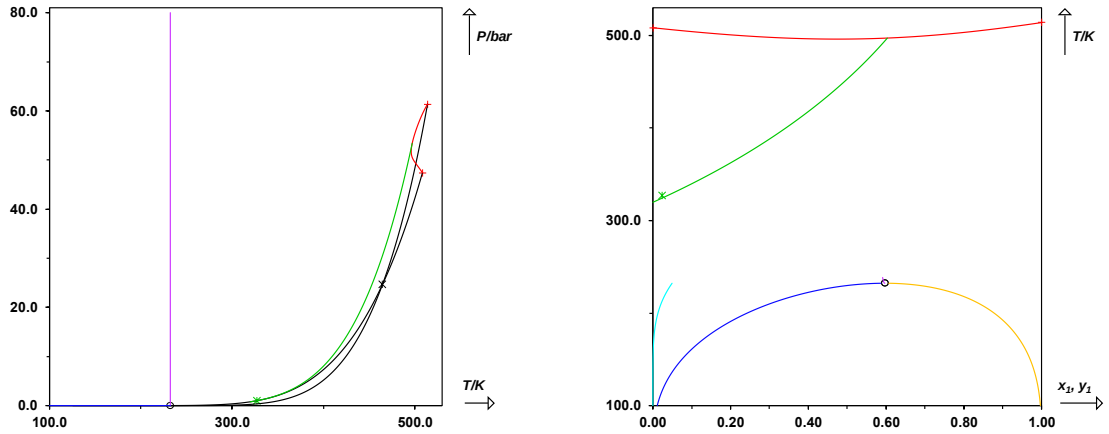
| | | |
|---|---|---|
| **CAS** | 64-17-5 | 109-94-4 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | WBJINCZRORDGAQ-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 508.40 |
| **$P_c$ / bar** | 61.37 | 47.40 |
| **ω** | 0.644 | 0.285 |

Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 308
B/MPa = 330

*Deviations*
MAPE on x = 11 %
MAPE on y = 6.2 %
MAPE on $x_{az}$ = 34 %
MAPE on $P_{az}$ = 0.51 %
MAPE on $h^M$ = 15 %
MAPE on $c_P^M$ = 85 %



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**Isothermal phase equilibrium data**

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Nagata, Isamu - Ohta, Tatsuhiko - Ogura, Michio - Yasuda, Shuhei, Excess Gibbs free energies and heats of mixing for binary systems: ethyl formate with methanol, ethanol, 1-propanol, and 2-propanol, Journal of Chemical & Engineering Data 3 (1976) 310-313. doi:10.1021/je60070a020

**T / K =** **318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3292 | 0.9490 | 0.6870 |
| 0.4609 | 0.8450 | 0.4460 |
| 0.5064 | 0.7990 | 0.3880 |
| 0.5426 | 0.7520 | 0.3530 |
| 0.6038 | 0.6310 | 0.2850 |
| 0.6245 | 0.5900 | 0.2670 |
| 0.6309 | 0.5710 | 0.2600 |
| 0.6793 | 0.4180 | 0.2130 |
| 0.6879 | 0.3650 | 0.1950 |
| 0.7155 | 0.2270 | 0.1510 |
| 0.7297 | 0.1090 | 0.0950 |
| 0.7330 | 0.0500 | 0.0460 |

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**Isobaric phase equilibrium data**

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Soto, Ana - Hernández, Pablo - Ortega, Juan, Experimental VLE at 101.32 kPa in binary systems composed of ethyl methanoate and alkan-1-ols or alkan-2-ols and treatment of data using a correlation with temperature-dependent parameters, Fluid Phase Equilibria 1-2 (1998) 351-370. doi:10.1016/S0378-3812(98)00193-9

**P / bar =** **1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 350.48 | 0.9890 | 0.9540 |
| 348.98 | 0.9750 | 0.8880 |
| 347.66 | 0.9620 | 0.8310 |
| 345.88 | 0.9420 | 0.7620 |
| 344.03 | 0.9200 | 0.6900 |
| 341.69 | 0.8860 | 0.6080 |
| 340.01 | 0.8590 | 0.5520 |
| 338.14 | 0.8200 | 0.4920 |
| 336.53 | 0.7790 | 0.4430 |
| 335.43 | 0.7460 | 0.4120 |
| 334.39 | 0.7100 | 0.3830 |
| 333.62 | 0.6810 | 0.3610 |
| 333.03 | 0.6550 | 0.3440 |
| 332.40 | 0.6240 | 0.3260 |
| 331.83 | 0.5910 | 0.3080 |
| 331.32 | 0.5580 | 0.2930 |
| 330.89 | 0.5290 | 0.2800 |
| 330.53 | 0.5050 | 0.2690 |
| 330.25 | 0.4820 | 0.2590 |
| 329.96 | 0.4590 | 0.2490 |
| 329.63 | 0.4290 | 0.2380 |
| 329.36 | 0.4060 | 0.2300 |
| 329.08 | 0.3790 | 0.2180 |
| 328.81 | 0.3490 | 0.2090 |
| 328.56 | 0.3230 | 0.1980 |
| 328.27 | 0.2860 | 0.1820 |
| 328.11 | 0.2600 | 0.1710 |
| 327.84 | 0.2250 | 0.1550 |
| 327.71 | 0.2060 | 0.1460 |
| 327.58 | 0.1760 | 0.1310 |
| 327.48 | 0.1610 | 0.1230 |
| 327.34 | 0.1250 | 0.1040 |
| 327.27 | 0.1020 | 0.0880 |
| 327.24 | 0.0830 | 0.0740 |
| 327.19 | 0.0650 | 0.0610 |
| 327.23 | 0.0190 | 0.0220 |

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**Enthalpy of mixing**

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Kasprzycka-Guttman, T. - Wilczura, H., Thermodynamic properties of solutions: enthalpy of mixing of 2,4-lutidine + n-alkanes, Thermochimica Acta (1992) 25-30. doi:10.1016/0040-6031(92)80181-U

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 340.00 | 0.9298 |
| 604.00 | 0.8652 |
| 861.00 | 0.7886 |
| 976.00 | 0.7449 |
| 1162.0 | 0.6551 |
| 1245.0 | 0.5948 |
| 1280.0 | 0.5698 |
| 1330.0 | 0.5201 |
| 1350.0 | 0.4697 |
| 1356.0 | 0.4402 |
| 1353.0 | 0.4149 |
| 1342.0 | 0.3815 |
| 1328.0 | 0.3543 |
| 1290.0 | 0.3162 |
| 1223.0 | 0.2749 |
| 1127.0 | 0.2276 |
| 973.00 | 0.1719 |

| | |
|---|---|
| 708.00 | 0.1079 |
| 434.00 | 0.0588 |

Hu, Jianhua - Tamura, Katsutoshi - Murakami, Sachio, Excess thermodynamic properties of binary mixtures of ethyl formate with benzene, ethanol, and 2,2,2-trifluoroethan-1-ol at 298.15 K, Fluid Phase Equilibria 1-2 (1997) 197-212. doi:10.1016/S0378-3812(96)03230-X

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 104.60 | 0.9750 |
| 230.90 | 0.9500 |
| 458.40 | 0.9000 |
| 648.00 | 0.8500 |
| 815.00 | 0.8000 |
| 959.00 | 0.7500 |
| 1080.0 | 0.7000 |
| 1181.0 | 0.6500 |
| 1262.0 | 0.6000 |
| 1323.0 | 0.5500 |
| 1363.0 | 0.5000 |
| 1383.0 | 0.4500 |
| 1378.0 | 0.4000 |
| 1349.0 | 0.3500 |
| 1292.0 | 0.3000 |
| 1205.0 | 0.2500 |
| 1079.0 | 0.2000 |
| 908.00 | 0.1500 |
| 683.00 | 0.1000 |
| 381.60 | 0.0500 |
| 205.70 | 0.0250 |

Nagata, Isamu - Ohta, Tatsuhiko - Ogura, Michio - Yasuda, Shuhei, Excess Gibbs free energies and heats of mixing for binary systems: ethyl formate with methanol, ethanol, 1-propanol, and 2-propanol, Journal of Chemical & Engineering Data 3 (1976) 310-313. doi:10.1021/je60070a020

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 235.72 | 0.9487 |
| 298.10 | 0.9322 |
| 696.68 | 0.8186 |
| 969.66 | 0.7093 |
| 1117.0 | 0.6073 |
| 1188.2 | 0.5110 |
| 1205.4 | 0.5024 |
| 1206.2 | 0.4053 |
| 1091.1 | 0.3105 |
| 1077.3 | 0.2911 |
| 928.63 | 0.2172 |
| 786.28 | 0.1639 |
| 603.32 | 0.1154 |
| 301.03 | 0.0500 |

Nagata, Isamu - Ohta, Tatsuhiko - Ogura, Michio - Yasuda, Shuhei, Excess Gibbs free energies and heats of mixing for binary systems: ethyl formate with methanol, ethanol, 1-propanol, and 2-propanol, Journal of Chemical & Engineering Data 3 (1976) 310-313. doi:10.1021/je60070a020

**T / K = 318.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 249.11 | 0.9473 |
| 784.61 | 0.8027 |
| 1020.3 | 0.7006 |
| 1169.4 | 0.6062 |
| 1223.4 | 0.4568 |
| 1213.3 | 0.4112 |
| 1138.4 | 0.3328 |
| 1140.1 | 0.3086 |
| 895.14 | 0.2005 |
| 812.24 | 0.1701 |
| 565.64 | 0.1056 |

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**Heat capacity of mixing**

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Hu, Jianhua - Tamura, Katsutoshi - Murakami, Sachio, Excess thermodynamic properties of binary mixtures of ethyl formate with benzene, ethanol, and 2,2,2-trifluoroethan-1-ol at 298.15 K, Fluid Phase Equilibria 1-2 (1997) 197-212. doi:10.1016/S0378-3812(96)03230-X

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.8100 | 0.9750 |
| 1.590 | 0.9500 |
| 3.170 | 0.9000 |
| 4.650 | 0.8500 |
| 5.680 | 0.8000 |
| 6.720 | 0.7500 |
| 7.530 | 0.7000 |
| 8.240 | 0.6500 |
| 8.720 | 0.6000 |

| | |
|---|---|
| 9.080 | 0.5500 |
| 9.180 | 0.5000 |
| 9.130 | 0.4500 |
| 8.810 | 0.4000 |
| 8.330 | 0.3500 |
| 7.590 | 0.3000 |
| 6.640 | 0.2500 |
| 5.390 | 0.2000 |
| 3.930 | 0.1500 |
| 2.300 | 0.1000 |
| 0.8300 | 0.0500 |
| 0.3000 | 0.0250 |

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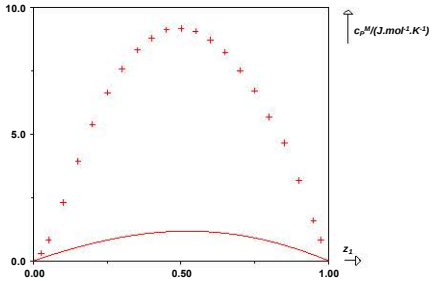
**Azeotropic point**

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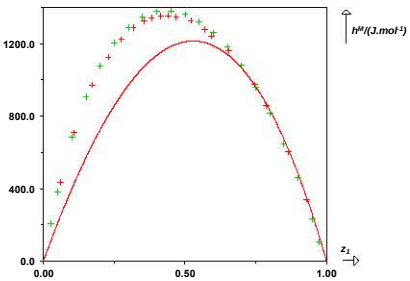
Soto, Ana - Hernández, Pablo - Ortega, Juan, Experimental VLE at 101.32 kPa in binary systems composed of ethyl methanoate and alkan-1-ols or alkan-2-ols and treatment of data using a correlation with temperature-dependent parameters, Fluid Phase Equilibria 1-2 (1998) 351-370. doi:10.1016/S0378-3812(98)00193-9

| T / K | P / bar | $x_1$ |
|---|---|---|
| 327.23 | 1.013 | 0.0235 |

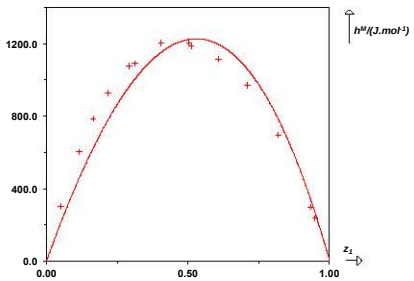
T/K = 298.15 - P/bar = 1.0132



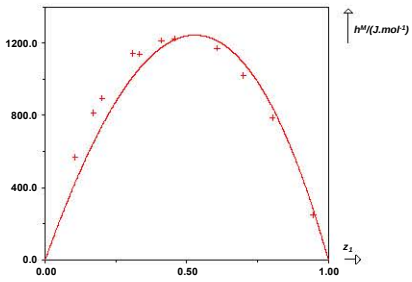

T/K = 298.15 - P/bar = 1.0132 1.0132



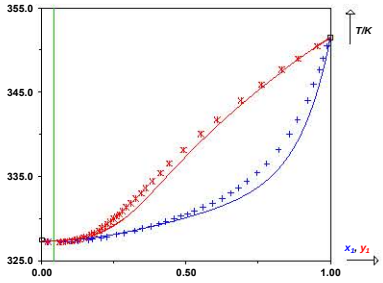

T/K = 308.15 - P/bar = 1.0132



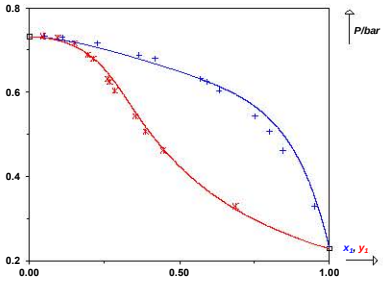

T/K = 318.15 - P/bar = 1.0132



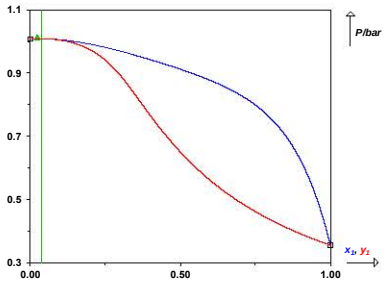

P/bar = 1.01320




T/K = 318.15




T/K = 327.23



## NITROMETHANE (1) + 1-BUTANOL (2)

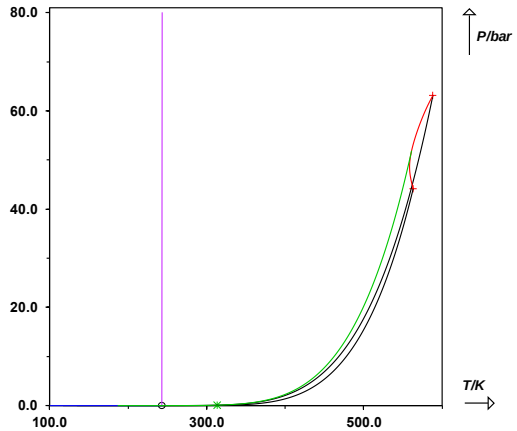
| | | |
|---|---|---|
| **CAS** | 75-52-5 | 71-36-3 |
| **InChiKey** | LYGJENNIWJXYER-UHFFFAOYSA-N | LRHPLDYGYMQRHN-UHFFFAOYSA-N |
| **$T_c$ / K** | 588.15 | 563.10 |
| **$P_c$ / bar** | 63.10 | 44.14 |
| **ω** | 0.348 | 0.588 |

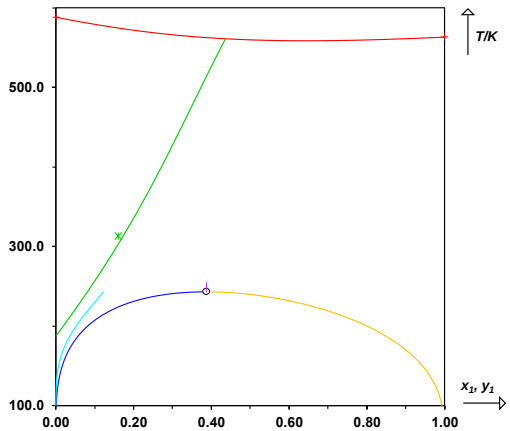
Non ideal with enthalpic causes

**PPR78 results**

*Parameters*
A/MPa = 280
B/MPa = 326

*Deviations*
MAPE on x = 60 %
MAPE on y = 38 %
MAPE on $x_{az}$ = 4.9 %
MAPE on $P_{az}$ = 16 %
MAPE on $h^M$ = 50 %
MAPE on $c_P^M$ = 98 %



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**Isothermal phase equilibrium data**

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Sazonov, V.P. - Filippov, V.V., Study of the thermodynamic properties of the nitromethane-butyl alcohol system, Vestn. Leningr. Univ. Ser. 4 Fiz. Khim. 10 (1977) 151-153.

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0080 | 0.0060 | 0.2390 |
| 0.0097 | 0.0120 | 0.3780 |
| 0.0131 | 0.0240 | 0.5420 |
| 0.0209 | 0.0600 | 0.7220 |
| 0.0288 | 0.1170 | 0.8080 |
| 0.0364 | 0.2330 | 0.8570 |
| 0.0379 | 0.3430 | 0.8670 |
| 0.0392 | 0.4470 | 0.8700 |
| 0.0395 | 0.5480 | 0.8730 |
| 0.0396 | 0.6360 | 0.8750 |
| 0.0397 | 0.7390 | 0.8760 |
| 0.0399 | 0.8260 | 0.8780 |
| 0.0400 | 0.9160 | 0.8970 |
| 0.0393 | 0.9580 | 0.9200 |
| 0.0373 | 0.9950 | 0.9830 |

Sazonov, V.P. - Filippov, V.V., Study of the thermodynamic properties of the nitromethane-butyl alcohol system, Vestn. Leningr. Univ. Ser. 4 Fiz. Khim. 10 (1977) 151-153.

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.0292 | 0.0060 | 0.1500 | |
| 0.0329 | 0.0120 | 0.2500 | |
| 0.0393 | 0.0240 | 0.3790 | |
| 0.0552 | 0.0600 | 0.5720 | |
| 0.0743 | 0.1170 | 0.6960 | |
| 0.0943 | 0.2330 | 0.7770 | |
| 0.1015 | 0.3430 | 0.8020 | |
| 0.1059 | 0.4470 | 0.8090 | |
| 0.1067 | 0.5480 | 0.8160 | |
| 0.1073 | 0.6360 | 0.8180 | |
| 0.1077 | 0.7390 | 0.8220 | |
| 0.1079 | 0.8260 | 0.8340 | |
| 0.1079 | 0.8400 | 0.8400 | AZEO |
| 0.1072 | 0.9160 | 0.8750 | |
| 0.1056 | 0.9580 | 0.9150 | |
| 0.1020 | 0.9950 | 0.9800 | |

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**Enthalpy of mixing**

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Feng, Hui - Wang, Yanru - Shi, Jun - Benson, George C. - Lu, Benjamin C.-Y., Excess enthalpies of (methyl formate or nitroethane + an n-alkane) and of (nitromethane + butan-1-ol or hexan-1-ol or ethan-1,2-diol), The Journal of Chemical Thermodynamics 2 (1991) 169-174. doi:10.1016/S0021-9614(05)80294-0

**T / K = 294.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 454.00 | 0.0499 |
| 996.00 | 0.1275 |
| 1395.0 | 0.2073 |
| 1620.0 | 0.2580 |
| 1738.0 | 0.3143 |
| 1885.0 | 0.4112 |
| 1938.0 | 0.4954 |
| 1930.0 | 0.5684 |
| 1902.0 | 0.6417 |
| 1842.0 | 0.7078 |
| 1735.0 | 0.7625 |
| 1404.0 | 0.8496 |
| 1161.0 | 0.8942 |
| 928.00 | 0.9245 |

Trampe, D. Mark - Eckert, Charles A., Calorimetric measurement of partial molar excess enthalpies at infinite dilution, Journal of Chemical & Engineering Data 1 (1991) 112-118. doi:10.1021/je00001a033

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 37.09 | 0.9977 |
| 33.00 | 0.9979 |
| 30.78 | 0.9981 |
| 26.97 | 0.9983 |
| 23.35 | 0.9985 |
| 19.46 | 0.9988 |
| 15.75 | 0.9990 |
| 11.67 | 0.9993 |
| 7.780 | 0.9995 |
| 3.930 | 0.9998 |

Rebelo, Luís P. N. - Najdanovic-Visak, Vesna - Visak, Zoran P. - Nunes da Ponte, M. - Troncoso, Jacobo - Cerdeiriña, Claudio A. - Romaní, Luis, Two ways of looking at Prigogine and Defay's equation, Physical Chemistry Chemical Physics 11 (2002) 2251-2259. doi:10.1039/b200292b

**T / K = 298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 833.00 | 0.1021 |
| 1598.0 | 0.2115 |
| 2163.0 | 0.3575 |
| 2332.0 | 0.4458 |
| 2382.0 | 0.5102 |
| 2378.0 | 0.5642 |
| 2365.0 | 0.6176 |
| 2313.0 | 0.6573 |
| 2146.0 | 0.7262 |
| 1922.0 | 0.7789 |
| 967.00 | 0.9105 |

Sharma, V.K. - Singh, J., Thermodynamics of molecular interactions in binary mixtures containing nitromethane: Molar excess volumes and molar excess enthalpies, Indian J. Chem. Sect. A 1 (1999) 65-69.

**T / K =** **308.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| 534.00 | 0.0681 |
| 1047.0 | 0.1432 |
| 1415.0 | 0.2054 |
| 1737.0 | 0.2682 |
| 2056.0 | 0.3432 |
| 2294.0 | 0.4161 |
| 2466.0 | 0.4973 |
| 2512.0 | 0.5402 |
| 2507.0 | 0.6181 |
| 2416.0 | 0.6767 |
| 2259.0 | 0.7302 |
| 1844.0 | 0.8141 |
| 1261.0 | 0.8902 |
| 568.00 | 0.9562 |

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**Heat capacity of mixing**

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Cerdeiriña, C.A. - Tovar, C.A. - González, D. - Carballo, E. - Romani, L., Thermodynamics of the nitromethane + 1-butanol system near the upper critical point, Fluid Phase Equilibria 1-2 (2001) 101-115. doi:10.1016/S0378-3812(00)00485-4

**T / K =** **288.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 3.372 | 0.0543 |
| 5.754 | 0.1027 |
| 10.51 | 0.2050 |
| 16.12 | 0.3067 |
| 18.42 | 0.3367 |
| 11.30 | 0.8281 |
| 4.683 | 0.8983 |
| 1.836 | 0.9384 |
| 0.4777 | 0.9688 |
| -1.182 | 0.9878 |

Cerdeiriña, C.A. - Tovar, C.A. - González, D. - Carballo, E. - Romani, L., Thermodynamics of the nitromethane + 1-butanol system near the upper critical point, Fluid Phase Equilibria 1-2 (2001) 101-115. doi:10.1016/S0378-3812(00)00485-4

**T / K =** **293.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 3.407 | 0.0543 |
| 5.747 | 0.1027 |
| 10.26 | 0.2050 |
| 15.03 | 0.3067 |
| 16.48 | 0.3367 |
| 20.52 | 0.4063 |
| 26.02 | 0.5054 |
| 27.17 | 0.5372 |
| 27.74 | 0.5705 |
| 27.54 | 0.5910 |
| 25.52 | 0.6501 |
| 22.25 | 0.6926 |
| 17.24 | 0.7432 |
| 9.605 | 0.8281 |
| 3.983 | 0.8983 |
| 1.571 | 0.9384 |
| 0.3589 | 0.9688 |
| -1.007 | 0.9878 |

Cerdeiriña, C.A. - Tovar, C.A. - González, D. - Carballo, E. - Romani, L., Thermodynamics of the nitromethane + 1-butanol system near the upper critical point, Fluid Phase Equilibria 1-2 (2001) 101-115. doi:10.1016/S0378-3812(00)00485-4

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 3.355 | 0.0543 |
| 5.654 | 0.1027 |
| 9.987 | 0.2050 |
| 14.07 | 0.3067 |
| 15.23 | 0.3367 |

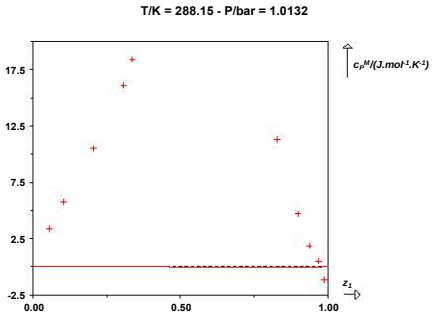
| | |
|---|---|
| 17.91 | 0.4063 |
| 20.79 | 0.5054 |
| 21.04 | 0.5372 |
| 21.13 | 0.5705 |
| 20.95 | 0.5910 |
| 19.34 | 0.6501 |
| 17.40 | 0.6926 |
| 14.20 | 0.7432 |
| 8.314 | 0.8281 |
| 3.279 | 0.8983 |
| 1.260 | 0.9384 |
| 0.2525 | 0.9688 |
| -0.1247 | 0.9878 |

