

Benchmark Database Containing Binary-System-High-Quality- Certified Data for Cross-Comparing Thermodynamic Models and Assessing Their Accuracy

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Article

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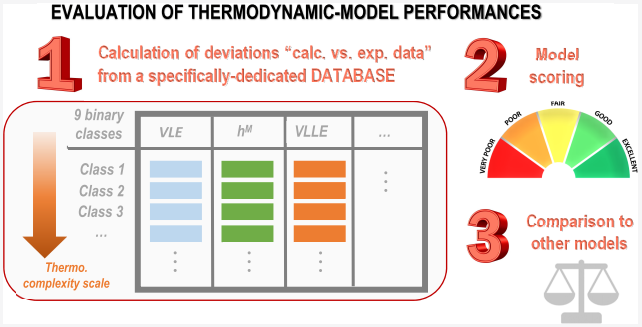
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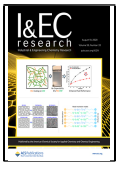
ABSTRACT: In the last two centuries, equations of state (EoSs) have become a key tool for the correlation and prediction of thermodynamic properties of fluids. They not only can be applied to pure substances as well as to mixtures but also constitute the heart of commercially available computer-aided-process-design software. In the last 20 years, thousands of publications have been devoted to the development of sophisticated models or to the improvement of already existing EoSs. Chemical engineering thermodynamics is thus a field under steady development, and to assess the accuracy of a thermodynamic model or to cross-compare two models, it is necessary to confront model predictions with experimental data. In this context, the importance of a reliable free-to-access benchmark database is pivotal and becomes absolutely necessary. The goal of this paper is thus to present a database, specifically designed to assess the accuracy of a thermodynamic model or cross-compare models, to explain how it was developed and to enlighten how to use it. A total of 200 nonelectrolytic binary systems have been selected and divided into nine groups according to the associating character of the components, i.e., their ability to be involved in a hydrogen bond (the nature and strength of the association phenomena are indeed considered a measure of the complexity to model the thermodynamic properties of mixtures). The methodology for assessing the performance of a given model is then described. As an illustration, the Peng−Robinson EoS with classical van der Waals mixing rules and a temperature-dependent binary interaction parameter (k_{ij}) have been used to correlate the numerous data included in the proposed database, and its performance has been assessed following the proposed methodology.



1. INTRODUCTION

Commercially available computer-aided-process-design software requires thermodynamic models to design, develop, analyze, and optimize chemical processes. As a result of their great potential, equations of state (EoSs) represent the cornerstone of thermodynamic models.[1] Indeed, combining an EoS and ideal-gas heat capacities enables one to calculate not only phase equilibria but also all of the thermodynamic properties needed for energy and exergy balances (enthalpy, entropy, exergy, heat capacities, etc.). It can be argued that in 2020, chemical engineering thermodynamics is a field under steady growth since new models are continuously under development. In the academic community, it is often assumed that the accuracy of incoming models is increasing over the years, as they become more sophisticated. However, the industry sometimes seems skeptical when weighing the value gained using a more complex model and rarely updates[2] or replaces its thermodynamic models with newer ones unless a clear advantage is evident. As a rule of thumb, it takes 10 years[3] for a new model to be conceived, developed, validated, and accepted by the industry. It is believed that such a time lapse is extensive because, among other reasons, developers usually do not confront model predictions to experimental data that cover a wide range of compositions, temperatures, and pressures. Moreover, the comparison between experimental data and model predictions is often limited to phase equilibria, ignoring other properties like enthalpies and heat capacities. For a new model, the absence of serious validation seems to be the major obstacle to its industrialization. Although scientists spend a great deal of time building and revising EoS, and much journal space is dedicated to introducing these valuable tools, the

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question of their accuracy inevitably arises because these models are, by definition, a simplification of reality.

In this paper, to address the relevant issue of model reliability, it was decided to build a high-quality reference database usable for assessing the accuracy of a thermodynamic model or to cross-compare the performances of two different models.

This work was conducted with the full support of the working party (WP) on thermodynamics and transport properties (https://wp-ttp.dk/) of the European Federation of Chemical Engineering (https://efce.info/). In 2010, this WP published[3] a paper entitled: "Industrial requirements for thermodynamics and transport properties" and one of the many conclusions, which fully justifies this work, was "new models are published very frequently, but unfortunately most, if not all, of these models are tested against only a few data sets. The issue of having large, standardized set of data against which all models may be tested is a very pertinent one that needs addressing and will be of great benefit, as it will allow models to be compared on equal footing."

In the first part of this paper devoted to the building of a benchmark database, a total of 200 nonelectrolytic binary systems was selected to cover all categories of mixtures and divided into nine groups according to the associating character of the components, i.e., to their ability to be involved in a hydrogen bond. The nature and strength of the association phenomena are indeed considered a measure of the complexity to model the thermodynamic properties of mixtures. In the second part of this paper, it is explained how to assess the accuracy of an EoS and to grade it with the proposed database. In particular, the exact procedure that has to be used to unambiguously calculate the deviations between model predictions and experimental data is discussed in detail and emphasis is given to the selection of specified and calculated variables. For illustration purposes, in the last part, the Peng–Robinson (PR) EoS with classical van der Waals mixing rules and a temperature-dependent k_{ij} is scored after being used to correlate the various data of the proposed database. The grades are then interpreted through a discussion dealing with the accuracy of such a thermodynamic model.

2. CRITERION TO BUILD A BENCHMARK DATABASE

2.1. Literature Review. Two databases that contain a vast number of experimental data points are widely used by researchers in the area of applied thermodynamics. The first one is the Dortmund Data Bank (DDB) (http://www.ddbst.com/ddb.html), which provides the largest data bank worldwide for thermophysical properties of pure components and their mixtures. In February 2020, the DDB contained 8.7 million data points for approximately 75 000 components from 88 200 references. The second one, provided by the National Institute of Standards and Technology (NIST), also contains pure-component and mixture data, divided into 90 Nation's Standard Reference Data (SRD) databases (https://www.nist.gov/srd). The trustworthiness of the data is assessed by experts, so that they can be used with confidence to make significant decisions.

Although extremely useful, such databases cannot be used as such to assess the accuracy of a thermodynamic model. First, they are so comprehensive that a model evaluation procedure accounting for all of the data would require an excessive amount of time. Second, the different types of systems (e.g., those that form ideal solutions, that contain size-asymmetric components, etc.) and data (e.g., vapor–liquid equilibrium (VLE) data, liquid–liquid equilibrium (LLE) data, etc.) are not equitably distributed; an evaluation over these data would lead to biased conclusions about the model efficiency. Our goal is thus to build a subdatabase from these very complete databases after a strict selection of the systems and data so that the diversity of molecular interactions and all kinds of fluid-phase behavior are represented.

To the best of our knowledge, the unique benchmark database for nonelectrolytic and nonpolymeric systems available in the literature is the one proposed by Danner and Gess in 1990.[4] This database that embeds data for 104 binary systems shows the following characteristics.

- Only subcritical VLE data are available.
- Data quality is ensured by performing consistency tests.
- Pure compounds are classified according to their polarity, from nonpolar to strongly polar, leading to the definition of nine classes of binary systems.
- For a given class, binary systems are categorized with respect to their deviations from ideality and there is an even distribution between ideal and nonideal systems.

In our opinion, such a database has many desirable features, including the classification scheme of the binary systems. However, several weak points can be pointed out: VLE data are limited to the subcritical domain and other types of phase equilibrium data, e.g., LLE, vapor–liquid–liquid equilibrium (VLLE), or derived properties like enthalpies and heat capacities are not included. Moreover, such a database was made available by their authors "on a 5 1/4 or 3 1/2 in. MS-DOS formatted floppy disk", and we cannot assert that it is still possible to get a copy or to read this support.

This short literature review makes it possible to conclude that the time has come to propose a revised version of the database developed by Danner and Gess,[4] which we hope will be widely adopted by others for assessing the accuracy of a thermodynamic model or cross-comparing two models. To guide the reader over the understanding of the choices we made to build this database, the following sections aim to address three questions.

1. Which thermophysical properties should be included?
2. Which binary systems?
3. How many systems and how many data?

2.2. Which Thermophysical Properties Should Be Included? To answer this question, we must be aware of the industrial needs. The paper by Hendriks et al.[3] explains that simultaneous description of different thermodynamic properties and phase equilibrium types (VLE, LLE, VLLE) is of great importance. It is also stated that thermodynamic modelers should no longer be satisfied with EoSs that are capable of reproducing VLE data with a reasonable accuracy at low pressures but are either untested or fail to reproduce other regions of the phase space and other properties.

As explained below, we followed these recommendations, but we have decided to go one step further in the selection of the thermophysical properties.

First, it is indisputable that a good reproduction of phase equilibrium data is mandatory to ensure that processes meet their compositional specifications. However, depending on the temperature and pressure conditions, phase equilibrium data may involve two subcritical compounds, a subcritical and a supercritical compound or possibly two supercritical compounds. In the two latter cases, binary critical points appear on

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the corresponding phase diagrams. For some systems, azeotropic behavior and three-phase VLLE can occur as well. To consider such a diversity, it was decided to embed all kinds of phase equilibrium data in the developed database, i.e., VLE, LLE, VLLE, and azeotropic data points, and to cover a very wide range of compositions, temperatures, and pressures. Binary critical points were also included because we know by experience that a good representation of the critical lines[5] leads to an accurate restitution of phase diagrams on the entire temperature and pressure ranges. Such lines indeed fix the global topology[6] of the isothermal and isobaric phase diagrams for any fixed temperature or pressure, respectively. Convinced by the importance of critical points, special emphasis was given to binary systems for which such data were available.

A proper reproduction of energetic mixing properties (enthalpy and heat capacity changes on mixing) contributes to a good quantification of utility needs and energy losses in a chemical engineering process. Such knowledge is typically required for performing heat integration in chemical plants. Unlike phase equilibrium properties, the calculation of enthalpy and heat capacity changes on mixing (hereafter simply called mixing enthalpy and mixing heat capacity) with an EoS involves the derivative of the EoS expression with respect to the temperature. Consequently, h^M data help determine the temperature dependence of the phase equilibrium, which supports their value. As a matter of fact, a good reproduction of experimental phase diagrams does not ensure accurate estimations of mixing properties and, consequently, of energy-balance terms. The same conclusion was drawn by Agarwal et al.,[7] who wrote: "...if you are modeling a system with significant excess enthalpies 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." This highlights the necessity of considering mixing enthalpy and mixing heat capacity data for evaluating model performances. In his Ph.D. thesis, Qian[8] reached the same conclusion but also demonstrated that it was possible for the Peng−Robinson (PR) EoS with temperature-dependent binary interaction parameters (BIPs) to accurately correlate both fluid-phase equilibria and mixing properties if both types of data were included in the regression procedure. Eventually, we decided to include both mixing enthalpy and mixing heat capacity data in the proposed benchmark database.

To conclude this section, we want to emphasize that we intentionally did not incorporate excess volume data in the proposed database. This is because we know by experience that volume change on mixing is generally small (and often very small). As a direct consequence, the calculated density of a phase mainly depends on the accuracy with which the density of the pure components is calculated but is only slightly influenced by the mixing rules used. This implies that before grading a thermodynamic model with the proposed database, it is necessary to provide information on how the model behaves to correlate/predict the properties of pure compounds and in particular the vapor pressures, the liquid densities, the enthalpies of vaporization, and the liquid heat capacities.

It was also decided to exclude electrolytic systems and to only consider fluid-state binary systems, meaning that the proposed database does not include liquid−solid, solid−solid, or adsorption[9] equilibrium data.

2.3. Which Binary Systems Should Be Included? The Danner and Gess database retained our attention as it not only compiles experimental data but also provides a classification for binary systems, revealing their thermodynamic complexity (here, thermodynamic complexity means a measure of the nonideal character of a system inducing difficulties for a model to reproduce thermodynamic macroscopic properties). In the paper by Danner and Gess, pure compounds were categorized with respect to their polarity and were classified as nonpolar, weakly polar, strongly polar, or very strongly polar. Such authors define polarity as the ability of a molecule to donate or accept a hydrogen atom and the presence of hydrogen bonding. Starting from these four categories of pure compounds, Danner and Gess defined nine classes of binary systems (nonpolar/nonpolar, nonpolar/weakly polar, etc.), and for each class, their database includes a variety of systems ranging from ideal to highly nonideal. We were totally convinced by this approach and decided to propose a somehow similar classification of binary systems but giving more emphasis on the associating character of the pure compounds, i.e., on their ability to be involved in a hydrogen bond, rather than on their polarity. Indeed, the various publications devoted to the CPA[10−12] or SAFT[13−24] EoSs clearly indicate that an actual scientific challenge for EoSs is their ability to properly describe the very complex association phenomena.

2.3.1. Definition of the "Associating Character" of a Pure Component. In this paper, "association" means association only by hydrogen bonding. In classical physical chemistry,[25] hydrogen bonds are defined as an attractive interaction between a hydrogen atom from a molecule or a molecular fragment A−H in which A is more electronegative than H and a highly electronegative atom (denoted B) in the same or a different molecule that possesses a lone pair of electrons. There is no strict cutoff for an ability to participate in hydrogen bonding, but nitrogen (N), oxygen (O), or fluor (F) atoms participate the most effectively. From the definition above, the formation of a hydrogen bond can be regarded as the electrostatic interaction between a partial positive charge (δ^+) located on the labile hydrogen atom and a partial negative charge (δ^-) located on B that possesses a lone pair of electrons (see Figure 1). The distance between the atoms H and B is classically taken as indication of the hydrogen-bond strength; it typically varies between 160 and 200 pm.

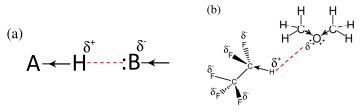


Figure 1. (a) Illustration of the definition of a hydrogen bond (red dashed line). The arrows indicate the more electronegative atom, i.e., the direction in which the shared pair of electrons (of the covalent bond) is shifted. (b) Case of the pentafluoroethane−dimethyl ether system.

To create an association by hydrogen bonding, it is needed the conjunction of (i) a labile hydrogen atom and (ii) a lone pair of electrons. It thus becomes possible to classify the pure components into four categories according to their associating character, i.e., depending on whether they have a labile hydrogen atom and/or a lone pair of electrons or none of them.

- Category 1 (associating character denoted NA for "nonassociating"): The molecule has neither a labile hydrogen atom nor a lone pair of electrons. It is

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Table 1. . Definition of the 10 Families of Binary Systems and the 9 Corresponding Binary Association Codes (BACs)

component 1	component 2	binary association code (BAC)	type of exhibited association
nonassociating (NA) nonpolar	nonassociating (NA) nonpolar	1	mixtures without association
hydrogen-acceptor (HA) polar but nonassociating	nonassociating (NA) nonpolar	2	
hydrogen-donor (HD) polar but nonassociating	nonassociating (NA) nonpolar	3	
hydrogen-acceptor (HA) polar but nonassociating	hydrogen-acceptor (HA) polar but nonassociating	4	
hydrogen-donor (HD) polar but nonassociating	hydrogen-donor (HD) polar but nonassociating		
self-associating (SA) polar and associating	nonassociating (NA) nonpolar	5	mixtures in which self-association takes place (but tends to be broken)
hydrogen-donor (HD) polar but nonassociating	hydrogen-acceptor (HA) polar but nonassociating	6	mixtures in which cross-association takes place alone
self-associating (SA) polar and associating	hydrogen-donor (HD) polar but nonassociating	7	
self-associating (SA) polar and associating	hydrogen-acceptor (HA) polar but nonassociating	8	mixtures in which both cross-association and self-association take place
self-associating (SA) polar and associating	self-associating (SA) polar and associating	9	

nonpolar. Molecules like alkanes and monohalogenated compounds are included in this family. In short, this category includes nonpolar/nonassociating components.

- Category 2 (associating character denoted HA for "hydrogen-acceptor"): The molecule possesses a lone pair of electrons (on an electronegative atom) but no labile hydrogen atom. Consequently, the molecule is polar. Ketones, aldehydes, ether, and ternary amines belong to this family. In short, this category includes polar but nonassociating components.
- Category 3 (associating character denoted HD for "hydrogen-donor"): The molecule has a labile hydrogen atom but does not possess a lone pair of electrons and thus is polar. Di- or trihalogenated compounds or the ones with a terminal alkyne group belong to this family. The labile hydrogen earns its acidity from the electronegativity of its closest neighbors. In short, this category includes polar but nonassociating components.
- Category 4 (associating character denoted SA for "self-associating"): The molecule possesses both a labile hydrogen atom and a lone pair of electrons. It is strongly polar. Such molecules fulfill the two necessary and sufficient conditions to establish a hydrogen bond. They are thus self-associating. Water, alcohols, and carboxylic acids belong to this family. In short, this category includes polar and associating components.

Table S1 of the file ie0c01734_si_011.pdf which is part of the Supporting Information lists the 107 pure compounds included in the proposed database and indicates for each of them the corresponding associating character among nonassociating (NA), hydrogen-acceptor (HA), hydrogen-donor (HD), or self-associating (SA).

2.3.2. Definition of Binary Association Codes (BACs) to Describe Association in Solution. With this associating character coding, the binary systems in the database were immediately divided into the following ten families by performing all of the possible combinations (see Table 1), and a binary association code (BAC) was assigned to each family. From our experience, much less experimental data are reported for HA/HA and HD/HD binary systems than for any other family. The lack of experimental data on HD/HD binary systems can be explained by noticing that HD molecules are mostly refrigerants that are generally encountered as pure compounds in chemical processes. Therefore, it was decided to merge HA/HA and HD/HD families, which are both nonassociating mixtures, into a single family, thus reducing the number of BACs to nine.

From Table 1, it is possible to determine at a glance in which binary systems hydrogen bonds occur. Indeed, the requirement for the existence of a hydrogen bond remains to be the presence of both a labile hydrogen atom and a lone pair of electrons. In the case when the labile hydrogen atom and the lone pair of electrons originate from two different species, the hydrogen bond is said to be formed by "cross-association" between compounds 1 and 2. The last column of Table 1 highlights that all types of binary systems (those in which nonassociation, self-association, cross-association, or both cross-association and self-association are taking place) are included in the proposed database. In other words, four categories of binary systems based on the type of association they exhibit can be distinguished.

- Binary systems having a small BAC value (from 1 to 4) cannot exhibit association and are expected to be easily correlated by any sophisticated-enough thermodynamic model. In that sense, the BAC plays the role of a thermodynamic-complexity degree (for a small BAC value, the thermodynamic complexity is low, and this complexity increases with the BAC).
- In binary systems belonging to the BAC_5, an nonassociating (NA) component faces an self-associating (SA) component so that self-association (at least partially) persists in the mixture. The nonassociating molecules tend to break the hydrogen-bond network, while SA molecules tend to resist so that liquid-phase partial immiscibility is often observed in this family (these two compounds do not like being mixed together and often prefer to be each one in a separate liquid phase). In Table 1, such systems are thus considered as

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Table 2. Overview of How the Deviations from Ideality Are Distributed Among the Nine Binary Association Codes (BACs) for the 200 Binary Systems of the Proposed Database[a]

binary association code (BAC)	deviations from ideality not assessed[b] (%)	ideal (%)	nonideal with enthalpic causes (%)	nonideal with entropic causes (%)	nonideal with enthalpic and entropic causes (%)	nonideal with nonassessed causes[c] (%)
1 (NA-NA)	38	15	15	4	19	8
2 (HA-NA)	29	29	13	4	17	8
3 (HD-NA)	10	30	15	0	10	35
4 (HA-HA or HD-HD)	32	32	14	5	9	9
5 (SA-NA)	33	11	22	0	22	11
6 (HD-HA)	28	16	4	0	28	24
7 (SA-HD)	44	0	6	25	25	0
8 (SA-HA)	23	15	27	4	23	8
9 (SA-SA)	9	30	22	9	17	13

[a]The abbreviations used for the associating character of a pure compound are NA for nonassociating, HA for hydrogen-acceptor, HD for hydrogen-donor, and SA for self-associating. [b]Nonavailability of subcritical VLE data (refer to Figure 2). [c]Nonavailability of h^M data (refer to Figure 2).

"mixtures in which self-association tends to be broken". All binary systems of water + alkane or alcohol + alkane types belong to this family.

- BAC_6 results from the mixing of a component that has a labile hydrogen atom with another component that possesses a lone pair of electrons, causing a cross-association phenomenon. The two components do not exhibit association when they are pure, but their mixture exhibits hydrogen bonding. Consequently, these two molecules are more attracted to each other in a mixture than when they are pure; therefore, such mixtures usually exhibit negative deviations from ideality.
- For binary association codes 7−9, more complex phenomena occur as a self-associating compound is mixed with another molecule likely to generate a hydrogen bonding with it. Therefore, it is not always possible to determine a priori how the mixture is going to behave (thermodynamically) and if the mixing leads to an intensification or a relaxation of hydrogen bonding.

2.3.3. Quantification of Deviations from Ideality. For each class of binary system, identified by its BAC, our motivation is to include in the proposed database a large variety of binary systems revealing the variety of deviation-from-ideality types. This section aims to explain how such deviations were sorted from both quantitative and qualitative viewpoints. Qualitatively, a system will be considered ideal if it is formed by molecules having (i) similar sizes, (ii) similar shapes, and (iii) showing similar energetic interactions (nature and strength), regardless of the temperature, pressure, and composition.[26] On the contrary, a system is considered nonideal if a noticeable departure from the three aforementioned criteria is observed. If deviations from ideality are the consequence of a difference in molecular sizes and/or shapes only, the excess enthalpy (h^E) is negligible and the solution is called athermal; consequently, the excess Gibbs energy is proportional to the mixture excess entropy ($g^E \approx Ts^E$) and it is said that deviations from ideality originate from entropic effects. In the same way, if deviations from ideality are solely caused by a difference in energetic interactions, the excess entropy (s^E) is negligible and the solution is called regular; consequently, $g^E \approx h^E$. In such a case, deviations from ideality are the consequence of enthalpic effects. Naturally, both effects may coexist in a nonideal solution and, in this case, it is said that deviations from ideality are the consequence of combined effects (of enthalpic and entropic natures). Such an overview of the possible causes of deviations from ideality is important as many thermodynamic models are built by summing the contributions of an enthalpic (related to the energetic interactions in the system) and an entropic (related to the size of the molecules) term. To provide a benchmark database for EoS model evaluation, it is necessary to include mixture data spanning the whole range of departure-from-ideality types (from ideal to nonideal, including enthalpic, entropic, and combined effects). Doing so, our database will allow the identification of model failures in their enthalpic and/or entropic modeling patterns.

Quantitative information on how deviations from ideality were quantified and how the origin of such deviations was assessed is now detailed. To start, it is worth recalling that to determine the magnitude of the deviations from ideality, the activity coefficients have to be calculated from experimental VLE data. It can be done easily using the VLE relationship stemming from the $\gamma-\varphi$ approach:

$$\gamma_i(T, x) = P_{exp} \cdot y_{i,exp} / [P_i^{sat}(T_{exp}) \cdot x_{i,exp}] \quad (1)$$

Equation 1 however requires a correlation to estimate the vapor pressure of component i, so that only subcritical VLE data ($T < T_{c,i}$) can be used to estimate the deviations from ideality. In the case subcritical VLE data are not available for a system included in our database, the message deviations from ideality not assessed is reported for such a system in Table 2.

For each binary system for which subcritical VLE data were available, a set of four parameters (p_1, p_2, p_3, p_4) of the Margules excess Gibbs energy model was fit over both VLE data and enthalpy of mixing data (when available).

$$\begin{cases} \dfrac{g^E(T, \boldsymbol{x})}{RT} = x_1 \cdot x_2 \cdot A(T) \\ A(T) = p_1 - p_2 T - p_3 \ln T + P_4 \exp\left(\dfrac{1}{T}\right) \end{cases} \quad (2)$$

The p_i parameters were determined to minimize the mean average percent error (MAPE) between calculated and experimental VLE and h^M data. The mathematical expression of h^E (and thus h^M) can be straightforwardly derived from eq 2

$$h^E = g^E - T\left(\frac{\partial g^E}{\partial T}\right)_x \quad (3)$$

For VLE calculations, the $\gamma-\varphi$ approach was used assuming that the gas phase is perfect and by neglecting the Poynting

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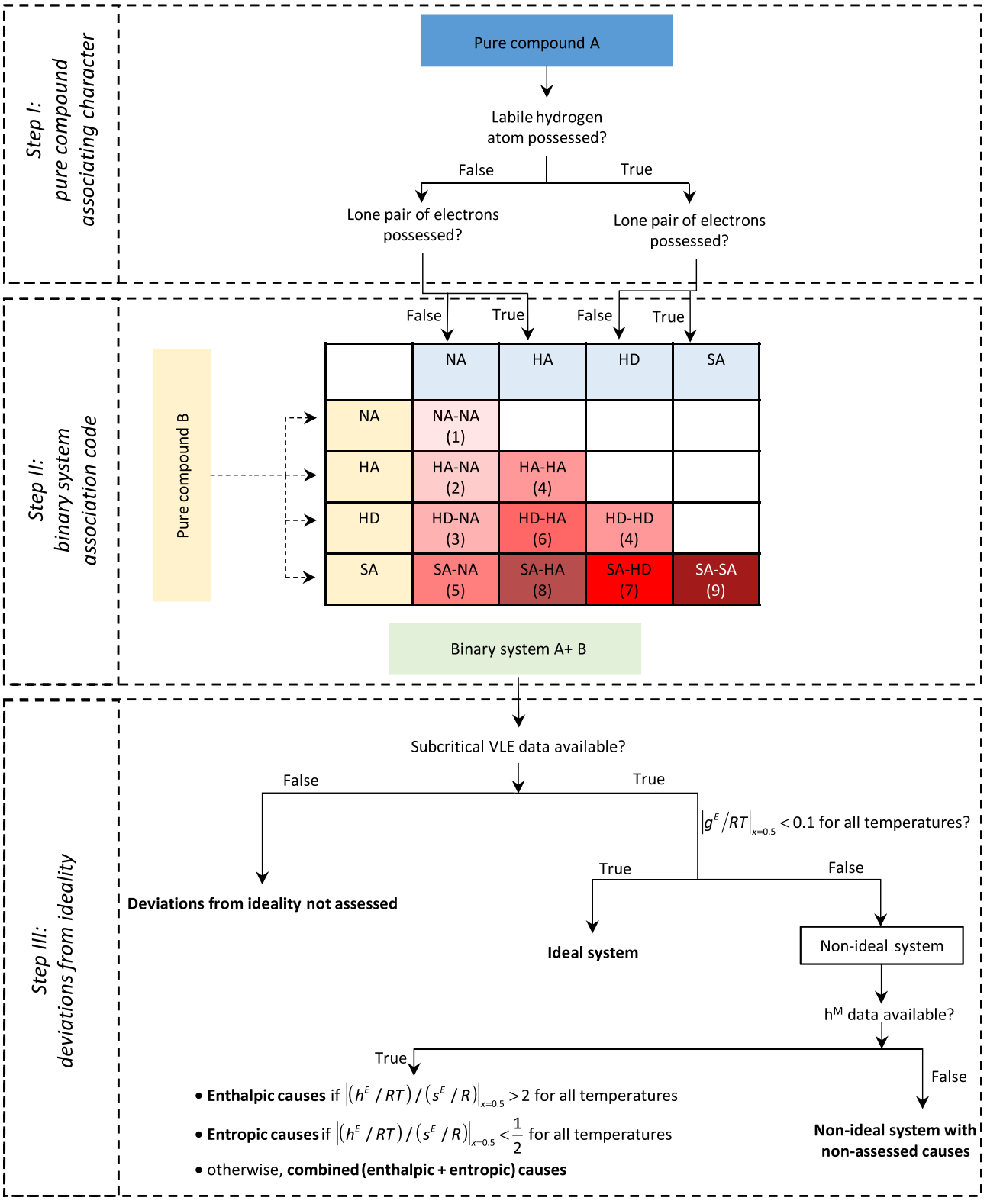


Figure 2. Procedure followed to build the proposed database.

factor. In other words, the following classical VLE relation, especially suitable to correlate subcritical data, was used:

$$Py_i = P_i^{sat} x_i \gamma_i \quad (4)$$

The vapor pressures were calculated by means of correlations extracted from the DIPPR database.

Once the four parameters (p_1, p_2, p_3, p_4) have been fit, the magnitude of the deviations from ideality can be estimated. For each temperature involved in the regression procedure, g^E, h^E, and s^E were calculated at the unique composition $x_1 = 0.50$. Based on our experience, a binary system can be considered ideal (see Table 2) if $|g^E/RT|_{x=0.5} < 0.1$ for each of the

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Table 3. Overview of the Distribution of the Different Types of Experimental Data among the Nine Binary Association Codes (BACs) for the 200 Binary Systems of the Proposed Database[a]

binary association code (BAC)	subcritical liquid-phase[b] composition	subcritical vapor-phase (or second liquid phase[c]) composition	supercritical liquid-phase[b] composition	supercritical vapor-phase (or second liquid phase[c]) composition	azeotropic point	critical point	enthalpy of mixing	heat capacity of mixing	three-phase line	sum	%
1 (NA-NA)	1323	1336	2293	2203	11	252	1314	231	16	8979	18.8
2 (HA-NA)	1406	1406	1195	1148	22	319	1532	27	0	7055	14.7
3 (HD-NA)	1087	1087	306	306	44	49	258	30	0	3167	6.6
4 (HA-HA or HD-HD)	904	904	561	561	7	60	454	15	0	3466	7.2
5 (SA-NA)	1237	1219	343	378	35	130	1525	155	25	5047	10.5
6 (HD-HA)	1112	1112	410	410	18	63	466	99	0	3690	7.7
7 (SA-HD)	741	711	0	0	13	0	498	26	0	1989	4.2
8 (SA-HA)	2140	2119	915	881	42	193	1408	144	12	7854	16.4
9 (SA-SA)	2299	2287	149	149	33	50	1115	507	13	6602	13.8
sum	12 249	12 181	6172	6036	225	1116	8570	1234	66	47 849	
%	25.6	25.5	12.9	12.6	0.47	2.33	17.91	2.58	0.14		

[a]The abbreviations used for the associating character of a pure compound are NA for nonassociating, HA for hydrogen-acceptor, HD for hydrogen-donor, and SA for self-associating. [b]Liquid phase refers indifferently to a VLE or an LLE data point. For an LLE, it designates the composition of the α-liquid phase. [c]Second liquid phase designates the composition of the β-liquid phase in the case of an LLE.

considered temperatures. If not, the system is declared nonideal.

For nonideal systems, the origin of the deviations from ideality (entropic, enthalpic, or combined) was only evaluated when h^M experimental data were available and thus included in the regression procedure. We indeed noticed that the calculation of the excess enthalpy and entropy of a binary system could be very uncertain when the four p_i parameters were determined over VLE data only. For nonideal systems, when h^M data were lacking, the systems were thus declared (see Table 2): nonideal with nonassessed causes. In turn, when h^M data were available:

1. If $|(h^E/RT)/(s^E/R)|_{x=0.5} > 2$ for all temperatures, it was considered that nonideality stemmed from enthalpic effects. In Table 2, the system is labeled nonideal with enthalpic causes.
2. If $|(h^E/RT)/(s^E/R)|_{x=0.5} < 1/2$ for all temperatures, it was considered that nonideality stemmed from entropic effects. In Table 2, the system is labeled nonideal with entropic causes.
3. Otherwise, deviations from ideality are the consequence of combined effects, i.e., both enthalpic and entropic effects, and none is dominant. In Table 2, the system is labeled nonideal with enthalpic and entropic causes.

An overview of how the deviations from ideality are distributed among the nine BACs can be found in Table 2, whereas the different steps that were followed to build the proposed database are summarized in Figure 2.

2.4. How Many Systems and How Many Data Should Be Included? Commercial databases, especially the Dortmund Data Bank, report VLE data for tens of thousands of binary systems. It would be impractical to cross-compare EoS on such a huge number of data; therefore, our objective is to work with a much smaller number of wisely chosen binary systems to cover all categories of mixtures. For each of the nine families of binary systems—defined each by a distinct BAC—our objective is to consider systems, deemed as good representative of their family. Among these systems, our objective is to reach a distribution of one-fourth of systems containing high-pressure VLE data (for which deviations from ideality cannot be assessed), one-fourth of ideal systems, and half of nonideal systems. The nonideal systems should include similar numbers of systems for which the origin of the deviations from ideality could not be assessed due to a lack of h^M data or stem from enthalpic, entropic, or (enthalpic + entropic) effects. To have a meaningful representation of such a diversity, it was found acceptable to include around 20 binary systems per BAC.

Another key point is to only retain high-quality-certified data explaining why the consistency of the data was checked with the help of four consistency tests: the point test,[27] the integral test,[28] the differential test, and the infinite-dilution test,[29] all performed with the Data Preparation Package (DPP), which is a software package for the regression of thermophysical property models commercialized by Dechema. It is however worth noting that the aforementioned tests only apply to VLE data when both compounds are subcritical. As a direct consequence, among the many data included in our benchmark database, only the quality of the subcritical data can be guaranteed. For an ideal binary system, passing the point test was considered as a sufficient consistency condition, while for nonideal systems, the point test and two of the three remaining tests had to be passed to keep the experimental data in our database. Indeed, as explained by Wisniak et al.,[30] the quality of the equilibrium data should be checked using simultaneously several of the available consistency tests.

In the end, the proposed database comprises 200 binary systems and contains about 30 000 experimental data points (around 18 000 VLE/LLE data points, 8500 h^M data, 1500 c_P^M data, and 2000 data points relative to critical points, azeotropic points, or three-phase lines).

2.5. Built Database. An extensive screening of thousands of binary systems was first realized, and a complex strategy was developed to only keep the 200 systems that met our criteria in terms of (i) types of association, (ii) deviations from ideality, and (iii) quality, quantity, and diversity of the experimental data. Indeed, as previously discussed, we made our best in order that the selected systems are such that phase equilibrium data (VLE, LLE, VLLE, azeotrope) and mixing properties (h^M, c_P^M) are abundant in large temperature, pressure, and composition ranges.

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Ind. Eng. Chem. Res. 2020, 59, 14981−15027

As previously stated, an overview of how the deviations from ideality are distributed among the nine BACs can be found in Table 2. Similarly, an overview of how the different types of data are distributed among the nine BACs can be found in Table 3. For each BAC, Tables 4−12 detail the list of the selected binary systems, specify the origin of the deviations from ideality, and list the references in which the experimental data can be found. A scan of the 958 original references from which the data were extracted was realized, and the authors are committed to sending a copy of an article to any reader of this paper that would, e.g., necessitate more details on the used experimental setup.

Table 4. List of the 26 Binary Systems for Which the Binary Association Code Is BAC = 1 (NA-NA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	methane	propane	31−43
	methane	*n*-hexane	41, 44−51
	methane	*n*-heptane	41, 52−55
	nitrogen	ethane	56−63
	methane	*n*-decane	64−69
	ethane	*n*-heptane	70−75
	nitrogen	*n*-pentane	76−78
	nitrogen	*n*-decane	79, 80
	methane	*n*-tetracosane	81−84
	ethane	*n*-hexatriacontane	85−87
ideal	*n*-hexane	cyclohexane	88−100
	benzene	toluene	101−110
	propane	isopentane	111
	cyclohexane	methylcyclohexane	89, 110, 112−115
nonideal with nonassessed causes	ethane	propane	116−128
	methane	*n*-butane	41, 51, 129−133
nonideal with enthalpic causes	argon	methane	134−143
	n-heptane	monochlorobenzene	144−150
	cyclohexane	monochlorobenzene	113, 150−155
	1,2-dichloroethane	carbon tetrachloride	156−161
nonideal with entropic causes	1,2-dichloroethane	toluene	105, 162−166
nonideal with enthalpic and entropic causes	nitrogen	methane	61, 134, 142, 143, 167−175
	methane	ethane	39, 41, 60, 61, 176−180
	benzene	*n*-heptane	89, 110, 145, 181−197
	benzene	cyclohexane	91, 100, 191, 198−215
	ethylene	xenon	216−218

[a]Such a BAC corresponds to a binary system involving a nonassociating (NA) molecule + another nonassociating (NA) molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

Remark. Table 3 shows that the proposed database contains information for 225 azeotropic points. Some of them can however not be found in the original publications from which the data were extracted. We indeed decided on some azeotropic systems to interpolate the experimental VLE data to determine the temperature, pressure, and composition of the azeotropic point.

Several Excel files are available as Supporting Information.

- The first one, named ie0c01734_si_001.xlsx, is a light Excel file that only contains the experimental data and the corresponding references. This file comprises 201 sheets. The first one, named "ReadMe", provides an overview of the database and explains how it is organized. The other 200 sheets each contain the data related to a given binary system.
- The nine others, one for each BAC, and named ie0c01734_si_002.xlsx (BAC_1), ie0c01734_si_003.xlsx (BAC_2), ie0c01734_si_004.xlsx (BAC_3), ie0c01734_si_005.xlsx (BAC_4), ie0c01734_si_006.xlsx (BAC_5), ie0c01734_si_007.xlsx (BAC_6), ie0c01734_si_008.xlsx (BAC_7), ie0c01734_si_009.xlsx (BAC_8), ie0c01734_si_010.xlsx (BAC_9) are large-size Excel files that provide figures to have a visualization of the experimental data (as a complement to data tables) and the singularities of the binary systems. These files contain several sheets. Here also, the first one, named ReadMe, provides an overview of the database and explains how it is organized, whereas the other sheets each contain the data related to a given binary system.

3. GRADING OF A THERMODYNAMIC MODEL BY MEANS OF THE PROPOSED DATABASE TO ASSESS ITS ACCURACY

This section focuses initially on the methodology that has to be followed to evaluate the deviations between model predictions and experimental data (in particular, which property of each data set must be specified and which property must be calculated from the thermodynamic model and compared to an experimental value). It is then explained how a thermodynamic model may be graded. The methodology described hereafter to assess the accuracy of a model is specific, but we believe this approach is necessary to fairly compare the scores obtained by two thermodynamic models. It is exactly what happens with the grading of students: the professor establishes a very detailed marking scheme before marking the examination papers.

3.1. Evaluation of the Deviations between Model Predictions and Experimental Data. To fairly cross-compare two thermodynamic models, we are convinced that the deviations between model predictions and experimental data have to be calculated in the same way, i.e., following the same procedure. However, in accordance with Gibbs's phase rule, there is no unique way to perform a fluid-phase equilibrium (VLE, LLE, VLLE, critical point, azeotropic point) calculation. It is always necessary to first determine the variance (also called the number of degrees of freedom) of the system and then to specify a number of intensive variables equal to the variance and finally to calculate the other intensive variables (those that will be compared to the experimental data). The variables that are specified and those that are calculated can however be freely chosen. To fix the ideas, let us consider the VLE calculation of a binary system for which the temperature T, pressure P, and composition of the liquid (x_1) and gas (y_1) phases were experimentally measured. For such a system, the number of degrees of freedom (the variance) is equal to 2 and it is thus necessary to specify two variables among (T,P,x_1,y_1) and to calculate the other two. The arbitrary

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Table 5. List of the 24 Binary Systems for Which the Binary Association Code Is BAC = 2 (HA-NA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	carbon dioxide	toluene	219−233
	carbon dioxide	*n*-decane	234−245
	methane	carbon dioxide	35, 179, 246−255
	carbon dioxide	cyclopentane	256, 257
	nitrogen	carbon dioxide	58, 247−249, 253, 258−269
	methane	hydrogen sulfide	270−272
	carbon dioxide	*n*-dotriacontane	273−275
ideal	methyl *tert*-butyl ether	*n*-heptane	276−280
	ethyl acetate	toluene	281−284
	carbon tetrachloride	1,4-dioxane	285−290
	methyl ethyl ketone	benzene	291−294
	methyl *tert*-pentyl ether	*n*-heptane	295−298
	methyl *tert*-butyl ether	toluene	299−302
	1,2,3,4-tetrahydronaphthalene	quinoline	303, 304
nonideal with nonassessed causes	ethylene	carbon dioxide	305−311
	carbon dioxide	propane	35, 42, 127, 259, 312−320
nonideal with enthalpic causes	acetone	*n*-hexane	321−327
	n-pentane	acetone	321, 325, 327−329
	acetone	cyclohexane	98, 198, 330−337
nonideal with entropic causes	benzene	*n*-methyl-2-pyrrolidone	338−343
nonideal with enthalpic and entropic causes	carbon dioxide	ethane	179, 317, 344−353
	carbon dioxide	*n*-butane	127, 261, 306, 316−319, 354−361
	n-hexane	methyl ethyl ketone	187, 294, 362−365
	acetone	benzene	198, 286, 366−374

[a]Such a BAC corresponds to a binary system involving a hydrogen-acceptor (HA) molecule + a nonassociating (NA) molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

Table 6. List of the 20 Binary Systems for Which the Binary Association Code Is BAC = 3 (HD-NA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	ethylene	dichloromethane	375
	nitrogen	chlorodifluoromethane	376−379
ideal	chloroform	benzene	105, 371, 380−386
	chloroform	1,2-dichloroethane	387−389
	chloroform	carbon tetrachloride	390−393
	1,1,1-trifluoroethane	2,3,3,3-tetrafluoropropene	394
	ethyl fluoride	1,1,1,2-tetrafluoroethane	395
	propylene	chlorodifluoromethane	396
nonideal with nonassessed causes	difluoromethane	propane	397−401
	trifluoromethane	ethane	402, 403
	carbon tetrafluoride	chlorodifluoromethane	404, 405
	pentafluoroethane	propane	398, 400, 406−408
	carbon tetrafluoride	trifluoromethane	409
	hexafluoroethane	1,1,1,2-tetrafluoroethane	396, 410
	decafluorobutane	1,1,1,3,3-pentafluorobutane	411
nonideal with enthalpic causes	chlorodifluoromethane	dichlorodifluoromethane	412−417
	dichloromethane	carbon tetrachloride	157, 160, 391, 418
	chloroform	*n*-hexane	419−425
nonideal with enthalpic and entropic causes	chloroform	*n*-heptane	419, 422, 423, 425−427
	dichloromethane	*n*-pentane	428−430

[a]Such a BAC corresponds to a binary system involving a hydrogen-donor (HD) molecule + a nonassociating (NA) molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

choice made in this paper is to specify T and P (i.e., to fix T and P to their experimental values) and to calculate, in turn, x_1 and y_1. There are thus no deviations between model predictions and experimental values of T and P but instead deviations over x_1 and y_1. Specifying T and P and calculating x_1 and y_1 are somehow similar to a T,P-flash calculation.[989] For each property available in the proposed database, Table 13 reports the variance and the specified and calculated variables. In other words, Table 13 dictates the methodology that has to be strictly followed to evaluate the deviations between model predictions and experimental data by means of the proposed database.

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Table 7. List of the 22 Binary Systems for Which the Binary Association Code Is BAC = 4 (HA-HA or HD-HD)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	carbon dioxide	dimethyl ether	431−433
	carbon dioxide	hydrogen sulfide	434−437
	carbon dioxide	ethyl acetate	438−442
	carbon dioxide	carbon disulfide	443, 444
	carbon dioxide	dimethyl carbonate	445−450
	carbon monoxide	carbon dioxide	451−453
	oxygen	carbon dioxide	264, 265, 454−457
ideal	pentafluoroethane	1,1,1,2-tetrafluoroethane	458−462
	chlorodifluoromethane	1,1,1,2-tetrafluoroethane	463, 464
	difluoromethane	1,1,1,2-tetrafluoroethane	458, 459, 461, 462, 465−469
	1,1,1,2-tetrafluoroethane	1,1-difluoroethane	396, 470, 471
	ethyl acetate	1,4-dioxane	285, 472−474
	dimethyl carbonate	diethyl carbonate	475−477
	1,2-epoxybutane	dimethyl carbonate	478
nonideal with nonassessed causes	dimethyl ether	sulfur dioxide	479−481
	trifluoromethane	chlorodifluoromethane	482, 483
nonideal with enthalpic causes	diethyl ether	acetone	383, 484, 485
	carbon disulfide	acetone	486−488
	triethylamine	1,4-dioxane	489, 490
nonideal with entropic causes	thiophene	sulfolane	491
nonideal with enthalpic and entropic causes	tetrahydrofuran	*N*,*N*-dimethylformamide	492, 493
	n-butyl acetate	*N*,*N*-dimethylformamide	494, 495

[a]Such a BAC corresponds to a binary system involving two hydrogen-acceptor (HA) molecules or two hydrogen-donor (HD) molecules. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

Table 8. List of the 18 Binary Systems for Which the Binary Association Code Is BAC = 5 (SA-NA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	*n*-butane	water	496−500
	water	benzene	501−505
	ethane	1-propanol	506−511
	nitrogen	ammonia	512−514
	ethane	water	497
	nitrogen	water	515−525
ideal	diethylamine	benzene	145, 526, 527
	diethylamine	monochlorobenzene	145, 528
nonideal with nonassessed causes	ethane	methanol	508, 529−534
	propane	methanol	535−539
nonideal with enthalpic causes	1-propanol	benzene	200, 540−548
	ethanol	benzene	190, 193, 208, 380, 545, 548−558
	isopropanol	2,2,4-trimethylpentane	559−566
	2-butanol	cyclohexane	567−572
nonideal with enthalpic and entropic causes	1-propanol	*n*-hexane	573−579
	ethanol	*n*-heptane	580−596
	methanol	*n*-hexane	579, 588, 597−605
	methanol	benzene	545, 548, 555, 606−616

[a]Such a BAC corresponds to a binary system involving a self-associating (SA) molecule + a nonassociating (NA) molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

Table 13 highlights that for systems of variance equal to 2 (two-phase equilibrium binary systems), we arbitrarily decided that temperature and pressure should be specified, whereas phase compositions should be calculated. For systems of unitary variance (binary critical point, binary azeotropic point, binary three-phase equilibrium), we decided that the temperature should be specified and that other variables (critical pressure and composition, azeotropic pressure and composition, three-phase pressure and compositions) should be calculated.