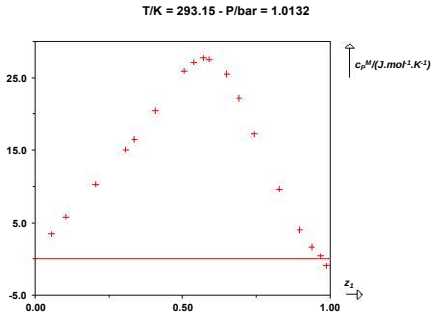
Cerdeiriña, C.A. - Tovar, C.A. - González, D. - Carballo, E. - Romani, L., Thermodynamics of the nitromethane + 1-butanol system near the upper critical point, Fluid Phase Equilibria 1-2 (2001) 101-115. doi:10.1016/S0378-3812(00)00485-4

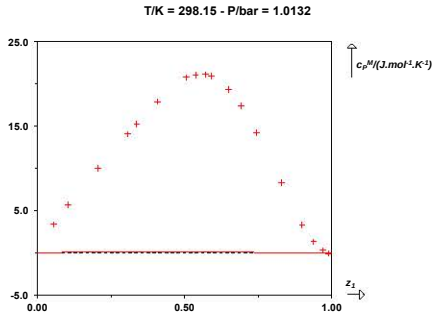
**T / K =** **308.15**

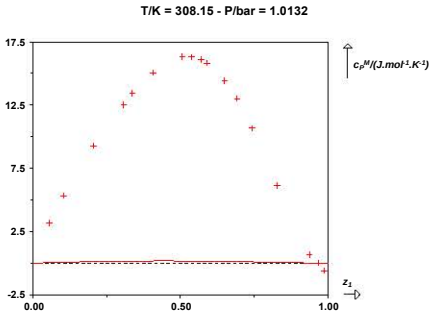
**P / bar =** **UNKNOWN (1.0132)**

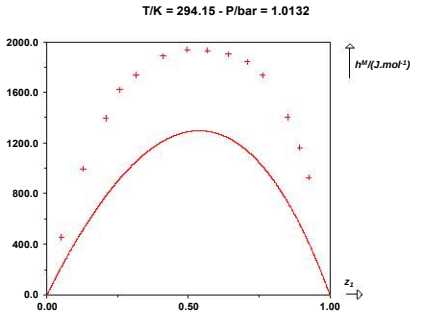
| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 3.182 | 0.0543 |
| 5.349 | 0.1027 |
| 9.293 | 0.2050 |
| 12.50 | 0.3067 |
| 13.41 | 0.3367 |
| 15.03 | 0.4063 |
| 16.33 | 0.5054 |
| 16.30 | 0.5372 |
| 16.08 | 0.5705 |
| 15.81 | 0.5910 |
| 14.42 | 0.6501 |
| 13.01 | 0.6926 |
| 10.66 | 0.7432 |
| 6.134 | 0.8281 |
| 0.6459 | 0.9384 |
| 0.0078 | 0.9688 |
| -0.5749 | 0.9878 |

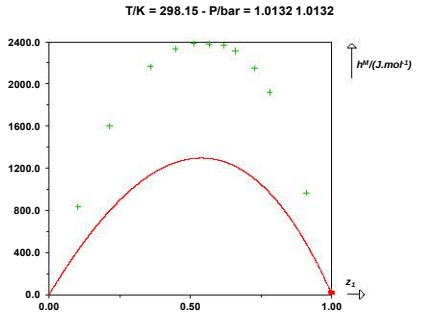

T/K = 288.15 - P/bar = 1.0132
$c_p^M/(J.mol^{-1}.K^{-1})$
$z_1$

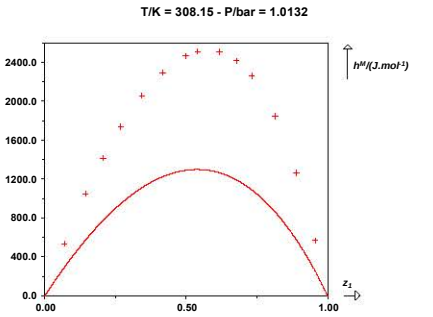

T/K = 293.15 - P/bar = 1.0132
$c_p^M/(J.mol^{-1}.K^{-1})$
$z_1$

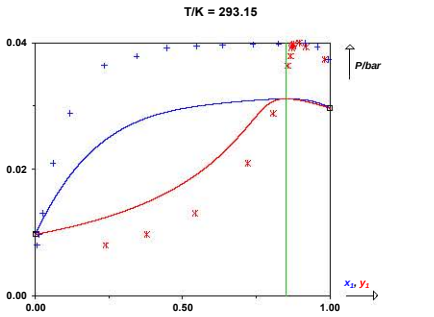

T/K = 298.15 - P/bar = 1.0132
$c_p^M/(J.mol^{-1}.K^{-1})$
$z_1$

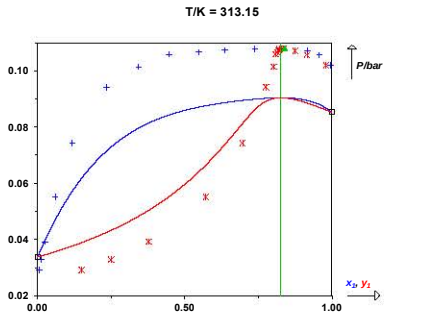

T/K = 308.15 - P/bar = 1.0132
$c_p^M/(J.mol^{-1}.K^{-1})$
$z_1$


T/K = 294.15 - P/bar = 1.0132
$h^M/(J.mol^{-1})$
$z_1$


T/K = 298.15 - P/bar = 1.0132 1.0132
$h^M/(J.mol^{-1})$
$z_1$


T/K = 308.15 - P/bar = 1.0132
$h^M/(J.mol^{-1})$
$z_1$


T/K = 293.15
P/bar
$x_1, y_1$


T/K = 313.15
P/bar
$x_1, y_1$

## ETHANOL (1) + WATER (2)

| | | |
|---|---|---|
| **CAS** | 64-17-5 | 7732-18-5 |
| **InChiKey** | LFQSCWFLJHTTHZ-UHFFFAOYSA-N | XLYOFNOQVPJJNP-UHFFFAOYSA-N |
| **$T_c$ / K** | 514.00 | 647.10 |
| **$P_c$ / bar** | 61.37 | 220.64 |
| **ω** | 0.644 | 0.345 |

Non ideal with enthalpic and entropic causes

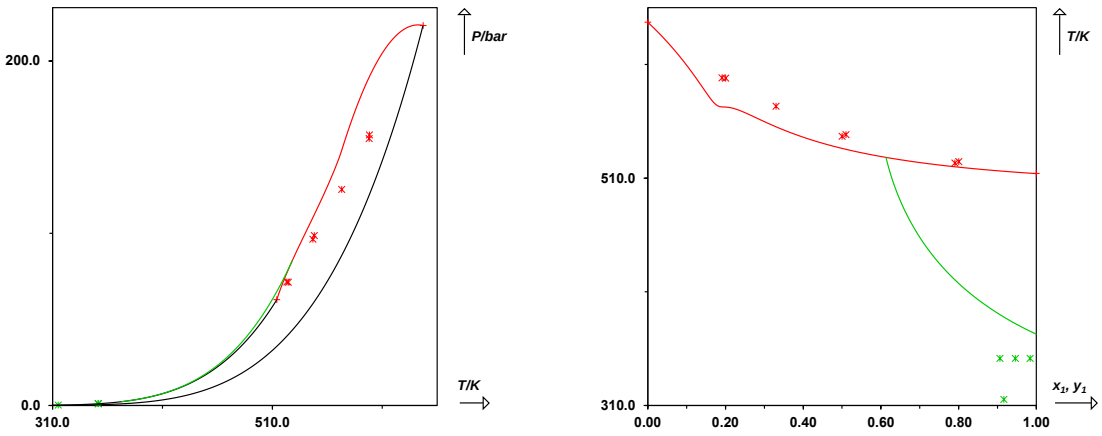
**PPR78 results**

*Parameters*

A/MPa = 830.01
B/MPa = -181.04

*Deviations*

MAPE on x = 34 %
MAPE on y = 17 %
MAPE on $x_c$ = 39 %
MAPE on $P_c$ = 11 %
MAPE on $h^M$ = 72 %
MAPE on $c_P^M$ = 92 %



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**Isothermal phase equilibrium data**

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Hall, D.J. - Mash, C.J. - Pemberton, R.C., Vapor liquid equilibriums for the systems water-methanol, water-ethanol, methanol-ethanol, and water-methanol-ethanol at 298.15 K determined by a rapid transpiration method (1979) 1-13.

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0444 | 0.0550 | 0.3230 |
| 0.0561 | 0.1246 | 0.4970 |
| 0.0640 | 0.2142 | 0.5790 |
| 0.0699 | 0.3941 | 0.6480 |
| 0.0736 | 0.5496 | 0.7005 |
| 0.0757 | 0.7006 | 0.7685 |
| 0.0770 | 0.7842 | 0.8185 |
| 0.0783 | 0.8396 | 0.8585 |
| 0.0780 | 0.8790 | 0.8895 |
| 0.0788 | 0.9365 | 0.9390 |

Dobson, Hilyard John Eglinton, CCCXCVII.—The partial pressures of aqueous ethyl alcohol, J. Chem. Soc., Trans. 0 (1925) 2866-2873. doi:10.1039/CT9252702866

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0442 | 0.0523 | 0.3164 |
| 0.0513 | 0.0916 | 0.4334 |
| 0.0579 | 0.1343 | 0.5037 |
| 0.0609 | 0.1671 | 0.5449 |
| 0.0629 | 0.2022 | 0.5683 |
| 0.0671 | 0.2848 | 0.6105 |
| 0.0682 | 0.3368 | 0.6286 |
| 0.0719 | 0.4902 | 0.6790 |
| 0.0743 | 0.5820 | 0.7095 |
| 0.0774 | 0.7810 | 0.8161 |

Pemberton, R.C - Mash, C.J, Thermodynamic properties of aqueous non-electrolyte mixtures II. Vapour pressures and excess Gibbs energies for water + ethanol at 303.15 to 363.15 K determined by an accurate static method, The Journal of Chemical Thermodynamics 9 (1978) 867-888. doi:10.1016/0021-9614(78)90160-X

**T / K = 303.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0441 | 0.0043 | 0.0412 |
| 0.0480 | 0.0152 | 0.1280 |
| 0.0520 | 0.0273 | 0.2043 |
| 0.0578 | 0.0463 | 0.2975 |
| 0.0639 | 0.0678 | 0.3753 |
| 0.0733 | 0.1099 | 0.4743 |
| 0.0819 | 0.1711 | 0.5479 |
| 0.0872 | 0.2469 | 0.5907 |
| 0.0909 | 0.3239 | 0.6194 |
| 0.0930 | 0.3866 | 0.6406 |
| 0.0940 | 0.4176 | 0.6508 |
| 0.0966 | 0.5049 | 0.6797 |
| 0.0987 | 0.5809 | 0.7087 |
| 0.1000 | 0.6343 | 0.7329 |
| 0.1020 | 0.7246 | 0.7810 |
| 0.1034 | 0.8084 | 0.8337 |
| 0.1039 | 0.8579 | 0.8705 |
| 0.1043 | 0.8906 | 0.8979 |
| 0.1044 | 0.8993 | 0.9056 |
| 0.1045 | 0.9244 | 0.9284 |
| 0.1046 | 0.9537 | 0.9556 |
| 0.1047 | 0.9731 | 0.9739 |
| 0.1047 | 0.9815 | 0.9819 |

Vu, Dung T. - Lira, Carl T. - Asthana, Navinchandra S. - Kolah, Aspi K. - Miller, Dennis J., Vapor−Liquid Equilibria in the Systems Ethyl Lactate + Ethanol and Ethyl Lactate + Water, Journal of Chemical & Engineering Data 4 (2006) 1220-1225. doi:10.1021/je050537y

**T / K = 313.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0783 | 0.0050 | 0.0360 |
| 0.0808 | 0.0070 | 0.0690 |
| 0.0827 | 0.0100 | 0.0960 |
| 0.0855 | 0.0140 | 0.1330 |
| 0.0897 | 0.0200 | 0.1810 |
| 0.0932 | 0.0260 | 0.2210 |
| 0.0985 | 0.0350 | 0.2690 |
| 0.1064 | 0.0500 | 0.3320 |
| 0.1172 | 0.0750 | 0.4070 |
| 0.1217 | 0.0850 | 0.4210 |
| 0.1301 | 0.1080 | 0.4780 |
| 0.1312 | 0.1110 | 0.4740 |
| 0.1377 | 0.1360 | 0.5190 |
| 0.1425 | 0.1580 | 0.5410 |
| 0.1493 | 0.2010 | 0.5730 |
| 0.1551 | 0.2560 | 0.5980 |
| 0.1579 | 0.3190 | 0.6120 |
| 0.1637 | 0.4180 | 0.6550 |
| 0.1657 | 0.4480 | 0.6600 |
| 0.1696 | 0.5180 | 0.6970 |
| 0.1721 | 0.5830 | 0.7300 |

| | | |
|---|---|---|
| 0.1751 | 0.6820 | 0.7670 |
| 0.1771 | 0.7480 | 0.8050 |
| 0.1781 | 0.8280 | 0.8410 |
| 0.1795 | 0.8920 | 0.8930 |
| 0.1800 | 0.9430 | 0.9600 |

Kurihara, Kiyofumi - Minoura, Tsuyoshi - Takeda, Kouichi - Kojima, Kazuo, Isothermal Vapor-Liquid Equilibria for Methanol + Ethanol + Water, Methanol + Water, and Ethanol + Water, Journal of Chemical & Engineering Data 3 (1995) 679-684. doi:10.1021/je00019a033

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2033 | 0.0874 | 0.4341 |
| 0.2090 | 0.0967 | 0.4549 |
| 0.2280 | 0.1411 | 0.5120 |
| 0.2366 | 0.1756 | 0.5372 |
| 0.2434 | 0.2065 | 0.5562 |
| 0.2457 | 0.2253 | 0.5636 |
| 0.2503 | 0.2552 | 0.5761 |
| 0.2544 | 0.2856 | 0.5890 |
| 0.2582 | 0.3133 | 0.6008 |
| 0.2626 | 0.3535 | 0.6133 |
| 0.2648 | 0.3773 | 0.6226 |
| 0.2669 | 0.3999 | 0.6311 |
| 0.2690 | 0.4258 | 0.6397 |
| 0.2728 | 0.4691 | 0.6563 |
| 0.2754 | 0.4987 | 0.6660 |
| 0.2770 | 0.5218 | 0.6741 |
| 0.2788 | 0.5421 | 0.6840 |
| 0.2810 | 0.5692 | 0.6971 |
| 0.2822 | 0.5907 | 0.7050 |
| 0.2845 | 0.6242 | 0.7205 |
| 0.2871 | 0.6697 | 0.7434 |
| 0.2883 | 0.6868 | 0.7523 |
| 0.2920 | 0.7586 | 0.7940 |
| 0.2925 | 0.7811 | 0.8081 |
| 0.2941 | 0.8299 | 0.8429 |
| 0.2949 | 0.8454 | 0.8555 |
| 0.2948 | 0.8559 | 0.8639 |
| 0.2948 | 0.8638 | 0.8699 |
| 0.2950 | 0.8713 | 0.8769 |
| 0.2952 | 0.8801 | 0.8849 |
| 0.2954 | 0.8911 | 0.8948 |
| 0.2953 | 0.9031 | 0.9065 |
| 0.2956 | 0.9136 | 0.9151 |
| 0.2957 | 0.9263 | 0.9273 |
| 0.2955 | 0.9528 | 0.9512 |

Pemberton, R.C - Mash, C.J, Thermodynamic properties of aqueous non-electrolyte mixtures II. Vapour pressures and excess Gibbs energies for water + ethanol at 303.15 to 363.15 K determined by an accurate static method, The Journal of Chemical Thermodynamics 9 (1978) 867-888. doi:10.1016/0021-9614(78)90160-X

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1292 | 0.0043 | 0.0478 |
| 0.1425 | 0.0152 | 0.1450 |
| 0.1556 | 0.0272 | 0.2259 |
| 0.1738 | 0.0463 | 0.3182 |
| 0.1909 | 0.0678 | 0.3893 |
| 0.2152 | 0.1098 | 0.4738 |
| 0.2359 | 0.1710 | 0.5355 |
| 0.2496 | 0.2468 | 0.5753 |
| 0.2593 | 0.3238 | 0.6044 |
| 0.2657 | 0.3884 | 0.6270 |
| 0.2684 | 0.4175 | 0.6370 |
| 0.2756 | 0.5049 | 0.6681 |
| 0.2813 | 0.5808 | 0.6989 |
| 0.2849 | 0.6343 | 0.7239 |
| 0.2901 | 0.7245 | 0.7735 |
| 0.2918 | 0.7638 | 0.7981 |
| 0.2935 | 0.8084 | 0.8286 |
| 0.2947 | 0.8579 | 0.8664 |
| 0.2951 | 0.8906 | 0.8942 |
| 0.2953 | 0.8993 | 0.9019 |

Mertl, I., Liquid-vapour equilibrium. IL. Phase equilibria in the ternary system ethyl acetate-ethanol-water, Collection of Czechoslovak Chemical Communications 2 (1972) 366-374. doi:10.1135/cccc19720366

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.4833 | 0.0620 | 0.3740 |
| 0.5320 | 0.0950 | 0.4390 |
| 0.5653 | 0.1310 | 0.4820 |
| 0.6012 | 0.1940 | 0.5240 |
| 0.6240 | 0.2520 | 0.5520 |
| 0.6473 | 0.3340 | 0.5830 |
| 0.6634 | 0.4010 | 0.6110 |
| 0.7011 | 0.5930 | 0.6910 |
| 0.7123 | 0.6800 | 0.7390 |
| 0.7235 | 0.7930 | 0.8160 |
| 0.7241 | 0.8100 | 0.8260 |
| 0.7259 | 0.9430 | 0.9410 |
| 0.7259 | 0.9470 | 0.9450 |

Pemberton, R.C - Mash, C.J, Thermodynamic properties of aqueous non-electrolyte mixtures II. Vapour pressures and excess Gibbs energies for water + ethanol at 303.15 to 363.15 K determined by an accurate static method, The Journal of Chemical Thermodynamics 9 (1978) 867-888. doi:10.1016/0021-9614(78)90160-X

**T / K = 343.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3276 | 0.0043 | 0.0512 |
| 0.3636 | 0.0152 | 0.1532 |
| 0.3982 | 0.0271 | 0.2348 |
| 0.4444 | 0.0462 | 0.3245 |
| 0.4857 | 0.0676 | 0.3906 |
| 0.5406 | 0.1097 | 0.4662 |
| 0.5859 | 0.1709 | 0.5216 |
| 0.6180 | 0.2467 | 0.5604 |
| 0.6411 | 0.3237 | 0.5904 |
| 0.6570 | 0.3883 | 0.6139 |
| 0.6634 | 0.4173 | 0.6244 |
| 0.6814 | 0.5047 | 0.6578 |
| 0.6952 | 0.5807 | 0.6907 |
| 0.7040 | 0.6342 | 0.7170 |
| 0.7159 | 0.7244 | 0.7681 |
| 0.7197 | 0.7637 | 0.7934 |
| 0.7232 | 0.8084 | 0.8247 |
| 0.7255 | 0.8578 | 0.8635 |
| 0.7262 | 0.8906 | 0.8917 |
| 0.7261 | 0.8993 | 0.8995 |
| 0.7259 | 0.9244 | 0.9229 |
| 0.7251 | 0.9537 | 0.9515 |
| 0.7243 | 0.9731 | 0.9713 |
| 0.7239 | 0.9815 | 0.9801 |

Pemberton, R.C - Mash, C.J, Thermodynamic properties of aqueous non-electrolyte mixtures II. Vapour pressures and excess Gibbs energies for water + ethanol at 303.15 to 363.15 K determined by an accurate static method, The Journal of Chemical Thermodynamics 9 (1978) 867-888. doi:10.1016/0021-9614(78)90160-X

**T / K = 363.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.7373 | 0.0043 | 0.0520 |
| 0.8191 | 0.0151 | 0.1539 |
| 0.8962 | 0.0269 | 0.2337 |
| 0.9967 | 0.0459 | 0.3200 |
| 1.083 | 0.0673 | 0.3823 |
| 1.196 | 0.1094 | 0.4530 |
| 1.288 | 0.1706 | 0.5058 |
| 1.356 | 0.2464 | 0.5449 |
| 1.407 | 0.3236 | 0.5763 |
| 1.442 | 0.3880 | 0.6010 |
| 1.456 | 0.4170 | 0.6123 |
| 1.496 | 0.5044 | 0.6480 |
| 1.526 | 0.5804 | 0.6830 |
| 1.545 | 0.6340 | 0.7106 |
| 1.570 | 0.7243 | 0.7639 |
| 1.578 | 0.7636 | 0.7901 |
| 1.585 | 0.8083 | 0.8224 |
| 1.589 | 0.8578 | 0.8618 |
| 1.590 | 0.8907 | 0.8903 |
| 1.590 | 0.8993 | 0.8981 |
| 1.589 | 0.9244 | 0.9216 |
| 1.586 | 0.9537 | 0.9506 |
| 1.584 | 0.9731 | 0.9708 |
| 1.582 | 0.9815 | 0.9797 |

Oh, Seung-Kyo - Campbell, Scott W., Total Pressure Measurements for Copper(II) Chloride + Methanol + Ethanol at 303.15 K, Journal of Chemical & Engineering Data 2 (1995) 504-508. doi:10.1021/je00018a033

**T / K = 523.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 53.02 | 0.1010 | 0.2600 |
| 58.06 | 0.2050 | 0.3620 |
| 64.47 | 0.3700 | 0.4750 |
| 69.64 | 0.5900 | 0.6200 |
| 71.02 | 0.6790 | 0.6930 |
| 71.23 | 0.6850 | 0.6970 |

Barr-David, Frank - Dodge, B. F., Vapor-Liquid Equilibrium at High Pressures. The Systems Ethanol-Water and 2-Propanol-Water., Journal of Chemical & Engineering Data 2 (1959) 107-121. doi:10.1021/je60002a003

**T / K = 523.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 40.82 | 0.0090 | 0.0440 |
| 45.85 | 0.0340 | 0.1350 |
| 49.50 | 0.0630 | 0.2060 |
| 52.68 | 0.0980 | 0.2640 |
| 54.81 | 0.1350 | 0.3060 |
| 57.02 | 0.1720 | 0.3400 |
| 59.16 | 0.2230 | 0.3760 |
| 61.50 | 0.2850 | 0.4170 |
| 62.74 | 0.3390 | 0.4460 |
| 64.81 | 0.4020 | 0.4870 |
| 66.53 | 0.4630 | 0.5300 |
| 69.15 | 0.5650 | 0.6050 |

| | | | |
|---|---|---|---|
| 71.15 | 0.6730 | 0.6900 | |
| 71.71 | 0.7900 | 0.7900 | CRIT |

Barr-David, Frank - Dodge, B. F., Vapor-Liquid Equilibrium at High Pressures. The Systems Ethanol-Water and 2-Propanol-Water., Journal of Chemical & Engineering Data 2 (1959) 107-121. doi:10.1021/je60002a003

**T / K = 548.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 61.36 | 0.0070 | 0.0290 |
| 67.91 | 0.0330 | 0.1120 |
| 73.08 | 0.0650 | 0.1770 |
| 77.22 | 0.1050 | 0.2330 |
| 80.88 | 0.1490 | 0.2770 |
| 84.12 | 0.2010 | 0.3220 |
| 88.39 | 0.2730 | 0.3770 |
| 92.73 | 0.3480 | 0.4290 |
| 93.98 | 0.3740 | 0.4410 |
| 95.98 | 0.4140 | 0.4650 |
| 97.98 | 0.4550 | 0.4860 |
| 98.60 | 0.5100 | 0.5100 CRIT |

Barr-David, Frank - Dodge, B. F., Vapor-Liquid Equilibrium at High Pressures. The Systems Ethanol-Water and 2-Propanol-Water., Journal of Chemical & Engineering Data 2 (1959) 107-121. doi:10.1021/je60002a003

**T / K = 573.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 88.46 | 0.0060 | 0.0240 |
| 95.29 | 0.0300 | 0.0870 |
| 101.35 | 0.0570 | 0.1380 |
| 105.83 | 0.0910 | 0.1860 |
| 112.66 | 0.1280 | 0.2280 |
| 118.59 | 0.1780 | 0.2760 |
| 123.07 | 0.2460 | 0.3150 |
| 125.48 | 0.3300 | 0.3300 CRIT |

Barr-David, Frank - Dodge, B. F., Vapor-Liquid Equilibrium at High Pressures. The Systems Ethanol-Water and 2-Propanol-Water., Journal of Chemical & Engineering Data 2 (1959) 107-121. doi:10.1021/je60002a003

**T / K = 598.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 123.97 | 0.0070 | 0.0180 |
| 133.55 | 0.0350 | 0.0750 |
| 140.10 | 0.0630 | 0.1140 |
| 143.76 | 0.0840 | 0.1340 |
| 150.65 | 0.1210 | 0.1730 |
| 155.13 | 0.1610 | 0.1910 |
| 157.06 | 0.1900 | 0.1920 |
| 157.06 | 0.1910 | 0.1910 CRIT |

Barr-David, Frank - Dodge, B. F., Vapor-Liquid Equilibrium at High Pressures. The Systems Ethanol-Water and 2-Propanol-Water., Journal of Chemical & Engineering Data 2 (1959) 107-121. doi:10.1021/je60002a003