The calculation of the deviations between model predictions and experimental data for mixing properties does not need to make arbitrary choices on the specified and calculated variables; there is indeed a unique way to perform the calculation. For such properties, the temperature, pressure, global composition z_1, and h^M (or c_P^M) are experimentally determined. Depending on (T,P,z_1), the binary system can be either in a one-phase or in a two-phase region so that a T,P-flash calculation has to be first performed at a specified temperature, pressure, and global composition to determine the number of phases in equilibrium, their composition, and their proportions. Once done, h^M or c_P^M can be straightforwardly calculated for the specified (T,P,z_1) values.[990] It is worth noting that the experimentalists who performed h^M or c_P^M measurements do not mention systematically the pressure at which the measurements were conducted although such a value is required to perform the calculation from an EoS. This usually happens for mixing properties related to a liquid phase on which the pressure has a negligible influence. When this happened, the assumed experimental pressure was determined by trial and errors so that the calculated physical state of the system agrees with the experimentally observed state. The first guessed pressure is always the atmospheric pressure. In the 10 Excel files ie0c01734_si_001.xlsx (complete database),

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Table 9. List of the 25 Binary Systems for Which the Binary Association Code Is BAC = 6 (HD-HA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	carbon dioxide	chlorodifluoromethane	376, 377, 483, 617
	carbon dioxide	1,1,1,2-tetrafluoroethane	618−621
	carbon dioxide	1,1,1,2,3,3,3-heptafluoropropane	622, 623
	trifluoromethane	carbon disulfide	483
	chloroform	diisopropyl ether	425, 490, 624, 625
	1,1,1-trifluoroethane	dimethyl ether	626
	chloroform	*n*-butyl ethyl ether	624, 627
ideal	carbon dioxide	difluoromethane	469, 628−630
	difluoromethane	dimethyl ether	631−633
	difluoromethane	sulfur dioxide	634
	ethyl acetate	trichloroethylene	635
nonideal with nonassessed causes	sulfur dioxide	1,1,1,2,3,3,3-heptafluoropropane	636
	chlorodifluoromethane	dimethyl ether	637
	chlorodifluoromethane	carbon disulfide	483
	pentafluoroethane	dimethyl ether	407, 638
	3-pentanone	1,1,2,2-tetrachloroethane	639
	dimethyl ether	1,1,1,3,3,3-hexafluoropropane	640, 641
nonideal with enthalpic causes	dichloromethane	carbon disulfide	642, 643
nonideal with enthalpic and entropic causes	acetone	chloroform	372, 374, 384, 420, 425, 490, 644−651
	chloroform	ethyl acetate	652−655
	chloroform	tetrahydrofuran	387, 425, 656−659
	chloroform	di-n-propyl ether	425, 624, 625, 627, 660, 661
	methyl acetate	chloroform	425, 652, 662, 663
	cyclopentanone	1,1,2,2-tetrachloroethane	664−666
	ethyl acetate	1,1,2,2-tetrachloroethane	667, 668

[a]Such a BAC corresponds to a binary system involving a hydrogen-donor (HD) molecule + a hydrogen-acceptor (HA) molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

Table 10. List of the 16 Binary Systems for Which the Binary Association Code Is BAC = 7 (SA-HD)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	chloroform	1-butanol	382, 669, 670
	1-propanol	trichloroethylene	671, 672
	trichloroethylene	1-butanol	672, 673
	isopropanol	trichloroethylene	671, 674
	2-butanol	trichloroethylene	673, 674
	1-hexyne	acetonitrile	675, 676
	isopropanol	chloroform	670, 677, 678
nonideal with enthalpic causes	ethanol	1-heptyne	679, 680
nonideal with entropic causes	ethanol	chloroform	382, 427, 670, 681−686
	chloroform	acetic acid	687−691
	methanol	halothane	692−694
	trichloroethylene	2-methoxyethanol	695, 696
nonideal with enthalpic and entropic causes	chloroform	acetonitrile	697−702
	ethyl formate	chloroform	652, 654
	chloroform	1-propanol	383, 670, 703, 704
	n-propyl formate	1,1,2,2-tetrachloroethane	667, 705

[a]Such a BAC corresponds to a binary system involving a self-associating (SA) molecule + a hydrogen-acceptor (HA) Molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

ie0c01734_si_002.xlsx (BAC_1), ie0c01734_si_003.xlsx (BAC_2), ie0c01734_si_004.xlsx (BAC_3), ie0c01734_si_005.xlsx (BAC_4), ie0c01734_si_006.xlsx (BAC_5), ie0c01734_si_007.xlsx (BAC_6), ie0c01734_si_008.xlsx (BAC_7), ie0c01734_si_009.xlsx (BAC_8), ie0c01734_si_010.xlsx (BAC_9)—available as Supporting Information—that contain all of the experimental data, the experimental pressure appears as unknown and the assumed experimental pressure is indicated in parentheses. For clarity, an example is given in Figure 3. In this example, the unknown (not stated) experimental pressure has to be replaced by the atmospheric pressure (1.0132 bar).

Lastly, for any calculated property X, the mean absolute percentage error (MAPE) was selected to quantify the deviation between experimental and calculated data:

$$\mathrm{MAPE}_X(\%) = \frac{1}{N_{\mathrm{data}}} \sum_{i=1}^{N_{\mathrm{data}}} 100 \times \left| \frac{X_i^{\mathrm{EXP}} - X_i^{\mathrm{MODEL}}}{X_i^{\mathrm{EXP}}} \right| \quad (5)$$

3.2. Treatment of "Out-of-Model" Data Points. It may happen that the isothermal or isobaric phase diagram, calculated with the thermodynamic model we want to grade, does not have the expected topology. To fix the ideas, it may happen that a model does not predict the existence of a homogeneous azeotrope that is however experimentally observed. In such a case, the MAPE on P_{az} and x_{az} cannot be evaluated and the corresponding experimental data point is said to be out of model (not calculable by the model). When such a situation arises, the experimental data point must be rejected, i.e., not taken into account in eq 5 to evaluate the $\mathrm{MAPE}_x(\%)$. In other words, we simply apply $N_{\mathrm{data}} = N_{\mathrm{data}} - 1$

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Table 11. List of the 26 Binary Systems for Which the Binary Association Code Is BAC = 8 (SA-HA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	carbon dioxide	water	706−724
	carbon dioxide	ethanol	219, 242, 507, 579, 725−739
	ethanol	methyl *tert*-butyl ether	280, 740−744
	carbon dioxide	2-methyl-1-propanol	745−750
	carbon monoxide	methanol	751−753
	carbon dioxide	1-pentanol	242, 747, 754−757
ideal	diethylamine	ethyl acetate	473, 474
	diethylamine	triethylamine	758−761
	2-methyl-2-propanol	methyl *tert*-butyl ether	762−765
	acetonitrile	1,4-dioxane	766−768
nonideal with nonassessed causes	dimethyl ether	water	433, 769−772
	carbon dioxide	methanol	220, 221, 242, 433, 579, 731, 736, 739, 751, 773−783
nonideal with enthalpic causes	methanol	ethyl acetate	784−791
	isopropanol	diisopropyl ether	561, 742, 792, 793
	methanol	*n*-butyl acetate	789, 794−796
	diethyl ether	ethanol	797−799
	methanol	1,4-dioxane	800−805
	methanol	thiophene	606
	ethanol	di-*n*-butyl ether	799, 806−808
nonideal with entropic causes	methanol	diisopropyl ether	742, 809−811
nonideal with enthalpic and entropic causes	methanol	methyl *tert*-butyl ether	277, 279, 280, 741, 810, 812−816
	ethanol	ethyl acetate	786, 789, 790, 808, 817−824
	acetone	water	335, 610, 825−836
	ethanol	methyl ethyl ketone	291, 837−844
	ethanol	acetone	586, 845−850
	methanol	acetone	331, 335, 830, 851−856

[a]Such a BAC corresponds to a binary system involving a self-associating (SA) molecule + a hydrogen-acceptor (HA) Molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component.

Table 12. List of the 23 Binary Systems for Which the Binary Association Code Is BAC = 9 (SA-SA)[a]

origin of the deviations from ideality	molecule 1	molecule 2	references
deviations from ideality not assessed	water	ethylenediamine	857−859
	water	1-pentanol	860−863
ideal	methanol	1-butanol	610, 864−868
	ethanol	acetic acid	824, 869−872
	methanol	ethanol	655, 868, 873−879
	2-methyl-2-propanol	1-butanol	880−882
	ethanol	3-methyl-1-butanol	883−885
	methanol	3-methyl-1-butanol	885−887
	methanol	1-propanol	596, 833, 868, 878, 879, 888−891
nonideal with nonassessed causes	ammonia	water	892−901
	ammonia	acetonitrile	902
	water	allyl alcohol	903, 904
nonideal with enthalpic causes	water	phenol	905−911
	methyl formate	methanol	912−916
	ethyl formate	water	917, 918
	ethanol	ethyl formate	916, 919−921
	1-butanol	nitromethane	879, 922−926
nonideal with entropic causes	water	2-butoxyethanol	927−932
	water	propylene glycol monomethyl ether	928
nonideal with enthalpic and entropic causes	ethanol	water	817, 833, 874, 933−953
	water	acetonitrile	954−963
	methanol	water	830, 936, 950, 951, 964−981
	isopropanol	water	586, 938, 982−988

[a]Such a BAC corresponds to a binary system involving a self-associating (SA) molecule + another self-associating (SA) molecule. Corresponding origin of the deviations from ideality and list of the references in which the experimental data can be found. By convention, molecule 1 refers to the more volatile component. [b]The following part of this article (Section 3) aims at explaining how the proposed database should be used to grade a thermodynamic model to assess its accuracy. For illustrative purposes, Section 4 clarifies the grading of the thermodynamic model: {Peng−Robinson EoS + classical VdW mixing rules + a temperature-dependent BIP} and opens a discussion around its accuracy.

in eq 5. Below are detailed all of the cases in which out-of-model data points could appear.

Case 1. At specified T and P ($T = T_{exp}$ and $P = P_{exp}$), a two-phase system is experimentally observed, whereas the model predicts a one-phase system. All of the experimental data points for which the model predicts a one-phase system are declared out of model. This case is illustrated in Figure 4a.

Case 2. At specified T and P ($T = T_{exp}$ and $P = P_{exp}$), a two-phase system is experimentally observed and a two-phase system is also predicted by the model. However, it was experimentally found that $y_{1,exp} > x_{1,exp}$ (respectively, $y_{1,exp} < x_{1,exp}$), and the model predicts the wrong topology, i.e., predicts $y_{1,cal} < x_{1,cal}$ (respectively, $y_{1,cal} > x_{1,cal}$). All of these experimental data points are declared out of model. This case, which typically appears when the azeotropic composition is not properly predicted by the model, is illustrated in Figure 4b.

Case 3. A homogeneous azeotrope is experimentally observed at $T = T_{exp}$, whereas the model predicts a different topology (a zeotropic behavior or a heterogeneous azeotrope). The experimental homogeneous azeotropic point is declared out of model. This case is illustrated in Figure 4b,c.

Case 4. A three-phase line (VLLE) is experimentally observed at $T = T_{exp}$, whereas the model does not predict such a behavior. The experimental three-phase line is thus declared out of model. This case is illustrated in Figure 4d.

Case 5. The number of calculated critical points at $T = T_{exp}$ is different from the number of critical points experimentally observed. For example, the binary system may exhibit two

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Table 13. Specified and Calculated Variables for the Different Binary-System Properties Involved in the Database

property	variance	measured variables	specified variables	calculated variables (to be compared with experimental data values)
critical point		T, P, x_1	T	P, x_1
azeotropic point	1	T, P, x_1	T	P, x_1
three-phase equilibrium data (VLLE)		T, P, x_1^α, x_1^β, y_1	T	P, x_1^α, x_1^β, y_1
two-phase equilibrium data (VLE or LLE)	2	$\begin{cases} T, P, x_1, y_1 \text{ for VLE} \\ T, P, x_1^\alpha, x_1^\beta \text{ for LLE} \end{cases}$	T, P	$\begin{cases} x_1, y_1 \text{ for VLE} \\ x_1^\alpha, x_1^\beta \text{ for LLE} \end{cases}$
enthalpy of mixing	N.A.[a]	T, P, z_1, h^M	T, P, z_1	h^M
heat capacity of mixing		T, P, z_1, c_p^M	T, P, z_1	c_p^M

[a]Not applicable because global variables (here, global mole fractions z_1 and $z_2 = 1 - z_1$) are involved. Let us indeed recall that the phase rule that defines the variance only considers intensive variables specific to one of the phases.

Enthalpy of mixing (Methane + Ethane system)

Miller, R. C. - Staveley, L. A. K., 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

Figure 3. Notation used in the files database.xlsx and BACi with visualization of the data.xlsx (i = 1−9) when the experimental pressure is not mentioned.

experimental critical points, whereas 1 or 0 are returned by the model (see, e.g., Figure 4e). The opposite may also happen: the binary system exhibits a unique critical point, but 2 are returned by the model (see, e.g., Figure 4f). In such cases, the experimental critical points are all declared out of model.

3.3. Grading of a Thermodynamic Model. Our objective is to give a unique mark over 20 to a given thermodynamic model to immediately be able to benchmark its accuracy against the accuracy of other models. A grade of 20/20 is the highest attainable mark. It is obtained only if the model is able to exactly reproduce (with 0% deviation) all of the experimental data available in the proposed database. In all other cases, a score lower than 20 will be assigned to the model. Once the MAPEs are calculated (see eq 5), the scoring of a thermodynamic model starts by giving a mark over 20 to each of the nine families of binary systems, each identified by its BAC. Such a mark is actually an average over 10 marks (one for each of the 10 calculated properties defined in the last column of Table 13), which are:

(1) critical pressure,
(2) critical composition,
(3) azeotropic pressure,
(4) azeotropic composition,
(5) liquid-phase composition (x_1, x_1^α),
(6) gas-phase (or second liquid phase) composition (y_1, x_1^β),
(7) three-phase pressure,
(8) three-phase compositions,
(9) mixing enthalpy, and
(10) mixing heat capacity.

Once done, a thermodynamic model is characterized by nine marks (one for each BAC). In a second step, the number of marks is reduced from 9 to 4 by averaging the marks obtained by some BACs to only retain four categories of binary systems based on the type of association they exhibit.

- The marks obtained by BAC_1 + BAC_2 + BAC_3 + BAC_4 are averaged because all of these systems do not exhibit association (see Table 1). In eq 6, the resulting average mark is noted $mark_{NA}$ (where NA stands for no association).
- The mark obtained by BAC_5 is kept as a single mark because in this type of system, and only in this one, self-association tends to be broken (see Table 1). In eq 6, $mark_{BAC_5}$ is noted $mark_{SA}$ (where SA stands for self-association).
- The mark obtained by BAC_6 is kept as a single mark because in this type of system, and only in this one, cross-association without the presence of self-association is observed. BAC_6 refers to binary systems in which cross-association takes place alone (see Table 1). In eq 6, $mark_{BAC_6}$ is noted $mark_{CA}$ (where CA stands for cross-association).
- The marks obtained by BAC_7 + BAC_8 + BAC_9 are averaged because all of these systems exhibit both cross-association and self-association (see Table 1). In eq 6, the resulting average mark is noted $mark_{CA+SA}$ (where CA+SA stands for "cross-association + self-association").

The unique final mark given to a thermodynamic model is obtained by averaging the 4 marks (see eq 6) relative to (i)

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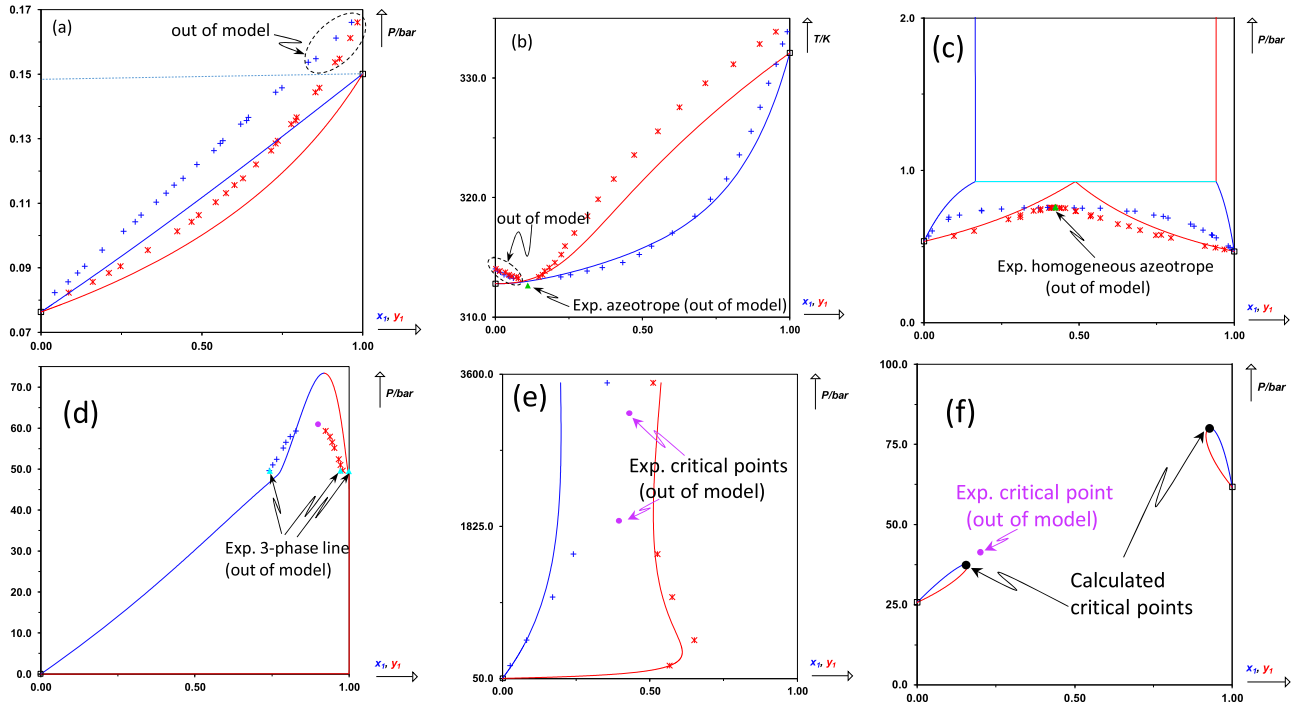


Figure 4. Illustration of all of the cases in which out-of-model data points can appear. For such exp. data points, the MAPE cannot be evaluated. (a) Experimental two-phase data points that are found to be one phase by the model. (b) An azeotropic system is predicted as a zeotropic system so that the homogeneous azeotrope is declared as out of model. In addition, for small mole fractions, $y_{1,\mathrm{exp}} > x_{1,\mathrm{exp}}$, whereas the model predicts the opposite. (c) A homogeneous azeotrope is predicted as heterogeneous. (d) A three-phase line is not predicted by the model. (e) Two critical points that are not predicted by the model are experimentally observed. (f) The model predicts two critical points, whereas only one is experimentally observed.

systems without association, (ii) systems in which self-association tends to be broken, (iii) systems in which cross-association takes place alone, and (iv) systems in which both cross-association and self-association take place.

$$\left\{\begin{array}{l}\textbf{Final mark of a thermodynamic model (over 20)} = \frac{1}{4}\times\underbrace{\left[\underbrace{mark_{NA}}_{\text{no association}} + \underbrace{mark_{SA}}_{\text{self-association}} + \underbrace{mark_{CA}}_{\text{cross-association}} + \underbrace{mark_{CA+SA}}_{\text{cross-association + self-association}}\right]}_{\text{average of 4 marks}} \\ \\ \text{with}: \left\{\begin{array}{l} mark_{NA} = \frac{mark_{BAC_1} + mark_{BAC_2} + mark_{BAC_3} + mark_{BAC_4}}{4} \\ mark_{SA} = mark_{BAC_5} \\ mark_{CA} = mark_{BAC_6} \\ mark_{CA+SA} = \frac{mark_{BAC_7} + mark_{BAC_8} + mark_{BAC_9}}{3} \end{array}\right. \end{array}\right. \quad (6)$$

The procedure aimed at giving a mark over 20 to a given BAC ($\mathrm{mark}_{\mathrm{BAC}_i}$) is now detailed. As previously stated, such mark is, in itself, the average value of 10 marks (in liquid-phase composition x (or x^{α}), gas-phase (or second liquid phase) composition y (or x^{β}), three-phase pressure P_{LLV}, three-phase composition z_{LLV}, critical pressure P_c, critical composition x_c, azeotropic pressure P_{az}, azeotropic composition x_{az}, mixing enthalpy h^{M}, mixing heat capacity c_P^{M}), each defined below.

(1) Mark in the liquid-phase composition (x for VLE and x^{α} for LLE):

$$\mathrm{Mark}_{x \text{ or } x^{\alpha}} = 20 - 0.5 \times \left[\frac{\text{MAPE on } x_1 \text{ or } x_1^{\alpha}\ (\%) + \text{MAPE on } x_2 \text{ or } x_2^{\alpha}\ (\%)}{2}\right] \quad (7)$$

where x_i (respectively, x_i^{α}) is the mole fraction of component i in the liquid phase (respectively, the α-liquid phase).

(2) Mark in the gas-phase (y) or second liquid-phase (x^{β}) composition:

$$\mathrm{Mark}_{y \text{ or } x^{\beta}} = 20 - 0.5 \times \left[\frac{\text{MAPE on } y_1 \text{ or } x_1^{\beta}\ (\%) + \text{MAPE on } y_2 \text{ or } x_2^{\beta}\ (\%)}{2}\right] \quad (8)$$

where y_i (respectively, x_i^{β}) is the mole fraction of component i in the gas or second liquid phase.

Remark: Very small (or close to 1) mole fractions may lead to huge percent deviations. As an example, at T/K = 377.59 K and P = 1.379 bar, the solubility of n-butane in water is $x_{1,\mathrm{exp}} = 0.000002$. In the case a model calculates $x_1 = 0.000082$, the corresponding 1/2 × (MAPE on x_1 + MAPE on x_2) relative to this unique data point is about 2000% even though the absolute deviation is extremely small ($|x_{1,\mathrm{exp}} - x_{1,\mathrm{cal}}| = 0.00008$). Such a data point can thus have a huge influence on the calculated $\mathrm{Mark}_{x \text{ or } x^{\alpha}}$ (or $\mathrm{Mark}_{y \text{ or } x^{\beta}}$). To avoid such a bias, if

$$\left\{\begin{array}{l} z_{1,\mathrm{exp}} < 0.01 \text{ or } z_{1,\mathrm{exp}} > 0.99 \\ \\ \text{and simultaneously:} \\ \quad 1/2 \times (\text{MAPE on } z_1 + \text{MAPE on } z_2) \\ \quad > 45\% \end{array}\right. \quad (9)$$

where z_1 stands for the mole fraction of component 1 in the liquid or gas phase of a two-phase system (VLE or LLE), the corresponding data point is rejected (we here mean, it is not taken into account in eq 5 to annihilate its influence on the calculated $\mathrm{Mark}_{x \text{ or } x^{\alpha}}$ (or $\mathrm{Mark}_{y \text{ or } x^{\beta}}$)).

(3) Mark in the three-phase pressure, P_{LLV}:

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$$\text{Mark}_{P_{\text{LLV}}} = 20 - 0.50 \times \text{MAPE on } P_{\text{LLV}}\ (\%) \quad (10)$$

(4) Mark in the three-phase composition, z_{LLV}:

$$\text{Mark}_{z_{\text{LLV}}} = 20 - 0.5 \times \sum_{i=1}^{2}\left[\frac{\text{MAPE on } x_i^{\alpha}\ (\%)+\text{MAPE on } x_i^{\beta}\ (\%)+\text{MAPE on } y_i\ (\%)}{6}\right] \quad (11)$$

where x_i^{α}, x_i^{β}, and y_i are the mole fractions of component i in each of the three equilibrium phases.

(5) Mark in critical pressure, P_c:

$$\text{Mark}_{P_c} = 20 - 0.75 \times \text{MAPE on } P_c\ (\%) \quad (12)$$

(6) Mark in critical composition, x_c:

$$\text{Mark}_{x_c} = 20 - 0.5 \times \left[\frac{\text{MAPE on } x_{1,c}\ (\%)+\text{MAPE on } x_{2,c}\ (\%)}{2}\right] \quad (13)$$

where $x_{i,c}$ is the mole fraction of component i at the critical point.

(7) Mark in azeotropic pressure, P_{az}:

$$\text{Mark}_{P_{az}} = 20 - 0.50 \times \text{MAPE on } P_{az}\ (\%) \quad (14)$$

(8) Mark in azeotropic composition, x_{az}:

$$\text{Mark}_{x_{az}} = 20 - 0.5 \times \left[\frac{\text{MAPE on } x_{1,az}\ (\%) + \text{MAPE on } x_{2,az}\ (\%)}{2}\right] \quad (15)$$

where $x_{i,az}$ is the mole fraction of component i at the azeotropic point.

(9) Mark in mixing enthalpy, h^M:

$$\text{Mark}_{h^M} = 20 - 0.25 \times \frac{1}{n_{h^M}}\sum_{i=1}^{n_{h^M}}\frac{1}{2}\left(100 \times \left|\frac{h_i^{M,EXP} - h_i^{M,MODEL}}{h_i^{M,EXP}}\right| + 100 \times \left|\frac{h_i^{M,EXP} - h_i^{M,MODEL}}{h_i^{M,MODEL}}\right|\right) \quad (16)$$

where n_{h^M} is the number of mixing enthalpy data points.

Remarks:

1. h^M goes to 0 when the mole fraction of the studied phase (z_1) goes to 0 or 1. In such cases, huge percent deviations and consequently very bad marks on h^M can be obtained. To avoid such a bias, if in eq 16

$$\frac{1}{2}\left(100\times\left|\frac{h_i^{M,EXP} - h_i^{M,MODEL}}{h_i^{M,EXP}}\right| + 100 \times \left|\frac{h_i^{M,EXP} - h_i^{M,MODEL}}{h_i^{M,MODEL}}\right|\right) > 80\%$$

this quantity is set to 80%.

2. Equation 16 highlights that we here decided to make the average between two MAPEs: one calculated with the classical definition (see eq 5) and one obtained by introducing $h_i^{M,MODEL}$ (i.e., the calculated value) at the denominator. This procedure is selected to obtain the same mark when calculated values of h^M are n times (e.g., twice) smaller or n times larger than the experimental values. To fix the ideas, let us assume that $h^{M,EXP} = 100$ J·mol^{-1}. If the calculated value is 50 times too small, let us say $h^{M,MODEL} = 2$ J·mol^{-1}, then eq 5 returns a MAPE_{h^M} (%) of 98%. In contrast, if the calculated value is 50 times too large, i.e., $h^{M,MODEL} = 5000$ J·mol^{-1}, then eq 5 returns a MAPE_{h^M} (%) of 4900%. As a direct consequence, the classical MAPE definition favors the case where $h^{M,MODEL}$ is 50 times below $h^{M,EXP}$. However, for both cases ($h^{M,MODEL} = 2$ J·mol^{-1} or $h^{M,MODEL} = 5000$ J·mol^{-1}), the average of the two MAPEs embedded in eq 16 is exactly the same. For the selected example,

$$\frac{1}{2}\left(100\times\left|\frac{h_i^{M,EXP} - h_i^{M,MODEL}}{h_i^{M,EXP}}\right| + 100 \times \left|\frac{h_i^{M,EXP} - h_i^{M,MODEL}}{h_i^{M,MODEL}}\right|\right) = 2499\%$$

3. In practice, h^M is used to evaluate molar enthalpies of the streams ($h_{\text{stream}} = z_1h_1 + z_2h_2 + h^M$) that are involved in the energy balance of a given process. The mark determined by eq 16 thus needs to capture the influence of h^M on such a balance. One possibility of reaching this target is to convert the difference $|h_i^{M,EXP} - h_i^{M,MODEL}|$ into terms of the temperature effect[990] ΔT_h through

$$\Delta T_h = \frac{|h_i^{M,EXP} - h_i^{M,MODEL}|}{c_P} \quad (17)$$

where c_P is the molar isobaric heat capacity of the mixture. ΔT_h quantifies the error made in the estimation of the final temperature of a mixture obtained by mixing two pure compounds at isobaric and adiabatic conditions. From our experience in process simulation, we decided to consider that $\Delta T_h = 1.4$ K was a good reference. In many cases, such a deviation is reached when h^M is estimated with a deviation of around 20%, and eq 16 is conceived so that with this deviation the mark is equal to 15/20.

(10) Mark in mixing heat capacity, c_P^M:

$$\text{Mark}_{c_P^M} = 20 - 0.10 \times \frac{1}{n_{c_P^M}}\sum_{i=1}^{n_{c_P^M}}\frac{1}{2}\left(100 \times \left|\frac{c_{P,i}^{M,EXP} - c_{P,i}^{M,MODEL}}{c_{P,i}^{M,EXP}}\right| + 100 \times \left|\frac{c_{P,i}^{M,EXP} - c_{P,i}^{M,MODEL}}{c_{P,i}^{M,MODEL}}\right|\right) \quad (18)$$

where $n_{c_P^M}$ is the number of mixing heat capacity data points. This mark was developed in a similar manner to Mark_{h^M} so that the following remarks apply.

Remarks:

1. Analogously to h^M, c_P^M goes to 0 when the mole fraction of the studied phase (z_1) goes to 0 or 1. In such cases, huge percent deviations and consequently very bad marks on c_P^M can be obtained. To avoid such a bias, if in eq 18

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$$\frac{1}{2}\left(100\times\left|\frac{c_{P,i}^{M,EXP}-c_{P,i}^{M,MODEL}}{c_{P,i}^{M,EXP}}\right|+100\times\left|\frac{c_{P,i}^{M,EXP}-c_{P,i}^{M,MODEL}}{c_{P,i}^{M,MODEL}}\right|\right)>200\%$$

this quantity is set to 200%.

2. The choice of eq 18 is based on the fact that for the data points embedded in the proposed database, we noticed that a deviation of 50% on c_P^M leads to an average deviation of only 2% on the molar isobaric heat capacity of the corresponding stream calculated as $c_{P,stream} = z_1c_{P,1} + z_2c_{P,2} + c_P^M$. As a consequence, eq 18 is developed so that a deviation of 50% on c_P^M leads to a good mark of 15/20.

Important remark: Any mark below 0 is raised to 0. Moreover, in the end:

$$\text{Mark}_{BAC_i} = \text{average}\begin{pmatrix}\text{Mark}_{x\text{ or }x^\alpha};\ \text{Mark}_{y\text{ or }x^\beta};\ \text{Mark}_{P_{LLV}};\ \text{Mark}_{z_{LLV}};\text{Mark}_{P_c};\\ \text{Mark}_{x_c};\ \text{Mark}_{P_{az}};\ \text{Mark}_{x_{az}};\ \text{Mark}_{h^M};\ \text{Mark}_{c_P^M}\end{pmatrix} \quad (19)$$

To conclude, 10 marks (at the most) are attributed to a given BAC. Obviously, when experimental data are missing for one or several properties, the corresponding mark(s) cannot be calculated and is(are) removed from eq 19. As an example, none of the binary systems embedded in BAC_2 contain three-phase equilibrium data so that $\text{Mark}_{P_{LLV}}$ and $\text{Mark}_{z_{LLV}}$ cannot be evaluated. For BAC_2, the given mark (eq 19) is the average of only 8 marks (instead of 10).

It is worth noting that the previous equations (from eq 7 to eq 18) give the greatest weight to the critical pressures that fix the topology of a binary system and are thus, in our view, extremely important, while less attention is given to mixing enthalpies and even less to mixing heat capacities. In practical terms, according to eq 12, a MAPE of 13% on the critical pressures leads to a Mark_{P_c} of 10/20 and a MAPE of 26% leads to a Mark_{P_c} of 0/20. By contrast, from eq 18, a similar MAPE of 13% on the mixing heat capacities leads to a $\text{Mark}_{c_P^M}$ of 18.7/20 and a MAPE of 26% leads to a $\text{Mark}_{c_P^M}$ of 17.4/20.

4. ILLUSTRATION: GRADING AND DISCUSSION AROUND THE ACCURACY OF THE PENG−ROBINSON EOS WITH CLASSICAL MIXING RULES AND A TEMPERATURE-DEPENDENT BIP

4.1. Model. In this section, it was decided to use the benchmark database developed in this study to assess the accuracy and to grade the Peng−Robinson[991,992] (PR) EoS with classical mixing rules and a temperature-dependent BIP (denoted k_{ij}). We found no reason to introduce a volume shift because all of the experimental properties contained in the database are unaffected by a temperature-independent volume translation.[993,994]

For a pure component, the PR EoS is

$$P = \frac{RT}{v-b_i} - \frac{a_i(T)}{v(v+b_i)+b_i(v-b_i)} \quad (20)$$

Although nonconsistent[995−997] at very high temperatures, it was decided to classically use the Soave-type[998] α-function proposed by Peng and Robinson[991] in 1978. An updated version has however recently been developed by Pina-Martinez[999] and co-workers (including Peng). We thus used

$$\begin{cases} R = 8.314472\ \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1} \\ X = [1+\sqrt[3]{4-2\sqrt{2}}+\sqrt[3]{4+2\sqrt{2}}]^{-1} \approx 0.253076587 \\ b_i = \Omega_b\frac{RT_{c,i}}{P_{c,i}} \text{ with } \Omega_b = \frac{X}{X+3} \approx 0.0777960739 \\ a_i(T) = a_{c,i}\alpha_i(T) \text{ with } \begin{cases} a_{c,i} = \Omega_a\frac{R^2T_{c,i}^2}{P_{c,i}} \text{ and} \\ \Omega_a = \frac{8(5X+1)}{49-37X} \approx 0.457235529 \\ \alpha_i(T) = \left[1+m_i\left(1-\sqrt{\frac{T}{T_{c,i}}}\right)\right]^2 \end{cases} \\ \text{if } \omega_i \le 0.491 \text{ then } m_i = 0.37464 + 1.54226\omega_i - 0.26992\omega_i^2 \\ \text{if } \omega_i > 0.491 \text{ then } m_i = 0.379642 + 1.48503\omega_i - 0.164423\omega_i^2 + 0.016666\omega_i^3 \end{cases} \quad (21)$$

where P is the pressure, R is the gas constant, T is the temperature, a_i and b_i are the cohesive parameter and the molar covolume of the pure component i, respectively, v is the molar volume, $T_{c,i}$ is the experimental critical temperature, $P_{c,i}$ is the experimental critical pressure, and ω_i is the experimental acentric factor of pure i. Such experimental properties were extracted from the DIPPR database, thus avoiding their estimation by group contribution methods.[1000]

To apply this EoS to a mixture, mixing rules are necessary to calculate the values of a and b of the mixture. Classical van der Waals one-fluid mixing rules[1001] are used in this study:

$$\begin{cases} a(T,z) = \sum_{i=1}^{N}\sum_{j=1}^{N} z_iz_j\sqrt{a_i(T)\cdot a_j(T)}\,[1-k_{ij}(T)] \\ b(z) = \sum_{i=1}^{N} z_ib_i \end{cases} \quad (22)$$

where z_i represents the mole fraction of component i and N is the number of components in the mixture (in this work, $N = 2$). The $k_{ij}(T)$ parameter is the BIP characterizing the molecular interactions between molecules i and j. In this study, the equation that gives the changes of k_{ij} with respect to temperature (see eq 23) is the one used in the well-established PPR78[1002−1007] and PR_2SRK[1008] models and contains two parameters (A_{ij} and B_{ij}) for the binary system $i + j$.

$$k_{ij}(T) = \frac{A_{ij}\left(\frac{298.15}{T}\right)^{B_{ij}/A_{ij}-1} - \left(\frac{\sqrt{a_i}}{b_i}-\frac{\sqrt{a_j}}{b_j}\right)^2}{2\times\frac{\sqrt{a_i}}{b_i}\times\frac{\sqrt{a_j}}{b_j}} \quad (23)$$

4.2. Fitting Procedure. The selected model is a correlative (i.e., nonpredictive) model, and for a given binary system, the two parameters involved in eq 23 have to be fitted against experimental data. In this work, it was decided that the two parameters would be determined, system by system, to ensure the best reproduction of the experimental data available in the proposed database by minimizing an objective function accounting for the deviations between experimental data (VLE data, LLE data, VLLE data, critical data, azeotropic

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Ind. Eng. Chem. Res. 2020, 59, 14981−15027

data, heat capacity of mixing data, and enthalpy of mixing data) and model predictions. The selected objective function expression is

$$F_{obj} = \frac{\left(\begin{array}{l} F_{obj,x \text{ or } x^{\alpha}} + F_{obj,y \text{ or } x^{\beta}} + F_{obj,P_{LLV}} + F_{obj,z_{LLV}} + F_{obj,P_c} \\ + F_{obj,x_c} + F_{obj,P_{az}} + F_{obj,x_{az}} + F_{obj,h^M} + F_{obj,c_P^M} \end{array}\right)}{n_{x \text{ or } x^{\alpha}} + n_{y \text{ or } x^{\beta}} + 2n_{triph} + 2n_{crit} + 2n_{az} + n_{h^M} + n_{c_P^M}} \quad (24)$$

- $F_{obj,x \text{ or } x^{\alpha}}$ quantifies the deviations on the liquid-phase composition for VLE data and on the α-liquid phase for LLE data:

$$\begin{cases} F_{obj,x \text{ or } x^{\alpha}} = 100 \sum_{i=1}^{n_{x \text{ or } x^{\alpha}}} 0.5\left(\frac{|\Delta x|}{x_{1,exp}(\text{or } x^{\alpha}_{1,exp})} + \frac{|\Delta x|}{x_{2,exp}(\text{or } x^{\alpha}_{2,exp})}\right)_i \\ \text{with } |\Delta x| = |x_{1,exp}(\text{or } x^{\alpha}_{1,exp}) - x_{1,cal}(\text{or } x^{\alpha}_{1,cal})| \end{cases} \quad (25)$$

where $n_{x \text{ or } x^{\alpha}}$ is the number of data points for which the liquid-phase composition x_1 (VLE data) or the α-liquid phase composition x_1^{α} (LLE data) is known.

Remark: As previously explained, very small mole fractions may lead to huge percent deviations. When this happens, the fitting algorithm is going to change the parameters to reduce this huge deviation to the detriment of other compositions. To avoid such a bias, if $x_{1,exp} < 0.01$ (or $x_{1,exp} < 0.99$) and simultaneously $50\left(\frac{|\Delta x|}{x_{1,exp}(\text{or } x^{\alpha}_{1,exp})} + \frac{|\Delta x|}{x_{2,exp}(\text{or } x^{\alpha}_{2,exp})}\right) > 45\%$, the corresponding deviation was not included in the calculation of $F_{obj,x \text{ or } x^{\alpha}}$.

- $F_{obj,y \text{ or } x^{\beta}}$ quantifies the deviations on the gas-phase composition for VLE data and on the β-liquid phase for LLE data:

$$\begin{cases} F_{obj,y \text{ or } x^{\beta}} = 100 \sum_{i=1}^{n_{y \text{ or } x^{\beta}}} 0.5\left(\frac{|\Delta y|}{y_{1,exp}(\text{or } x^{\beta}_{1,exp})} + \frac{|\Delta y|}{x_{2,exp}(\text{or } x^{\beta}_{2,exp})}\right)_i \\ \text{with } |\Delta y| = |y_{1,exp}(\text{or } x^{\beta}_{1,exp}) - y_{1,cal}(\text{or } x^{\beta}_{1,cal})| \end{cases} \quad (26)$$

where $n_{y \text{ or } x^{\beta}}$ is the number of data points for which the gas-phase composition y_1 (VLE data) or the β-liquid-phase composition x_1^{β} (LLE data) is known.

Remark: Here also, to avoid bias, if $y_{1,exp} > 0.99$ (or $y_{1,exp} > 0.01$) and simultaneously $50\left(\frac{|\Delta y|}{y_{1,exp}(\text{or } x^{\beta}_{1,exp})} + \frac{|\Delta y|}{x_{2,exp}(\text{or } x^{\beta}_{2,exp})}\right) > 45\%$, the corresponding deviation was not included in the calculation of $F_{obj,y \text{ or } x^{\beta}}$.

- $F_{obj,P_{LLV}}$ quantifies the deviations on the three-phase pressure (VLLE data):

$$F_{obj,P_{LLV}} = 100 \sum_{i=1}^{n_{triph}} \left(\frac{|P_{LLV,exp} - P_{LLV,cal}|}{P_{LLV,exp}}\right)_i \quad (27)$$

where n_{triph} is the number of three-phase pressure data.

- $F_{obj,z_{LLV}}$ quantifies the deviations on the three-phase composition (VLLE data):

$$F_{obj,z_{LLV}} = 100 \sum_{i=1}^{n_{triph}} \frac{1}{6}\left(\frac{|\Delta x^{\alpha}|}{x^{\alpha}_{1,exp}} + \frac{|\Delta x^{\alpha}|}{x^{\alpha}_{2,exp}} + \frac{|\Delta x^{\beta}|}{x^{\beta}_{1,exp}} + \frac{|\Delta x^{\beta}|}{x^{\beta}_{2,exp}} + \frac{|\Delta y|}{y_{1,exp}} + \frac{|\Delta y|}{y_{2,exp}}\right)_i \quad (28)$$

$$\text{with } \begin{cases} |\Delta x^{\alpha}| = |x^{\alpha}_{1,exp} - x^{\alpha}_{1,cal}| = |x^{\alpha}_{2,exp} - x^{\alpha}_{2,cal}| \\ |\Delta x^{\beta}| = |x^{\beta}_{1,exp} - x^{\beta}_{1,cal}| = |x^{\beta}_{2,exp} - x^{\beta}_{2,cal}| \\ |\Delta y| = |y_{1,exp} - y_{1,cal}| = |y_{2,exp} - y_{2,cal}| \end{cases}$$

n_{triph} being the number of three-phase composition data (VLLE data).

- F_{obj,P_c} quantifies the deviations on the critical pressure:

$$F_{obj,P_c} = 100 \sum_{i=1}^{n_{crit}} \left(\frac{|P_{c,exp} - P_{c,cal}|}{P_{c,exp}}\right)_i \quad (29)$$

where n_{crit} is the number of critical pressure data.

- F_{obj,x_c} quantifies the deviations on the critical composition:

$$F_{obj,x_c} = 100 \sum_{i=1}^{n_{crit}} 0.5\left(\frac{|\Delta x_c|}{x_{c1,exp}} + \frac{|\Delta x_c|}{x_{c2,exp}}\right)_i$$
$$|\Delta x_c| = |x_{c1,exp} - x_{c1,cal}| = |x_{c2,exp} - x_{c2,cal}| \quad (30)$$

where n_{crit} is the number of critical composition data.

- $F_{obj,P_{az}}$ quantifies the deviations on the azeotropic pressure:

$$F_{obj,P_{az}} = 100 \sum_{i=1}^{n_{az}} \left(\frac{|P_{az,exp} - P_{az,cal}|}{P_{az,exp}}\right)_i \quad (31)$$

where n_{az} is the number of azeotropic pressure data.

- $F_{obj,x_{az}}$ quantifies the deviations on the azeotropic composition:

$$F_{obj,x_{az}} = 100 \sum_{i=1}^{n_{az}} 0.5\left(\frac{|\Delta x_{az}|}{x_{az1,exp}} + \frac{|\Delta x_{az}|}{x_{az2,exp}}\right)_i$$
$$|\Delta x_{az}| = |x_{az1,exp} - x_{az1,cal}| = |x_{az2,exp} - x_{az2,cal}| \quad (32)$$

where n_{az} is the number of azeotropic composition data.

- F_{obj,h^M} quantifies the deviations on the mixing enthalpies:

$$F_{obj,h^M} = 100 \sum_{i=1}^{n_{h^M}} 0.5\left(\left|\frac{h^M_{exp} - h^M_{cal}}{h^M_{exp}}\right| + \left|\frac{h^M_{exp} - h^M_{cal}}{h^M_{cal}}\right|\right)_i \quad (33)$$

where n_{h^M} is the number of mixing enthalpy data points.

- F_{obj,c_P^M} quantifies the deviations on the mixing heat capacities:

$$F_{obj,c_P^M} = 100 \sum_{i=1}^{n_{c_P^M}} 0.5\left(\left|\frac{c^M_{P,exp} - c^M_{P,cal}}{c^M_{P,exp}}\right| + \left|\frac{c^M_{P,exp} - c^M_{P,cal}}{c^M_{P,cal}}\right|\right)_i \quad (34)$$

where $n_{c_P^M}$ is the number of mixing heat capacity data points.

Important remark: Section 3 of this paper, devoted to the grading of a thermodynamic model, dictates the methodology that has to be strictly followed to evaluate the deviations between model predictions and experimental data by means of

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Ind. Eng. Chem. Res. 2020, 59, 14981−15027

Table 14. Overview of the MAPE between Experimental Data and Values Calculated with the Model: {PR EoS + Classical Mixing Rules with a T-Dependent k_{ij}} for the 200 Binary Systems Included in the Proposed Database That Are Classified in Nine Binary Association Codes (BACs)[a]

		MAPE on									
		x	y	P_{LLV}	z_{LLV}	P_c	x_c	P_{az}	x_{az}	h^M	c_P^M
binary association code	type of association	eq 25	eq 26	eq 27	eq 28	eq 29	eq 30	eq 31	eq 32	eq 33	eq 34
1 (NA-NA)	mixtures without association	7.9%	7.9%	1.3%	42.7%	3.6%	12.9%	1.0%	5.0%	21.7%	34.7%
2 (HA-NA)		8.8%	6.8%	-	-	2.4%	9.0%	1.0%	6.1%	16.3%	160.3%
3 (HD-NA)		6.9%	5.7%	-	-	5.2%	15.8%	0.6%	3.7%	12.5%	70.5%
4 (HA-HA or HD-HD)		7.5%	7.2%	-	-	4.0%	11.1%	5.6%	9.6%	13.5%	104.5%
5 (SA-NA)	mixtures in which self-association tends to be broken	40.0%	14.9%	5.2%	69.9%	10.9%	46.0%	4.9%	13.8%	32.4%	200%
6 (HD-HA)	mixtures in which cross-association takes place alone	6.0%	6.1%	-	-	3.5%	21.5%	2.0%	9.6%	23.6%	43.1%
7 (SA-HD)	mixtures in which both cross-association and self-association take place	15.2%	12.3%	-	-	-	-	2.5%	9.6%	84.4%	188.0%
8 (SA-HA)		24.9%	15.7%	24.5%	39.1%	13.0%	28.4%	3.9%	11.0%	37.2%	164.4%
9 (SA-SA)		33.9%	22.6%	6.4%	32.7%	5.5%	13.2%	1.1%	24.4%	39.7%	182.4%

[a]The abbreviations used for the associating character of a pure compound are NA for nonassociating, HA for hydrogen-acceptor, HD for hydrogen-donor, and SA for self-associating.

the proposed database. If not, it becomes impossible to fairly compare two thermodynamic models.

In turn, the parameterization of the tested EoS (in the present case, the fitting procedure described above in Section 4.2) is not imposed and can be freely chosen. We are of the opinion that a researcher who wants to score a thermodynamic model (defined as the association of an EoS and a parameterization procedure) should be free to choose the number of adjustable parameters in the model, the experimental data to which such parameters are fitted, and the weighting given for each considered property during the fitting stage of the model parameters. In the previous section, a correlative model (the PR EoS with classical mixing rules and a T-dependent k_{ij}) was selected so that the experimental data of the proposed database were used to fit the parameters of eq 23. If our goal were to assess the accuracy of a predictive thermodynamic model in which the binary interaction parameters are determined by group contribution (e.g., PSRK,[1009,1010] VTPR,[1011,1012] UMR-PRU,[1013,1014] PPR78,[1002] MHV1-UNIFAC,[1015] etc.), the experimental data of the proposed database would not have been used for parameterization purposes.

From the above, an EoS may thus get different grades depending on its parameterization. For example, it would be possible in this paper to grade the PR EoS by setting all k_{ij} to 0. By doing so, a lower score than with temperature-dependent k_{ij} would be obtained. In short, a grade is in fact always given to a model, i.e., to the association of both {an equation of state + a selected parameterization}. The proposed database can thus be used to test the influence of the parameterization on EoS performance, and we know by experience[1016] that such an influence may be huge.