**T / K = 623.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 170.64 | 0.0080 | 0.0160 |
| 180.64 | 0.0330 | 0.0570 |
| 185.54 | 0.0520 | 0.0740 |

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**Isobaric phase equilibrium data**

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Voutsas, Epaminondas C. - Pamouktsis, Christos - Argyris, Dimitrios - Pappa, Georgia D., Measurements and thermodynamic modeling of the ethanol–water system with emphasis to the azeotropic region, Fluid Phase Equilibria 1-2 (2011) 135-141. doi:10.1016/j.fluid.2011.06.009

**P / bar = 0.1971**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 323.53 | 0.0760 | 0.4070 |
| 320.52 | 0.1410 | 0.5100 |
| 318.05 | 0.2600 | 0.5920 |
| 317.04 | 0.3900 | 0.6320 |
| 316.35 | 0.4990 | 0.6790 |
| 315.90 | 0.5990 | 0.7060 |
| 315.55 | 0.6880 | 0.7600 |
| 315.29 | 0.7990 | 0.8260 |
| 315.26 | 0.8050 | 0.8280 |
| 315.19 | 0.8410 | 0.8540 |
| 315.15 | 0.8830 | 0.8880 |
| 315.16 | 0.9130 | 0.9150 |

Jones, C. A. - Schoenborn, E. M. - Colburn, A. P., Equilibrium Still for Miscible Liquids, Industrial & Engineering Chemistry 6 (1943) 666-672. doi:10.1021/ie50402a009

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 368.65 | 0.0180 | 0.1790 |
| 363.75 | 0.0540 | 0.3375 |
| 358.55 | 0.1240 | 0.4700 |
| 356.85 | 0.1760 | 0.5140 |
| 355.90 | 0.2300 | 0.5420 |
| 355.15 | 0.2880 | 0.5700 |

| | | |
|---|---|---|
| 354.15 | 0.3850 | 0.6120 |
| 353.65 | 0.4400 | 0.6330 |
| 352.95 | 0.5140 | 0.6570 |
| 352.05 | 0.6730 | 0.7350 |
| 351.41 | 0.8400 | 0.8500 |

Hughes, H.E. - Maloney, J.O., Application of radioactive tracers to diffusional operations. Binary and ternary equilibrium data, Chem. Eng. Progr. 4 (1952) 192-200.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 372.08 | 0.0044 | 0.0510 |
| 370.20 | 0.0110 | 0.1230 |
| 365.45 | 0.0340 | 0.2610 |
| 361.47 | 0.0680 | 0.3830 |
| 360.62 | 0.0770 | 0.4110 |
| 358.64 | 0.1160 | 0.4640 |
| 357.90 | 0.1350 | 0.4760 |
| 357.49 | 0.1470 | 0.4990 |
| 356.62 | 0.1770 | 0.5160 |
| 356.57 | 0.1780 | 0.5190 |
| 356.09 | 0.2070 | 0.5360 |
| 355.65 | 0.2330 | 0.5440 |
| 355.71 | 0.2360 | 0.5410 |
| 355.14 | 0.2700 | 0.5620 |
| 354.99 | 0.2870 | 0.5720 |
| 354.05 | 0.3610 | 0.6050 |
| 354.07 | 0.3700 | 0.6010 |
| 353.06 | 0.4800 | 0.6450 |
| 351.31 | 0.9040 | 0.9000 |

Kojima, K. - Tochigi, K. - Seki, H. - Watase, K., Determination of vapor-liquid equilibriums from boiling point curves, Kagaku Kogaku (1968) 149-153. doi:10.1252/kakoronbunshu1953.32.149

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 363.15 | 0.0500 | 0.3372 |
| 359.08 | 0.1000 | 0.4521 |
| 357.12 | 0.1500 | 0.5056 |
| 356.05 | 0.2000 | 0.5359 |
| 355.29 | 0.2500 | 0.5589 |
| 354.67 | 0.3000 | 0.5794 |
| 354.14 | 0.3500 | 0.5987 |
| 353.67 | 0.4000 | 0.6177 |
| 353.25 | 0.4500 | 0.6371 |
| 352.90 | 0.5000 | 0.6558 |
| 352.57 | 0.5500 | 0.6765 |
| 352.28 | 0.6000 | 0.6986 |
| 352.00 | 0.6500 | 0.7250 |
| 351.75 | 0.7000 | 0.7550 |
| 351.57 | 0.7500 | 0.7840 |
| 351.45 | 0.8000 | 0.8167 |
| 351.37 | 0.8500 | 0.8591 |
| 351.35 | 0.9000 | 0.8959 |
| 351.39 | 0.9500 | 0.9474 |

Bloom, C. H. - Clump, C. W. - Koeckert, A. H., Simultaneous Measurement of Vapor-Liquid Equilibria and Latent Heats of Vaporization, Industrial & Engineering Chemistry 10 (1961) 829-832. doi:10.1021/ie50622a029

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 367.45 | 0.0210 | 0.1990 |
| 365.05 | 0.0330 | 0.2720 |
| 363.15 | 0.0500 | 0.3530 |
| 360.45 | 0.0850 | 0.4110 |
| 359.25 | 0.1050 | 0.4580 |
| 358.35 | 0.1250 | 0.4880 |
| 357.85 | 0.1350 | 0.4840 |
| 354.95 | 0.3150 | 0.5710 |
| 354.75 | 0.3210 | 0.5720 |
| 352.65 | 0.5560 | 0.6750 |
| 352.35 | 0.6020 | 0.6950 |
| 352.25 | 0.6430 | 0.7130 |
| 351.75 | 0.6890 | 0.7410 |
| 351.35 | 0.9870 | 0.9850 |

Stabnikov, V.N. - Matyushev, B.Z. - Protsyuk, T.B. - Yushchenko, N.M., Equilibrium in the ethyl alcohol-water system at atmospheric pressure, Pishch. Promst. Kiev (1972) 49-56.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 372.96 | 0.0010 | 0.0100 |
| 372.77 | 0.0020 | 0.0205 |
| 372.58 | 0.0030 | 0.0312 |
| 372.39 | 0.0040 | 0.0421 |
| 372.20 | 0.0050 | 0.0532 |
| 372.01 | 0.0060 | 0.0644 |
| 371.82 | 0.0070 | 0.0753 |
| 371.63 | 0.0080 | 0.0858 |
| 371.44 | 0.0090 | 0.0958 |
| 371.25 | 0.0100 | 0.1040 |
| 370.73 | 0.0120 | 0.1200 |
| 370.21 | 0.0140 | 0.1360 |
| 369.69 | 0.0160 | 0.1509 |
| 369.17 | 0.0180 | 0.1655 |

| | | | | | |
|---|---|---|---|---|---|
| 368.65 | 0.0200 | 0.1800 | 354.90 | 0.2900 | 0.5680 |
| 368.08 | 0.0220 | 0.1943 | 354.79 | 0.3000 | 0.5725 |
| 367.61 | 0.0240 | 0.2080 | 354.70 | 0.3100 | 0.5765 |
| 367.09 | 0.0260 | 0.2205 | 354.60 | 0.3200 | 0.5805 |
| 366.57 | 0.0280 | 0.2327 | 354.49 | 0.3300 | 0.5840 |
| 366.05 | 0.0300 | 0.2442 | 354.40 | 0.3400 | 0.5880 |
| 365.00 | 0.0350 | 0.2695 | 354.30 | 0.3500 | 0.5920 |
| 364.20 | 0.0400 | 0.2905 | 354.20 | 0.3600 | 0.5955 |
| 363.62 | 0.0450 | 0.3075 | 354.10 | 0.3700 | 0.5992 |
| 363.05 | 0.0500 | 0.3245 | 354.02 | 0.3800 | 0.6032 |
| 362.60 | 0.0550 | 0.3400 | 353.90 | 0.3900 | 0.6068 |
| 362.07 | 0.0600 | 0.3545 | 353.81 | 0.4000 | 0.6102 |
| 361.65 | 0.0650 | 0.3660 | 353.72 | 0.4100 | 0.6135 |
| 361.28 | 0.0700 | 0.3775 | 353.63 | 0.4200 | 0.6170 |
| 360.91 | 0.0750 | 0.3885 | 353.54 | 0.4300 | 0.6205 |
| 360.60 | 0.0800 | 0.3990 | 353.44 | 0.4400 | 0.6245 |
| 360.25 | 0.0850 | 0.4091 | 353.40 | 0.4500 | 0.6280 |
| 359.92 | 0.0900 | 0.4190 | 353.33 | 0.4600 | 0.6320 |
| 359.61 | 0.0950 | 0.4283 | 353.25 | 0.4700 | 0.6355 |
| 359.35 | 0.1000 | 0.4370 | 353.18 | 0.4800 | 0.6395 |
| 359.11 | 0.1050 | 0.4450 | 353.11 | 0.4900 | 0.6435 |
| 358.88 | 0.1100 | 0.4528 | 353.04 | 0.5000 | 0.6475 |
| 358.65 | 0.1150 | 0.4605 | 352.99 | 0.5100 | 0.6520 |
| 358.43 | 0.1200 | 0.4675 | 352.92 | 0.5200 | 0.6565 |
| 358.25 | 0.1250 | 0.4740 | 352.90 | 0.5300 | 0.6610 |
| 358.05 | 0.1300 | 0.4800 | 352.86 | 0.5400 | 0.6660 |
| 357.87 | 0.1350 | 0.4855 | 352.80 | 0.5500 | 0.6710 |
| 357.70 | 0.1400 | 0.4900 | 352.75 | 0.5600 | 0.6760 |
| 357.51 | 0.1450 | 0.4940 | 352.70 | 0.5700 | 0.6810 |
| 357.35 | 0.1500 | 0.4980 | 352.65 | 0.5800 | 0.6865 |
| 357.31 | 0.1550 | 0.5002 | 352.59 | 0.5900 | 0.6920 |
| 357.07 | 0.1600 | 0.5055 | 352.55 | 0.6000 | 0.6980 |
| 356.93 | 0.1650 | 0.5090 | 352.50 | 0.6100 | 0.7030 |
| 356.80 | 0.1700 | 0.5120 | 352.45 | 0.6200 | 0.7090 |
| 356.65 | 0.1750 | 0.5145 | 352.42 | 0.6300 | 0.7145 |
| 356.52 | 0.1800 | 0.5175 | 352.35 | 0.6400 | 0.7200 |
| 356.40 | 0.1850 | 0.5200 | 352.30 | 0.6500 | 0.7255 |
| 356.27 | 0.1900 | 0.5230 | 352.25 | 0.6600 | 0.7310 |
| 356.15 | 0.1950 | 0.5255 | 352.20 | 0.6700 | 0.7365 |
| 356.05 | 0.2000 | 0.5280 | 352.15 | 0.6800 | 0.7420 |
| 355.93 | 0.2100 | 0.5330 | 352.10 | 0.6900 | 0.7475 |
| 355.70 | 0.2200 | 0.5375 | 352.04 | 0.7000 | 0.7530 |
| 355.58 | 0.2300 | 0.5420 | 352.01 | 0.7100 | 0.7590 |
| 355.43 | 0.2400 | 0.5460 | 351.95 | 0.7200 | 0.7650 |
| 355.31 | 0.2500 | 0.5505 | 351.91 | 0.7300 | 0.7710 |
| 355.20 | 0.2600 | 0.5545 | 351.86 | 0.7400 | 0.7770 |
| 355.09 | 0.2700 | 0.5590 | 351.81 | 0.7500 | 0.7830 |
| 355.00 | 0.2800 | 0.5635 | 351.75 | 0.7600 | 0.7890 |

| | | |
|---|---|---|
| 351.72 | 0.7700 | 0.7950 |
| 351.68 | 0.7800 | 0.8015 |
| 351.65 | 0.7900 | 0.8080 |
| 351.62 | 0.8000 | 0.8155 |
| 351.59 | 0.8100 | 0.8225 |
| 351.55 | 0.8200 | 0.8300 |
| 351.52 | 0.8300 | 0.8385 |
| 351.49 | 0.8400 | 0.8470 |
| 351.46 | 0.8500 | 0.8560 |
| 351.43 | 0.8600 | 0.8645 |
| 351.39 | 0.8700 | 0.8730 |
| 351.36 | 0.8800 | 0.8806 |
| 351.33 | 0.8900 | 0.8905 |
| 351.35 | 0.9000 | 0.8990 |
| 351.40 | 0.9100 | 0.9075 |
| 351.45 | 0.9190 | 0.9158 |

Otsuki, H. - Williams, F.C., Effect of pressure on vapor-liquid equilibria for the system ethyl alcohol-water, Chem. Eng. Progr. Symp. Ser. (1953) 55-67.

**P / bar = 3.448**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 408.65 | 0.0076 | 0.0718 |
| 404.35 | 0.0230 | 0.1910 |
| 401.85 | 0.0392 | 0.2650 |
| 399.25 | 0.0590 | 0.3210 |
| 398.55 | 0.0675 | 0.3380 |
| 396.45 | 0.0866 | 0.3910 |
| 395.65 | 0.1010 | 0.4110 |
| 394.45 | 0.1200 | 0.4330 |
| 393.55 | 0.1350 | 0.4540 |
| 392.55 | 0.1840 | 0.4920 |
| 390.25 | 0.2630 | 0.5360 |
| 389.45 | 0.3240 | 0.5660 |
| 388.45 | 0.4210 | 0.6040 |
| 387.75 | 0.4960 | 0.6380 |
| 387.05 | 0.5880 | 0.6840 |
| 386.45 | 0.6880 | 0.7390 |
| 386.05 | 0.8060 | 0.8200 |

Otsuki, H. - Williams, F.C., Effect of pressure on vapor-liquid equilibria for the system ethyl alcohol-water, Chem. Eng. Progr. Symp. Ser. (1953) 55-67.

**P / bar = 6.895**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 435.25 | 0.0075 | 0.0570 |
| 433.55 | 0.0141 | 0.1090 |
| 430.15 | 0.0275 | 0.1850 |
| 427.15 | 0.0412 | 0.2550 |
| 424.75 | 0.0583 | 0.3100 |
| 424.55 | 0.0635 | 0.3140 |
| 422.65 | 0.0807 | 0.3560 |
| 420.95 | 0.1030 | 0.3860 |
| 419.25 | 0.1390 | 0.4260 |
| 417.95 | 0.1710 | 0.4560 |
| 415.85 | 0.2530 | 0.5070 |
| 414.65 | 0.3150 | 0.5400 |
| 413.05 | 0.4320 | 0.5940 |
| 412.15 | 0.5130 | 0.6340 |
| 411.35 | 0.5890 | 0.6730 |
| 410.65 | 0.6610 | 0.7170 |
| 410.05 | 0.7610 | 0.7850 |

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**Enthalpy of mixing**

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Friese, T. - Ulbig, P. - Schulz, S. - Wagner, K., Effect of NaCl or KCl on the Excess Enthalpies of Alkanol + Water Mixtures at Various Temperatures and Salt Concentrations 4 (1999) 701-714. doi:10.1021/je980303x

**T / K = 285.65**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -288.50 | 0.0250 |
| -534.30 | 0.0500 |
| -723.90 | 0.0750 |
| -854.90 | 0.1000 |
| -929.40 | 0.1250 |
| -958.50 | 0.1500 |
| -958.20 | 0.1750 |
| -938.50 | 0.2000 |
| -910.70 | 0.2250 |
| -879.30 | 0.2500 |
| -845.20 | 0.2750 |
| -806.80 | 0.3000 |
| -717.20 | 0.3600 |
| -635.70 | 0.4200 |
| -559.80 | 0.4800 |
| -490.50 | 0.5400 |
| -430.20 | 0.6000 |
| -381.30 | 0.6600 |
| -335.40 | 0.7200 |
| -291.60 | 0.7800 |
| -242.70 | 0.8400 |
| -178.20 | 0.9010 |
| -86.00 | 0.9590 |

Ott, J.B. - Stouffer, C.E. - Cornett, G.V. - Woodfield, B.F. - Wirthlin, R.C. - Christensen, J.J. - Deiters, U.K., Excess enthalpies for (ethanol + water) at 298.15 K and pressures of 0.4, 5, 10, and 15 MPa, The Journal of Chemical Thermodynamics 1 (1986) 1-12. doi:10.1016/0021-9614(86)90036-4

**T / K = 298.15**

**P / bar = 100.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -290.30 | 0.0303 |
| -580.10 | 0.0705 |
| -707.00 | 0.1005 |
| -755.90 | 0.1206 |
| -781.50 | 0.1412 |
| -788.20 | 0.1606 |
| -775.60 | 0.2012 |
| -725.60 | 0.2514 |
| -664.00 | 0.3012 |
| -599.60 | 0.3520 |
| -536.90 | 0.4027 |
| -480.90 | 0.4518 |
| -428.60 | 0.5023 |
| -384.20 | 0.5510 |
| -343.50 | 0.6020 |
| -310.60 | 0.6525 |
| -281.10 | 0.7012 |
| -256.70 | 0.7507 |
| -227.20 | 0.8005 |
| -197.00 | 0.8505 |
| -152.50 | 0.8999 |
| -93.20 | 0.9482 |

Friese, T. - Ulbig, P. - Schulz, S. - Wagner, K., Effect of NaCl or KCl on the Excess Enthalpies of Alkanol + Water Mixtures at Various Temperatures and Salt Concentrations 4 (1999) 701-714. doi:10.1021/je980303x

**T / K = 338.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -108.80 | 0.0250 |
| -188.60 | 0.0500 |
| -238.50 | 0.0750 |
| -261.90 | 0.1000 |
| -263.90 | 0.1250 |
| -253.30 | 0.1500 |
| -232.50 | 0.1750 |
| -208.90 | 0.2000 |
| -156.90 | 0.2500 |
| -100.60 | 0.3000 |
| -49.00 | 0.3500 |
| -2.800 | 0.4000 |
| 36.20 | 0.4500 |
| 66.70 | 0.5000 |
| 87.70 | 0.5500 |
| 99.50 | 0.6000 |
| 102.10 | 0.6500 |
| 96.80 | 0.7000 |
| 83.10 | 0.7500 |
| 42.30 | 0.8490 |
| 30.70 | 0.9010 |
| 23.70 | 0.9500 |

Ott, J.B. - Cornett, G.V. - Stouffer, C.E. - Woodfield, B.F. - Guanquan, C. - Christensen, J.J., Excess enthalpies of (ethanol+water) at 323.15, 333.15, 348.15, and 373.15 K and from 0.4 to 15 MPa, The Journal of Chemical Thermodynamics 9 (1986) 867-875. doi:10.1016/0021-9614(86)90121-7

**T / K = 373.15**

**P / bar = 10.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -8.700 | 0.0100 |
| -14.20 | 0.0198 |
| -16.40 | 0.0301 |
| -15.10 | 0.0403 |
| -11.50 | 0.0503 |
| 6.700 | 0.0736 |
| 39.80 | 0.1000 |
| 76.00 | 0.1241 |
| 120.40 | 0.1504 |
| 199.70 | 0.2002 |
| 270.60 | 0.2502 |
| 333.70 | 0.2999 |
| 387.90 | 0.3505 |
| 429.70 | 0.4011 |
| 458.40 | 0.4502 |
| 475.80 | 0.5007 |
| 474.30 | 0.5494 |
| 463.20 | 0.6006 |
| 438.40 | 0.6511 |
| 402.90 | 0.6999 |
| 356.20 | 0.7495 |
| 297.80 | 0.7996 |
| 230.00 | 0.8497 |
| 156.60 | 0.8993 |
| 85.50 | 0.9478 |

Ott, J.B - Stouffer, C.E - Cornett, G.V - Woodfield, B.F - Guanquan, Che - Christensen, J.J, Excess enthalpies

for (ethanol + water) at 398.15, 423.15, 448.15, and 473.15 K and at pressures of 5 and 15 MPa. Recommendations for choosing (ethanol + water) as an HmE reference mixture, The Journal of Chemical Thermodynamics 4 (1987) 337-348. doi:10.1016/0021-9614(87)90115-7

**T / K = 423.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 165.20 | 0.0504 |
| 331.90 | 0.1002 |
| 479.30 | 0.1508 |
| 602.90 | 0.2007 |
| 700.60 | 0.2507 |
| 780.90 | 0.3005 |
| 839.20 | 0.3512 |
| 878.80 | 0.4018 |
| 895.00 | 0.4509 |
| 894.90 | 0.5014 |
| 877.20 | 0.5501 |
| 839.80 | 0.6013 |
| 789.20 | 0.6518 |
| 718.60 | 0.7005 |
| 635.80 | 0.7501 |
| 533.40 | 0.8001 |
| 420.20 | 0.8501 |
| 293.80 | 0.8996 |
| 160.00 | 0.9480 |

Ott, J.B - Stouffer, C.E - Cornett, G.V - Woodfield, B.F - Guanquan, Che - Christensen, J.J, Excess enthalpies for (ethanol + water) at 398.15, 423.15, 448.15, and 473.15 K and at pressures of 5 and 15 MPa. Recommendations for choosing (ethanol + water) as an HmE reference mixture, The Journal of Chemical Thermodynamics 4 (1987) 337-348. doi:10.1016/0021-9614(87)90115-7

**T / K = 473.15**

**P / bar = 50.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 274.80 | 0.0504 |
| 506.00 | 0.1002 |
| 695.30 | 0.1508 |
| 847.20 | 0.2007 |
| 961.90 | 0.2507 |
| 1044.0 | 0.3005 |
| 1104.1 | 0.3512 |
| 1137.1 | 0.4018 |
| 1140.0 | 0.4509 |
| 1137.9 | 0.5014 |
| 1110.0 | 0.5501 |
| 1056.0 | 0.6013 |
| 984.80 | 0.6518 |
| 896.40 | 0.7005 |
| 785.10 | 0.7501 |
| 659.90 | 0.8001 |
| 514.50 | 0.8501 |
| 357.90 | 0.8996 |
| 187.00 | 0.9480 |

Wormald, C.J. - Lloyd, M.J., Excess enthalpies for (water + ethanol) atT= 398 K toT= 548 K andp= 15 MPa, The Journal of Chemical Thermodynamics 6 (1996) 615-626. doi:10.1006/jcht.1996.0058

**T / K = 538.00**

**P / bar = 150.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 1354.0 | 0.2000 |
| 1550.0 | 0.2500 |
| 1705.0 | 0.3000 |
| 1800.0 | 0.3500 |
| 1868.0 | 0.4000 |
| 1917.0 | 0.4500 |
| 1920.0 | 0.5000 |
| 1861.0 | 0.5500 |
| 1797.0 | 0.6000 |
| 1705.0 | 0.6500 |
| 1529.0 | 0.7000 |
| 1382.0 | 0.7500 |
| 1096.0 | 0.8000 |
| 916.00 | 0.8500 |
| 650.00 | 0.9000 |

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**Heat capacity of mixing**

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Benson, George C. - D'Arcy, Patrick J., Excess isobaric heat capacities of water-n-alcohol mixtures, Journal of Chemical & Engineering Data 4 (1982) 439-442. doi:10.1021/je00030a021

**T / K = 288.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 1.620 | 0.0102 |
| 2.380 | 0.0152 |
| 3.070 | 0.0198 |
| 3.240 | 0.0209 |
| 3.870 | 0.0252 |
| 4.530 | 0.0298 |
| 6.090 | 0.0412 |

| | |
|---|---|
| 7.010 | 0.0486 |
| 7.440 | 0.0519 |
| 7.560 | 0.0527 |
| 7.730 | 0.0543 |
| 8.940 | 0.0646 |
| 9.350 | 0.0688 |
| 11.45 | 0.0922 |
| 11.56 | 0.0930 |
| 11.95 | 0.0996 |
| 12.65 | 0.1100 |
| 13.14 | 0.1201 |
| 13.40 | 0.1275 |
| 13.70 | 0.1406 |
| 13.59 | 0.1502 |
| 13.91 | 0.1581 |
| 13.68 | 0.1695 |
| 13.81 | 0.1757 |
| 13.13 | 0.2021 |
| 13.31 | 0.2023 |
| 12.87 | 0.2280 |
| 12.80 | 0.2311 |
| 12.45 | 0.2434 |
| 12.47 | 0.2454 |
| 12.38 | 0.2465 |
| 12.49 | 0.2493 |
| 12.14 | 0.2704 |
| 12.06 | 0.2759 |
| 11.96 | 0.2775 |
| 11.75 | 0.2993 |
| 11.09 | 0.3406 |
| 10.42 | 0.3845 |
| 9.790 | 0.4217 |
| 9.620 | 0.4358 |
| 8.660 | 0.5082 |
| 8.470 | 0.5266 |
| 7.560 | 0.5955 |
| 6.730 | 0.6579 |
| 5.930 | 0.7142 |
| 5.740 | 0.7255 |
| 4.300 | 0.8121 |
| 3.690 | 0.8427 |
| 2.330 | 0.9054 |
| 1.230 | 0.9498 |

Ogawa, Hideo - Murakami, Sachio, Excess isobaric heat capacities for water + alkanol mixtures at 298.15 K, Thermochimica Acta 1 (1986) 145-154. doi:10.1016/0040-6031(86)85016-X

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 3.594 | 0.0250 |
| 6.966 | 0.0500 |
| 9.904 | 0.0750 |
| 12.01 | 0.1000 |
| 13.84 | 0.1501 |
| 13.85 | 0.1501 |
| 14.01 | 0.2001 |
| 13.66 | 0.2501 |
| 13.15 | 0.3001 |
| 12.59 | 0.3501 |
| 11.99 | 0.4001 |
| 11.31 | 0.4501 |
| 10.66 | 0.5001 |
| 9.993 | 0.5501 |
| 9.264 | 0.6001 |
| 8.489 | 0.6501 |
| 7.705 | 0.7001 |
| 6.832 | 0.7501 |
| 5.876 | 0.8001 |
| 4.780 | 0.8501 |
| 3.448 | 0.9000 |
| 1.848 | 0.9500 |

Grolier, J.-P.E. - Wilhelm, Emmerich, Excess volumes and excess heat capacities of water + ethanol at 298.15 K, Fluid Phase Equilibria 3-4 (1981) 283-287. doi:10.1016/0378-3812(81)85011-X

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 2.560 | 0.0189 |
| 4.470 | 0.0325 |
| 6.670 | 0.0494 |
| 8.840 | 0.0671 |
| 9.730 | 0.0757 |
| 10.60 | 0.0845 |
| 11.99 | 0.1011 |
| 13.39 | 0.1255 |
| 13.83 | 0.1414 |
| 14.08 | 0.1982 |
| 13.75 | 0.2323 |
| 12.82 | 0.3349 |
| 11.45 | 0.4305 |
| 10.32 | 0.5075 |
| 9.580 | 0.5602 |
| 7.780 | 0.6712 |

| | |
|---|---|
| 7.290 | 0.6918 |
| 6.370 | 0.7418 |
| 4.420 | 0.8324 |
| 2.120 | 0.9201 |

Benson, George C. - D'Arcy, Patrick J., Excess isobaric heat capacities of water-n-alcohol mixtures, Journal of Chemical & Engineering Data 4 (1982) 439-442. doi:10.1021/je00030a021

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 2.150 | 0.0149 |
| 3.190 | 0.0218 |
| 4.830 | 0.0334 |
| 5.800 | 0.0412 |
| 8.590 | 0.0632 |
| 9.720 | 0.0738 |
| 10.91 | 0.0851 |
| 11.27 | 0.0900 |
| 11.80 | 0.0994 |
| 12.80 | 0.1098 |
| 13.43 | 0.1242 |
| 13.96 | 0.1485 |
| 13.90 | 0.1485 |
| 13.95 | 0.1502 |
| 14.39 | 0.1757 |
| 14.48 | 0.2020 |
| 14.34 | 0.2024 |
| 14.36 | 0.2281 |
| 14.32 | 0.2503 |
| 14.13 | 0.2503 |
| 14.14 | 0.2525 |
| 14.00 | 0.2792 |
| 13.61 | 0.3056 |
| 13.81 | 0.3080 |
| 13.46 | 0.3355 |
| 13.37 | 0.3507 |
| 13.25 | 0.3507 |
| 13.00 | 0.3779 |
| 12.79 | 0.4048 |
| 12.49 | 0.4264 |
| 12.12 | 0.4567 |
| 11.46 | 0.5065 |
| 10.89 | 0.5465 |
| 10.82 | 0.5465 |
| 10.45 | 0.5707 |
| 10.09 | 0.6049 |
| 9.450 | 0.6432 |
| 9.330 | 0.6458 |
| 8.530 | 0.6952 |
| 7.650 | 0.7341 |
| 7.250 | 0.7561 |
| 6.150 | 0.8091 |
| 5.440 | 0.8337 |
| 4.200 | 0.8751 |
| 3.630 | 0.8946 |
| 3.600 | 0.8946 |
| 2.780 | 0.9222 |
| 2.030 | 0.9444 |

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**Critical point**

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Bazaev, A.R. - Abdulagatov, I.M. - Bazaev, E.A. - Abdurashidova, A., (p,v,T,x) Measurements of {(1−x)H2O+xC2H5OH} mixtures in the near-critical and supercritical regions, The Journal of Chemical Thermodynamics 3 (2007) 385-411. doi:10.1016/j.jct.2006.08.002

| T / K | P / bar | $x_1$ |
|---|---|---|
| 598.05 | 155.00 | 0.2000 |
| 546.84 | 96.50 | 0.5000 |
| 524.48 | 71.50 | 0.8000 |

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**Azeotropic point**

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Kojima, K. - Tochigi, K. - Seki, H. - Watase, K., Determination of vapor-liquid equilibriums from boiling point curves, Kagaku Kogaku (1968) 149-153. doi:10.1252/kakoronbunshu1953.32.149

| T / K | P / bar | $x_1$ |
|---|---|---|
| 351.39 | 1.013 | 0.9461 |

Bloom, C. H. - Clump, C. W. - Koeckert, A. H., Simultaneous Measurement of Vapor-Liquid Equilibria and Latent Heats of Vaporization, Industrial & Engineering Chemistry 10 (1961) 829-832. doi:10.1021/ie50622a029

| T / K | P / bar | $x_1$ |
|---|---|---|
| 351.35 | 1.013 | 0.9840 |

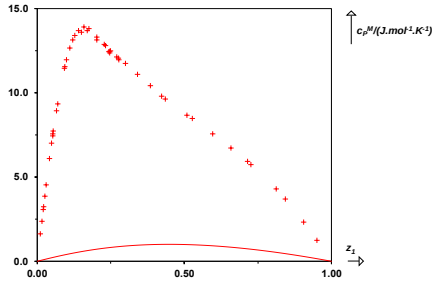
Stabnikov, V.N. - Matyushev, B.Z. - Protsyuk, T.B. - Yushchenko, N.M., Equilibrium in the ethyl alcohol-water system at atmospheric pressure, Pishch. Promst. Kiev (1972) 49-56.

| T / K | P / bar | $x_1$ |
|---|---|---|
| 351.40 | 1.013 | 0.9062 |

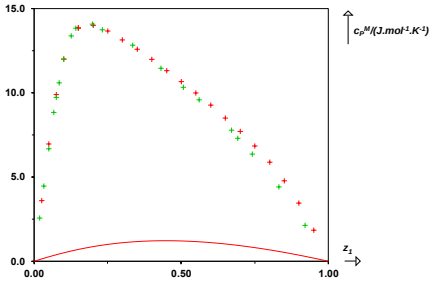
Voutsas, Epaminondas C. - Pamouktsis, Christos - Argyris, Dimitrios - Pappa, Georgia D., Measurements and thermodynamic modeling of the ethanol–water system with emphasis to the azeotropic region, Fluid Phase Equilibria 1-2 (2011) 135-141. doi:10.1016/j.fluid.2011.06.009

| T / K | P / bar | $x_1$ |
|---|---|---|
| 315.16 | 0.1971 | 0.9160 |

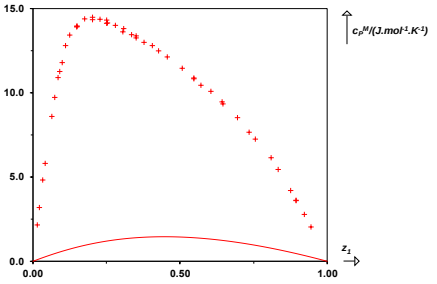
T/K = 288.15 - P/bar = 1.0132



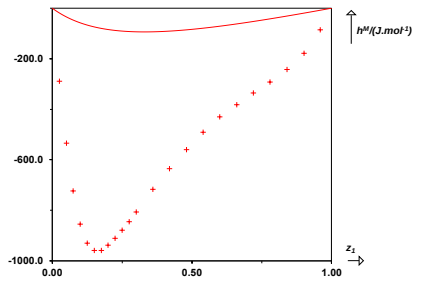

T/K = 298.15 - P/bar = 1.0132 1.0132



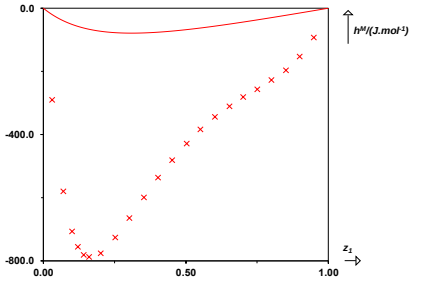

T/K = 308.15 - P/bar = 1.0132



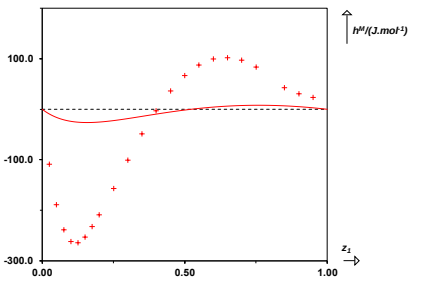

T/K = 285.65 - P/bar = 1.0132



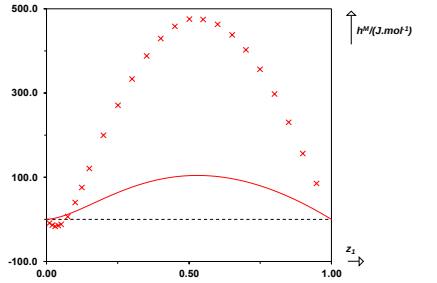

T/K = 298.15 - P/bar = 100.00



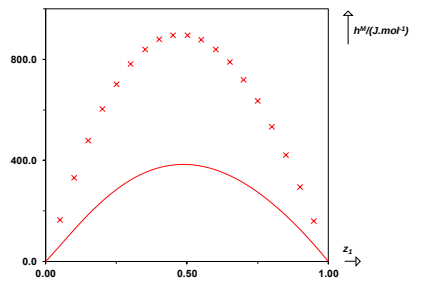

T/K = 338.15 - P/bar = 1.0132



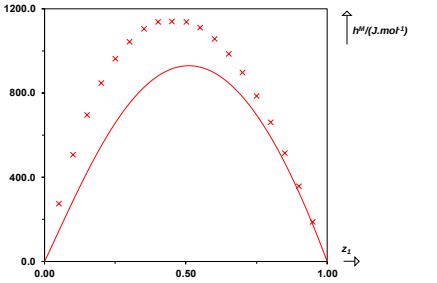

T/K = 373.15 - P/bar = 10.00



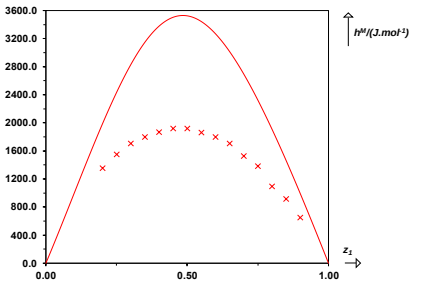

T/K = 423.15 - P/bar = 50.00



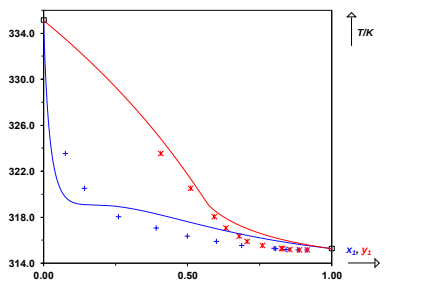

T/K = 473.15 - P/bar = 50.00



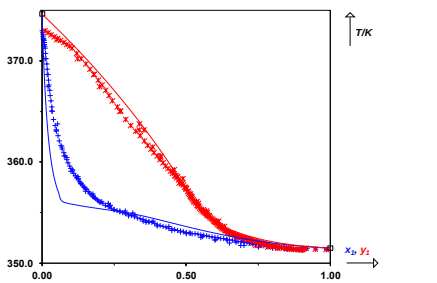

T/K = 538.00 - P/bar = 150.00



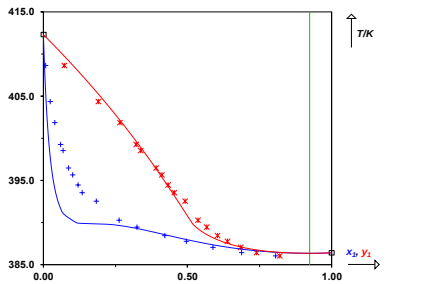

P/bar = 0.19710



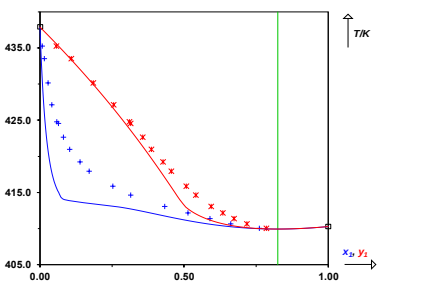

P/bar = 1.01330



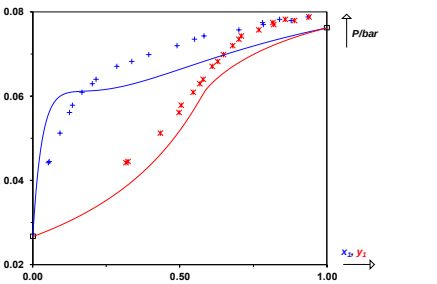

P/bar = 3.44770



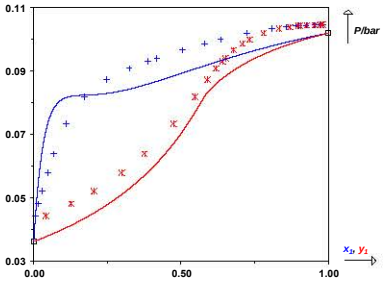

P/bar = 6.89540



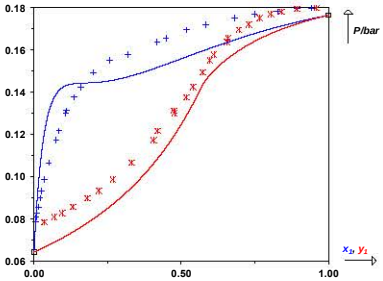

T/K = 298.15



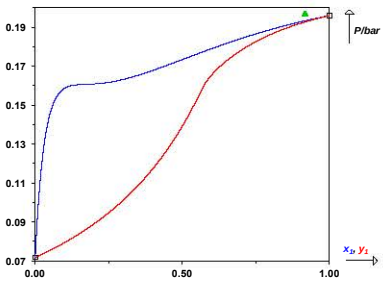
T/K = 303.15



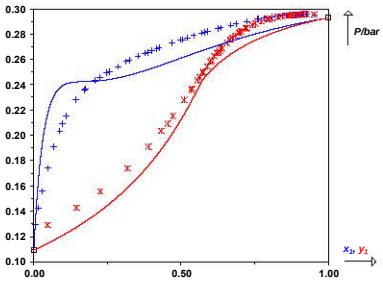

T/K = 313.15



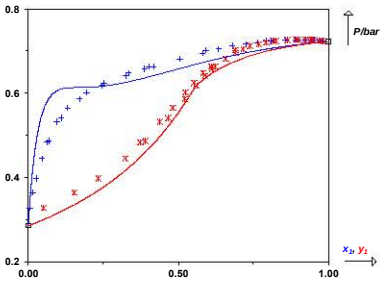

T/K = 315.16



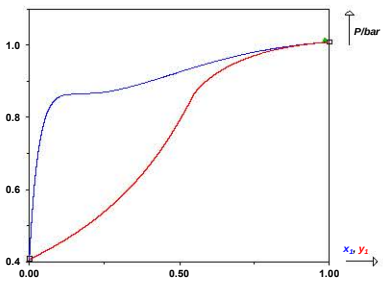

T/K = 323.15



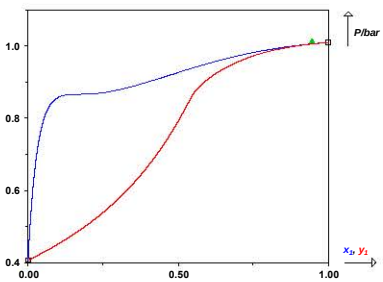

T/K = 343.15



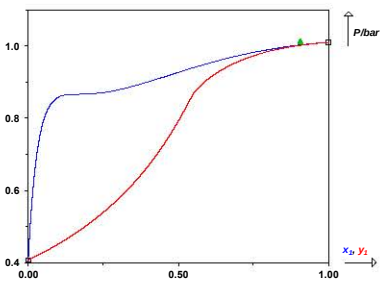

T/K = 351.35



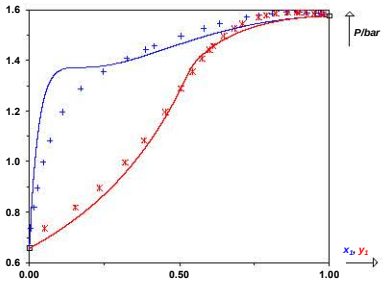

T/K = 351.39



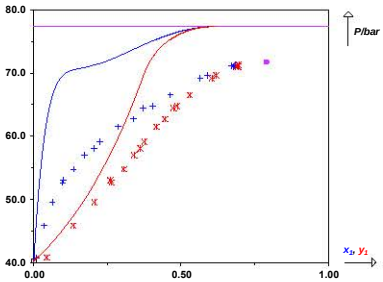

T/K = 351.40



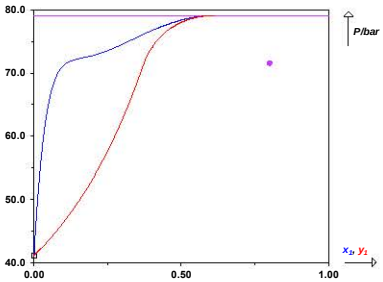

T/K = 363.15



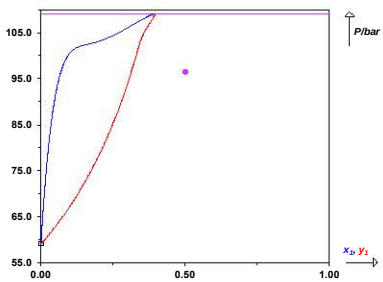

T/K = 523.15

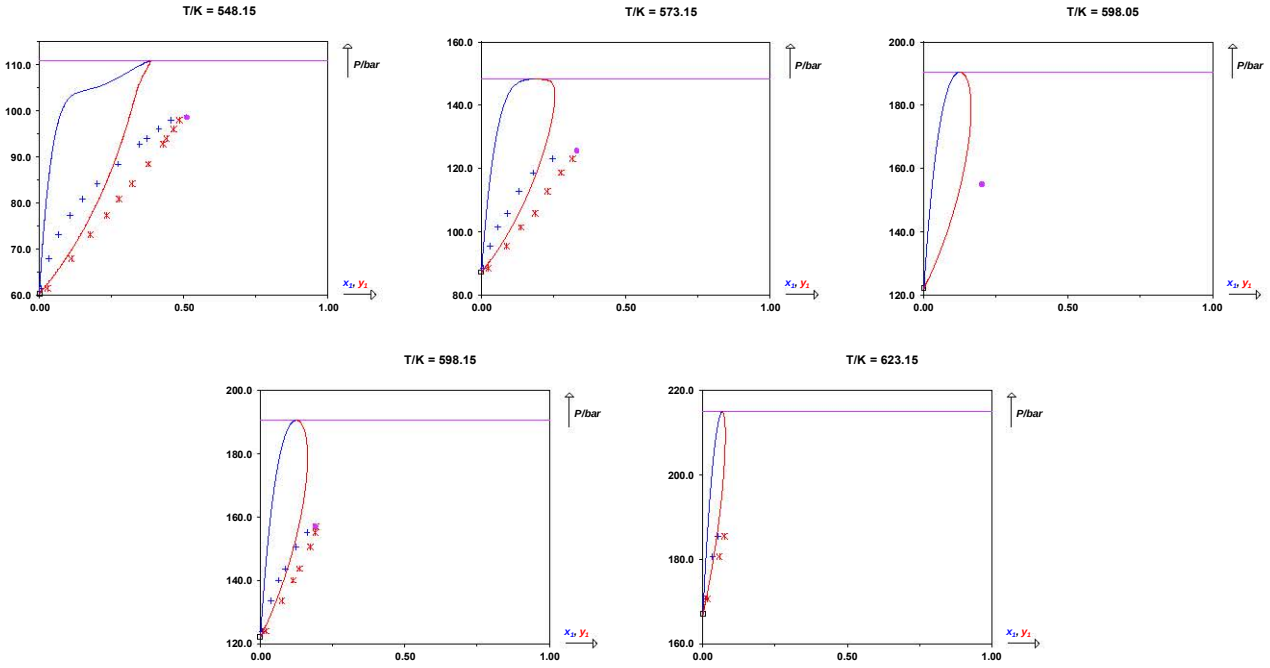



T/K = 524.48




T/K = 546.84




T/K = 548.15
P/bar
110.0
100.0
90.0
80.0
70.0
60.0
0.00
0.50
1.00
x1, y1
T/K = 573.15
P/bar
160.0
140.0
120.0
100.0
80.0
0.00
0.50
1.00
x1, y1
T/K = 598.05
P/bar
200.0
180.0
160.0
140.0
120.0
0.00
0.50
1.00
x1, y1
T/K = 598.15
P/bar
200.0
180.0
160.0
140.0
120.0
0.00
0.50
1.00
x1, y1
T/K = 623.15
P/bar
220.0
200.0
180.0
160.0
0.00
0.50
1.00
x1, y1

## WATER (1) + ACETONITRILE (2)

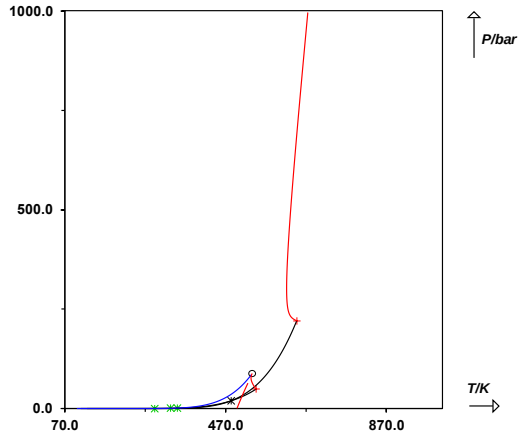
| | | |
|---|---|---|
| **CAS** | 7732-18-5 | 75-05-8 |
| **InChiKey** | XLYOFNOQVPJJNP-UHFFFAOYSA-N | WEVYAHXRMPXWCK-UHFFFAOYSA-N |
| **$T_c$ / K** | 647.10 | 545.50 |
| **$P_c$ / bar** | 220.64 | 48.50 |
| **ω** | 0.345 | 0.342 |

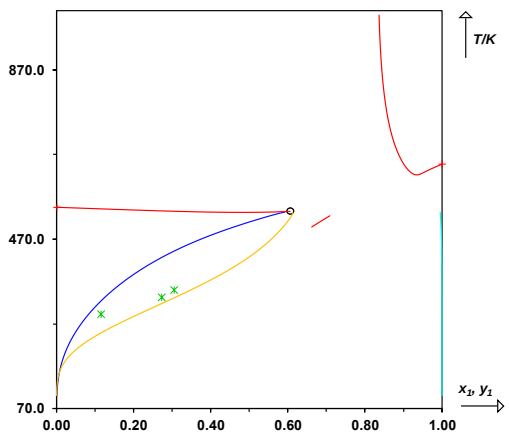
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 2130
B/MPa = 1630

*Deviations*
MAPE on x = 64 %
MAPE on y = 16 %
MAPE on $h^M$ = 77 %
MAPE on $c_P^M$ = 87 %



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**Isothermal phase equilibrium data**

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Vierk, Anna-Luise, Experimentelle Untersuchungen an den Zweistoffsystemen: Wasser-Acetonitril, Wasser-Dioxan, Äthanol-Acetonitril und Cyclohexan-Dioxan, Zeitschrift für anorganische Chemie 5-6 (1950) 283-296. doi:10.1002/zaac.19502610504

**T / K = 293.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.0840 | 0.9300 | 0.2063 | |
| 0.0953 | 0.8500 | 0.1706 | |
| 0.0976 | 0.8100 | 0.1530 | |
| 0.0989 | 0.6500 | 0.1415 | |
| 0.0996 | 0.3500 | 0.1406 | |
| 0.0999 | 0.2400 | 0.1295 | |
| 0.1000 | 0.1150 | 0.1150 | AZEO |
| 0.0997 | 0.0800 | 0.1110 | |

Park, S-Jin - Oh, Hyeog-Jong - Choi, Ho-Jun - Peak, Seung-Kwan - Fischer, K. - Gmehling, J., Phase equilibrium and excess molar volume for systems acrylonitrile+water, acetonitrile+water, and acrylonitrile+acetonitrile, Hwahak Konghak 5 (1997) 678-683.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1533 | 0.9913 | 0.7957 |
| 0.2088 | 0.9730 | 0.5745 |
| 0.2734 | 0.9429 | 0.4287 |
| 0.3510 | 0.8439 | 0.3201 |
| 0.3689 | 0.7246 | 0.2983 |
| 0.3752 | 0.5546 | 0.2882 |
| 0.3809 | 0.3388 | 0.2694 |
| 0.3802 | 0.1904 | 0.2295 |
| 0.3654 | 0.0692 | 0.1222 |
| 0.3585 | 0.0422 | 0.0861 |

Sugi, Hiroshi - Katayama, Takashi, Ternary Liquid-Liquid And Miscible Binary Vapor-Liquid Equilibrium Data For The Two Systems n-Hexane Ethanol Acetonitrile And Water Acetonitrile-Ethyl Acetate, Journal of Chemical Engineering of Japan 3 (1978) 167-172. doi:10.1252/jcej.11.167