4.3. System-by-System Results of the Fitting Procedure. A system-by-system analysis of the {PR EoS + classical mixing rules with a T-dependent k_{ij}} performances to correlate the data included in the proposed database can be found in Table S2 of the file ie0c01734_si_011.pdf, available as Supporting Information. This very detailed analysis (over 1000 pages) includes the following.

1. Information on how the system deviates from ideality.
2. Values of the A and B optimal parameters (see eq 23).
3. Values of the numerical values of the average deviations between experimental data and model correlation for the ten calculated properties.In the file ie0c01734_si_011.pdf of the Supporting Information,
   - *MAPE* on x refers to $F_{\text{obj, x or } x^\alpha}/n_{x \text{ or } x^\alpha}$ (see eq 25)
   - *MAPE* on y refers to $F_{\text{obj, y or } x^\beta}/n_{y \text{ or } x^\beta}$ (see eq 26)
   - *MAPE* on P_{LLV} refers to $F_{\text{obj, } P_{LLV}}/n_{\text{triph}}$ (see eq 27)
   - *MAPE* on Z_{LLV} refers to $F_{\text{obj, } Z_{LLV}}/n_{\text{triph}}$ (see eq 28)
   - *MAPE* on P_c refers to $F_{\text{obj, } P_c}/n_{crit}$ (see eq 29)
   - *MAPE* on x_c refers to $F_{\text{obj, } x_c}/n_{crit}$ (see eq 30)
   - *MAPE* on P_{az} refers to $F_{\text{obj, } P_{az}}/n_{az}$ (see eq 31)
   - *MAPE* on x_{az} refers to $F_{\text{obj, } x_{az}}/n_{az}$ (see eq 32)
   - *MAPE* on h^M refers to $F_{\text{obj, } h^M}/n_{h^M}$ (see eq 33)
   - *MAPE* on c_P^M refers to $F_{\text{obj, } c_P^M}/n_{c_P^M}$ (see eq 34)
4. The so-called global phase equilibrium diagram (GPED), calculated by the PR EoS, enabling one to immediately identify the binary system class according to the scheme proposed by van Konynenburg and Scott.[6]
5. All of the experimental data with the corresponding references.
6. All of the deviations between experimental data and model correlation graphically illustrated by hundreds of figures. Explanations on "how to read the charts" are available at the beginning of the file ie0c01734_si_011.pdf, available as Supporting Information..

4.4. Grading of the Model: {PR EoS + Classical Mixing Rules with a T-Dependent k_{ij}}. For each binary association code, the MAPEs on liquid-phase composition x, gas-phase composition y, three-phase pressure P_{LLV}, three-phase composition z_{LLV}, critical pressure P_c, critical composition x_c, azeotropic pressure P_{az}, azeotropic composition x_{az}, mixing enthalpy h^M, and mixing heat capacity c_P^M are resumed in Table 14. Such MAPEs make it possible to give a score over 20 to

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Ind. Eng. Chem. Res. 2020, 59, 14981−15027

each of the nine BACs by averaging the 10 marks in x, y, P_{LLV}, z_{LLV}, P_c, x_c, P_{az}, x_{az}, h^M, and c_P^M (see eq 19). Such marks can be found in Table 15. At the end, as previously explained, the marks obtained by BACs 1−4 and BACs 7−9 are averaged to only retain four categories (BAC_1−BAC_4; BAC_5; BAC_6; BAC_7−BAC_9) of binary systems based on the type of association they exhibit. By averaging the marks of these four categories of binary systems (see eq 6), the model {PR EoS + classical mixing rules with a T-dependent k_{ij}} receives the final mark of 12.3/20.

4.5. Discussion around the Accuracy of the Model: {PR EoS + Classical Mixing Rules with a *T*-Dependent k_{ij}}. At this step, it is possible to analyze the results obtained with the PR EoS coupled to classical mixing rules and a T-dependent k_{ij}. The marks reported in Table 15 are plotted in Figure 5 for each category of binary systems based on the type of association they exhibit.

Figure 5 and Table 15 highlight that with an excellent mark of 15.6/20, the binary systems that exhibit cross-association alone are those that are correlated with the highest accuracy by the model {PR EoS + classical mixing rules with a T-dependent k_{ij}}. For such binary systems, the two molecules form hydrogen bonds after mixing, thus stabilizing the liquid phase and preventing phase splitting. As a general rule, mixtures of this family exhibit negative deviations from ideality and belong to type-I in the classification scheme of van Konynenburg and Scott.

With the poorest rating of 8.4/20, binary systems belonging to BAC_5 cannot be accurately correlated with the PR EoS even when temperature-dependent BIPs are used. Three marks are equal to 0. In such systems, a nonassociating component is mixed with a self-associating compound so that self-association (partially) persists in the mixture. The nonassociating molecules tend to break the hydrogen-bond network, but the self-associating compounds withstand so that liquid-phase splitting is often observed in this family. As previously stated, such systems were thus classified as "mixtures in which self-association tends to be broken". As a general rule, they exhibit positive deviations from ideality and three-phase equilibrium at low temperature. Many of them belong to type-III systems in the classification scheme of van Konynenburg and Scott. All binary systems of water + alkane or alcohol + alkane belong to this family. They are generally considered by model developers as the most difficult systems to correlate. It can be reasonably thought that either the addition of an association term or the use of more-sophisticated mixing rules could help the PR EoS quantitatively reproduce the behavior of such systems.

Mixtures in which both cross-association and self-association take place fall into the middle scoring range by receiving a mark of 9.8/20. This is the result of two antagonistic effects: on the one hand, hydrogen bonds between two identical self-associating molecules are broken by dilution effect and this behavior is highly difficult to describe with the model {PR EoS + classical mixing rules with a T-dependent k_{ij}}, while, on the other hand, new hydrogen bonds are formed by cross-association; this latter behavior can be modeled accurately with the selected model, as explained above. Many of these systems belong to type-I systems in the classification scheme of van Konynenburg and Scott (although some may fall into type-III).

As expected, systems that do not exhibit association received a very good mark of 15.5/20. The identified weakness is the inaccurate correlation of the composition of the phases in

Table 15. Rating of the Nine Binary Association Codes to Finally Grade the Model {PR EoS + Classical Mixing Rules with a *T*-Dependent k_{ij}}[a]

binary association code (BAC)	type of association	mark on										binary association code mark	mark (over 20) by type of association	final mark of the PR EoS with classical MR and T-dependent BIPS
		x	y	P_{LLV}	z_{LLV}	P_c	x_c	P_{az}	x_{az}	h^M	c_P^M			
		eq 7	eq 8	eq 10	eq 11	eq 12	eq 13	eq 14	eq 15	eq 16	eq 18	eq 19	eq 6	eq 6
1 (NA-NA)	mixtures without association	16.0	16.1	19.3	0.0	17.3	13.6	19.5	17.5	14.6	16.5	15.0	$\underline{\text{Mark}_{NA}}$ = 15.5	12.3/20
2 (HA-NA)		15.6	16.6			18.2	15.5	19.5	16.9	15.9	4.0	15.3	no association	
3 (HD-NA)		16.5	17.2			16.1	12.1	19.7	18.2	16.9	13.0	16.2		
4 (HA-HA or HD-HD)		16.2	16.4			17.0	14.4	17.2	15.2	16.6	9.6	15.3		
5 (SA-NA)	mixtures in which self-association tends to be broken	0.0	12.6	17.4	0.0	11.8	0.0	17.5	13.1	11.9	0.0	8.4	$\underline{\text{Mark}_{SA}}$ = 8.4 self−association	
6 (HD-HA)	mixtures in which cross-association takes place alone	17.0	16.9			17.4	9.2	19.0	15.2	14.1	15.7	15.6	$\underline{\text{Mark}_{CA}}$ = 15.6 cross−association	
7 (SA-HD)	mixtures in which both cross-association and self-association take place	12.4	13.9					18.8	15.2	0.0	1.2	10.2	$\underline{\text{Mark}_{CA+SA}}$ = 9.8 cross−association+self−association	
8 (SA-HA)		7.5	12.2	7.7	0.45	10.3	5.8	18.0	14.5	10.7	3.6	9.1		
9 (SA-SA)		3.1	8.7	16.8	3.6	15.8	13.4	19.5	7.8	10.1	1.8	10.0		

[a]The abbreviations used for the associating character of a pure compound are NA for nonassociating, HA for hydrogen-acceptor, HD for hydrogen-donor, and SA for self-associating.

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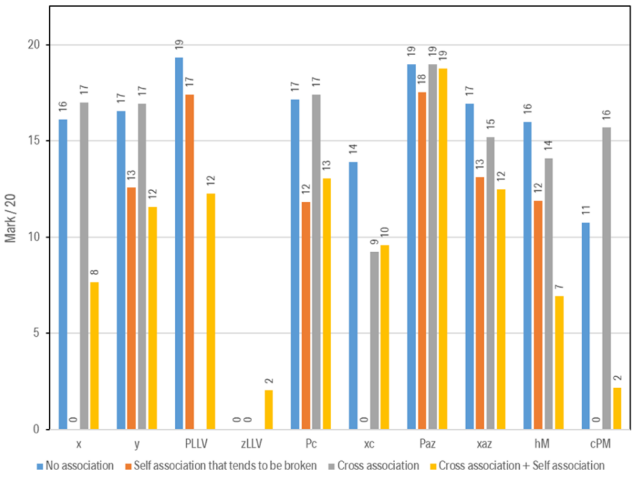


Figure 5. Overview of the accuracy of the model {PR EoS + classical mixing rules with a T-dependent k_{ij}} by plotting the marks in 10 properties for the four categories of binary systems based on the type of association they exhibit.

equilibrium when the system exhibits a three-phase line. This weakness highlights the difficulty in simultaneously correlating VLE and LLE data with a unique set of adjustable parameters. Nonassociating systems often belong to type-I systems but some fall into type-III, especially when the two compounds show a high size-asymmetry.

This analysis allows one to conclude that, with an overall score of 12.3/20, the PR EoS with classical mixing rules and a temperature-dependent k_{ij} can be safely used in process and product design applications as long as systems in which hydrogen bonds are broken without the possibility of forming new ones are not involved.

A similar analysis is possible from the viewpoint of system ideality.

Figure 6 shows that except for the liquid-phase composition (including the critical composition), all of the other properties are correlated with a similar accuracy for both ideal and nonideal systems. It is observed that deviations on mixing enthalpies can become huge when the deviations from ideality originate from entropic effects, but this result is not significant because in such a case experimental and calculated h^M values are both low.

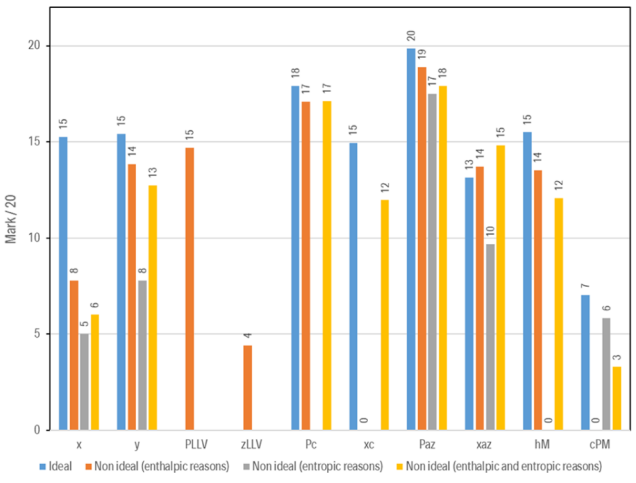


Figure 6. Marks in eight properties calculated for five categories of binary systems based on how they deviate from ideality (marks on VLLE data are not shown due to a lack of information on some categories of binary systems).

It is thus possible to conclude that deviations from ideality are not the key parameters to be accounted for when highlighting the strengths and the weaknesses of a model. A classification of the binary systems based on the type of association they exhibit, as the one proposed in this paper, is much more pertinent.

5. CONCLUSIONS

A benchmark database is presented in this paper to enable a proposed-standardized assessment of the performance of a given thermodynamic model or to compare two models. To classify a database's systems on the basis of their thermodynamic complexity, 107 pure components were first divided into four categories according to their associating character and nine classes of binary systems were defined combining these four pure-component categories. Each of these classes is identified by a binary association code (BAC). We are indeed convinced that binary systems must be classified according to the type of association they exhibit. For each class of systems, the proposed database includes a variety of binary systems ranging from ideal to highly nonideal. In the end, the proposed database embeds 200 binary mixtures uniformly distributed among the nine BACs and includes for each system both phase equilibrium data (VLE, LLE, VLLE, azeotropic data, critical data) and energetic data (h^M and c_P^M data). For each property, a detailed procedure explaining how deviations between model predictions and experimental data have to be estimated is provided.

Finally, the performances of the Peng–Robinson EoS with classical van der Waals mixing rules and a temperature-dependent binary interaction parameter were evaluated over the full database. In light of the obtained results, a discussion about the strengths and weaknesses of the model was conducted. Such a thermodynamic model got an overall respectable score of 12.3/20. Its main drawback is the poor correlation of systems in which hydrogen bonds are broken without the possibility of forming new ones. For such complex systems, the addition of an association term to the EoS and the selection of more sophisticated mixing rules could help improve the model efficiency.

Last but not the least, we hope that the proposed database will be widely adopted by the scientific community to identify the strengths and weaknesses of the many published thermodynamic models and to identify the remaining scientific obstacles that need to be overcome. We also hope that such a database will be used by model developers to test a new concept. As an example, experimental data of binary systems, the BAC of which is 7, 8, or 9, could be very useful to test the influence of various association schemes.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.iecr.0c01734.

Numerical values of the experimental data included in the proposed database with the corresponding references (light Excel file named: ie0c01734_si_001.xlsx) (XLSX)

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Ind. Eng. Chem. Res. 2020, 59, 14981−15027

Numerical values of the experimental data included in the proposed database with the corresponding references and with a visualization of the experimental data through graphs. Nine large-size Excel files (one for each BAC) are provided:

1. ie0c01734_si_002.xlsx (BAC_1) (XLSX)
2. ie0c01734_si_003.xlsx (BAC_2) (XLSX)
3. ie0c01734_si_004.xlsx (BAC_3) (XLSX)
4. ie0c01734_si_005.xlsx (BAC_4) (XLSX)
5. ie0c01734_si_006.xlsx (BAC_5) (XLSX)
6. ie0c01734_si_007.xlsx (BAC_6) (XLSX)
7. ie0c01734_si_008.xlsx (BAC_7) (XLSX)
8. ie0c01734_si_009.xlsx (BAC_8) (XLSX)
9. ie0c01734_si_010.xlsx (BAC_9) (XLSX)

List of the 107 pure compounds included in the proposed database with their corresponding associating character: NA, Non-Associating; HA, Hydrogen-Acceptor; HD, Hydrogen-Donor; SA, Self-Associating. Provided in Table S1 of the file ie0c01734_si_011.pdf (PDF)

System-by-system analysis of the {PR EoS + classical mixing rules with a T-dependent k_{ij}} performances to correlate the data included in the proposed database. Provided in Table S2 of the file ie0c01734_si_011.pdf (PDF)

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Notes

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REFERENCES

(1) Kontogeorgis, G. M.; Liang, X.; Arya, A.; Tsivintzelis, I. Equations of State in Three Centuries. Are We Closer to Arriving to a Single Model for All Applications? *Chem. Eng. Sci.: X* **2020**, *7*, No. 100060.

(2) Chen, C.-C.; Mathias, P. M. Applied Thermodynamics for Process Modeling. *AIChE J.* **2002**, *48*, 194−200.

(3) Hendriks, E.; Kontogeorgis, G. M.; Dohrn, R.; de Hemptinne, J.-C.; Economou, I. G.; Žilnik, L. F.; Vesovic, V. Industrial Requirements for Thermodynamics and Transport Properties. *Ind. Eng. Chem. Res.* **2010**, *49*, 11131−11141.

(4) Danner, R. P.; Gess, M. A. A Data Base Standard for the Evaluation of Vapor-Liquid-Equilibrium Models. *Fluid Phase Equilib.* **1990**, *56*, 285−301.

(5) Privat, R.; Jaubert, J.-N. Classification of Global Fluid-Phase Equilibrium Behaviors in Binary Systems. *Chem. Eng. Res. Des.* **2013**, *91*, 1807−1839.

(6) van Konynenburg, P. H.; Scott, R. L. Critical Lines and Phase Equilibria in Binary Van Der Waals Mixtures. *Philos. Trans. R. Soc., A* **1980**, *298*, 495−540.

(7) Agarwal, R.; Li, Y.-K.; Santollani, O.; Satyro, M. A.; Vieler, A. Uncovering the Realities of Simulation. Part II. *Chem. Eng. Prog.* **2001**, *97*, 64−72.

(8) Qian, J. *Développement Du Modèle E-PPR78 Pour Prédire Les Équilibres de Phases et Les Grandeurs de Mélange de Systèmes Complexes d'intérêt Pétrolier Sur de Larges Gammes de Températures et de Pressions*; Institut National Polytechnique de Lorraine: Nancy, 2011.

(9) Benkhedda, J.; Jaubert, J.-N.; Barth, D.; Perrin, L.; Bailly, M. Adsorption Isotherms of M-Xylene on Activated Carbon: Measurements and Correlation with Different Models. *J. Chem. Thermodyn.* **2000**, *32*, 401−411.

(10) Kontogeorgis, G. M.; Michelsen, M. L.; Folas, G. K.; Derawi, S.; von Solms, N.; Stenby, E. H. Ten Years with the CPA (Cubic-Plus-Association) Equation of State. Part 1. Pure Compounds and Self-Associating Systems. *Ind. Eng. Chem. Res.* **2006**, *45*, 4855−4868.

(11) Kontogeorgis, G. M.; Voutsas, E. C.; Yakoumis, I. V.; Tassios, D. P. An Equation of State for Associating Fluids. *Ind. Eng. Chem. Res.* **1996**, *35*, 4310−4318.

(12) Kontogeorgis, G. M.; Folas, G. K. *Thermodynamic Models for Industrial Applications*; John Wiley & Sons, Ltd.: Chichester, U.K., 2010.
(13) Gross, J.; Sadowski, G. Perturbed-Chain SAFT: An Equation of State Based on a Perturbation Theory for Chain Molecules. *Ind. Eng. Chem. Res.* **2001**, *40*, 1244−1260.
(14) Llovell, F.; Vega, L. F. Global Fluid Phase Equilibria and Critical Phenomena of Selected Mixtures Using the Crossover Soft-Saft Equation. *J. Phys. Chem. B* **2006**, *110*, 1350−1362.
(15) Llovell, F.; Vega, L. F. Prediction of Thermodynamic Derivative Properties of Pure Fluids through the Soft-Saft Equation of State. *J. Phys. Chem. B* **2006**, *110*, 11427−11437.
(16) Llovell, F.; Peters, C. J.; Vega, L. F. Second-Order Thermodynamic Derivative Properties of Selected Mixtures by the Soft-SAFT Equation of State. *Fluid Phase Equilib.* **2006**, *248*, 115−122.
(17) Llovell, F.; Vega, L. F. Phase Equilibria, Critical Behavior and Derivative Properties of Selected n-Alkane/n-Alkane and n-Alkane/1-Alkanol Mixtures by the Crossover Soft-SAFT Equation of State. *J. Supercrit. Fluids* **2007**, *41*, 204−216.
(18) Silva, G. M. C.; Justino, J.; Morgado, P.; Teixeira, M.; Pereira, L. M. C.; Vega, L. F.; Filipe, E. J. M. Detailed Surface Characterization of Highly Fluorinated Liquid Alcohols: Experimental Surface Tensions, Molecular Simulations and Soft-SAFT Theory. *J. Mol. Liq.* **2020**, *300*, No. 112294.
(19) Polishuk, I.; Garrido, J. M. Comparison of SAFT-VR-Mie and CP-PC-SAFT in Predicting Phase Behavior of Associating Systems IV. Methanol−Aliphatic Hydrocarbons. *J. Mol. Liq.* **2019**, *291*, No. 111321.
(20) Polishuk, I.; Privat, R.; Jaubert, J.-N. Novel Methodology for Analysis and Evaluation of SAFT-Type Equations of State. *Ind. Eng. Chem. Res.* **2013**, *52*, 13875−13885.
(21) Polishuk, I.; Garrido, J. M. Comparison of SAFT-VR-Mie and CP-PC-SAFT in Predicting Phase Behavior of Associating Systems III. Aliphatic Hydrocarbons - 1-Propanol, 1-Butanol and 1-Pentanol. *J. Mol. Liq.* **2019**, *279*, 492−502.
(22) Polishuk, I.; Garrido, J. M. Comparison of SAFT-VR-Mie and CP-PC-SAFT in Predicting Phase Behavior of Associating Systems II. Ammonia − Hydrocarbons. *J. Mol. Liq.* **2018**, *269*, 657−665.
(23) Polishuk, I.; Garrido, J. M. Comparison of SAFT-VR-Mie and CP-PC-SAFT in Predicting Phase Behavior of Associating Systems I. Ammonia−Water, Methanol, Ethanol and Hydrazine. *J. Mol. Liq.* **2018**, *265*, 639−653.
(24) Gil-Villegas, A.; Galindo, A.; Whitehead, P. J.; Mills, S. J.; Jackson, G.; Burgess, A. N. Statistical Associating Fluid Theory for Chain Molecules with Attractive Potentials of Variable Range. *J. Chem. Phys.* **1997**, *106*, 4168−4186.
(25) Atkins, P. W.; De Paula, J. *Atkins' Physical Chemistry*; Oxford University Press: Oxford, 2011.
(26) Privat, R.; Jaubert, J.-N. Discussion around the Paradigm of Ideal Mixtures with Emphasis on the Definition of the Property Changes on Mixing. *Chem. Eng. Sci.* **2012**, *82*, 319−333.
(27) Van Ness, H. C.; Byer, S. M.; Gibbs, R. E. Vapor-Liquid Equilibrium: Part I. An Appraisal of Data Reduction Methods. *AIChE J.* **1973**, *19*, 238−244.
(28) Redlich, O.; Kister, A. T. Algebraic Representation of Thermodynamic Properties and the Classification of Solutions. *Ind. Eng. Chem.* **1948**, *40*, 345−348.
(29) Kojima, K.; Man Moon, H.; Ochi, K. Thermodynamic Consistency Test of Vapor-Liquid Equilibrium Data. *Fluid Phase Equilib.* **1990**, *56*, 269−284.
(30) Wisniak, J.; Ortega, J.; Fernández, L. A Fresh Look at the Thermodynamic Consistency of Vapour-Liquid Equilibria Data. *J. Chem. Thermodyn.* **2017**, *105*, 385−395.
(31) Poon, D. P. L.; Lu, B. C.-Y. Phase Equilibria for Systems Containing Nitrogen, Methane, and Propane. In *Advances in Cryogenic Engineering*; Timmerhaus, K. D., Ed.; Springer, 1995; pp 292−299.
(32) Wichterle, I.; Kobayashi, R. Vapor-Liquid Equilibrium of Methane-Propane System at Low Temperatures and High Pressures. *J. Chem. Eng. Data* **1972**, *17*, 4−9.
(33) Price, A. R.; Kobayashi, R. Low Temperature Vapor-Liquid Equilibrium in Light Hydrocarbon Mixtures: Methane-Ethane-Propane System. *J. Chem. Eng. Data* **1959**, *4*, 40−52.
(34) Wichterle, I.; Kobayashi, R. Vapor-Liquid Equilibrium of Methane-Ethane-Propane System at Low Temperatures and High Pressures. *J. Chem. Eng. Data* **1972**, *17*, 13−18.
(35) Webster, L. A.; Kidnay, A. J. Vapor−Liquid Equilibria for the Methane−Propane−Carbon Dioxide Systems at 230 K and 270 K. *J. Chem. Eng. Data* **2001**, *46*, 759−764.
(36) Akers, W. W.; Burns, J. F.; Fairchild, W. R. Low-Temperature Phase Equilibria: Methane-Propane System. *Ind. Eng. Chem.* **1954**, *46*, 2531−2534.
(37) Reamer, H. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane-Propane System. *Ind. Eng. Chem.* **1950**, *42*, 534−539.
(38) Watanabe, K.; Kuroki, M.; Ogura, M.; Saito, I. Vapour-Liquid-Equilibrium of LNG. *TEION KOGAKU* **1969**, *4*, 292−301.
(39) Miller, R. C.; Staveley, L. A. K. Excess Enthalpies for Some Binary Liquid Mixtures of Low-Molecular-Weight Alkanes. In *Advances in Cryogenic Engineering*; Timmerhaus, K. D.; Weitzel, D. H., Eds.; Springer: Boston, 1960; pp 493−500.
(40) Cutler, A. J. B.; Morrison, J. A. Excess Thermodynamic Functions for Liquid Mixtures of Methane + Propane. *Trans. Faraday Soc.* **1965**, *61*, 429.
(41) 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. *J. Chem. Thermodyn.* **1978**, *10*, 559−566.
(42) Roof, J. G.; Baron, J. D. Critical Loci of Binary Mixtures of Propane with Methane, Carbon Dioxide, and Nitrogen. *J. Chem. Eng. Data* **1967**, *12*, 292−293.
(43) Sage, B. H.; Lacey, W. N.; Schaafsma, J. G. Phase Equilibria in Hydrocarbon Systems II. Methane-Propane System. *Ind. Eng. Chem.* **1934**, *26*, 214−217.
(44) Lin, Y.-N.; Chen, R. J. J.; Chappelear, P. S.; Kobayashi, R. Vapor-Liquid Equilibrium of the Methane-n-Hexane System at Low Temperature. *J. Chem. Eng. Data* **1977**, *22*, 402−408.
(45) Kandil, M. E.; Thoma, M. J.; Syed, T.; Guo, J.; Graham, B. F.; Marsh, K. N.; Huang, S. H.; May, E. 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. *J. Chem. Eng. Data* **2011**, *56*, 4301−4309.
(46) Stepanova, G. S.; Vybornova, Y. I. Phase Equilibriums of Methane-Hexane System. *Tr., Vses. Nauchno-Issled. Inst. Prir. Gazov* **1962**, 203−208.
(47) Shim, J.; Kohn, J. P. Multiphase and Volumetric Equilibria of Methane-n-Hexane Binary System at Temperatures Between -110° and 150 °C. *J. Chem. Eng. Data* **1962**, *7*, 3−8.
(48) Poston, R. S.; McKetta, J. J. Vapor-Liquid Equilibrium in the Methane-n-Hexane System. *J. Chem. Eng. Data* **1966**, *11*, 362−363.
(49) Gunn, R. D.; McKetta, J. J.; Ata, N. Measurement and Prediction of High-Pressure Phase Equilibria with a Dilute Component in the Gas Phase: The Methane-n-Hexane System. *AIChE J.* **1974**, *20*, 347−353.
(50) 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 Equilib.* **1997**, *129*, 285−305.
(51) 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; Gas Processors Association, 1976; pp 1−19.
(52) Chang, H. L.; Hurt, L. J.; Kobayashi, R. Vapor-Liquid Equilibria of Light Hydrocarbons at Low Temperatures and High Pressures: The Methane-n-Heptane System. *AIChE J.* **1966**, *12*, 1212−1216.
(53) Reamer, H. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