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ | |
|---|---|---|---|
| 0.3386 | 0.9700 | 0.5791 | |
| 0.4305 | 0.9346 | 0.4582 | |
| 0.4896 | 0.8873 | 0.4011 | |
| 0.5226 | 0.8156 | 0.3645 | |
| 0.5350 | 0.7470 | 0.3450 | |
| 0.5478 | 0.5853 | 0.3268 | |
| 0.5521 | 0.5157 | 0.3208 | |
| 0.5576 | 0.4060 | 0.3078 | |
| 0.5602 | 0.3280 | 0.2889 | |
| 0.5622 | 0.2720 | 0.2720 | AZEO |
| 0.5614 | 0.2511 | 0.2646 | |
| 0.5593 | 0.1996 | 0.2437 | |
| 0.5493 | 0.1214 | 0.1901 | |
| 0.5253 | 0.0529 | 0.1061 | |

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**Isobaric phase equilibrium data**

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Acosta, Jhoany - Arce, Alberto - Rodil, Eva - Soto, Ana, A thermodynamic study on binary and ternary mixtures of acetonitrile, water and butyl acetate, Fluid Phase Equilibria 1-2 (2002) 83-98. doi:10.1016/S0378-3812(02)00171-1

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 372.77 | 0.9994 | 0.9864 |
| 371.86 | 0.9969 | 0.9545 |
| 371.51 | 0.9967 | 0.9398 |
| 370.42 | 0.9936 | 0.9045 |
| 369.07 | 0.9894 | 0.8539 |
| 367.92 | 0.9866 | 0.8148 |
| 366.81 | 0.9831 | 0.7758 |
| 365.98 | 0.9805 | 0.7445 |
| 364.89 | 0.9766 | 0.7079 |
| 363.57 | 0.9716 | 0.6706 |
| 362.09 | 0.9639 | 0.6213 |
| 360.43 | 0.9566 | 0.5811 |
| 358.96 | 0.9471 | 0.5445 |
| 357.11 | 0.9325 | 0.4946 |
| 354.78 | 0.9031 | 0.4479 |
| 353.12 | 0.8657 | 0.4123 |
| 351.64 | 0.7932 | 0.3833 |
| 350.87 | 0.7036 | 0.3654 |
| 350.61 | 0.6551 | 0.3631 |
| 350.31 | 0.5944 | 0.3567 |
| 350.07 | 0.5167 | 0.3470 |
| 349.86 | 0.4590 | 0.3387 |
| 349.74 | 0.3997 | 0.3290 |
| 349.66 | 0.3232 | 0.3113 |
| 349.68 | 0.2886 | 0.3018 |
| 349.72 | 0.2511 | 0.2868 |
| 349.82 | 0.2234 | 0.2741 |
| 349.92 | 0.2090 | 0.2614 |
| 350.07 | 0.1795 | 0.2490 |

| | | |
|---|---|---|
| 350.25 | 0.1610 | 0.2351 |
| 350.53 | 0.1353 | 0.2154 |
| 350.79 | 0.1182 | 0.1993 |
| 351.11 | 0.1016 | 0.1811 |
| 351.56 | 0.0821 | 0.1569 |
| 352.08 | 0.0626 | 0.1292 |
| 353.04 | 0.0356 | 0.0819 |
| 353.64 | 0.0214 | 0.0524 |

Conner, Albert Z. - Elving, Philip J. - Steingiser, Samuel, Vapor-Liquid Equilibria in Binary System Acetaldehyde Dibutyl Acetal–n–Butanol, Industrial & Engineering Chemistry 3 (1948) 497-499. doi:10.1021/ie50459a032

**P / bar = 3.009**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 385.60 | 0.7140 | 0.4580 |
| 385.35 | 0.5550 | 0.4440 |
| 385.27 | 0.4930 | 0.4170 |
| 385.22 | 0.4460 | 0.4110 |
| 385.16 | 0.3270 | 0.3860 |
| 385.18 | 0.3420 | 0.3820 |
| 385.32 | 0.2930 | 0.3580 |
| 385.66 | 0.2550 | 0.3250 |

Conner, Albert Z. - Elving, Philip J. - Steingiser, Samuel, Vapor-Liquid Equilibria in Binary System Acetaldehyde Dibutyl Acetal–n–Butanol, Industrial & Engineering Chemistry 3 (1948) 497-499. doi:10.1021/ie50459a032

**P / bar = 3.921**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 396.36 | 0.7410 | 0.5080 |
| 395.20 | 0.6430 | 0.4760 |
| 394.88 | 0.5290 | 0.4460 |
| 394.81 | 0.4990 | 0.4380 |
| 394.95 | 0.4470 | 0.4230 |
| 394.88 | 0.3780 | 0.3980 |
| 394.94 | 0.3410 | 0.3840 |
| 395.06 | 0.2970 | 0.3520 |
| 395.36 | 0.2560 | 0.3410 |

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**Enthalpy of mixing**

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Stokes, R.H, Excess partial molar enthalpies for (acetonitrile + water) from 278 to 318 K, The Journal of Chemical Thermodynamics 9 (1987) 977-983. doi:10.1016/0021-9614(87)90044-9

**T / K = 278.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -4.600 | 0.9987 |
| -13.30 | 0.9960 |
| -24.90 | 0.9919 |
| -37.20 | 0.9864 |
| -46.00 | 0.9808 |
| -51.20 | 0.9752 |
| -53.00 | 0.9698 |
| -51.90 | 0.9643 |
| -48.20 | 0.9590 |
| -38.20 | 0.9509 |
| -17.70 | 0.9398 |
| 9.200 | 0.9287 |
| 40.10 | 0.9175 |
| 73.10 | 0.9063 |
| 107.20 | 0.8950 |
| 141.60 | 0.8836 |
| 175.40 | 0.8723 |
| 208.10 | 0.8609 |
| 239.90 | 0.8494 |
| 270.60 | 0.8379 |
| 300.00 | 0.8264 |
| 327.80 | 0.8149 |
| 354.50 | 0.8034 |
| 380.40 | 0.7918 |
| 405.00 | 0.7802 |
| 428.70 | 0.7687 |
| 451.80 | 0.7572 |
| 474.30 | 0.7456 |
| 495.90 | 0.7340 |
| 516.90 | 0.7224 |
| 537.50 | 0.7109 |
| 557.30 | 0.6994 |
| 586.50 | 0.6842 |
| 611.30 | 0.6683 |
| 635.70 | 0.6522 |
| 661.90 | 0.6343 |
| 689.40 | 0.6145 |
| 717.40 | 0.5933 |
| 745.60 | 0.5709 |
| 773.70 | 0.5469 |
| 802.80 | 0.5200 |
| 830.70 | 0.4913 |
| 857.40 | 0.4596 |
| 881.00 | 0.4250 |
| 898.80 | 0.3873 |
| 907.80 | 0.3444 |
| 901.40 | 0.2973 |

| | |
|---|---|
| 881.30 | 0.2586 |
| 856.60 | 0.2307 |
| 819.20 | 0.2011 |
| 764.60 | 0.1697 |
| 685.20 | 0.1363 |
| 570.40 | 0.1005 |
| 403.10 | 0.0623 |
| 227.90 | 0.0318 |
| 128.30 | 0.0170 |
| 65.20 | 0.0084 |
| 15.60 | 0.0020 |

Nakamura, Masanori - Tamura, Katsutoshi - Murakami, Sachio, Isotope effects on thermodynamic properties: mixtures of x(D2O or H2O) + (1 − x)CH3CN at 298.15 K, Thermochimica Acta (1995) 127-136. doi:10.1016/0040-6031(94)02086-4

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -8.500 | 0.9750 |
| 30.70 | 0.9500 |
| 180.60 | 0.9000 |
| 326.10 | 0.8500 |
| 454.70 | 0.8000 |
| 568.80 | 0.7500 |
| 669.70 | 0.7000 |
| 758.90 | 0.6500 |
| 840.60 | 0.6000 |
| 909.70 | 0.5500 |
| 969.40 | 0.5000 |
| 1015.2 | 0.4500 |
| 1045.6 | 0.4000 |
| 1058.5 | 0.3500 |
| 1044.3 | 0.3000 |
| 1001.2 | 0.2500 |
| 926.90 | 0.2000 |

Stokes, R.H, Excess partial molar enthalpies for (acetonitrile + water) from 278 to 318 K, The Journal of Chemical Thermodynamics 9 (1987) 977-983. doi:10.1016/0021-9614(87)90044-9

**T / K = 308.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -1.200 | 0.9978 |
| -2.100 | 0.9946 |
| -2.200 | 0.9927 |
| -1.800 | 0.9895 |
| 0.8000 | 0.9842 |
| 5.400 | 0.9793 |
| 20.10 | 0.9692 |
| 40.30 | 0.9594 |
| 64.50 | 0.9497 |
| 91.30 | 0.9403 |
| 119.80 | 0.9310 |
| 149.10 | 0.9219 |
| 208.20 | 0.9042 |
| 266.20 | 0.8871 |
| 320.20 | 0.8709 |
| 371.30 | 0.8550 |
| 418.50 | 0.8398 |
| 462.10 | 0.8251 |
| 503.00 | 0.8110 |
| 540.60 | 0.7973 |
| 575.70 | 0.7840 |
| 608.80 | 0.7712 |
| 639.50 | 0.7588 |
| 652.50 | 0.7544 |
| 666.50 | 0.7485 |
| 668.00 | 0.7468 |
| 694.50 | 0.7364 |
| 695.00 | 0.7357 |
| 725.40 | 0.7224 |
| 756.90 | 0.7077 |
| 792.60 | 0.6903 |
| 828.40 | 0.6719 |
| 869.00 | 0.6497 |
| 910.80 | 0.6250 |
| 954.90 | 0.5977 |
| 1000.7 | 0.5654 |
| 1047.7 | 0.5263 |
| 1091.2 | 0.4817 |
| 1128.9 | 0.4259 |
| 1139.1 | 0.3931 |
| 1141.7 | 0.3574 |
| 1129.9 | 0.3167 |
| 1092.7 | 0.2703 |
| 1013.5 | 0.2172 |
| 859.40 | 0.1560 |
| 736.00 | 0.1216 |
| 563.90 | 0.0843 |
| 475.00 | 0.0683 |
| 381.80 | 0.0523 |
| 270.50 | 0.0349 |
| 146.90 | 0.0178 |

Schedemann, A., Weiterentwicklung von thermodynamischen Vorhersagemethoden als Grundlage für die Lösungsmittelauswahl bei der Flüssig-Flüssig-Extraktion und der Absorption (2013)

**T / K =** **363.15**

**P / bar =** **16.87**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| 276.29 | 0.9410 |
| 560.65 | 0.8822 |
| 806.54 | 0.8233 |
| 1020.4 | 0.7643 |
| 1198.5 | 0.7055 |
| 1345.8 | 0.6466 |
| 1461.5 | 0.5879 |
| 1547.7 | 0.5288 |
| 1594.6 | 0.4703 |
| 1605.0 | 0.4114 |
| 1570.1 | 0.3524 |
| 1484.6 | 0.2936 |
| 1340.3 | 0.2348 |
| 1125.7 | 0.1763 |
| 820.48 | 0.1173 |
| 442.24 | 0.0590 |

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**Heat capacity of mixing**

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De Visser, Cees - Heuvelsland, Wim J. M. - Dunn, Lawrence A. - Somsen, Gus, Some properties of binary aqueous liquid mixtures. Apparent molar volumes and heat capacities at 298.15 K over the whole mole fraction range, Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases 0 (1978) doi:10.1039/f19787401159

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 2.200 | 0.9760 |
| 4.000 | 0.9530 |
| 4.900 | 0.9200 |
| 4.800 | 0.9000 |
| 5.800 | 0.8500 |
| 6.800 | 0.7970 |
| 6.900 | 0.7500 |
| 7.700 | 0.7200 |
| 8.700 | 0.6360 |
| 8.900 | 0.6010 |
| 9.100 | 0.5780 |
| 9.020 | 0.4960 |
| 9.400 | 0.4000 |
| 8.800 | 0.3290 |
| 7.400 | 0.2440 |
| 5.700 | 0.1750 |
| 3.500 | 0.1080 |
| 1.900 | 0.0600 |

Nakamura, Masanori - Tamura, Katsutoshi - Murakami, Sachio, Isotope effects on thermodynamic properties: mixtures of x(D2O or H2O) + (1 − x)CH3CN at 298.15 K, Thermochimica Acta (1995) 127-136. doi:10.1016/0040-6031(94)02086-4

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 2.150 | 0.9750 |
| 3.510 | 0.9500 |
| 4.710 | 0.9000 |
| 5.250 | 0.8499 |
| 5.910 | 0.7999 |
| 6.610 | 0.7499 |
| 7.230 | 0.6999 |
| 7.830 | 0.6499 |
| 8.280 | 0.5999 |
| 8.540 | 0.5499 |
| 8.680 | 0.4999 |
| 8.620 | 0.4499 |
| 8.400 | 0.3999 |
| 7.930 | 0.3499 |
| 7.360 | 0.2999 |
| 6.490 | 0.2499 |
| 5.430 | 0.1999 |
| 4.090 | 0.1499 |
| 2.570 | 0.0999 |
| 1.050 | 0.0500 |

Benson, George C. - D'Arcy, Patrick J. - Handa, Yash Paul, Thermodynamics of aqueous mixtures of nonelectrolytes. V. Isobaric heat capacities and ultrasonic speeds for water + ethanenitrile mixtures at 25°C, Thermochimica Acta 3 (1981) 295-301. doi:10.1016/0040-6031(81)80328-0

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.5060 | 0.9948 |
| 1.314 | 0.9853 |
| 2.070 | 0.9755 |
| 2.770 | 0.9643 |

| | |
|---|---|
| 3.390 | 0.9509 |
| 3.790 | 0.9392 |
| 4.040 | 0.9301 |
| 4.240 | 0.9202 |
| 4.440 | 0.9089 |
| 4.530 | 0.9009 |
| 4.900 | 0.8737 |
| 4.980 | 0.8612 |
| 5.140 | 0.8523 |
| 5.340 | 0.8309 |
| 5.730 | 0.8023 |
| 5.930 | 0.7843 |
| 6.080 | 0.7719 |
| 6.370 | 0.7523 |
| 6.690 | 0.7305 |
| 7.060 | 0.7012 |
| 7.060 | 0.6950 |
| 7.680 | 0.6441 |
| 8.090 | 0.6047 |
| 8.050 | 0.5999 |
| 8.260 | 0.5541 |
| 8.300 | 0.5098 |
| 8.380 | 0.4973 |
| 8.180 | 0.4617 |
| 8.290 | 0.4501 |
| 7.540 | 0.3403 |
| 7.130 | 0.3049 |
| 6.060 | 0.2398 |
| 5.150 | 0.2013 |
| 3.660 | 0.1469 |
| 2.880 | 0.1231 |
| 2.280 | 0.1029 |
| 1.730 | 0.0837 |
| 0.9400 | 0.0548 |
| 0.3100 | 0.0280 |

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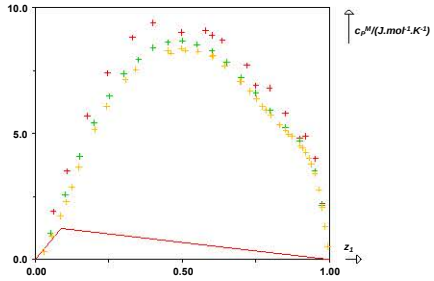
**Azeotropic point**

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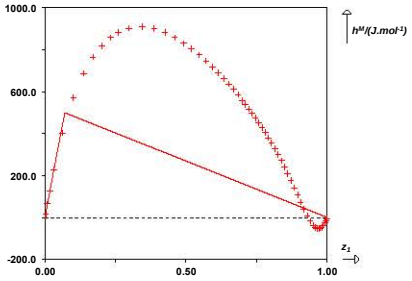
Acosta, Jhoany - Arce, Alberto - Rodil, Eva - Soto, Ana, A thermodynamic study on binary and ternary mixtures of acetonitrile, water and butyl acetate, Fluid Phase Equilibria 1-2 (2002) 83-98. doi:10.1016/S0378-3812(02)00171-1

| T / K | P / bar | $x_1$ |
|---|---|---|
| 349.66 | 1.013 | 0.3050 |

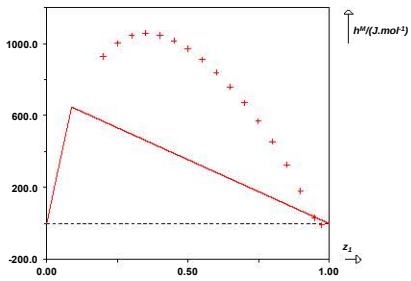
T/K = 298.15 - P/bar = 1.0132 1.0132 1.0132



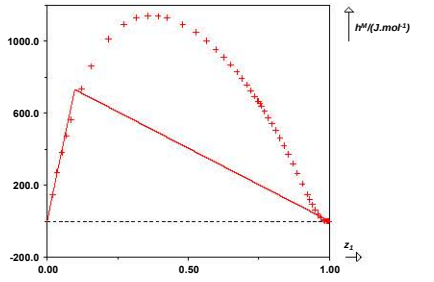

T/K = 278.15 - P/bar = 1.0132



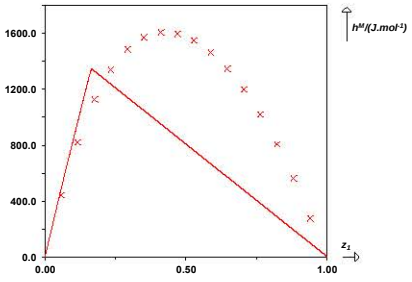

T/K = 298.15 - P/bar = 1.0132



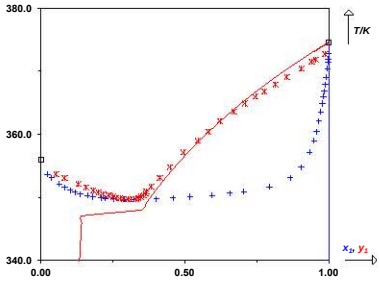

T/K = 308.15 - P/bar = 1.0132



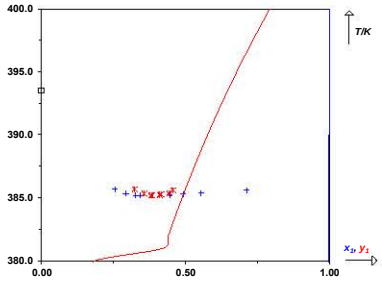

T/K = 363.15 - P/bar = 16.8700



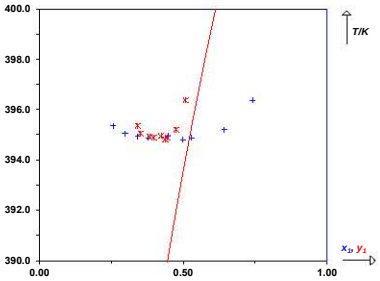

P/bar = 1.01320



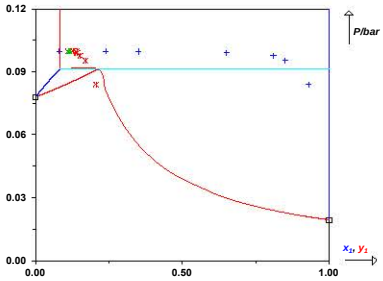

P/bar = 3.00930



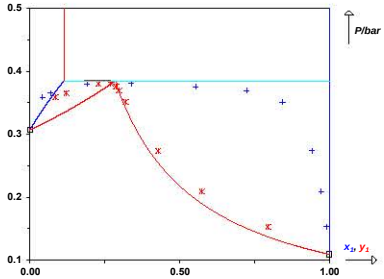

P/bar = 3.92130



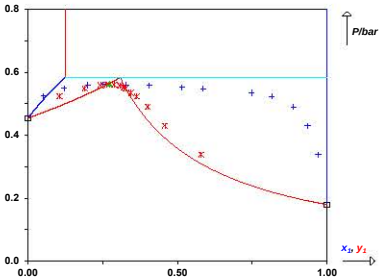

T/K = 293.15



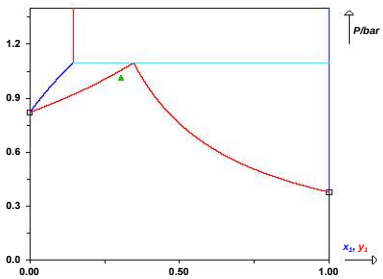

T/K = 323.15




T/K = 333.15




T/K = 349.66



## METHANOL (1) + WATER (2)

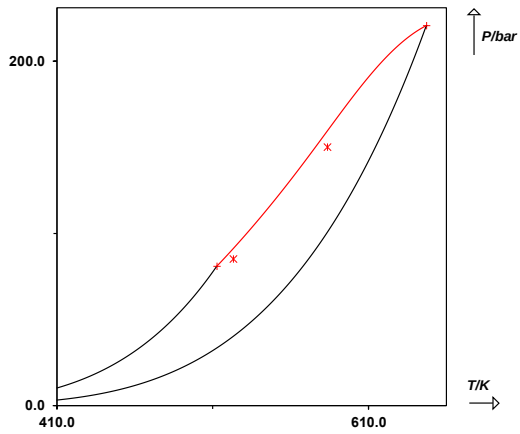
| | | |
|---|---|---|
| **CAS** | 67-56-1 | 7732-18-5 |
| **InChiKey** | OKKJLVBELUTLKV-UHFFFAOYSA-N | XLYOFNOQVPJJNP-UHFFFAOYSA-N |
| **$T_c$ / K** | 512.50 | 647.10 |
| **$P_c$ / bar** | 80.84 | 220.64 |
| **ω** | 0.566 | 0.345 |

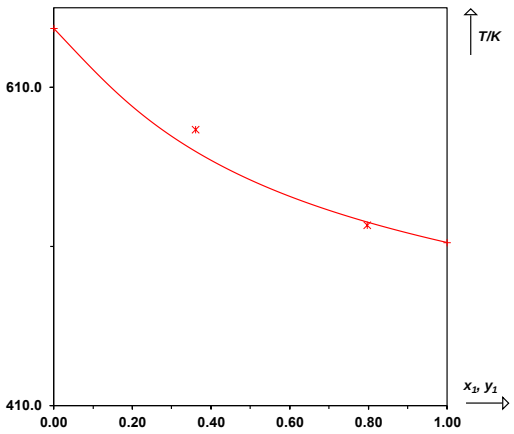
Non ideal with enthalpic and entropic causes

**PPR78 results**

*Parameters*
A/MPa = 557
B/MPa = -125

*Deviations*
MAPE on x = 15 %
MAPE on y = 9.8 %
MAPE on $x_c$ = 14 %
MAPE on $P_c$ = 6.7 %
MAPE on $h^M$ = 91 %
MAPE on $c_P^M$ = 93 %



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**Isothermal phase equilibrium data**

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Jinyan Fu - Kun Wang - Ying Hu, Studies on the Vapor-Liquid Equilibrium and Vapor-Liquid-Liquid Equilibrium for a Methanol-Methyl Methacrylate-WaterTernary System (I) Three Different Binary Systems, Huagong Xuebao 1 (1988) 64-76.

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0565 | 0.1029 | 0.5002 |
| 0.0757 | 0.2021 | 0.6533 |
| 0.0916 | 0.3032 | 0.7370 |
| 0.1033 | 0.4028 | 0.7927 |
| 0.1137 | 0.5019 | 0.8360 |
| 0.1252 | 0.6096 | 0.8760 |
| 0.1357 | 0.7073 | 0.9089 |
| 0.1457 | 0.8016 | 0.9390 |
| 0.1575 | 0.9000 | 0.9695 |

Maximo, Guilherme J. - Meirelles, Antonio J.A. - Batista, Eduardo A.C., Boiling point of aqueous d-glucose and d-fructose solutions: Experimental determination and modeling with group-contribution method, Fluid Phase Equilibria 1 (2010) 32-41. doi:10.1016/j.fluid.2010.08.018

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0583 | 0.1000 | 0.5070 |
| 0.0760 | 0.2000 | 0.6540 |
| 0.0900 | 0.3000 | 0.7330 |
| 0.1020 | 0.4000 | 0.7890 |
| 0.1133 | 0.5000 | 0.8330 |
| 0.1243 | 0.6000 | 0.8710 |
| 0.1352 | 0.7000 | 0.9060 |
| 0.1461 | 0.8000 | 0.9390 |
| 0.1575 | 0.9000 | 0.9700 |

Jinyan Fu - Kun Wang - Ying Hu, Studies on the Vapor-Liquid Equilibrium and Vapor-Liquid-Liquid Equilibrium for a Methanol-Methyl Methacrylate-WaterTernary System (I) Three Different Binary Systems, Huagong Xuebao 1 (1988) 64-76.

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0981 | 0.1029 | 0.4872 |
| 0.1291 | 0.2021 | 0.6394 |
| 0.1545 | 0.3032 | 0.7234 |
| 0.1736 | 0.4028 | 0.7801 |
| 0.1903 | 0.5019 | 0.8247 |
| 0.2084 | 0.6096 | 0.8666 |
| 0.2253 | 0.7073 | 0.9014 |
| 0.2416 | 0.8016 | 0.9336 |
| 0.2601 | 0.9000 | 0.9666 |

McGlashan, M. L. - Williamson, A. G., Isothermal liquid-vapor equilibriums for system methanol-water, Journal of Chemical & Engineering Data 2 (1976) 196-199. doi:10.1021/je60069a019

**T / K = 308.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0733 | 0.0408 | 0.2490 |
| 0.1087 | 0.1387 | 0.5274 |
| 0.1401 | 0.2488 | 0.6738 |
| 0.1640 | 0.3603 | 0.7559 |
| 0.1835 | 0.4694 | 0.8084 |
| 0.2058 | 0.6012 | 0.8611 |
| 0.2268 | 0.7239 | 0.9071 |
| 0.2398 | 0.7951 | 0.9316 |
| 0.2576 | 0.8880 | 0.9636 |
| 0.2586 | 0.9005 | 0.9683 |
| 0.2680 | 0.9406 | 0.9815 |

Jinyan Fu - Kun Wang - Ying Hu, Studies on the Vapor-Liquid Equilibrium and Vapor-Liquid-Liquid Equilibrium for a Methanol-Methyl Methacrylate-WaterTernary System (I) Three Different Binary Systems, Huagong Xuebao 1 (1988) 64-76.

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1639 | 0.1029 | 0.4750 |
| 0.2125 | 0.2021 | 0.6260 |
| 0.2516 | 0.3032 | 0.7103 |
| 0.2813 | 0.4028 | 0.7679 |
| 0.3073 | 0.5019 | 0.8137 |
| 0.3354 | 0.6096 | 0.8573 |
| 0.3618 | 0.7073 | 0.8940 |
| 0.3868 | 0.8016 | 0.9283 |
| 0.4148 | 0.9000 | 0.9638 |

Yao, Jia - Li, Haoran - Han, Shijun, Vapor–liquid equilibrium data for methanol–water–NaCl at 45°C, Fluid Phase Equilibria 1-2 (1999) 253-260. doi:10.1016/S0378-3812(99)00204-6

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1477 | 0.0753 | 0.3986 |
| 0.1819 | 0.1358 | 0.5384 |
| 0.2189 | 0.2171 | 0.6466 |
| 0.2476 | 0.2926 | 0.7082 |
| 0.2767 | 0.3805 | 0.7641 |
| 0.3007 | 0.4731 | 0.8073 |

| | | |
|---|---|---|
| 0.3258 | 0.5563 | 0.8397 |
| 0.3518 | 0.6507 | 0.8743 |
| 0.3814 | 0.7604 | 0.9136 |
| 0.4095 | 0.8739 | 0.9538 |
| 0.4278 | 0.9354 | 0.9773 |

Kurihara, Kiyofumi - Minoura, Tsuyoshi - Takeda, Kouichi - Kojima, Kazuo, Isothermal Vapor-Liquid Equilibria for Methanol + Ethanol + Water, Methanol + Water, and Ethanol + Water, Journal of Chemical & Engineering Data 3 (1995) 679-684. doi:10.1021/je00019a033

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2912 | 0.2470 | 0.6710 |
| 0.3062 | 0.2842 | 0.7029 |
| 0.3114 | 0.2940 | 0.7109 |
| 0.3279 | 0.3338 | 0.7373 |
| 0.3532 | 0.4028 | 0.7772 |
| 0.3628 | 0.4316 | 0.7873 |
| 0.3809 | 0.4872 | 0.8100 |
| 0.3934 | 0.5314 | 0.8254 |
| 0.4016 | 0.5513 | 0.8326 |
| 0.4061 | 0.5688 | 0.8410 |
| 0.4205 | 0.6145 | 0.8569 |
| 0.4492 | 0.6989 | 0.8890 |
| 0.4594 | 0.7290 | 0.8991 |
| 0.4733 | 0.7730 | 0.9160 |

Dulitskaya, K.A., Vapor pressure of binary systems. I, Zh. Obshch. Khim. 1-2 (1945) 9-21.

**T / K = 323.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1907 | 0.0873 | 0.3783 |
| 0.2620 | 0.1900 | 0.5883 |
| 0.3260 | 0.3417 | 0.7076 |
| 0.3813 | 0.4943 | 0.7807 |
| 0.4440 | 0.6919 | 0.8655 |
| 0.4973 | 0.8492 | 0.9349 |

Jinyan Fu - Kun Wang - Ying Hu, Studies on the Vapor-Liquid Equilibrium and Vapor-Liquid-Liquid Equilibrium for a Methanol-Methyl Methacrylate-WaterTernary System (I) Three Different Binary Systems, Huagong Xuebao 1 (1988) 64-76.

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.2652 | 0.1029 | 0.4635 |
| 0.3398 | 0.2021 | 0.6131 |
| 0.3977 | 0.3032 | 0.6976 |
| 0.4429 | 0.4028 | 0.7559 |
| 0.4822 | 0.5019 | 0.8029 |
| 0.5240 | 0.6096 | 0.8481 |
| 0.5640 | 0.7073 | 0.8867 |
| 0.6018 | 0.8016 | 0.9231 |
| 0.6429 | 0.9000 | 0.9610 |

Kurihara, Kiyofumi - Minoura, Tsuyoshi - Takeda, Kouichi - Kojima, Kazuo, Isothermal Vapor-Liquid Equilibria for Methanol + Ethanol + Water, Methanol + Water, and Ethanol + Water, Journal of Chemical & Engineering Data 3 (1995) 679-684. doi:10.1021/je00019a033

**T / K = 328.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3071 | 0.1587 | 0.5660 |
| 0.3337 | 0.1980 | 0.6154 |
| 0.3904 | 0.2961 | 0.7019 |
| 0.4022 | 0.3171 | 0.7182 |
| 0.4084 | 0.3339 | 0.7280 |
| 0.4214 | 0.3610 | 0.7432 |
| 0.4276 | 0.3733 | 0.7504 |
| 0.4424 | 0.4137 | 0.7693 |
| 0.4518 | 0.4346 | 0.7799 |
| 0.4674 | 0.4753 | 0.7947 |
| 0.4818 | 0.5078 | 0.8079 |
| 0.5050 | 0.5669 | 0.8315 |
| 0.5110 | 0.5897 | 0.8401 |
| 0.5197 | 0.6030 | 0.8495 |
| 0.5223 | 0.6091 | 0.8502 |
| 0.5266 | 0.6217 | 0.8557 |
| 0.5425 | 0.6600 | 0.8709 |
| 0.5496 | 0.6781 | 0.8770 |
| 0.5598 | 0.7032 | 0.8866 |
| 0.5921 | 0.7808 | 0.9183 |

Jinyan Fu - Kun Wang - Ying Hu, Studies on the Vapor-Liquid Equilibrium and Vapor-Liquid-Liquid Equilibrium for a Methanol-Methyl Methacrylate-WaterTernary System (I) Three Different Binary Systems, Huagong Xuebao 1 (1988) 64-76.

**T / K = 333.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3337 | 0.1029 | 0.4579 |
| 0.4256 | 0.2021 | 0.6069 |
| 0.4956 | 0.3032 | 0.6914 |
| 0.5498 | 0.4028 | 0.7501 |
| 0.5977 | 0.5019 | 0.7976 |
| 0.6495 | 0.6096 | 0.8436 |
| 0.6959 | 0.7073 | 0.8831 |
| 0.7434 | 0.8016 | 0.9205 |

| | | |
|---|---|---|
| 0.7947 | 0.9000 | 0.9596 |

McGlashan, M. L. - Williamson, A. G., Isothermal liquid-vapor equilibriums for system methanol-water, Journal of Chemical & Engineering Data 2 (1976) 196-199. doi:10.1021/je60069a019

**T / K = 338.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3903 | 0.0854 | 0.3926 |
| 0.3920 | 0.0874 | 0.4018 |
| 0.4496 | 0.1328 | 0.4963 |
| 0.5030 | 0.1816 | 0.5718 |
| 0.5728 | 0.2586 | 0.6512 |
| 0.7264 | 0.4920 | 0.7842 |
| 0.7784 | 0.5815 | 0.8242 |
| 0.8462 | 0.7043 | 0.8747 |
| 0.9071 | 0.8028 | 0.9180 |
| 0.9696 | 0.9030 | 0.9605 |

Nagatani, M. - Fujino, K., Measurement of isothermal vapor-liquid equilibria for methanol-water system, Fukuoka Daigaku Kogaku Shuho (2000) 147-152.

**T / K = 338.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.3283 | 0.0481 | 0.2804 |
| 0.3819 | 0.0827 | 0.3848 |
| 0.3995 | 0.0970 | 0.4323 |
| 0.4012 | 0.1001 | 0.4352 |
| 0.4119 | 0.1073 | 0.4499 |
| 0.4126 | 0.1089 | 0.4589 |
| 0.4131 | 0.1090 | 0.4492 |
| 0.4531 | 0.1388 | 0.5118 |
| 0.4596 | 0.1450 | 0.5254 |
| 0.4768 | 0.1623 | 0.5515 |
| 0.4793 | 0.1644 | 0.5545 |
| 0.4914 | 0.1732 | 0.5676 |
| 0.4971 | 0.1814 | 0.5767 |
| 0.5032 | 0.1857 | 0.5799 |
| 0.5052 | 0.1900 | 0.5857 |
| 0.5656 | 0.2551 | 0.6512 |
| 0.5694 | 0.2600 | 0.6537 |
| 0.5824 | 0.2782 | 0.6672 |
| 0.5865 | 0.2830 | 0.6709 |
| 0.6370 | 0.3451 | 0.7098 |
| 0.6370 | 0.3542 | 0.7166 |
| 0.6413 | 0.3620 | 0.7122 |
| 0.6445 | 0.3667 | 0.7244 |
| 0.6968 | 0.4483 | 0.7640 |
| 0.6992 | 0.4527 | 0.7644 |
| 0.7021 | 0.4594 | 0.7694 |
| 0.7050 | 0.4624 | 0.7709 |
| 0.7659 | 0.5677 | 0.8173 |
| 0.7729 | 0.5781 | 0.8216 |
| 0.8216 | 0.6648 | 0.8592 |
| 0.8291 | 0.6790 | 0.8656 |
| 0.9003 | 0.7924 | 0.9100 |
| 0.8985 | 0.7937 | 0.9145 |
| 0.9033 | 0.7995 | 0.9171 |
| 0.9101 | 0.8115 | 0.9220 |

Bao, Z. - Liu, M. - Yang, J. - Wang, N., Measurement and Correlation of Moderate Pressure Vapor-Liquid Equilibrium Data for Methanol - Water Binary System, Huagong Xuebao 2 (1995) 230-233.

**T / K = 403.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 3.920 | 0.0990 | 0.3520 |
| 4.720 | 0.1960 | 0.5060 |
| 5.550 | 0.3460 | 0.6370 |
| 6.310 | 0.4920 | 0.7230 |
| 6.820 | 0.6430 | 0.7970 |
| 7.480 | 0.7930 | 0.8810 |
| 7.900 | 0.8910 | 0.9380 |
| 8.150 | 0.9420 | 0.9670 |

Schröder, W., Messungen von Siedegleichgewichten bei Überdruck: Messungen von Siedegleichgewichten bei Überdruck, Chemie Ingenieur Technik 8 (1958) 523-525. doi:10.1002/cite.330300809

**T / K = 413.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 5.096 | 0.0960 | 0.3440 |
| 6.799 | 0.2750 | 0.5790 |
| 7.879 | 0.4440 | 0.7020 |
| 8.826 | 0.5950 | 0.7860 |
| 9.933 | 0.7910 | 0.8800 |
| 10.59 | 0.9460 | 0.9620 |

Pryanikova, R.O. - Efremova, G.D., Liquid-vapor equilibrium and volume behavior of the methanol-water system at high temperatures and pressures, Fiz. Khim. Rastvorov (1972) 228-233.

**T / K = 523.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 40.53 | 0.0100 | 0.0300 |
| 45.60 | 0.0700 | 0.2270 |
| 50.66 | 0.1250 | 0.3500 |
| 55.73 | 0.1800 | 0.4500 |
| 60.80 | 0.2600 | 0.5550 |

| | | |
|---|---|---|
| 65.86 | 0.3350 | 0.6550 |
| 70.93 | 0.4500 | 0.7350 |

Pryanikova, R.O. - Efremova, G.D., Liquid-vapor equilibrium and volume behavior of the methanol-water system at high temperatures and pressures, Fiz. Khim. Rastvorov (1972) 228-233.

**T / K = 548.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 60.80 | 0.0200 | 0.0750 |
| 65.86 | 0.0550 | 0.2000 |
| 70.93 | 0.1000 | 0.2950 |
| 75.99 | 0.1450 | 0.3800 |
| 81.06 | 0.1950 | 0.4550 |
| 86.13 | 0.2400 | 0.5250 |

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**Isobaric phase equilibrium data**

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Yang, Changsheng - Sun, Feizhong - Ma, Shengyong - Yin, Xia - Zeng, Hao, Organic Salt Effect on Vapor–Liquid Equilibrium of the Methanol + Water System at Subatmospheric Pressure, Journal of Chemical & Engineering Data 10 (2012) 2696-2701. doi:10.1021/je300613v

**P / bar = 0.6662**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 358.06 | 0.0200 | 0.1390 |
| 355.88 | 0.0390 | 0.2350 |
| 352.16 | 0.0750 | 0.3660 |
| 346.11 | 0.1600 | 0.5380 |
| 342.54 | 0.2460 | 0.6380 |
| 341.06 | 0.2890 | 0.6740 |
| 339.77 | 0.3320 | 0.7060 |
| 338.16 | 0.3930 | 0.7440 |
| 336.93 | 0.4490 | 0.7690 |
| 335.03 | 0.5360 | 0.8160 |
| 333.76 | 0.6200 | 0.8490 |
| 331.93 | 0.7070 | 0.8880 |
| 330.31 | 0.8190 | 0.9350 |
| 328.20 | 0.9480 | 0.9830 |

Lesteva, T.M. - Ogorodnikov, S.K. - Kazakova, S.V., Liquid-vapor equilibrium in the trimethylcarbinol-methanol-water system at a pressure of 760 mm. V, J. Appl. Chem. USSR 7 (1970) 1582-1586.

**P / bar = 1.013**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 360.55 | 0.1000 | 0.3860 |
| 354.95 | 0.2000 | 0.5570 |
| 351.05 | 0.3000 | 0.6610 |
| 348.35 | 0.4000 | 0.7260 |
| 346.25 | 0.5000 | 0.7750 |
| 344.45 | 0.6000 | 0.8230 |
| 342.95 | 0.7000 | 0.8670 |
| 341.15 | 0.8000 | 0.9130 |
| 339.45 | 0.9000 | 0.9560 |

Hirata, M. - Suda, S., Vapor-liquid equilibrium under pressurized conditions; experimental apparatus and methanol-water system, Kagaku Kogaku 8 (1967) 759-766. doi:10.1252/kakoronbunshu1953.31.759

**P / bar = 8.106**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 438.25 | 0.0300 | 0.1430 |
| 434.25 | 0.0580 | 0.2320 |
| 429.35 | 0.1060 | 0.3430 |
| 425.25 | 0.1540 | 0.4340 |
| 421.45 | 0.2300 | 0.5140 |
| 418.05 | 0.3090 | 0.5760 |
| 415.15 | 0.3910 | 0.6310 |
| 411.45 | 0.5180 | 0.7200 |
| 408.95 | 0.6180 | 0.7850 |
| 406.95 | 0.7160 | 0.8460 |
| 404.65 | 0.8400 | 0.9100 |
| 404.55 | 0.8500 | 0.9140 |

Hirata, M. - Suda, S., Vapor-liquid equilibrium under pressurized conditions; experimental apparatus and methanol-water system, Kagaku Kogaku 8 (1967) 759-766. doi:10.1252/kakoronbunshu1953.31.759

**P / bar = 11.35**

| T / K | $x_1$ | $y_1$ |
|---|---|---|
| 451.05 | 0.0380 | 0.1640 |
| 447.85 | 0.0670 | 0.2410 |
| 443.25 | 0.1040 | 0.3380 |
| 438.75 | 0.1710 | 0.4340 |
| 434.85 | 0.2400 | 0.5120 |
| 431.35 | 0.3290 | 0.5830 |
| 427.45 | 0.4430 | 0.6640 |
| 425.25 | 0.5110 | 0.7100 |
| 421.15 | 0.6700 | 0.8040 |
| 420.05 | 0.7170 | 0.8250 |
| 417.65 | 0.8450 | 0.9080 |

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**Enthalpy of mixing**

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Bose, E., Remarks on thermochemical statement of Julius Thomsens, Phys. Z. 14 (1906) 503-505.

**T / K = 273.15**

**P / bar =** **UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -243.63 | 0.0288 |
| -485.11 | 0.0588 |
| -636.97 | 0.0903 |
| -783.47 | 0.1233 |
| -883.09 | 0.1579 |
| -948.16 | 0.1942 |
| -988.20 | 0.2324 |
| -994.68 | 0.2727 |
| -988.93 | 0.3151 |
| -970.28 | 0.3600 |
| -945.07 | 0.4074 |
| -914.24 | 0.4576 |
| -870.13 | 0.5109 |
| -809.79 | 0.5675 |
| -743.42 | 0.6279 |
| -658.23 | 0.6923 |
| -555.15 | 0.7612 |
| -420.93 | 0.8350 |
| -245.41 | 0.9144 |

Cochran, S.W. - Holste, J.C. - Marsh, K.N. - Gammon, B.E. - Hall, K.R., Enthalpies of water + methanol mixtures between 180 K and 320 K, Fluid Phase Equilibria (1993) 171-181. doi:10.1016/0378-3812(93)87110-M

**T / K =** **288.15**

**P / bar =** **1.013**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -26.80 | 0.0035 |
| -79.80 | 0.0103 |
| -131.40 | 0.0171 |
| -181.70 | 0.0240 |
| -230.80 | 0.0309 |
| -278.10 | 0.0378 |
| -323.60 | 0.0447 |
| -367.30 | 0.0516 |
| -429.20 | 0.0619 |
| -504.70 | 0.0756 |
| -572.10 | 0.0893 |
| -632.00 | 0.1030 |
| -685.60 | 0.1168 |
| -731.50 | 0.1304 |
| -771.00 | 0.1440 |
| -805.60 | 0.1575 |
| -834.30 | 0.1710 |
| -858.50 | 0.1845 |
| -878.90 | 0.1979 |
| -895.60 | 0.2113 |
| -908.70 | 0.2245 |
| -918.70 | 0.2376 |
| -926.60 | 0.2508 |
| -932.40 | 0.2641 |
| -937.60 | 0.2824 |
| -938.60 | 0.2939 |
| -938.60 | 0.3060 |
| -937.50 | 0.3188 |
| -934.60 | 0.3324 |
| -930.10 | 0.3467 |
| -924.70 | 0.3618 |
| -918.00 | 0.3776 |
| -909.80 | 0.3945 |
| -899.80 | 0.4124 |
| -887.90 | 0.4314 |
| -874.20 | 0.4515 |
| -858.40 | 0.4730 |
| -840.40 | 0.4959 |
| -819.70 | 0.5205 |
| -795.90 | 0.5467 |
| -768.80 | 0.5748 |
| -737.30 | 0.6052 |
| -701.00 | 0.6379 |
| -659.20 | 0.6733 |
| -609.30 | 0.7118 |
| -548.70 | 0.7536 |
| -493.90 | 0.7876 |
| -452.00 | 0.8116 |
| -404.90 | 0.8367 |
| -351.60 | 0.8630 |
| -290.70 | 0.8907 |
| -220.80 | 0.9199 |
| -140.40 | 0.9507 |
| -49.60 | 0.9831 |

Tomaszkiewicz, Iwona - Randzio, Stanisław.L. - Gierycz, Paweł, Excess enthalpy in the methanol-water system at 278.15, 298.15 and 323.15 k under pressures of 0.1, 20 and 39 mpa, Thermochimica Acta 2 (1986) 281-289. doi:10.1016/0040-6031(86)85164-4

**T / K =** **298.15**

**P / bar =** **390.00**

| $h^M$ / J.mol$^{-1}$ | $z_1$ |
|---|---|
| -564.00 | 0.0980 |
| -795.00 | 0.1910 |
| -869.00 | 0.2520 |
| -892.00 | 0.3390 |
| -849.00 | 0.4400 |

| | |
|---|---|
| -787.00 | 0.5200 |
| -726.00 | 0.6040 |

Cochran, S.W. - Holste, J.C. - Marsh, K.N. - Gammon, B.E. - Hall, K.R., Enthalpies of water + methanol mixtures between 180 K and 320 K, Fluid Phase Equilibria (1993) 171-181. doi:10.1016/0378-3812(93)87110-M

| | |
|---|---|
| **T / K =** | **318.15** |
| **P / bar =** | **1.013** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| -13.50 | 0.0023 |
| -39.80 | 0.0068 |
| -69.90 | 0.0121 |
| -107.90 | 0.0189 |
| -148.30 | 0.0264 |
| -206.20 | 0.0377 |
| -278.50 | 0.0527 |
| -344.30 | 0.0678 |
| -403.80 | 0.0828 |
| -457.20 | 0.0978 |
| -504.60 | 0.1129 |
| -545.70 | 0.1278 |
| -581.60 | 0.1428 |
| -613.20 | 0.1577 |
| -640.60 | 0.1727 |
| -663.60 | 0.1876 |
| -682.60 | 0.2022 |
| -698.50 | 0.2169 |
| -711.50 | 0.2316 |
| -721.80 | 0.2463 |
| -725.40 | 0.2553 |
| -729.70 | 0.2606 |
| -731.10 | 0.2670 |
| -735.80 | 0.2750 |
| -735.80 | 0.2793 |
| -740.20 | 0.2893 |
| -739.40 | 0.2924 |
| -743.20 | 0.3039 |
| -741.80 | 0.3062 |
| -744.80 | 0.3181 |
| -743.00 | 0.3208 |
| -745.10 | 0.3315 |
| -743.10 | 0.3365 |
| -741.80 | 0.3532 |
| -739.30 | 0.3708 |
| -735.50 | 0.3896 |
| -729.50 | 0.4097 |
| -721.90 | 0.4313 |
| -712.20 | 0.4545 |
| -700.40 | 0.4794 |
| -686.10 | 0.5062 |
| -669.00 | 0.5352 |
| -649.30 | 0.5666 |
| -625.60 | 0.6009 |
| -596.30 | 0.6382 |
| -560.00 | 0.6791 |
| -513.90 | 0.7241 |
| -454.00 | 0.7739 |
| -373.70 | 0.8293 |
| -293.90 | 0.8751 |
| -228.60 | 0.9079 |
| -158.50 | 0.9395 |
| -95.00 | 0.9653 |
| -33.90 | 0.9882 |

Hynek, V. - Degrange, S. - Polednicek, M. - Majer, V. - Quint, J. - Grolier, J.P.E., Combined flow-mixing power-compensation calorimeter and vibrating tube densimeter for measurements at superambient condition, J. Solution Chem. 6 (1999) 631-666. doi:10.1023/A:1021759810070

| | |
|---|---|
| **T / K =** | **523.15** |
| **P / bar =** | **200.00** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 65.00 | 0.0160 |
| 128.00 | 0.0320 |
| 168.00 | 0.0430 |
| 238.00 | 0.0660 |
| 259.00 | 0.0750 |
| 304.00 | 0.0890 |
| 394.00 | 0.1190 |
| 457.00 | 0.1400 |
| 520.00 | 0.1680 |
| 612.00 | 0.2260 |
| 743.00 | 0.3270 |
| 826.00 | 0.4130 |
| 835.00 | 0.4470 |
| 840.00 | 0.4890 |
| 824.00 | 0.5480 |
| 759.00 | 0.6200 |
| 733.00 | 0.6660 |

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**Heat capacity of mixing**

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Benson, George C. - D'Arcy, Patrick J., Excess isobaric heat capacities of water-n-alcohol mixtures, Journal of

Chemical & Engineering Data 4 (1982) 439-442. doi:10.1021/je00030a021

**T / K = 288.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 1.0000 | 0.0130 |
| 1.450 | 0.0192 |
| 1.850 | 0.0250 |
| 2.200 | 0.0303 |
| 2.840 | 0.0410 |
| 3.270 | 0.0489 |
| 3.370 | 0.0513 |
| 3.870 | 0.0614 |
| 4.170 | 0.0686 |
| 4.310 | 0.0725 |
| 4.600 | 0.0809 |
| 4.900 | 0.0908 |
| 5.140 | 0.1010 |
| 5.470 | 0.1201 |
| 5.480 | 0.1243 |
| 5.650 | 0.1489 |
| 5.650 | 0.1725 |
| 5.600 | 0.1892 |
| 5.500 | 0.2046 |
| 5.340 | 0.2255 |
| 5.060 | 0.2503 |
| 4.930 | 0.2716 |
| 4.720 | 0.2909 |
| 4.470 | 0.3194 |
| 4.410 | 0.3239 |
| 4.230 | 0.3411 |
| 4.010 | 0.3719 |
| 3.610 | 0.4069 |
| 3.500 | 0.4310 |
| 3.260 | 0.4629 |
| 3.030 | 0.4862 |
| 2.810 | 0.5235 |
| 2.540 | 0.5455 |
| 2.410 | 0.5731 |
| 2.370 | 0.5847 |
| 2.020 | 0.6304 |
| 1.870 | 0.6474 |
| 1.770 | 0.6698 |
| 1.530 | 0.7007 |
| 1.430 | 0.7253 |
| 1.120 | 0.7658 |
| 0.9000 | 0.8001 |
| 0.6600 | 0.8375 |
| 0.5400 | 0.8531 |
| 0.3900 | 0.8843 |
| 0.1500 | 0.9366 |