Methane- n-Heptane System. *Ind. Eng. Chem. Chem. Eng. Data Ser.* **1956**, *1*, 29−42.
(54) 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 Equilib.* **1996**, *114*, 161−174.
(55) 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; Gas Processors Association, 1976; pp 1−14.
(56) Stryjek, R.; Chappelear, P. S.; Kobayashi, R. Low-Temperature Vapor-Liquid Equilibriums of Nitrogen-Ethane System. *J. Chem. Eng. Data* **1974**, *19*, 340−343.
(57) Grausø, L.; Fredenslund, A.; Mollerup, J. Vapour-Liquid Equilibrium Data for the Systems C2H6 + N2, C2H4 + N2, C3H8 + N2, and C3H6 + N2. *Fluid Phase Equilib.* **1977**, *1*, 13−26.
(58) Brown, T. S.; Sloan, E. D.; Kidnay, A. J. Vapor-Liquid Equilibria in the Nitrogen + Carbon Dioxide + Ethane System. *Fluid Phase Equilib.* **1989**, *51*, 299−313.
(59) 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 Equilib.* **1986**, *25*, 303−322.
(60) Gupta, M. K.; Gardner, G. C.; Hegarty, M. J.; Kidnay, A. J. Liquid-Vapor Equilibriums for the N2 + CH4 + C2H6 System from 260 to 280 K. *J. Chem. Eng. Data* **1980**, *25*, 313−318.
(61) Ellington, R. T.; Eakin, B. E.; Parent, J. D.; Gami, D. C.; Bloomer, O. T. In *Vapor−Liquid Phase Equilibriums in the Binary Systems of CH_4, C_2H_6, and N_2*, Thermodynamic and Transport Properties of Gases, Liquids and Solids, Symposium on Thermal Properties, 1959; pp 180−194.
(62) Guedes, H. J. R.; Zollweg, J. A.; Filipe, E. J. M.; Martins, L. F. G.; Calado, J. C. G. Thermodynamics of Liquid (Nitrogen + Ethane). *J. Chem. Thermodyn.* **2002**, *34*, 669−678.
(63) Yu, P.; Elshayal, I. M.; Lu, B. C.-Y. Liquid-Liquid-Vapor Equilibria in the Nitrogen-Methane-Ethane System. *Can. J. Chem. Eng.* **1969**, *47*, 495−498.
(64) Koonce, K. T.; Kobayashi, R. A Method for Determining the Solubility of Gases in Relatively Nonvolatile Liquids: Solubility of Methane in n-Decane. *J. Chem. Eng. Data* **1964**, *9*, 490−494.
(65) Lentz, H.; Nuennerich, P. Die Bestimmung Der Zusammensetzung Koexistierender Phasen Binärer Mischungen Aus Nodenlinien Und Volumen. *Chem. Ing. Tech.* **2001**, *73*, 1162−1164.
(66) Reamer, H. H.; Olds, R. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. *Ind. Eng. Chem.* **1942**, *34*, 1526−1531.
(67) Lavender, H. M.; Sage, B. H.; Lacey, W. N. Gas-Liquid Equilibrium Constants, Methane-Decane System. *Oil Gas J.* **1940**, *39*, 48−49.
(68) Lin, H.-M.; Sebastian, H. M.; Simnick, J. J.; Chao, K.-C. Gas-Liquid Equilibrium in Binary Mixtures of Methane with N-Decane, Benzene, and Toluene. *J. Chem. Eng. Data* **1979**, *24*, 146−149.
(69) Wiese, H. C.; Reamer, H. H.; Sage, B. H. Phase Equilibriums in Hydrocarbon Systems. Phase Behavior in the Methane-Propane-n-Decane System. *J. Chem. Eng. Data* **1970**, *15*, 75−82.
(70) Kay, W. B. Liquid-Vapor Phase Equilibrium Relations in the Ethane-n-Heptane System. *Ind. Eng. Chem.* **1938**, *30*, 459−465.
(71) Cota, H. M.; Thodos, G. Critical Temperatures and Critical Pressures of Hydrocarbon Mixtures. Methane Ethane-n-Butane System. *J. Chem. Eng. Data* **1962**, *7*, 62−65.
(72) Mehra, V. S.; Thodos, G. Vapor-Liquid Equilibrium in the Ethane-n-Heptane System. *J. Chem. Eng. Data* **1965**, *10*, 211−214.
(73) Ekiner, O.; Thodos, G. Critical Temperatures and Pressures of the Ethane-n-Heptane System. *Can. J. Chem. Eng.* **1965**, *43*, 205−208.
(74) Mehra, V. S.; Thodos, G. Vapor-Liquid Equilibrium Constants for the Ethane-Butane-n-Heptane System at 300° and 350°F. *J. Chem. Eng. Data* **1968**, *13*, 155−160.
(75) Singh, H.; Lucien, F. P.; Foster, N. R. Critical Properties for Binary Mixtures of Ethane Containing Low Concentrations of N-Alkane. *J. Chem. Eng. Data* **2000**, *45*, 131−135.
(76) 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; Gas Processors Association, 1971; pp 1−10.
(77) Kalra, H.; Robinson, D. B.; Besserer, G. J. The Equilibrium Phase Properties of the Nitrogen-n-Pentane System. *J. Chem. Eng. Data* **1977**, *22*, 215−218.
(78) Silva-Oliver, G.; Eliosa-Jiménez, G.; García-Sánchez, F.; Avendaño-Gómez, J. R. High-Pressure Vapor−Liquid Equilibria in the Nitrogen−n-Pentane System. *Fluid Phase Equilib.* **2006**, *250*, 37−48.
(79) Azarnoosh, A.; McKetta, J. J. Nitrogen-n-Decane System in the Two-Phase Region. *J. Chem. Eng. Data* **1963**, *8*, 494−496.
(80) García-Sánchez, F.; Eliosa-Jiménez, G.; Silva-Oliver, G.; García-Flores, B. E. Vapor-Liquid Equilibrium Data for the Nitrogen + n-Decane System from (344 to 563) K and at Pressures up to 50 MPa. *J. Chem. Eng. Data* **2009**, *54*, 1560−1568.
(81) Flöter, E.; de Loos, T. W.; de Swaan Arons, J. High Pressure Solid-Fluid and Vapour-Liquid Equilibria in the System (Methane + Tetracosane). *Fluid Phase Equilib.* **1997**, *127*, 129−146.
(82) Huang, C.-P.; Jan, D.-S.; Tsai, F.-N. Modeling of Methane Solubility in Heavy N-Paraffins. *J. Chem. Eng. Jpn.* **1992**, *25*, 182−186.
(83) Arnaud, J. F.; Ungerer, P.; Behar, E.; Moracchini, G.; Sanchez, J. Excess Volumes and Saturation Pressures for the System Methane + N-Tetracosane at 374 K. Representation by Improved EOS Mixing Rules. *Fluid Phase Equilib.* **1996**, *124*, 177−207.
(84) Suleiman, D.; Eckert, C. A. Phase Equilibria of Alkanes in Natural Gas Systems. 1. Alkanes in Methane. *J. Chem. Eng. Data* **1995**, *40*, 2−11.
(85) Schwarz, C. E.; Nieuwoudt, I.; Knoetze, J. H. Phase Equilibria of Long Chain N-Alkanes in Supercritical Ethane: Review, Measurements and Prediction. *J. Supercrit. Fluids* **2008**, *46*, 226−232.
(86) Tsai, F. N.; Huang, S. H.; Lin, H. M.; Chao, K. C. Solubility of Methane, Ethane, and Carbon Dioxide in n-Hexatriacontane. *J. Chem. Eng. Data* **1987**, *32*, 467−469.
(87) Gasem, K. A. M.; Bufkin, B. A.; Raff, A. M.; Robinson, R. L. Solubilities of Ethane in Heavy Normal Paraffins at Pressures to 7.8 MPa and Temperatures from 348 to 423 K. *J. Chem. Eng. Data* **1989**, *34*, 187−191.
(88) Martin, M.; Youings, J. Vapour Pressures and Excess Gibbs Free Energies of Cyclohexane + N-Hexane, + n-Heptane and + n-Octane at 298.15 K. *Aust. J. Chem.* **1980**, *33*, 2133.
(89) Benson, G. C.; Benson, G. C.; Anand, S. C.; Kiyohara, O. Thermodynamic Properties of Some Cycloalkane-Cycloalkanol Systems at 298. 15.Deg.K. II. *J. Chem. Eng. Data* **1974**, *19*, 258−261.
(90) 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. AA.* **1963**, *37*, 938−943.
(91) Ridgway, K.; Butler, P. A. Physical Properties of the Ternary System Benzene-Cyclohexane-Hexane. *J. Chem. Eng. Data* **1967**, *12*, 509−515.
(92) Myers, H. S. [Vapor-Liquid] Equilibrium for Naphthenes and Paraffins. *Pet. Refin.* **1957**, *36*, 175−178.
(93) 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. *J. Chem. Thermodyn.* **1982**, *14*, 1183−1190.
(94) Ewing, M. B.; Marsh, K. N. The Enthalpy of Mixing of N-Hexane + Cyclohexane at 288.15 and 318.15 K. *J. Chem. Thermodyn.* **1970**, *2*, 295−296.
(95) 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. *J. Chem. Thermodyn.* **1978**, *10*, 25−34.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(96) Heintz, A.; Lichtenthaler, R. N. An Isothermal Flow Calorimeter for Pressures to 600 Bar. *Ber. Bunsenges. Phys. Chem.* **1979**, *83*, 853−856.
(97) Gmehling, J.; Meents, B. Excess Enthalpy. Cyclohexane-Hexane System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1992**, 144.
(98) 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* **1995**, *1*, 181−190.
(99) Saito, A.; Tanaka, R. Excess Volumes and Heat Capacities of Binary Mixtures Formed from Cyclohexane, Hexane, and Heptane at 298.15 K. *J. Chem. Thermodyn.* **1988**, *20*, 859−865.
(100) Hissong, D. W.; Kay, W. B. Critical Properties of Hydrocarbons. II. Correlational Studies. *Proc. Am. Pet. Inst. Refin. Dep.* **1968**, *48*, 397−463.
(101) Kassmann, K.-D.; Knapp, H. Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Benzene, Toluene and n-Butyraldehyde. *Ber. Bunsenges. Phys. Chem.* **1986**, *90*, 452−458.
(102) Saito, S. *Separation of Hydrocarbons. 2. Vapor−Liquid Equilibriums of Normal Paraffin−Aromatic Systems*; Asahi Garasu Kogyo Gijutsu Shoreikai, 1969; Vol. *15*, pp 397−407.
(103) Jin, Z.; Hu, A.; Liu, K. VLE of Binary and Ternary Systems for BTX Mixtures. *Chem. Eng. China* **1991**, *19* (6), 56−60.
(104) Schuberth, H. Phasengleichgewichtsmessungen. II. Vorausberechnung von Gleichgewichtsdaten Dampfförmig-Flüssig Idealer Binärer Systeme Und Prüfung Derselben Mittels Einer Neuen Gleichgewichtsapparatur. *J. Prakt. Chem.* **1958**, *6*, 129−138.
(105) Baud, E. Thermal Analysis of Binary Mixtures. *Bull. Soc. Chim. Fr.* **1915**, *17*, 329−345.
(106) Hsu, K.-Y.; 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. *J. Chem. Thermodyn.* **1975**, *7*, 435−442.
(107) 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. *J. Chem. Thermodyn.* **1969**, *1*, 397−407.
(108) Diaz Pena, M.; Menduina, C. Semicontinuous Calorimeter for Measuring Heats of Mixing. *An. Quim.* **1973**, *69*, 857−868.
(109) Fortier, J. L.; Benson, G. C. Heat Capacities of Some Binary Aromatic Hydrocarbon Mixtures Containing Benzene or Toluene. *J. Chem. Eng. Data* **1979**, *24*, 34−37.
(110) Kay, W. B.; Hissong, D. The Critical Properties of Hydrocarbons. I. Simple Mixtures. *Proc., Am. Pet. Inst., Refin. Dep.* **1967**, *47*, 653−722.
(111) Vaughan, W. E.; Collins, F. C. P-V-T-x Relations of the System Propane-Isopentane. *Ind. Eng. Chem.* **1942**, *34*, 885−890.
(112) Zhang, X.; Zheng, Y.; Zhao, W. Measurement and Correlation of Vapor Liquid Equilibrium Data for Benzene Cyclohexane Methyl Cyclohexane DMF Systems. *Nat. Gas Chem. Ind.* **1997**, *22*, 52−55.
(113) Harsted, B. S.; Thomsen, E. S. Excess Enthalpies from Flow Microcalorimetry 3. Excess Enthalpies for Binary Liquid Mixtures of Aliphatic and Aromatic Hydrocarbons, Carbon Tetrachloride, Chlorobenzene, and Carbon Disulphide. *J. Chem. Thermodyn.* **1975**, *7*, 369−376.
(114) 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. *J. Chem. Thermodyn.* **1980**, *12*, 1139−1148.
(115) Tamura, K. Excess Heat Capacities of the Mixtures Containing Methylcyclohexane at 298.15 K. *Fluid Phase Equilib.* **2001**, *182*, 303−312.
(116) Djordjevich, L.; Budenholzer, R. A. Vapor-Liquid Equilibrium Data for Ethane-Propane System at Low Temperatures. *J. Chem. Eng. Data* **1970**, *15*, 10−12.
(117) Hirata, M.; Suda, S.; Hakuta, T.; Nagahama, K. Light Hydrocarbon Vapor-Liquid Equilibria. *Mem. Fac. Technol., Tokyo Metrop. Univ.* **1969**, *19*, 103−122.
(118) 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.* **1970**, *15*, 35−36.
(119) Blanc, C. J.; Setier, J. C. B. Vapor-Liquid Equilibria for the Ethane-Propane System at Low Temperature. *J. Chem. Eng. Data* **1988**, *33*, 111−115.
(120) Clark, A. Q.; Stead, K. (Vapour + Liquid) Phase Equilibria of Binary, Ternary, and Quaternary Mixtures of CH4, C2H6, C3H8, C4H10, and CO2. *J. Chem. Thermodyn.* **1988**, *20*, 413−427.
(121) Kahre, L. C. Liquid Density of Light Hydrocarbon Mixtures. *J. Chem. Eng. Data* **1973**, *18*, 267−270.
(122) Pöll, H.; Huemer, H.; Moser, F. Eine Apparatur Zur Bestimmung von Dampf-Flüssigkeits-Gleichgewichten Unter Erhöhtem Druck. *Monatsh. Chem.* **1980**, *111*, 1159−1164.
(123) Mikšovský, J.; Wichterle, I. Liquid-Vapor Equilibrium. LXX. Vapor -Liquid Equilibriums in the Ethane-Propane System at High Pressures. *Collect. Czech. Chem. Commun.* **1975**, *40*, 365−370.
(124) Matschke, D. E.; Thodos, G. Vapor-Liquid Equilibriums for the Ethane-Propane System. *J. Chem. Eng. Data* **1962**, *7*, 232−234.
(125) 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. *J. Chem. Thermodyn.* **1997**, *29*, 149−178.
(126) Horstmann, S.; Fischer, K.; Gmehling, J. Experimental Determination of Critical Data of Mixtures and Their Relevance for the Development of Thermodynamic Models. *Chem. Eng. Sci.* **2001**, *56*, 6905−6913.
(127) Van Poolen, L. J.; Holcomb, C. D. Critical Temperatures, Pressures, and Densities for the Mixtures CO2−C3H8, CO2−NC4H10, C2H6−C3H8, and C3H8−NC4H10. *Fluid Phase Equilib.* **1999**, *165*, 157−168.
(128) Uchytil, P.; Wichterle, I. 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 Equilib.* **1983**, *15*, 209−217.
(129) Kahre, L. C. Low-Temperature K Data for Methane-Butane. *J. Chem. Eng. Data* **1974**, *19*, 67−71.
(130) Elliot, D. G.; Chen, R. J. J.; Chappelear, P. S.; Kobayashi, R. Vapor-Liquid Equilibrium of Methane-Butane System at Low Temperatures and High Pressures. *J. Chem. Eng. Data* **1974**, *19*, 71−77.
(131) Wiese, H. C.; Jacobs, J.; Sage, B. H. Phase Equilibriums in the Hydrocarbon Systems. Phase Behavior in the Methane-Propane-n-Butane System. *J. Chem. Eng. Data* **1970**, *15*, 82−91.
(132) Sage, R. H.; Hicks, B. L.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. *Ind. Eng. Chem.* **1940**, *32*, 1085−1092.
(133) Rigas, T. J.; Mason, D. F.; Thodos, G. Vapor-Liquid Equilibria. Microsampling Technique Applied to a New Variable-Volume Cell. *Ind. Eng. Chem.* **1958**, *50*, 1297−1300.
(134) Sprow, F. B.; Prausnitz, J. M. Vapor-Liquid Equilibria for Five Cryogenic Mixtures. *AIChE J.* **1966**, *12*, 780−784.
(135) Calado, J. C. G.; Staveley, L. A. K. Excess Gibbs Energy of Argon-Methane Liquid Mixtures at 115.77°K. *J. Chem. Phys.* **1972**, *56*, 4718−4719.
(136) 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. BB.* **1976**, *50*, 298.
(137) Kehlen, H.; Schneider, F.-U.; Haufe, S.; Barnitzke, W. Auswertung von Taudruckmessungen Binärer Systeme Im Mitteldruckbereich. *Z. Phys. Chem.* **1983**, *264O*, 801−806.
(138) Christiansen, L. J.; Fredenslund, A. Vapour-Liquid Equilibria of the CH4-Ar-CO System. *Cryogenics* **1974**, *14*, 10−14.
(139) Christiansen, L. J.; Fredenslund, A.; Mollerup, J. Vapour-Liquid Equilibrium of the CH4-Ar, CH4-CO, and Ar-CO Systems at Elevated Pressures. *Cryogenics* **1973**, *13*, 405−413.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(140) Lewis, K. L.; Saville, G.; Staveley, L. A. K. Excess Enthalpies of Liquid Oxygen + Argon, Oxygen + Nitrogen, and Argon + Methane. *J. Chem. Thermodyn.* **1975**, *7*, 389−400.
(141) 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. *J. Chem. Thermodyn.* **1977**, *9*, 483−490.
(142) 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. *J. Chem. Thermodyn.* **1977**, *9*, 121−131.
(143) Wormald, C. J.; Lewis, K. L.; Mosedale, S. 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. *J. Chem. Thermodyn.* **1977**, *9*, 27−42.
(144) Paul, H. I.; Krug, J.; Knapp, H. Measurements of VLE, vE and HE for Binary Mixtures of n-Alkanes with Chloro-Alkylbenzenes. *Fluid Phase Equilib.* **1988**, *39*, 307−324.
(145) Bayles, J. W.; Letcher, T. M. Thermodynamics of Some Binary Liquid Mixtures Containing Aliphatic Amines. *J. Chem. Eng. Data* **1971**, *16*, 266−271.
(146) Al-Hayan, M. N. M.; Al-Kandary, J. A. M. Isobaric Vapour−Liquid Equilibria for Binary Mixtures of n-Heptane with Bromobenzene, Chlorobenzene and Fluorobenzene at Atmospheric Pressure. *Fluid Phase Equilib.* **2006**, *240*, 109−113.
(147) 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.* **1976**, *18*, 47−49.
(148) Wilhelm, E.; Inglese, A.; Grolier, J.-P. E.; Kehiaian, H. V. Enthalpy of Mixing of Chlorobenzene, 1,2-Dichlorobenzene, and 1,3-Dichlorobenzene with Some n-Alkanes. *Ber. Bunsen-Ges. Phys. Chem.* **1978**, *82*, 384−388.
(149) 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.* **1973**, *70*, 367−373.
(150) Bendiab, H.; Roux-Desgranges, G.; Roux, A. H.; Grolier, J.-P. E.; Patterson, D. Excess Heat Capacities of Ternary Systems Containing Chlorobenzene or Chloronaphthalene. *J. Solution Chem.* **1994**, *23*, 307−323.
(151) 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. *J. Chem. Thermodyn.* **1980**, *12*, 1051−1055.
(152) Rolemberg, M. P.; Krähenbühl, M. A. Vapor−Liquid Equilibria of Binary and Ternary Mixtures of Benzene, Cyclohexane, and Chlorobenzene at 40.0 KPa and 101.3 KPa. *J. Chem. Eng. Data* **2001**, *46*, 256−260.
(153) Tanaka, R.; Murakami, S.; Fujishiro, R. Excess Enthalpies of Mixing of a Polar Liquid + a Non-Polar Liquid at 298.15 K. *J. Chem. Thermodyn.* **1974**, *6*, 209−218.
(154) Amaya, K. 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. *Bull. Chem. Soc. Jpn.* **1961**, *34*, 1278−1285.
(155) Anantaraman, A. V.; Bhattacharyya, S. N.; Palit, S. R. Weak Dipolar Interaction in Solutions. Systems: Cyclohexane+chlorobenzene and Carbon Tetrachloride+chlorobenzene. *Trans. Faraday Soc.* **1961**, *57*, 40.
(156) Munoz Embid, J.; Berro, C.; Otin, S.; Kehiaian, H. 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. *J. Chem. Eng. Data* **1990**, *35*, 266−271.
(157) Azpiazu, Y.; Royo, F.; Gutiérrez Losa, C. Vapour Pressures of (Tetrachloromethane + α,ω-Dichloroalkane). *J. Chem. Thermodyn.* **1984**, *16*, 561−565.
(158) Sagnes, M.; Sanchez, V. Vapor-Liquid Equilibriums for Fourteen Systems Consisting of Chlorinated Hydrocarbons and Alcohols. *J. Chem. Eng. Data* **1971**, *16*, 351−354.
(159) Baños, I.; Valero, J.; Gracia, M.; Losa, C. G. Conformational Equilibrium and Calorimetric Behaviour of Systems Containing 1,2-Dichloroethane. *Ber. Bunsenges. Phys. Chem.* **1983**, *87*, 866−871.
(160) Marongiu, B. Excess Enthalpies of Alpha,Omega-Dichloroalkane (C1 - C6) + Tetrachloromethane. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1988**, 1−6.
(161) Wilhelm, E.; Faradjzadeh, A.; Grolier, J.-P. E. Molar Excess Heat Capacities and Excess Volumes of 1,2-Dichloroethane + Cyclooctane, + Mesitylene, and + Tetrachloromethane. *J. Chem. Thermodyn.* **1979**, *11*, 979−984.
(162) Ellis, S. R. M.; Contractor, R. M. Vapor-Liquid Equilibriums at Reduced Pressure. *Chem. Eng. Lond.* **1964**, *15*, 10−13.
(163) Rollet, A. P.; Toledano, P.; Elkaim, G.; Sonez, M. Ebulliometry of Volatile Solutes. II. *Publ. Sci. Univ. Alger, Ser. B* **1956**, *2*, 403−425.
(164) Tschamler, H. Über Binäre Flüssige Mischungen VI: Mischungswärmen, Molwärmen, Volumeffekte Und Zustands-Diagramme von 1,2-Dichloräthan Mit Benzol Und n-Alkylbenzolen. *Monatsh. Chem.* **1948**, *79*, 499−507.
(165) 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* **1996**, *2*, 111−120.
(166) Wilhelm, E.; Grolier, J.-P. E.; Ghassemi, M. H. K. Molar Heat Capacities of Binary Liquid Mixtures: 1,2-Dichlorethane + Benzene, + Toluene, and + p-Xylene. *Ber. Bunsenges. Phys. Chem.* **1977**, *81*, 925−930.
(167) Parrish, W. R.; Hiza, M. J. Liquid-Vapor Equilibria in the Nitrogen-Methane System between 95 and 120 K. In *Advances in Cryogenic Engineering*; Timmerhaus, K. D., Eds.; Springer: Boston, MA, 1995; pp 300−308.
(168) Han, X. H.; Zhang, Y. J.; Gao, Z. J.; Xu, Y. J.; Wang, Q.; Chen, G. M. Vapor−Liquid Equilibrium for the Mixture Nitrogen (N2) + Methane (CH4) in the Temperature Range of (110 to 125) K. *J. Chem. Eng. Data* **2012**, *57*, 1621−1626.
(169) Stryjek, R.; Chappelear, P. S.; Kobayashi, R. Low-Temperature Vapor-Liquid Equilibriums of Nitrogen-Methane System. *J. Chem. Eng. Data* **1974**, *19*, 334−339.
(170) Cines, M. R.; Roach, J. T.; Hogan, R. J.; Roland, C. H. Nitrogen-Methane Vapor-Liquid Equilibria. *Chem. Eng. Prog., Symp. Ser.* **1953**, *49*, 1−10.
(171) Bloomer, O. T.; Parent, J. D. Liquid-Vapor Phase Behavior of the Methane-Nitrogen System. *Chem. Eng. Prog., Symp. Ser.* **1953**, *49*, 11−24.
(172) 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* **1975**, *15*, 531−540.
(173) Brandt, L. W.; Stroud, L. Phase Equilibria in Natural Gas Systems. Apparatus with Windowed Cell for 800 P.S.I.G. and Temperatures to —320° F. *Ind. Eng. Chem.* **1958**, *50*, 849−852.
(174) 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. *J. Chem. Thermodyn.* **1976**, *8*, 785−792.
(175) Klein, R. R.; Bennett, C. O.; Dodgge, B. F. Experimental Heats of Mixing for Gaseous Nitrogen and Methane. *AIChE J.* **1971**, *17*, 958−965.
(176) Gomes de Azevedo, E. J. S.; Calado, J. C. G. Thermodynamics of Liquid Methane+ethane. *Fluid Phase Equilib.* **1989**, *49*, 21−34.
(177) 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. *J. Chem. Thermodyn.* **1977**, *9*, 167−178.
(178) Wichterle, I.; Kobayashi, R. Vapor-Liquid Equilibrium of Methane-Ethane System at Low Temperatures and High Pressures. *J. Chem. Eng. Data* **1972**, *17*, 9−12.
(179) Wei, M. S.-W.; Brown, T. S.; Kidnay, A. J.; Sloan, E. D. Vapor + Liquid Equilibria for the Ternary System Methane + Ethane + Carbon Dioxide at 230 K and Its Constituent Binaries at

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

Temperatures from 207 to 270 K. *J. Chem. Eng. Data* **1995**, *40*, 726−731.
(180) Davalos, J.; Anderson, W. R.; Phelps, R. E.; Kidnay, A. J. Liquid-Vapor Equilibria at 250.00K for Systems Containing Methane, Ethane, and Carbon Dioxide. *J. Chem. Eng. Data* **1976**, *21*, 81−84.
(181) Werner, G.; Schuberth, H. Das Phasengleichgewicht Flüssig-Flüssig Des Systems Benzol/n-Heptan/Acetonitril Sowie Die Phasengleichgewichte Dampfförmig-Flüssig Der Entsprechenden Binären Systeme Bei 20,0 °C. *J. Prakt. Chem.* **1966**, *31*, 225−239.
(182) Harris, K. R.; Dunlop, P. J. Vapour Pressures and Excess Gibbs Energies of Mixtures of Benzene with Chlorobenzene, n-Hexane, and n-Heptane at 25°C. *J. Chem. Thermodyn.* **1970**, *2*, 805−811.
(183) 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* **1986**, *7*, 54−58.
(184) Messow, U.; Schuetze, D.; Pfestorf, R.; Kuchenbecker, D.; Suehnel, K. Thermodynamische Untersuchungen an Lösungsmittel/n-Paraffin-Systemen. *Z. Phys. Chem.* **1977**, *258*, 24−32.
(185) Palmer, D. A.; Smith, B. D. Thermodynamic Excess Property Measurements for Acetonitrile-Benzene-n-Heptane System at 45°C. *J. Chem. Eng. Data* **1972**, *17*, 71−76.
(186) 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.* **1971**, *20*, 292−296.
(187) Hanson, D. O.; Van Winkle, M. Alteration of the Relative Volatility of Hexane-1-Hexene by Oxygenated and Chlorinated Solvents. *J. Chem. Eng. Data* **1967**, *12*, 319−325.
(188) Brown, I. Liquid-Vapour Equilibria. III. The Systems Benzene-n-Heptane, n-Hexane-Chlorobenzene, and Cyclohexane-Nitrobenzene. *Aust. J. Chem.* **1952**, *5*, 530.
(189) Brown, I.; Ewald, A. Liquid-Vapour Equilibria II. The System Benzene-Heptane. *Aust. J. Chem.* **1951**, *4*, 198.
(190) Nielsen, R. L.; Weber, J. H. Vapor-Liquid Equilibria at Subatmospheric Pressures. Binary and Ternary Systems Containing Ethyl Alcohol, Benzene, and n-Heptane. *J. Chem. Eng. Data* **1959**, *4*, 145−151.
(191) Sieg, L. Flüssigkeit-Dampf-Gleichgewichte in Binären Systemen von Kohlenwasserstoffen Verschiedenen Typs: Flüssigkeit-Dampf-Gleichgewichte in Binären Systemen von Kohlenwasserstoffen Verschiedenen Typs. *Chem. Ing. Tech.* **1950**, *22*, 322−326.
(192) Michishita, T.; Arai, Y.; Saito, S. Vapor-Liquid Equilibriums of Hydrocarbons at Atmospheric Pressure. *Chem. Eng.* **1971**, *35*, 111.
(193) Wang, Q.; Chen, G.; Han, S. Study on the Vapor-Liquid Equilibria under Pressure for Binary Systems. *Ranliao Huaxue Xuebao* **1990**, *18*, 185−192.
(194) Vilcu, R.; Stanciu, F. Excess Thermodynamic Functions from Calorimetric Data. *Rev. Roum. Chim.* **1966**, *11*, 175−182.
(195) Hammerl, I.; Raetzsch, M. T. Enthalpies of Mixing of Normal Paraffins with Aromatics. *Wiss. Z. Tech. Hochsch. Chem. "Carl Schorlemmer" Leuna-Merseburg* **1973**, *15*, 175−178.
(196) Tanaka, R. Excess Heat Capacities for Mixture of Benzene with N-Heptane at 293.15, 298.15, and 303.15 K. *J. Chem. Eng. Data* **1987**, *32*, 176−177.
(197) Karbalai Ghassemi, M. H.; Grolier, J. P. E. Excess Heat Capacity. Cyclohexane-n-Hexane System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1976**, *1976*, 95−96.
(198) Tasić, A.; Djordjević, B.; Grozdanić, D.; Afgan, N.; Malić, D. Vapour—Liquid Equilibria of the Systems Acetone—Benzene, Benzene—Cyclohexane and Acetone—Cyclohexane at 25°C. *Chem. Eng. Sci.* **1978**, *33*, 189−197.
(199) Mentzer, R. A.; Greenkorn, R. A.; Chao, K. C. Bubble Pressures and Vapor-Liquid Equilibria for Four Binary Hydrocarbon Mixtures. *J. Chem. Thermodyn.* **1982**, *14*, 817−830.
(200) Kurihara, K.; Uchiyama, M.; Kojima, K. Isothermal Vapor−Liquid Equilibria for Benzene + Cyclohexane + 1-Propanol and for Three Constituent Binary Systems. *J. Chem. Eng. Data* **1997**, *42*, 149−154.
(201) 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. *Collect. Czech. Chem. Commun.* **1963**, *28*, 1771−1779.
(202) Scatchard, G.; Wood, S. E.; Mochel, J. M. Vapor−Liquid Equilibrium. III. Benzene−Cyclohexane Mixtures. *J. Phys. Chem. A.* **1939**, *43*, 119−130.
(203) Dong, J.; Feng, C.; Li, Y. 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. *J. Chem. Eng. Data* **2011**, *56*, 2386−2392.
(204) Wiśniewska, B.; Gregorowicz, J.; Malanowski, S. Development of a Vapour-Liquid Equilibrium Apparatus to Work at Pressures up to 3 MPa. *Fluid Phase Equilib.* **1993**, *86*, 173−186.
(205) 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. Exactas, Fis., Quim. Nat. Zaragoza* **1992**, *47*, 183−190.
(206) Rao, V. N. K.; Swami, D. R.; Rao, M. N. Vapor-Liquid Equilibria of Benzene−n-Hexane and Benzene-Cyclohexane Systems. *AIChE J.* **1957**, *3*, 191−197.
(207) Elliott, K.; Wormald, C. J. A Precision Differential Flow Calorimeter the Excess Enthalpy of Benzene + Cyclohexane between 280.15 K and 393.15 K. *J. Chem. Thermodyn.* **1976**, *8*, 881−893.
(208) Yan, W.-D.; Lin, R.-S.; Yen, W.-H. Excess Enthalpies of Seven Binary Liquid Systems. *Thermochim. Acta* **1990**, *169*, 171−184.
(209) 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. *J. Therm. Anal. Calorim.* **2005**, *79*, 85−88.
(210) van Ness, H. C.; Abbott, M. M. Excess Enthalpy. Benzene-Cyclohexane System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1974**, *1974*, 160−161.
(211) Lohmann, J.; Bölts, R.; Gmehling, J. Excess Enthalpy Data for Seven Binary Systems at Temperatures between 50 and 140 °C. *J. Chem. Eng. Data* **2001**, *46*, 208−211.
(212) Tanaka, R. Determination of Excess Heat Capacities of (Benzene + Tetrachloromethane and + Cyclohexane) between 293.15 and 303.15 K by Use of a Picker Flow Calorimeter. *J. Chem. Thermodyn.* **1982**, *14*, 259−268.
(213) Páramo, R.; Zouine, M.; Casanova, C. New Batch Cells Adapted To Measure Saturated Heat Capacities of Liquids. *J. Chem. Eng. Data* **2002**, *47*, 441−448.
(214) D'arcy, P. J.; Hazlett, J. D.; Kiyohara, O.; Benson, G. C. Excess Heat Capacities of Mixtures of Benzene with Cyclohexane at 298.15 K. *Thermochim. Acta* **1977**, *21*, 297−300.
(215) Grolier, J.-P. E.; Wilhelm, E.; Hamedi, M. H. Molar Heat Capacity and Isothermal Compressibility of Binary Liquid Mixtures: Carbon Tetrachloride + Benzene, Carbon Tetrachloride + Cylohexane and Benzene + Cylohexane. *Ber. Bunsenges. Phys. Chem.* **1978**, *82*, 1282−1290.
(216) Calado, J. C. G.; Soares, V. A. M. Thermodynamics of Liquid Ethylene + Xenon at 161.38 K. *J. Chem. Thermodyn.* **1977**, *9*, 911−913.
(217) Da Ponte, M. N.; Chokappa, D.; Calado, J. C. G.; Zollweg, J.; Streett, W. B. Vapor-Liquid Equilibrium in the Xenon + Ethene System. *J. Phys. Chem. B.* **1986**, *90*, 1147−1152.
(218) 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. *J. Chem. Thermodyn.* **1987**, *19*, 35−38.
(219) Wu, W.; Ke, J.; Poliakoff, M. Phase Boundaries of CO2 + Toluene, CO2 + Acetone, and CO2 + Ethanol at High Temperatures and High Pressures. *J. Chem. Eng. Data* **2006**, *51*, 1398−1403.
(220) Naidoo, P.; Ramjugernath, D.; Raal, J. D. A New High-Pressure Vapour−Liquid Equilibrium Apparatus. *Fluid Phase Equilib.* **2008**, *269*, 104−112.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(221) Zhang, J. C.; Wu, X. Y.; Cao, W. L. Phase Equilibrium Properties of Supercritical Carbon Dioxide in Binary System. *Gaodeng Xuexiao Huaxue Xuebao* **2002**, *23*, 10−13.
(222) 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 Des. Dev.* **1986**, *25*, 584−589.
(223) Fink, S. D.; Hershey, H. C. Modeling the Vapor-Liquid Equilibria of 1,1,1-Trichloroethane + Carbon Dioxide and Toluene + Carbon Dioxide at 308, 323, and 353 K. *Ind. Eng. Chem. Res.* **1990**, *29*, 295−306.
(224) 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* **1990**, *28*, 438−443.
(225) Kim, C.-H.; Vimalchand, P.; Donohue, M. D. Vapor-Liquid Equilibria for Binary Mixtures of Carbon Dioxide with Benzene, Toluene and p-Xylene. *Fluid Phase Equilib.* **1986**, *31*, 299−311.
(226) Morris, W. O.; Donohue, M. D. Vapor-Liquid Equilibria in Mixtures Containing Carbon Dioxide, Toluene, and 1-Methylnaphthalene. *J. Chem. Eng. Data* **1985**, *30*, 259−263.
(227) Ng, H.-J.; Robinson, D. B. Equilibrium-Phase Properties of the Toluene-Carbon Dioxide System. *J. Chem. Eng. Data* **1978**, *23*, 325−327.
(228) 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. *J. Chem. Thermodyn.* **1987**, *19*, 845−856.
(229) 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. *J. Chem. Thermodyn.* **1986**, *18*, 647−656.
(230) 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. *J. Chem. Thermodyn.* **1983**, *15*, 747−755.
(231) 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. *J. Chem. Thermodyn.* **1985**, *17*, 1−10.
(232) Reaves, J. T.; Griffith, A. T.; Roberts, C. B. Critical Properties of Dilute Carbon Dioxide + Entrainer and Ethane + Entrainer Mixtures. *J. Chem. Eng. Data* **1998**, *43*, 683−686.
(233) Zhang, H.; Liu, Z.; Han, B. Critical Points and Phase Behavior of Toluene-CO2 and Toluene-H2-CO2 Mixture in CO2-Rich Region. *J. Supercrit. Fluids* **2000**, *18*, 185−192.
(234) Jiménez-Gallegos, R.; Galicia-Luna, L. A.; Elizalde-Solis, O. Experimental Vapor−Liquid Equilibria for the Carbon Dioxide + Octane and Carbon Dioxide + Decane Systems. *J. Chem. Eng. Data* **2006**, *51*, 1624−1628.
(235) Iwai, Y.; Hosotani, N.; Morotomi, T.; Koga, Y.; Arai, Y. High-Pressure Vapor-Liquid Equilibria for Carbon Dioxide + Linalool. *J. Chem. Eng. Data* **1994**, *39*, 900−902.
(236) Nagarajan, N.; Robinson, R. L. Equilibrium Phase Compositions, Phase Densities, and Interfacial Tensions for Carbon Dioxide + Hydrocarbon Systems. 2. Carbon Dioxide + n-Decane. *J. Chem. Eng. Data* **1986**, *31*, 168−171.
(237) Reamer, H. H.; Sage, B. H. Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the n-Decane-CO2 System. *J. Chem. Eng. Data* **1963**, *8*, 508−513.
(238) Inomata, H.; Tuchiya, K.; Arai, K.; Saito, S. Measurement of Vapor-Liquid Equilibria at Elevated Temperatures and Pressures Using a Flow Type Apparatus. *J. Chem. Eng. Jpn.* **1986**, *19*, 386−391.
(239) Sebastian, H. M.; Simnick, J. J.; Lin, H.-M.; Chao, K.-C. Vapor-Liquid Equilibrium in Binary Mixtures of Carbon Dioxide + n-Decane and Carbon Dioxide + n-Hexadecane. *J. Chem. Eng. Data* **1980**, *25*, 138−140.
(240) 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. *J. Chem. Thermodyn.* **1983**, *15*, 173−180.
(241) 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. *J. Chem. Thermodyn.* **1986**, *18*, 53−61.
(242) Gurdial, G. S.; Foster, N. R.; Yun, S. L. J.; Tilly, K. D. Phase Behavior of Supercritical Fluid—Entrainer Systems. *Supercritical Fluid Engineering Science*; ACS Symposium Series; ACS Publications, 1992; Vol. *514*, pp 34−45.
(243) Gulari, Es.; Saad, H.; Bae, Y. C. Effect of Critical Phenomena on Transport Properties in the Supercritical Region. *Supercritical Fluids*; ACS Symposium Series; ACS Publications, 1987; Vol. *329*, pp 2−14.
(244) Juntarachat, N.; Bello, S.; Privat, R.; Jaubert, J.-N. Validation of a New Apparatus Using the Dynamic Method for Determining the Critical Properties of Binary Mixtures Containing CO_2 and a N-Alkane. *Fluid Phase Equilib.* **2012**, *325*, 66−70.
(245) Polikhronidi, N. G.; Batyrova, R. G.; Abdulagatov, I. M.; Stepanov, G. V. Isochoric Heat Capacity of CO_2 + N-Decane Mixtures in the Critical Region. *Int. J. Thermophys.* **2006**, *27*, 729−759.
(246) Mraw, S. C.; Hwang, S.-C.; Kobayashi, R. Vapor-Liquid Equilibrium of the Methane-Carbon Dioxide System at Low Temperatures. *J. Chem. Eng. Data* **1978**, *23*, 135−139.
(247) Al-Sahhaf, T. A.; Kidnay, A. J.; Sloan, E. D. Liquid + Vapor Equilibriums in the Nitrogen + Carbon Dioxide + Methane System. *Ind. Eng. Chem. Fundam.* **1983**, *22*, 372−380.
(248) Somait, F. A.; Kidnay, A. J. Liquid-Vapor Equilibriums at 270.00 K for Systems Containing Nitrogen, Methane, and Carbon Dioxide. *J. Chem. Eng. Data* **1978**, *23*, 301−305.
(249) Xu, N.; Dong, J.; Wang, Y.; Shi, J. High Pressure Vapor Liquid Equilibria at 293 K for Systems Containing Nitrogen, Methane and Carbon Dioxide. *Fluid Phase Equilib.* **1992**, *81*, 175−186.
(250) Xu, N.; Dong, J.; Wang, Y.; Shi, J. Vapor Liquid Equilibria For N2-CH4-CO2 System Near Critical Region. *Huagong Xuebao* **1992**, *43*, 640−644.
(251) Lee, J. I.; Mather, A. E. The Excess Enthalpy of Gaseous Mixtures of Carbon Dioxide with Methane. *Can. J. Chem. Eng.* **1972**, *50*, 95−100.
(252) Barry, A. O.; Kaliaguine, S. C.; Ramalho, R. S. Direct Determination of Enthalpy of Mixing for the Binary Gaseous System Methane-Carbon Dioxide by an Isothermal Flow Calorimeter. *J. Chem. Eng. Data* **1982**, *27*, 258−264.
(253) Arai, Y.; Kaminishi, G.-I.; Saito, S. The Experimental Determination Of The P-V-T-X Relations For The Carbon Dioxide-Nitrogen And The Carbon Dioxide-Methane Systems. *J. Chem. Eng. Jpn.* **1971**, *4*, 113−122.
(254) Mraw, S. C.; Hwang, S. C.; Kobayashi, R. *The Vapor-Liquid Equilibrium of the CH_4−CO_2 System at Low Temperatures*, GPA Research Report; Gas Processors Association, 1977; pp 1−18.
(255) Hwang, S. C.; Lin, H. M.; Chappelear, P. S.; Kobayashi, R. *Dew-Point Values for the Methane−Carbon Dioxide System*, GPA Research Report; Gas Processors Association, 1976; pp 1−14.
(256) Shah, N. N.; Zollweg, J. A.; Streett, W. B. Vapor-Liquid Equilibrium in the System Carbon Dioxide + Cyclopentane from 275 to 493 K at Pressures to 12.2 MPa. *J. Chem. Eng. Data* **1991**, *36*, 188−192.
(257) Eckert, C. J.; Sandler, S. I. Vapor-Liquid Equilibria for the Carbon Dioxide-Cyclopentane System at 37.7, 45.0, and 60.0.Degree.C. *J. Chem. Eng. Data* **1986**, *31*, 26−28.
(258) Zhang, Z.; Guo, L.; Yang, X.; Knapp, H. Vapor And Liquid Equilibrium For Nitrogen - Ethane - Carbon Dioxide Ternary System. *Huagong Xuebao* **1999**, *50*, 392−398.
(259) Yucelen, B.; Kidnay, A. J. Vapor−Liquid Equilibria in the Nitrogen + Carbon Dioxide + Propane System from 240 to 330 K at Pressures to 15 MPa. *J. Chem. Eng. Data* **1999**, *44*, 926−931.
(260) 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. *Int. J. Thermophys.* **1994**, *15*, 1211−1219.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(261) 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 Equilib.* **1989**, *53*, 7−14.
(262) Al-Sahhaf, T. A. Vapor—Liquid Equilibria for the Ternary System N2 + CO2 + CH4 at 230 and 250 K. *Fluid Phase Equilib.* **1990**, *55*, 159−172.
(263) Yorizane, M.; Yoshimura, S.; Masuoka, H. Vapor Liquid Equilibrium at High Pressures. N2-CO2, H2-CO2 Systems. *Chem. Eng.* **1970**, *34*, 953−957.
(264) Zenner, G. H.; Dana, L. I. Liquid-Vapor Equilibrium Compositions of Carbon Dioxideoxygen-Nitrogen Mixtures. *Chem. Eng. Prog., Symp. Ser.* **1963**, *59*, 36−41.
(265) 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. *J. Soc. Chem. Ind., Jpn.* **1966**, *69*, 175−178.
(266) Krichevskii, I. R.; Khazanova, N. E.; Lesnevskaya, L. S.; Sandalova, L. Y. Liquid-Gas Equilibrium in the Nitrogen-Carbon Dioxide System under Elevated Pressures. *Khim. Prom-sti.* **1962**, 169−171.
(267) Bian, B.; Wang, Y.; Shi, J.; Zhao, E.; Lu, B. 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 Equilib.* **1993**, *90*, 177−187.
(268) Lee, J. I.; Mather, A. E. Excess Enthalpy of Gaseous Mixtures of Nitrogen and Carbon Dioxide. *J. Chem. Eng. Data* **1972**, *17*, 189−192.
(269) Hejmadi, A. V.; Katz, D. L.; Powers, J. E. Experimental Determination of the Enthalpy of Mixing of N + CO2 under Pressure. *J. Chem. Thermodyn.* **1971**, *3*, 483−496.
(270) Reamer, H. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems - Volumetric and Phase Behavior of the Methane-Hydrogen Sulfide System. *Ind. Eng. Chem.* **1951**, *43*, 976−981.
(271) Kohn, J. P.; Kurata, F. Heterogeneous Phase Equilibria of the Methane—Hydrogen Sulfide System. *AIChE J.* **1958**, *4*, 211−217.
(272) Barry, A. O.; Kaliaguine, S. C.; Ramalho, R. S. Excess Enthalpies of the Binary System Methane-Hydrogen Sulfide by Flow Calorimetry. *J. Chem. Eng. Data* **1982**, *27*, 436−439.
(273) Fall, D. J.; Luks, K. D. Phase Equilibria Behavior of the Systems Carbon Dioxide + N-Dotriacontane and Carbon Dioxide + n-Docosane. *J. Chem. Eng. Data* **1984**, *29*, 413−417.
(274) Tsai, F. N.; Yau, J. S. Solubility of Carbon Dioxide in N-Tetracosane and in n-Dotriacontane. *J. Chem. Eng. Data* **1990**, *35*, 43−45.