Benson, George C. - D'Arcy, Patrick J. - Kiyohara, Osamu, Thermodynamics of aqueous mixtures of nonelectrolytes II. Isobaric heat capacities of water-n-alcohol mixtures at 25°C, Journal of Solution Chemistry 12 (1980) 931-938. doi:10.1007/BF00646404

**T / K = 298.15**

**P / bar = UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 0.7050 | 0.0094 |
| 1.486 | 0.0204 |
| 2.060 | 0.0290 |
| 2.750 | 0.0400 |
| 3.210 | 0.0491 |
| 3.380 | 0.0510 |
| 3.840 | 0.0597 |
| 4.280 | 0.0690 |
| 4.730 | 0.0794 |
| 5.180 | 0.0912 |
| 5.460 | 0.1008 |
| 5.490 | 0.1018 |
| 6.240 | 0.1312 |
| 6.290 | 0.1449 |
| 6.770 | 0.1852 |
| 6.750 | 0.2014 |
| 6.740 | 0.2017 |
| 6.750 | 0.2334 |
| 6.540 | 0.2744 |
| 6.290 | 0.2989 |
| 6.230 | 0.3053 |
| 5.980 | 0.3362 |
| 5.540 | 0.3824 |
| 5.490 | 0.3949 |
| 5.430 | 0.4001 |
| 4.920 | 0.4565 |
| 4.500 | 0.5054 |
| 4.500 | 0.5069 |
| 4.100 | 0.5533 |
| 3.710 | 0.5981 |
| 3.600 | 0.6049 |
| 3.260 | 0.6483 |
| 2.800 | 0.6967 |
| 2.700 | 0.6967 |
| 2.310 | 0.7475 |
| 1.820 | 0.7972 |

| | |
|---|---|
| 1.680 | 0.7986 |
| 1.400 | 0.8467 |
| 0.6600 | 0.9011 |
| 0.7200 | 0.9077 |
| 0.4700 | 0.9375 |
| 0.2400 | 0.9582 |

Ogawa, Hideo - Murakami, Sachio, Excess isobaric heat capacities for water + alkanol mixtures at 298.15 K, Thermochimica Acta 1 (1986) 145-154. doi:10.1016/0040-6031(86)85016-X

**T / K =** **298.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 1.775 | 0.0250 |
| 3.305 | 0.0500 |
| 4.550 | 0.0750 |
| 5.479 | 0.1000 |
| 6.093 | 0.1250 |
| 6.497 | 0.1501 |
| 6.808 | 0.2001 |
| 6.690 | 0.2501 |
| 6.388 | 0.3001 |
| 6.016 | 0.3501 |
| 5.624 | 0.4001 |
| 5.204 | 0.4501 |
| 4.823 | 0.5001 |
| 4.365 | 0.5501 |
| 3.937 | 0.6001 |
| 3.496 | 0.6501 |
| 3.026 | 0.7001 |
| 2.049 | 0.8001 |
| 1.114 | 0.9000 |

Benson, George C. - D'Arcy, Patrick J., Excess isobaric heat capacities of water-n-alcohol mixtures, Journal of Chemical & Engineering Data 4 (1982) 439-442. doi:10.1021/je00030a021

**T / K =** **308.15**

**P / bar =** **UNKNOWN (1.0132)**

| $c_P^M$ / J.mol$^{-1}$.K$^{-1}$ | $x_1$ |
|---|---|
| 1.100 | 0.0155 |
| 1.530 | 0.0220 |
| 1.830 | 0.0262 |
| 2.230 | 0.0323 |
| 2.290 | 0.0334 |
| 3.020 | 0.0452 |
| 3.190 | 0.0481 |
| 3.420 | 0.0534 |
| 3.470 | 0.0537 |
| 4.570 | 0.0740 |
| 4.880 | 0.0810 |
| 5.680 | 0.1006 |
| 5.860 | 0.1063 |
| 6.470 | 0.1249 |
| 7.040 | 0.1492 |
| 7.170 | 0.1601 |
| 7.300 | 0.1704 |
| 7.460 | 0.1758 |
| 7.660 | 0.2084 |
| 7.730 | 0.2170 |
| 7.780 | 0.2235 |
| 7.810 | 0.2451 |
| 7.810 | 0.2645 |
| 7.790 | 0.2715 |
| 7.530 | 0.3105 |
| 7.540 | 0.3262 |
| 7.390 | 0.3449 |
| 7.340 | 0.3451 |
| 7.370 | 0.3567 |
| 7.190 | 0.3660 |
| 7.250 | 0.3737 |
| 7.180 | 0.3773 |
| 6.800 | 0.4138 |
| 6.830 | 0.4216 |
| 6.510 | 0.4587 |
| 6.360 | 0.4604 |
| 5.940 | 0.5095 |
| 5.820 | 0.5194 |
| 5.440 | 0.5541 |
| 4.890 | 0.6125 |
| 4.360 | 0.6563 |
| 4.040 | 0.6887 |
| 3.920 | 0.7002 |
| 3.830 | 0.7057 |
| 3.790 | 0.7064 |
| 3.100 | 0.7612 |
| 2.510 | 0.8064 |
| 1.960 | 0.8503 |
| 1.930 | 0.8527 |
| 0.7700 | 0.9471 |

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**Critical point**

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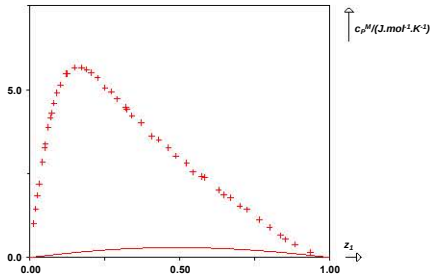
Musso, E. - Tesser, R. - Basile, G. - Di Serio, M. - Santacesaria, E., Description of the liquid–liquid equilibrium in binary and multicomponent CFC/lubricating oil mixtures by means of an extended Flory–Huggins model, Journal of Fluorine Chemistry 1 (2000) 41-51. doi:10.1016/S0022-1139(99)00255-9

| T / K | P / bar | $x_1$ |
|---|---|---|
| 523.15 | 85.08 | 0.7970 |

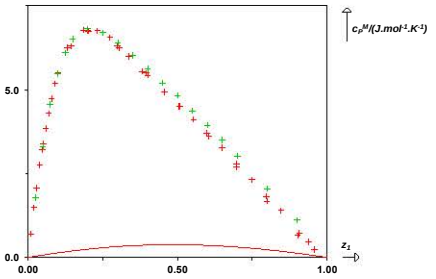
Bazaev, A. R. - Abdulagatov, I. M. - Magee, J. W. - Bazaev, E.A. - Ramazanova, A. E. - Abdurashidova, A. A., PVTx Measurements for a H2O + Methanol Mixture in the Subcritical and Supercritical Regions, International Journal of Thermophysics 3 (2004) 805-838. doi:10.1023/B:IJOT.0000034238.64651.32

| T / K | P / bar | $x_1$ |
|---|---|---|
| 583.50 | 150.00 | 0.3600 |

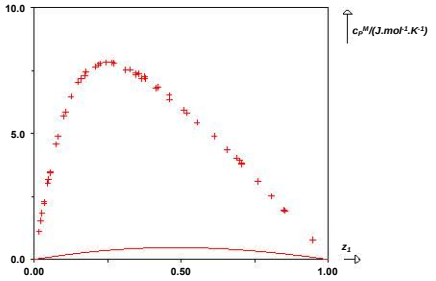
T/K = 288.15 - P/bar = 1.0132



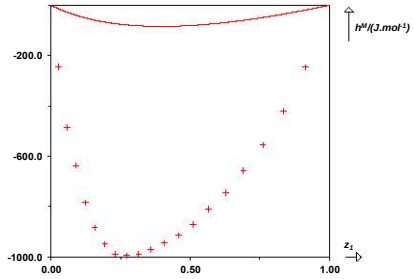

T/K = 298.15 - P/bar = 1.0132 1.0132



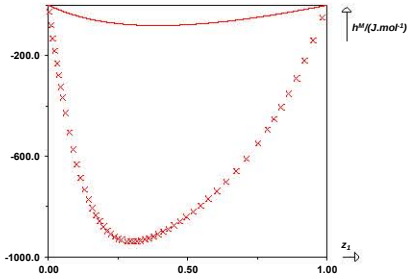

T/K = 308.15 - P/bar = 1.0132



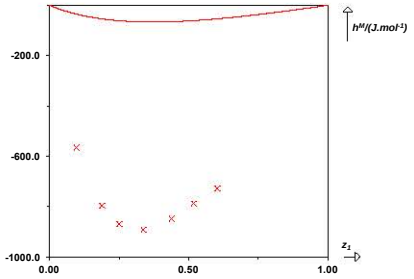

T/K = 273.15 - P/bar = 1.0132



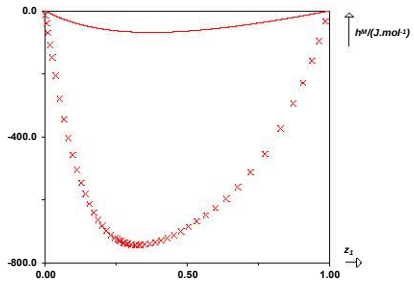

T/K = 288.15 - P/bar = 1.0132



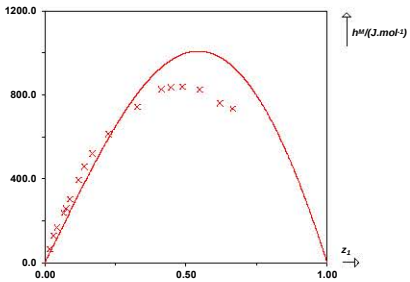

T/K = 298.15 - P/bar = 390.00



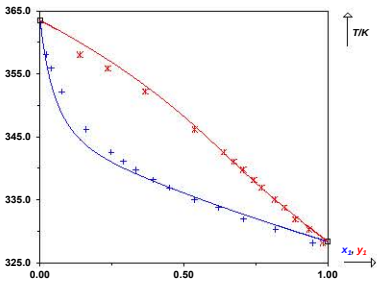

T/K = 318.15 - P/bar = 1.0132



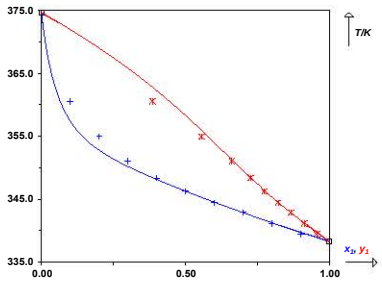

T/K = 523.15 - P/bar = 200.00



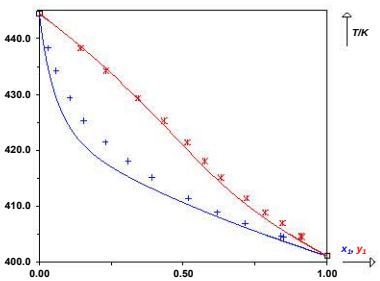

P/bar = 0.66620



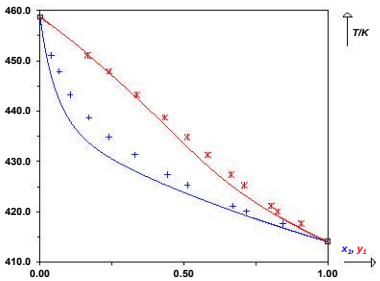

P/bar = 1.01330



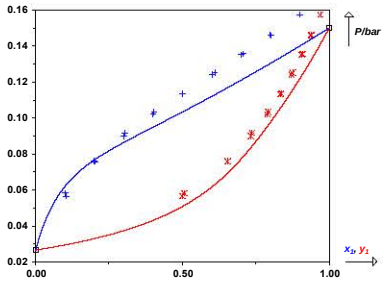

P/bar = 8.10600



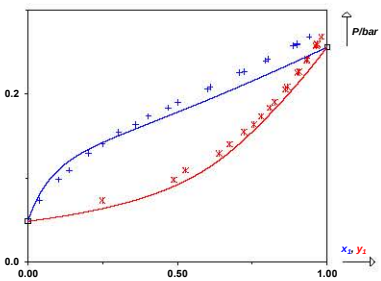

P/bar = 11.34800



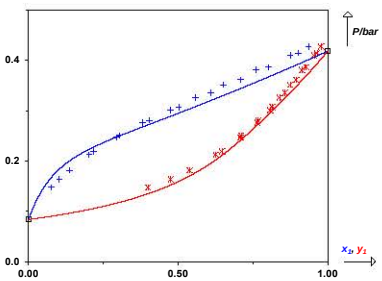

T/K = 298.15



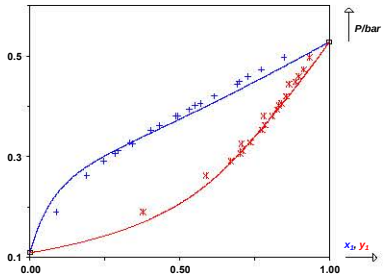

T/K = 308.15



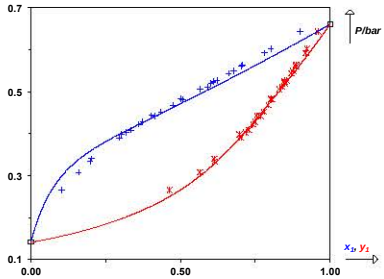

T/K = 318.15



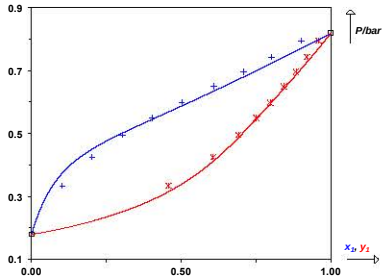
T/K = 323.15



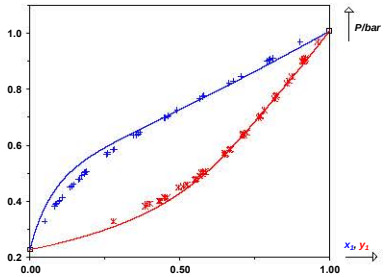

T/K = 328.15



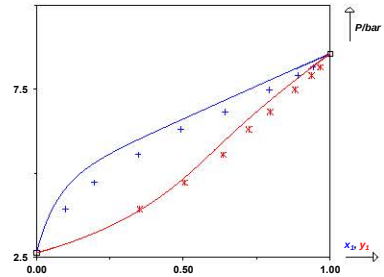

T/K = 333.15



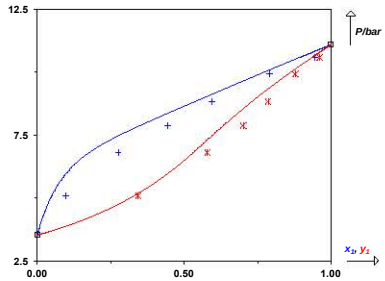

T/K = 338.15



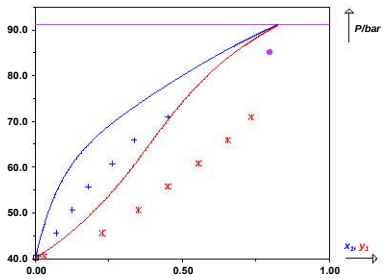

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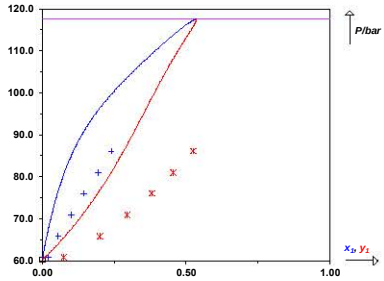

T/K = 413.15



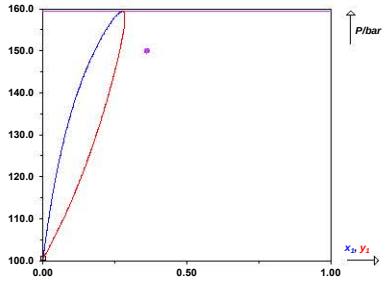

T/K = 523.15




T/K = 548.15




T/K = 583.50



## WATER (1) + 2-BUTOXYETHANOL (2)

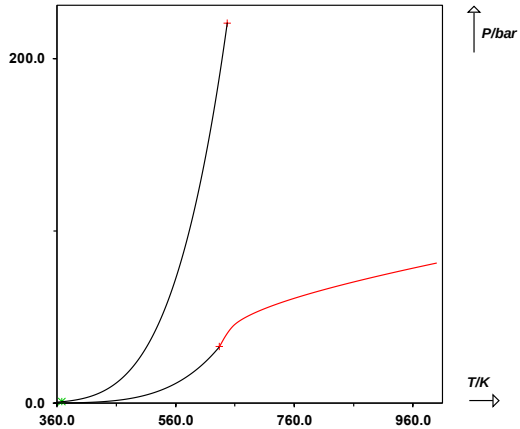
| | | |
|---|---|---|
| **CAS** | 7732-18-5 | 111-76-2 |
| **InChiKey** | XLYOFNOQVPJJNP-UHFFFAOYSA-N | POAOYUHQDCAZBD-UHFFFAOYSA-N |
| **$T_c$ / K** | 647.10 | 633.90 |
| **$P_c$ / bar** | 220.64 | 32.70 |
| **ω** | 0.345 | 0.514 |

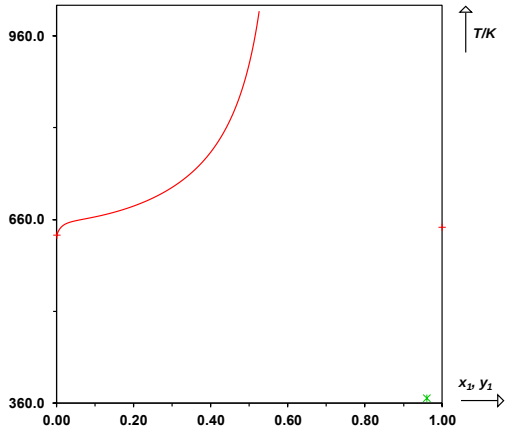
Non ideal with entropic causes

**PPR78 results**

*Parameters*
A/MPa = 7150
B/MPa = -1730

*Deviations*
MAPE on x = 130 %
MAPE on y = 39 %
MAPE on $h^M$ = 98 %



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**Isothermal phase equilibrium data**

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Scatchard, George. - Wilson, Grant M., Vapor-Liquid Equilibrium. XIII. The System Water-Butyl Glycol from 5 to 85°, Journal of the American Chemical Society 2 (1964) 133-137. doi:10.1021/ja01056a004

**T / K = 278.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0019 | 0.0742 | 0.8923 |
| 0.0032 | 0.1477 | 0.9432 |
| 0.0044 | 0.2139 | 0.9603 |
| 0.0057 | 0.3073 | 0.9721 |
| 0.0075 | 0.5072 | 0.9827 |
| 0.0082 | 0.6836 | 0.9864 |
| 0.0085 | 0.7885 | 0.9874 |
| 0.0086 | 0.8986 | 0.9880 |

Scatchard, George. - Wilson, Grant M., Vapor-Liquid Equilibrium. XIII. The System Water-Butyl Glycol from 5 to 85°, Journal of the American Chemical Society 2 (1964) 133-137. doi:10.1021/ja01056a004

**T / K = 298.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0072 | 0.0741 | 0.8526 |
| 0.0123 | 0.1473 | 0.9206 |
| 0.0165 | 0.2135 | 0.9441 |
| 0.0212 | 0.3069 | 0.9606 |
| 0.0280 | 0.5068 | 0.9755 |
| 0.0308 | 0.6834 | 0.9806 |

Scatchard, George. - Wilson, Grant M., Vapor-Liquid Equilibrium. XIII. The System Water-Butyl Glycol from 5 to 85°, Journal of the American Chemical Society 2 (1964) 133-137. doi:10.1021/ja01056a004

**T / K = 318.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0230 | 0.0734 | 0.8103 |
| 0.0384 | 0.1465 | 0.8957 |
| 0.0510 | 0.2125 | 0.9261 |
| 0.0658 | 0.3058 | 0.9477 |
| 0.0866 | 0.5061 | 0.9673 |
| 0.0936 | 0.6833 | 0.9742 |
| 0.0966 | 0.7882 | 0.9757 |
| 0.0972 | 0.8985 | 0.9752 |

Scatchard, George. - Wilson, Grant M., Vapor-Liquid Equilibrium. XIII. The System Water-Butyl Glycol from 5 to 85°, Journal of the American Chemical Society 2 (1964) 133-137. doi:10.1021/ja01056a004

**T / K = 338.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0622 | 0.0724 | 0.7665 |
| 0.1023 | 0.1446 | 0.8684 |
| 0.1348 | 0.2105 | 0.9061 |
| 0.1736 | 0.3036 | 0.9332 |
| 0.2291 | 0.5046 | 0.9583 |
| 0.2509 | 0.6822 | 0.9670 |
| 0.2553 | 0.7878 | 0.9690 |

Chiavone-Filho, Osvaldo - Proust, Patricio - Rasmussen, Peter, Vapor-liquid equilibria for glycol ether + water systems, Journal of Chemical & Engineering Data 1 (1993) 128-131. doi:10.1021/je00009a031

**T / K = 358.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0538 | 0.0188 | 0.2160 |
| 0.0642 | 0.0257 | 0.3416 |
| 0.0753 | 0.0338 | 0.4366 |
| 0.0881 | 0.0442 | 0.5233 |
| 0.1019 | 0.0537 | 0.5924 |
| 0.1236 | 0.0735 | 0.6730 |
| 0.1466 | 0.0935 | 0.7279 |
| 0.1747 | 0.1208 | 0.7729 |
| 0.2197 | 0.1595 | 0.8293 |
| 0.3035 | 0.2404 | 0.8855 |
| 0.3837 | 0.3205 | 0.9126 |
| 0.4546 | 0.3973 | 0.9339 |
| 0.5258 | 0.5150 | 0.9472 |
| 0.5724 | 0.6441 | 0.9564 |
| 0.5909 | 0.7609 | 0.9590 |
| 0.5939 | 0.8456 | 0.9613 |
| 0.5936 | 0.8671 | 0.9603 |
| 0.5934 | 0.9308 | 0.9604 |
| 0.5950 | 0.9812 | 0.9609 |

Scatchard, George. - Wilson, Grant M., Vapor-Liquid Equilibrium. XIII. The System Water-Butyl Glycol from 5 to 85°, Journal of the American Chemical Society 2 (1964) 133-137. doi:10.1021/ja01056a004

**T / K = 358.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1466 | 0.0703 | 0.7193 |
| 0.2369 | 0.1413 | 0.8380 |
| 0.3108 | 0.2067 | 0.8836 |
| 0.4006 | 0.2992 | 0.9168 |
| 0.5325 | 0.5016 | 0.9481 |
| 0.5853 | 0.6806 | 0.9591 |
| 0.5944 | 0.7870 | 0.9616 |

Escobedo-Alvarado, Gonzalo N. - Sandler, Stanley I., Vapor–Liquid Equilibrium of Two Aqueous Systems that Exhibit Liquid–Liquid Phase Separation, Journal of Chemical & Engineering Data 2 (1999) 319-322. doi:10.1021/je980228q

**T / K = 363.18**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0946 | 0.0243 | 0.4436 |
| 0.1391 | 0.0499 | 0.6153 |
| 0.1619 | 0.0677 | 0.6861 |
| 0.2179 | 0.1084 | 0.7942 |
| 0.2596 | 0.1358 | 0.8364 |
| 0.3079 | 0.1726 | 0.8688 |
| 0.3997 | 0.2444 | 0.9097 |
| 0.4470 | 0.2783 | 0.9191 |
| 0.4953 | 0.3154 | 0.9288 |
| 0.5459 | 0.3651 | 0.9355 |
| 0.5820 | 0.4040 | 0.9391 |
| 0.6217 | 0.4571 | 0.9435 |
| 0.6468 | 0.4958 | 0.9472 |
| 0.6685 | 0.5414 | 0.9492 |
| 0.6978 | 0.6292 | 0.9545 |
| 0.7088 | 0.6642 | 0.9554 |
| 0.7190 | 0.7415 | 0.9628 |
| 0.7237 | 0.7798 | 0.9656 |
| 0.7258 | 0.8126 | 0.9661 |
| 0.7247 | 0.9887 | 0.9697 |
| 0.7175 | 0.9942 | 0.9803 |
| 0.7085 | 0.9976 | 0.9893 |

Chiavone-Filho, Osvaldo - Proust, Patricio - Rasmussen, Peter, Vapor-liquid equilibria for glycol ether + water systems, Journal of Chemical & Engineering Data 1 (1993) 128-131. doi:10.1021/je00009a031

**T / K = 368.15**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.0871 | 0.0196 | 0.2165 |
| 0.1020 | 0.0272 | 0.3334 |
| 0.1201 | 0.0344 | 0.4329 |
| 0.1389 | 0.0486 | 0.5132 |
| 0.1647 | 0.0597 | 0.5993 |
| 0.1992 | 0.0790 | 0.6787 |
| 0.2385 | 0.1072 | 0.7352 |
| 0.2932 | 0.1468 | 0.7906 |
| 0.3794 | 0.2034 | 0.8431 |
| 0.4770 | 0.2707 | 0.8806 |
| 0.6162 | 0.3626 | 0.9194 |
| 0.7508 | 0.4867 | 0.9419 |
| 0.8332 | 0.6249 | 0.9503 |
| 0.8662 | 0.7486 | 0.9567 |
| 0.8704 | 0.8244 | 0.9575 |
| 0.8726 | 0.8666 | 0.9574 |
| 0.8709 | 0.9031 | 0.9592 |
| 0.8714 | 0.9565 | 0.9589 |
| 0.8720 | 0.9837 | 0.9590 |

Escobedo-Alvarado, Gonzalo N. - Sandler, Stanley I., Vapor–Liquid Equilibrium of Two Aqueous Systems that Exhibit Liquid–Liquid Phase Separation, Journal of Chemical & Engineering Data 2 (1999) 319-322. doi:10.1021/je980228q

**T / K = 371.19**

| P / bar | $x_1$ | $y_1$ |
|---|---|---|
| 0.1195 | 0.0223 | 0.3604 |
| 0.1357 | 0.0284 | 0.4302 |
| 0.1747 | 0.0477 | 0.5664 |
| 0.2059 | 0.0672 | 0.6401 |
| 0.2619 | 0.0970 | 0.7246 |
| 0.3341 | 0.1330 | 0.7907 |
| 0.3985 | 0.1652 | 0.8312 |
| 0.4810 | 0.2061 | 0.8674 |
| 0.5549 | 0.2482 | 0.8928 |
| 0.6237 | 0.2897 | 0.9101 |
| 0.7031 | 0.3429 | 0.9252 |
| 0.7739 | 0.3985 | 0.9355 |
| 0.8295 | 0.4546 | 0.9427 |
| 0.9218 | 0.5991 | 0.9590 |
| 0.9540 | 0.6952 | 0.9626 |
| 0.9623 | 0.7251 | 0.9653 |
| 0.9705 | 0.7554 | 0.9664 |
| 0.9780 | 0.8347 | 0.9666 |
| 0.9800 | 0.8377 | 0.9669 |
| 0.9800 | 0.9839 | 0.9665 |
| 0.9774 | 0.9888 | 0.9670 |
| 0.9709 | 0.9928 | 0.9719 |
| 0.9673 | 0.9946 | 0.9753 |
| 0.9555 | 0.9976 | 0.9872 |

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**Enthalpy of mixing**

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Onken, U., Die thermodynamischen Funktionen des Systems Wasser/Butylglykol, Z. Elektrochem. 2 (1959) 321-327.

**T / K = 293.15**

**P / bar = UNKNOWN (1.0132)**

| $h^M$ / J.mol$^{-1}$ | $x_1$ |
|---|---|
| -297.68 | 0.4238 |
| -406.54 | 0.5805 |

| | |
|---|---|
| -495.30 | 0.7007 |
| -499.90 | 0.7087 |
| -500.74 | 0.8017 |
| -426.22 | 0.9091 |
| -311.71 | 0.9656 |

Lim, Kyung-Hee - Whiting, Wallace B. - Smith, Duane H., Excess Enthalpies and Liquid-Liquid Equilibrium Phase Compositions of the Nonionic Amphiphile 2-Butoxyethanol and Water, Journal of Chemical & Engineering Data 2 (1994) 399-403. doi:10.1021/je00014a048

| **T / K =** | **321.62** |
|---|---|
| **P / bar =** | **1.010** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| -0.6500 | 0.0684 |
| -14.01 | 0.1835 |
| -46.68 | 0.3168 |
| -122.16 | 0.4467 |
| -159.43 | 0.5205 |
| -189.58 | 0.5805 |
| -218.44 | 0.6449 |
| -239.54 | 0.6965 |
| -246.38 | 0.7185 |
| -250.93 | 0.7386 |
| -253.33 | 0.7569 |
| -254.13 | 0.7737 |
| -254.25 | 0.7892 |
| -252.81 | 0.8034 |
| -250.12 | 0.8166 |
| -246.69 | 0.8289 |
| -240.62 | 0.8403 |
| -236.68 | 0.8509 |
| -231.27 | 0.8609 |
| -226.53 | 0.8702 |
| -220.62 | 0.8790 |
| -215.31 | 0.8873 |
| -209.13 | 0.8951 |
| -194.22 | 0.9127 |
| -181.02 | 0.9281 |
| -167.12 | 0.9418 |
| -154.44 | 0.9539 |
| -141.96 | 0.9647 |
| -137.23 | 0.9687 |
| -131.99 | 0.9726 |
| -126.92 | 0.9763 |
| -120.93 | 0.9798 |
| -113.99 | 0.9833 |
| -104.11 | 0.9866 |
| -98.38 | 0.9882 |
| -89.11 | 0.9898 |
| -79.52 | 0.9913 |
| -68.83 | 0.9928 |
| -57.31 | 0.9943 |
| -43.70 | 0.9958 |
| -30.83 | 0.9972 |

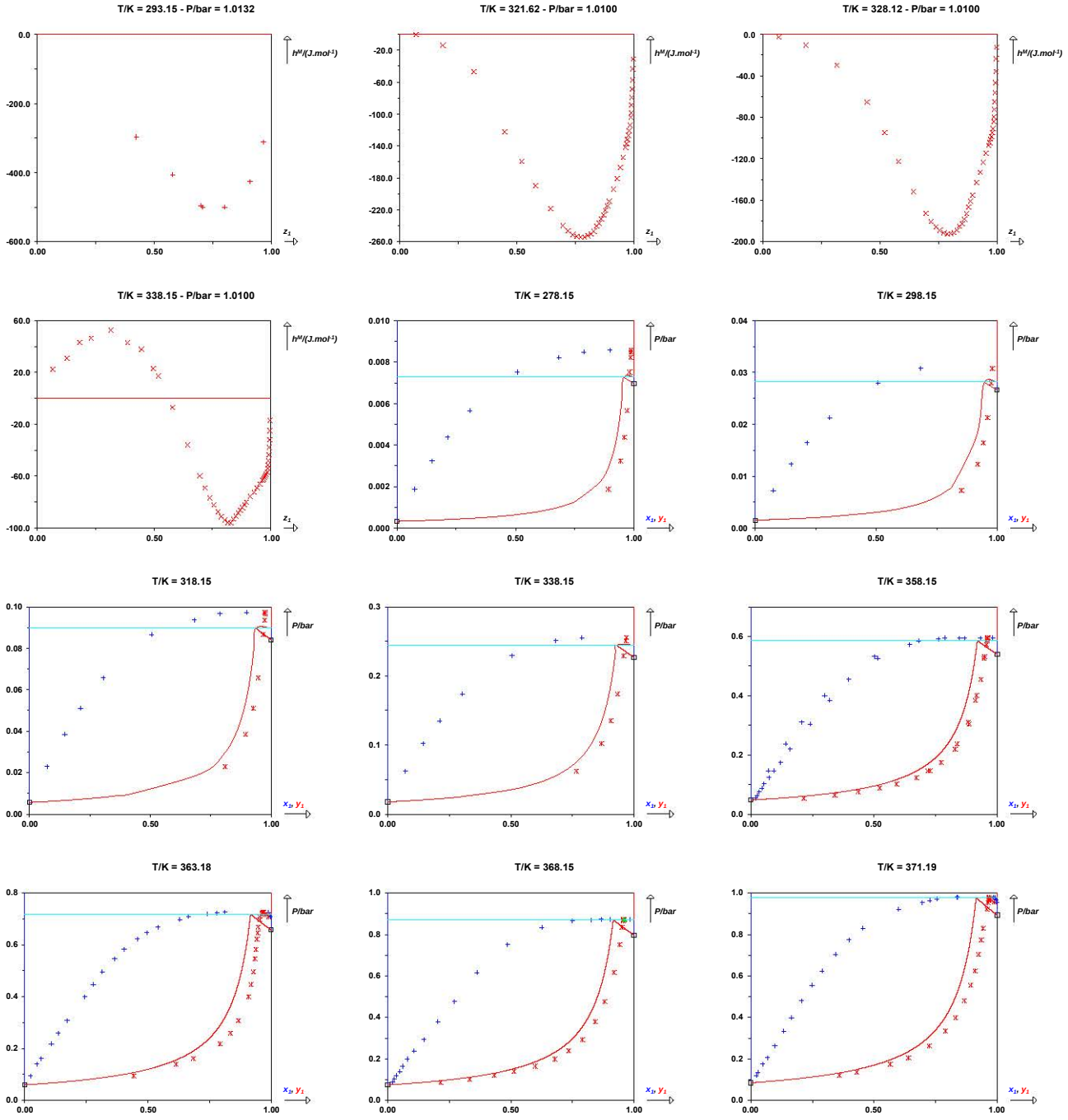
Lim, Kyung-Hee - Whiting, Wallace B. - Smith, Duane H., Excess Enthalpies and Liquid-Liquid Equilibrium Phase Compositions of the Nonionic Amphiphile 2-Butoxyethanol and Water, Journal of Chemical & Engineering Data 2 (1994) 399-403. doi:10.1021/je00014a048

| **T / K =** | **328.12** |
|---|---|
| **P / bar =** | **1.010** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| -2.680 | 0.0683 |
| -10.72 | 0.1834 |
| -29.80 | 0.3167 |
| -65.63 | 0.4465 |
| -94.94 | 0.5204 |
| -122.59 | 0.5804 |
| -151.59 | 0.6448 |
| -173.01 | 0.6963 |
| -180.42 | 0.7184 |
| -185.78 | 0.7385 |
| -189.32 | 0.7568 |
| -191.43 | 0.7736 |
| -192.56 | 0.7891 |
| -192.27 | 0.8033 |
| -191.00 | 0.8165 |
| -189.01 | 0.8288 |
| -185.17 | 0.8402 |
| -182.51 | 0.8508 |
| -178.27 | 0.8608 |
| -172.78 | 0.8702 |
| -166.55 | 0.8790 |
| -161.00 | 0.8872 |
| -155.31 | 0.8950 |
| -143.02 | 0.9126 |
| -133.28 | 0.9281 |
| -123.59 | 0.9417 |
| -114.90 | 0.9538 |
| -107.13 | 0.9647 |
| -104.28 | 0.9687 |
| -101.23 | 0.9726 |
| -98.50 | 0.9763 |
| -95.07 | 0.9798 |

| | |
|---|---|
| -90.74 | 0.9833 |
| -84.27 | 0.9866 |
| -79.49 | 0.9882 |
| -72.55 | 0.9897 |
| -65.11 | 0.9913 |
| -56.42 | 0.9928 |
| -46.69 | 0.9943 |
| -36.10 | 0.9958 |
| -23.61 | 0.9972 |
| -12.72 | 0.9986 |

Lim, Kyung-Hee - Whiting, Wallace B. - Smith, Duane H., Excess Enthalpies and Liquid-Liquid Equilibrium Phase Compositions of the Nonionic Amphiphile 2-Butoxyethanol and Water, Journal of Chemical & Engineering Data 2 (1994) 399-403. doi:10.1021/je00014a048

| | |
|---|---|
| **T / K =** | **338.15** |
| **P / bar =** | **1.010** |
| $h^M$ / J.mol$^{-1}$ | $z_1$ |
| 22.13 | 0.0684 |
| 30.99 | 0.1291 |
| 43.18 | 0.1835 |
| 46.29 | 0.2324 |
| 52.33 | 0.3168 |
| 42.84 | 0.3872 |
| 37.74 | 0.4467 |
| 23.04 | 0.4977 |
| 16.99 | 0.5205 |
| -6.940 | 0.5805 |
| -35.90 | 0.6449 |
| -59.92 | 0.6965 |
| -69.12 | 0.7185 |
| -76.65 | 0.7386 |
| -82.17 | 0.7569 |
| -87.40 | 0.7737 |
| -91.47 | 0.7892 |
| -93.90 | 0.8034 |
| -95.82 | 0.8166 |
| -95.92 | 0.8289 |
| -93.17 | 0.8403 |
| -90.93 | 0.8509 |
| -88.51 | 0.8609 |
| -86.35 | 0.8702 |
| -84.12 | 0.8790 |
| -82.19 | 0.8873 |
| -80.17 | 0.8951 |
| -75.77 | 0.9127 |
| -72.48 | 0.9281 |
| -69.05 | 0.9418 |
| -66.06 | 0.9539 |
| -63.06 | 0.9647 |
| -62.02 | 0.9687 |
| -60.85 | 0.9726 |
| -59.90 | 0.9763 |
| -58.67 | 0.9798 |
| -56.93 | 0.9833 |
| -53.95 | 0.9866 |
| -51.52 | 0.9882 |
| -47.93 | 0.9898 |
| -43.69 | 0.9913 |
| -37.85 | 0.9928 |
| -31.87 | 0.9943 |
| -24.92 | 0.9958 |
| -17.01 | 0.9972 |


T/K = 293.15 - P/bar = 1.0132
T/K = 321.62 - P/bar = 1.0100
T/K = 328.12 - P/bar = 1.0100
T/K = 338.15 - P/bar = 1.0100
T/K = 278.15
T/K = 298.15
T/K = 318.15
T/K = 338.15
T/K = 358.15
T/K = 363.18
T/K = 368.15
T/K = 371.19
hᴹ/(J.mol⁻¹)
P/bar
z₁
x₁, y₁

## WATER (1) + PROPYLENE GLYCOL MONOMETHYL ETHER (2)

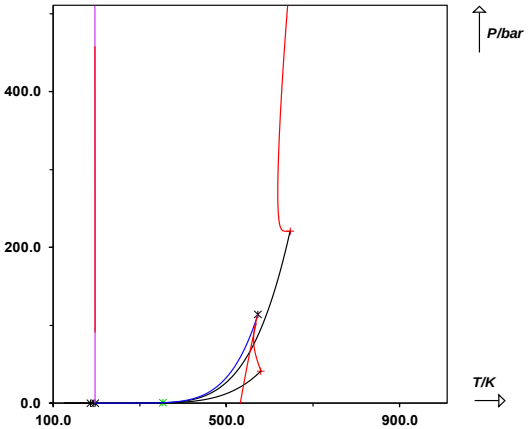
| | | |
|---|---|---|
| **CAS** | 7732-18-5 | 107-98-2 |
| **InChiKey** | XLYOFNOQVPJJNP-UHFFFAOYSA-N | ARXJGSRGQADJSQ-UHFFFAOYSA-N |
| **$T_c$ / K** | 647.10 | 579.80 |
| **$P_c$ / bar** | 220.64 | 41.13 |
| **ω** | 0.345 | 0.443 |

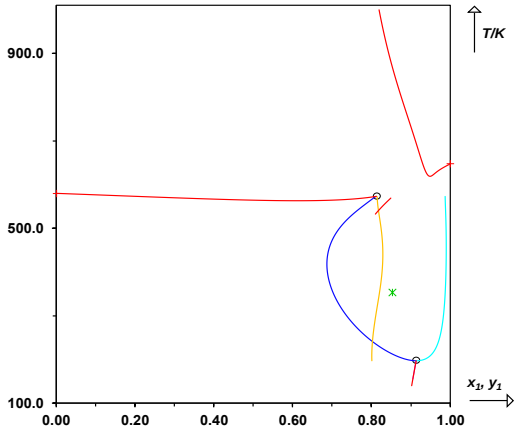
Non ideal with entropic causes

PPR78

*Parameters*
A/MPa = 814
B/MPa = -358

*Deviations*
MAPE on x = 22 %
MAPE on y = 5.6 %
MAPE on $h^M$ = 50 %



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**Isothermal phase equilibrium data**

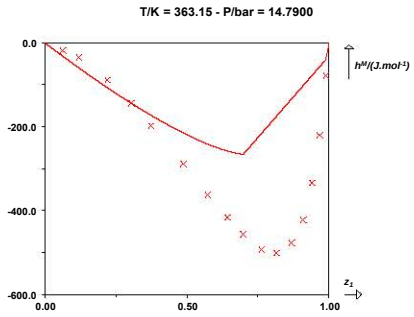
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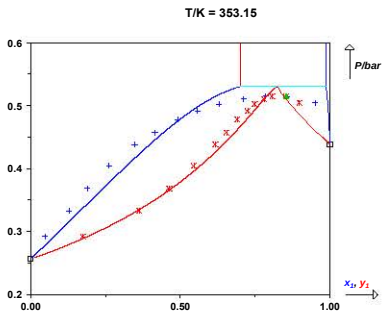
Chiavone-Filho, Osvaldo - Proust, Patricio - Rasmussen, Peter, Vapor-liquid equilibria for glycol ether + water systems, Journal of Chemical & Engineering Data 1 (1993) 128-131. doi:10.1021/je00009a031

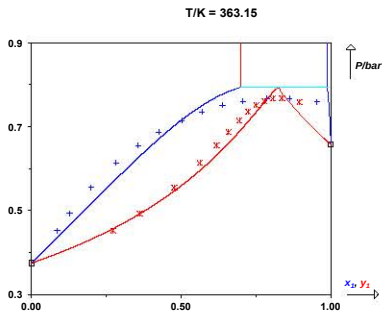
| **T / K =** | **353.15** | | |
|---|---|---|---|
| P / bar | $x_1$ | $y_1$ | |
| 0.2923 | 0.0471 | 0.1746 | |
| 0.3330 | 0.1285 | 0.3623 | |
| 0.3690 | 0.1895 | 0.4629 | |
| 0.4043 | 0.2617 | 0.5453 | |
| 0.4383 | 0.3470 | 0.6171 | |
| 0.4575 | 0.4150 | 0.6547 | |
| 0.4781 | 0.4908 | 0.6906 | |
| 0.4917 | 0.5580 | 0.7255 | |
| 0.5023 | 0.6289 | 0.7488 | |
| 0.5111 | 0.7112 | 0.7792 | |
| 0.5150 | 0.7859 | 0.8074 | |
| 0.5146 | 0.8534 | 0.8534 | AZEO |
| 0.5146 | 0.8564 | 0.8544 | |
| 0.5045 | 0.9499 | 0.8982 | |

Chiavone-Filho, Osvaldo - Proust, Patricio - Rasmussen, Peter, Vapor-liquid equilibria for glycol ether + water systems, Journal of Chemical & Engineering Data 1 (1993) 128-131. doi:10.1021/je00009a031

| **T / K =** | **363.15** | |
|---|---|---|
| P / bar | $x_1$ | $y_1$ |
| 0.4526 | 0.0844 | 0.2723 |
| 0.4934 | 0.1268 | 0.3611 |
| 0.5553 | 0.1982 | 0.4770 |
| 0.6138 | 0.2822 | 0.5620 |
| 0.6547 | 0.3564 | 0.6183 |
| 0.6865 | 0.4249 | 0.6572 |
| 0.7141 | 0.5013 | 0.6933 |
| 0.7357 | 0.5691 | 0.7236 |
| 0.7517 | 0.6375 | 0.7508 |
| 0.7605 | 0.7063 | 0.7778 |
| 0.7669 | 0.7861 | 0.8061 |
| 0.7668 | 0.8604 | 0.8364 |
| 0.7590 | 0.9524 | 0.8954 |


T/K = 363.15 - P/bar = 14.7900
0.0
-200.0
-400.0
-600.0
0.00
0.50
1.00
$h^{M}$/(J.mol$^{-1}$)
$z_1$


T/K = 353.15
0.6
0.5
0.4
0.3
0.2
0.00
0.50
1.00
P/bar
$x_1$, $y_1$


T/K = 363.15
0.9
0.7
0.5
0.3
0.00
0.50
1.00
P/bar
$x_1$, $y_1$

# Résumés


**« Développement d'équations d'état cubiques adaptées à la représentation de mélanges contenant des molécules polaires (eau, alcools, amines…) et des hydrocarbures. »**

L'objectif principal de ce travail de thèse est de développer un modèle thermodynamique de type équation d'état cubique, permettant de prédire avec un maximum de précision les propriétés thermodynamiques des corps purs (des comportements de phases aux propriétés énergétiques - enthalpie, capacité calorifique - en incluant les propriétés volumiques) et des mélanges (équilibres de phases dans les régions sub- et supercritiques, points critiques, propriétés énergétiques, densités …), y compris les plus complexes.
Concernant les corps purs tout d'abord : en nous appuyant sur la connaissance acquise par les études publiées pendant près d'un siècle et demi sur les équations d'état cubiques, nous avons identifié deux leviers pour accroître la précision de ces modèles. Le premier concerne la sélection d'une fonction α optimale (cette fonction est une quantité clef apparaissant dans le terme attractif du modèle) dont le bon paramétrage permet de représenter précisément les propriétés à saturation des corps purs, telles que la pression de saturation, l'enthalpie de vaporisation et la capacité calorifique du liquide à saturation. Afin que la fonction α puisse être extrapolée au domaine des hautes températures, nous avons défini les contraintes mathématiques que celle-ci doit respecter. Le second levier est le paramètre de translation volumique, paramètre clef pour la bonne représentation des densités liquides. Ces réflexions et les études associées sont à la base du développement des modèles tc-RK et tc-PR, utilisant une fonction α extrapolable à haute température ainsi qu'un paramètre de translation volumique, garantissant une précision jusqu'alors inégalée des propriétés sub- et supercritiques des corps purs prédites par des équations d'état cubiques.
Afin d'étendre les modèles tc-RK et tc-PR aux mélanges, il a été nécessaire de développer des règles de mélange appropriées pour deux paramètres de l'équation d'état des mélanges : le covolume et le paramètre attractif. Des règles de mélanges récemment proposées qui combinent équation d'état et modèle de coefficient d'activité ont été adoptées. Les valeurs optimales des paramètres universels de ces règles de mélange ont été identifiées dans le cadre de cette thèse. Une règle de mélange linéaire pour le paramètre de translation volumique du mélange a été sélectionnée ; il a été prouvé que cette règle de mélange garantit l'invariance des propriétés d'équilibre de phases et des propriétés énergétiques entre les modèles translatés et non translatés.
Afin de définir le modèle de coefficient d'activité optimal à intégrer dans la nouvelle règle de mélange, une base de données de 200 systèmes binaires a été développée. Ces systèmes binaires ont été sélectionnés afin d'être représentatifs des différents types d'interactions qui peuvent exister dans les mélanges non électrolytiques. La base de données accorde une place significative aux systèmes dits associés, qui sont certainement parmi les plus difficiles à modéliser par une équation d'état.
*In fine*, cette thèse pose toutes les bases du développement d'une équation d'état cubique des mélanges. Le choix du modèle de coefficient d'activité optimal, la détermination des paramètres d'interactions binaires des 200 systèmes de la base de données et leur prédiction constituent des suites possibles de ce travail.



Mots-clés : équation d'état cubique, fonction alpha, translation volumique, règles de mélange, banque de données de systèmes binaires



« Development of cubic equations of state adapted to the representation of mixtures containing polar molecules (water, alcohols, amines, etc.) and hydrocarbons. »

The main objective of this thesis work is to develop a cubic equation of state thermodynamic model able to accurately predict the thermodynamic properties of pure compounds (from phase equilibrium data to energetic properties – enthalpy, heat capacity – and volume properties) and mixtures (phase equilibria in sub- and supercritical regions, critical points, energetic properties, densities…), including the most complex ones.
Starting with pure compounds: relying on the knowledge collected all through the years from Van der Waals seminal work about cubic equations of state, we identified two levers to increase cubic-model accuracy. First is the selection of the optimal α function (this function is a key quantity involved in the model attractive term) the proper parameterization of which entails an accurate representation of pure-compound saturation properties such as saturation pressure, enthalpy of vaporization, saturated-liquid heat capacity. In order to safely extrapolate an α functions to the high temperature domain, we defined the mathematical constraints that it should satisfy. The second lever is the volume translation parameter, a key parameter for an accurate description of liquid densities. These studies led to the development of the tc-PR and tc-RK models, using an α function that correctly extrapolates to the high temperature domain so as a volume translation parameter, ensuring the most accurate estimations of pure-compound sub- and supercritical property from a cubic equation of state.
In order to extend the tc-PR and tc-RK models to mixtures, it was necessary to develop adequate mixing rules for both equation of state parameters: the covolume and the attractive parameter. Recently proposed mixing rules combining an equation of state and an activity coefficient model have been retained. Optimal values of the mixing rules universal parameters have been identified in the framework of this thesis. A linear mixing rule for the volume translation parameter has been selected; it has been proven that this mixing rule does not change the phase equilibrium and energetic properties when switching from a translated to an untranslated model.
In order to define the optimal activity coefficient model to include in the new mixing rule, a 200 binary-system database has been developed. These binary systems have been selected to be representative of the different kinds of interactions that can exist in non-electrolytic mixtures. The database includes in particular systems containing associating compounds, which are certainly among the most difficult ones to model with an equation of state.
*In fine*, this thesis sets all the bases for the development of a cubic equation of state for mixtures. The selection of the optimal activity-coefficient model, the estimation of binary interaction parameters for the 200 binary systems from the database and their prediction are possible continuations of this work.



Keywords : cubic equation of state, alpha function, volume translation, mixing rules, binary systems database