(275) Spee, M.; Schneider, G. M. Fluid Phase Equilibrium Studies on Binary and Ternary Mixtures of Carbon Dioxide with Hexadecane, 1-Dodecanol, 1,8-Octanediol and Dotriacontane at 393.2 K and at Pressures up to 100 MPa. *Fluid Phase Equilib.* **1991**, *65*, 263−274.
(276) Segovia, J. J.; Martín, M. C.; Chamorro, C. R.; Montero, E. A.; Villamañán, M. A. Excess Thermodynamic Functions for Ternary Systems Containing Fuel Oxygenates and Substitution Hydrocarbons: 2. Total-Pressure Data and GE for Methyl Tert-Butyl Ether/n-Heptane/1-Hexene at 313.15 K. *Fluid Phase Equilib.* **1998**, *152* (), 265−276. DOI: 10.1016/S0378-3812(98)00384-7.
(277) 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* **1995**, *33*, 527−534.
(278) Wisniak, J.; Magen, E.; Shachar, M.; Zeroni, I.; Reich, R.; Segura, H. Isobaric Vapor−Liquid Equilibria in the Systems Methyl 1,1-Dimethylethyl Ether + Hexane and + Heptane. *J. Chem. Eng. Data* **1997**, *42*, 243−247.
(279) 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). *J. Solution Chem.* **1991**, *20*, 153−163.
(280) Han, K.; Xia, S.; Ma, P.; Yan, F.; Liu, T. Measurement of Critical Temperatures and Critical Pressures for Binary Mixtures of Methyl Tert-Butyl Ether (MTBE)+alcohol and MTBE+alkane. *J. Chem. Thermodyn.* **2013**, *62*, 111−117.
(281) 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. *J. Chem. Eng. Data* **1962**, *7*, 26−28.
(282) 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 Equilib.* **1995**, *111*, 71−88.
(283) Gmehling, J.; Meents, B. Excess Enthalpy. Ethyl Ethanoate-Toluene System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1992**, 177.
(284) Jiménez, E.; et al. Excess Heat Capacities and Excess Volumes of (an n-Alkylalkanoate + Heptane or Decane or Toluene). *J. Chem. Thermodyn.* **1994**, *26*, 817−827.
(285) Steinbrecher, M.; Bittrich, H.-J. Das Isotherme Flüssigkeits-Dampf-Gleichgewicht Der Binären Systeme Zwischen Den Komponenten Tetrachlormethan, Äthylacetat Und Dioxan. *Z. Phys. Chem.* **1966**, *232O*, 313−324.
(286) Drobig, J.; Lindenau, E. A New Apparatus to Determine the Isothermal Liquid-Vapor Equilibrium. *Wiss. Z. Tech. Hochsch. Chem. "Carl Schorlemmer" Leuna-Merseburg* **1966**, *8*, 144−147.
(287) Guillen, M. D.; Gutierrez Losa, C. Excess Enthalpies and Excess Volumes of N-Hexane + and of Tetrachloromethane + Furan, + 1,4-Dioxane, + Tetrahydrofuran, and + Tetrahydropyran. *J. Chem. Thermodyn.* **1978**, *10*, 567−576.
(288) Murakami, S.; Benson, G. C. An Isothermal Dilution Calorimeter for Measuring Enthalpies of Mixing. *J. Chem. Thermodyn.* **1969**, *1*, 559−572.
(289) Becker, F.; Kiefer, M.; Koukol, H. Kontinuierliche Bestimmung von Mischungswärmen Durch Quasi-Isotherme Wärmeflußkalorimetrie. *Z. Phys. Chem.* **1972**, *80*, 29−43.
(290) McKinnon, I.; Williamson, A. Heats of Mixing of CCl4 with Dioxane. *Aust. J. Chem.* **1964**, *17*, 1374.
(291) Ohta, T.; Koyabu, J.; Nagata, I. Vapor—Liquid Equilibria for the Ternary Ethanol—2-Butanone—Benzene System at 298.15 K. *Fluid Phase Equilib.* **1981**, *7*, 65−73.
(292) 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. *J. Chem. Thermodyn.* **1978**, *10*, 1101−1106.
(293) 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**, *16*, 195−201.
(294) Kiyohara, O.; Benson, G. C.; Grolier, J.-P. E. Thermodynamic Properties of Binary Mixtures Containing Ketones I. Excess Enthalpies of Some Aliphatic Ketones + n-Hexane, + Benzene, and + Tetrachloromethane. *J. Chem. Thermodyn.* **1977**, *9*, 315−323.
(295) Chamorro, C. R.; Segovia, J. J.; Martín, M. C.; Montero, E. A.; Villamañán, M. 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 Equilib.* **1999**, *156*, 73−87.
(296) Mejía, A.; Segura, H.; Cartes, M. Vapor−Liquid Equilibrium in the Binary Systems 2-Butanol + Tert-Amyl Methyl Ether, 2-Butanol + Heptane, and Heptane + Tert-Amyl Methyl Ether. *J. Chem. Eng. Data* **2011**, *56*, 2256−2265.
(297) Kammerer, K.; Lichtenthaler, R. N. Excess Enthalpy HE of Binary Mixtures Containing Alkanes, Methanol and Tert-Amyl-Methyl Ether (TAME). *Thermochim. Acta* **1996**, *271*, 49−58.
(298) Tong, Z.; Benson, G. C.; Wang, L. L.; Lu, B. C.-Y. Excess Enthalpies of Ternary Mixtures Consisting of a Normal Alkane, Methyl Tert-Butyl Ether, and Tert-Amyl Methyl Ether. *J. Chem. Eng. Data* **1996**, *41*, 865−869.
(299) Vorenberg, D. G.; Raal, J. D.; Ramjugernath, D. Vapor−Liquid Equilibrium Measurements of MTBE and TAME with Toluene. *J. Chem. Eng. Data* **2005**, *50*, 56−59.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(300) Plura, J.; Matouš, J.; Novák, J. P.; Šobr, J. Vapour-Liquid Equilibrium in the Methyl Tert-Butyl Ether-n-Hexane and Methyl Tert-Butyl Ether-Toluene Systems. *Collect. Czech. Chem. Commun.* **1979**, *44*, 3627−3631.
(301) Reich, R.; Cartes, M.; Wisniak, J.; Segura, H. Phase Equilibria in the Systems Methyl 1,1-Dimethylethyl Ether + Benzene and + Toluene. *J. Chem. Eng. Data* **1998**, *43*, 299−303.
(302) Letcher, T. M.; Domańska, U. 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. *J. Chem. Thermodyn.* **1997**, *29*, 721−730.
(303) Niesen, V. G.; Yesavage, V. F. Vapor-Liquid Equilibria for m-Cresol/Tetralin and Tetralin/Quinoline at Temperatures between 523 and 598 K. *J. Chem. Eng. Data* **1988**, *33*, 253−258.
(304) Mahmood, S.; Zhao, Q.; Kabadi, V. N. High-Temperature VLE for the Tetralin−Quinoline System. *J. Chem. Eng. Data* **2001**, *46*, 994−999.
(305) Mollerup, J. Vapour/Liquid Equilibrium in Ethylene + Carbon Dioxide and Ethane + Carbon Dioxide. *J. Chem. Soc., Faraday Trans. 1* **1975**, *71*, 2351.
(306) Nagahama, K.; Konishi, H.; Hoshino, D.; Hirata, M. Binary Vapor-Liquid Equilibria Of Carbon Dioxide-Light Hydrocarbons At Low Temperature. *J. Chem. Eng. Jpn.* **1974**, *7*, 323−328.
(307) Bae, H. K.; Nagahama, K.; Hirata, M. Isothermal Vapor-Liquid Equilibriums for the Ethylene-Carbon Dioxide System at High Pressure. *J. Chem. Eng. Data* **1982**, *27*, 25−27.
(308) 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. *Proc. R. Soc. London, Ser. A* **1951**, *209*, 1−14.
(309) Wormald, C. J.; Eyears, J. M. Excess Molar Enthalpies of (Carbon Dioxide + Ethene) in the Liquid and near-Critical Regions. *J. Chem. Thermodyn.* **2001**, *33*, 775−786.
(310) Rowlinson, J. S.; Sutton, J. R.; Weston, J. F. In *Liquid−Vapor Equilibrium in the Ternary System Carbon Dioxide-Nitrous Oxide-Ethylene*, Proceedings of the Conference on Thermodynamic and Transport Properties of Fluids, 1958; pp 10−14.
(311) 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.* **1979**, *53*, 1594−1597.
(312) Kim, J. H.; Kim, M. S. Vapor−Liquid Equilibria for the Carbon Dioxide+propane System over a Temperature Range from 253.15 to 323.15K. *Fluid Phase Equilib.* **2005**, *238*, 13−19.
(313) Reamer, H. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Propane-Carbon Dioxide System. *Ind. Eng. Chem.* **1951**, *43*, 2515−2520.
(314) Tanaka, K.; Higashi, Y.; Akasaka, R.; Kayukawa, Y.; Fujii, K. Measurements of the Vapor−Liquid Equilibrium for the CO2 + R290 Mixture. *J. Chem. Eng. Data* **2009**, *54*, 1029−1033.
(315) Niesen, V. G.; Rainwater, J. C. Critical Locus, (Vapor + Liquid) Equilibria, and Coexisting Densities of (Carbon Dioxide + Propane) at Temperatures from 311 K to 361 K. *J. Chem. Thermodyn.* **1990**, *22*, 777−795.
(316) Poettmann, F. H.; Katz, D. L. Phase Behavior of Binary Carbon Dioxide-Paraffin Systems. *Ind. Eng. Chem.* **1945**, *37*, 847−853.
(317) Morrison, G.; Kincaid, J. M. Critical Point Measurements on Nearly Polydisperse Fluids. *AIChE J.* **1984**, *30*, 257−262.
(318) Juntarachat, N.; Bello, S.; Privat, R.; Jaubert, J.-N. Validation of a New Apparatus Using the Dynamic Method for Determining the Critical Properties of Binary Gas/Gas Mixtures. *J. Chem. Eng. Data* **2013**, *58*, 671−676.
(319) Horstmann, S.; Fischer, K.; Gmehling, J. Experimental Determination of Critical Points of Pure Components and Binary Mixtures Using a Flow Apparatus. *Chem. Eng. Technol.* **1999**, *22*, 839−842.
(320) Ke, J.; George, M. W.; Poliakoff, M.; Han, B.; Yan, H. How Does the Critical Point Change during the Hydrogenation of Propene in Supercritical Carbon Dioxide? *J. Phys. Chem. B* **2002**, *106*, 4496−4502.
(321) Rall, W.; Schäfer, K. Thermodynamische Untersuchungen an Flüssigen Mischsystemen von Aceton Und N-Pentan Sowie von Aceton Und n-Hexan. *Z. Elektrochem.* **1959**, *63*, 1019−1024.
(322) Kudryavtseva, L. S.; Susarev, M. P. Liquid-Vapor Equilibriums in the Systems Acetone-Hexane and Hexane-Ethyl Alcohol at 35, 45, and 55 and 760mmHg. *Zh. Prikl. Khim.* **1963**, *36*, 1419−1424.
(323) 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. *Z. Phys. Chem.* **1982**, *263O*, 151−160.
(324) Acosta, J.; Arce, A.; Martínez-Ageitos, J.; Rodil, E.; Soto, A. Vapor−Liquid Equilibrium of the Ternary System Ethyl Acetate + Hexane + Acetone at 101.32 KPa. *J. Chem. Eng. Data* **2002**, *47*, 849−854.
(325) Schaefer, K. Excess Enthalpies of Acetone + N-Alkane (C3-C6) Binary Mixtures. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1978**, *1*, 74−77.
(326) Singh, P. P.; Malik, R.; Maken, S.; Acree, W. E.; Tucker, S. A. Thermochemical Investigations of Associated Solutions. 10. Excess Enthalpies and Excess Volumes of Ternary Acetone + Bromoform + n-Hexane Mixtures. *Thermochim. Acta* **1990**, *162*, 291−309.
(327) Kay, W. B. P-T-x Diagrams in the Critical Region. Acetone-n-Alkane Systems. *J. Phys. Chem. C.* **1964**, *68*, 827−831.
(328) Campbell, S. W.; Wilsak, R. A.; Thodos, G. Isothermal Vapor-Liquid Equilibrium Measurements for the n-Pentane-Acetone System at 372.7, 397.7, and 422.6 K. *J. Chem. Eng. Data* **1986**, *31*, 424−430.
(329) Hajjar, R. F.; Cherry, R. H.; Kay, W. B. Critical Properties of the Vapor—Liquid Equilibria of the Binary System Acetone—n-Pentane. *Fluid Phase Equilib.* **1986**, *25*, 137−146.
(330) Puri, P. S.; Polak, J.; Ruether, J. A. Vapor-Liquid Equilibriums of Acetone-Cyclohexane and Acetone-Isopropanol Systems at 25°C. *J. Chem. Eng. Data* **1974**, *19*, 87−89.
(331) 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* **1965**, *38*, 371−375.
(332) Crespo Colin, A.; Compostizo, A.; Díaz Peña, M. Excess Gibbs Energy and Excess Volume of (Cyclohexane + 2-Propanone) and of (Cyclohexane+2-Butanone). *J. Chem. Thermodyn.* **1984**, *16*, 497−502.
(333) Mejía, A.; Segura, H.; Cartes, M.; Calvo, C. Vapor−Liquid Equilibria and Interfacial Tensions for the Ternary System Acetone +2,2′-Oxybis[Propane]+cyclohexane and Its Constituent Binary Systems. *Fluid Phase Equilib.* **2008**, *270*, 75−86.
(334) Pfeffer, T.; Löwen, B.; Schulz, S. 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 Equilib.* **1995**, *106*, 139−167.
(335) 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. *Thermochim. Acta* **1995**, *262*, 69−82.
(336) Marongiu, B. Excess Enthalpy. 2-Propanone-Cyclohexane System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1987**, *1987*, 1−6.
(337) Singh, P. P.; Malik, R.; Maken, S.; Acree, W. E.; Zvaigzni, A. I. Thermochemical Investigations of Associated Solutions. *Thermochim. Acta* **1990**, *165*, 113−127.
(338) Linek, J.; Wichterle, I.; Marsh, K. N. Vapor-Liquid Equilibria for N-Methyl-2-Pyrrolidone + Benzene, +Toluene, +Heptane, and +Methylcyclohexane. *J. Chem. Eng. Data* **1996**, *41*, 1212−1218.
(339) Blanco, B.; Beltrán, S.; Cabezas, J. L.; Coca, J. Phase Equilibria of Binary Systems Formed by Hydrocarbons from Petroleum Fractions and the Solvents N-Methylpyrrolidone and N,N-Dimethyl-

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

formamide. 1. Isobaric Vapor - Liquid Equilibria. *J. Chem. Eng. Data* **1997**, *42*, 938−942.
(340) 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 Equilib.* **1989**, *46*, 95−102.
(341) 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. *J. Chem. Thermodyn.* **1999**, *31*, 1585−1595.
(342) Chhikara, Y.; Yadav, J. S.; Sharma, D.; 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. *J. Chem. Thermodyn.* **2011**, *43*, 737−749.
(343) Gmehling, J.; Meents, B. Excess Enthalpy. 1-Methyl-2-Pyrrolidinone - Benzene System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1992**, 211.
(344) Brown, T. S.; Kidnay, A. J.; Sloan, E. D. Vapor—Liquid Equilibria in the Carbon Dioxide-Ethane System. *Fluid Phase Equilib.* **1988**, *40*, 169−184.
(345) Wallis, K. P.; Clancy, P.; Zollweg, J. A.; Streett, W. B. Excess Thermodynamic Properties for {xCO2 + (1 − x)C2H6} (I): Experiment and Theory. *J. Chem. Thermodyn.* 1984, *16* (9), 811−823. DOI: 10.1016/0021-9614(84)90028-4.
(346) Ohgaki, K.; Katayama, T. Isothermal Vapor-Liquid Equilibrium Data for the Ethane—Carbon Dioxide System at High Pressures. *Fluid Phase Equilib.* **1977**, *1*, 27−32.
(347) 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. *J. Chem. Thermodyn.* **1988**, *20*, 323−331.
(348) 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. *J. Chem. Thermodyn.* **1997**, *29*, 75−85.
(349) Khazanova, N. E.; Lesnevskaya, L. S.; Zakharova, A. V. Liquid-Vapor Equilibrium in the Ethane-CO2 System. *Khim. Prom-sti.* **1966**, *44*, 364−365.
(350) Gil, L.; Otín, S. F.; Embid, J. M.; Gallardo, M. A.; Blanco, S.; Artal, M.; Velasco, I. Experimental Setup to Measure Critical Properties of Pure and Binary Mixtures and Their Densities at Different Pressures and Temperatures. *J. Supercrit. Fluids* **2008**, *44*, 123−138.
(351) 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**, *10*, 213−219.
(352) Goodwin, A. R. H.; Moldover, M. R. Phase Border and Density Determinations in the Critical Region of (Carbon Dioxide +ethane) Determined from Dielectric Permittivity Measurements. *J. Chem. Thermodyn.* **1997**, *29*, 1481−1494.
(353) Horstmann, S.; Fischer, K.; Gmehling, J.; Kolář, P. 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. *J. Chem. Thermodyn.* **2000**, *32*, 451−464.
(354) Kalra, H.; Krishnana, T. R.; Robinson, D. B. Equilibrium-Phase Properties of Carbon Dioxide-Butane and Nitrogen-Hydrogen Sulfide Systems at Subambient Temperatures. *J. Chem. Eng. Data* **1976**, *21*, 222−225.
(355) Weber, L. A. Vapour-Liquid Equilibria Measurements for Carbon Dioxide with Normal and Isobutane from 250 to 280 K. *Cryogenics* **1985**, *25*, 338−342.
(356) Niesen, V. G. (Vapor + Liquid) Equilibria and Coexisting Densities of (Carbon Dioxide + n-Butane) at 311 to 395 K. *J. Chem. Thermodyn.* **1989**, *21*, 915−923.
(357) Hsu, J. 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. *J. Chem. Eng. Data* **1985**, *30*, 485−491.
(358) Pozo de Fernandez, M. E.; Zollweg, J. A.; Streett, W. B. Vapor-Liquid Equilibrium in the Binary System Carbon Dioxide + n-Butane. *J. Chem. Eng. Data* **1989**, *34*, 324−328.
(359) Weber, L. A. Simple Apparatus for Vapor-Liquid Equilibrium Measurements with Data for the Binary Systems of Carbon Dioxide with n-Butane and Isobutane. *J. Chem. Eng. Data* **1989**, *34*, 171−175.
(360) Olds, R. H.; Reamer, H. H.; Sage, B. H.; Lacey, W. N. The N-Butane−Carbon Dioxide System. *Ind. Eng. Chem.* **1949**, *41*, 475−482.
(361) Leu, A. D.; Robinson, D. B. Equilibrium Phase Properties of the N-Butane-Carbon Dioxide and Isobutane-Carbon Dioxide Binary Systems. *J. Chem. Eng. Data* **1987**, *32*, 444−447.
(362) Lladosa, E.; Martínez, N. F.; Montón, J. B.; de la Torre, J. Measurements and Correlation of Vapour−Liquid Equilibria of 2-Butanone and Hydrocarbons Binary Systems at Two Different Pressures. *Fluid Phase Equilib.* **2011**, *307*, 24−29.
(363) Murakami, S.; Amaya, K.; Fujishiro, R. Heats of Mixing for Binary Mixtures. The Energy of Hydrogen Bonding between Alcohol and Ketone Molecules. *Bull. Chem. Soc. Jpn.* **1964**, *37*, 1776−1780.
(364) Kreglewski, A.; Kay, W. B. Critical Constants of Conformed Mixtures. *J. Phys. Chem D.* **1969**, *73*, 3359−3366.
(365) 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* **1975**, *1975*, 139−156.
(366) 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. *Collect. Czech. Chem. Commun.* **1971**, *36*, 2547−2567.
(367) Müller, E.; Stage, H. *Experimentelle Vermessung von Dampf-Flüssigkeits-Phasengleichgewichten Dargestellt Am Beispiel Des Siedeverhaltens von Fettsäuren*; Springer-Verlag, 1961.
(368) Free, K. W.; Hutchinson, H. P. Isobaric Vapor-Liquid Equilibria for the Ternary System Acetone-Benzene-Chlorobenzene. *J. Chem. Eng. Data* **1959**, *4*, 193−197.
(369) 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 Metrop. Univ.* **1971**, *21*, 1883−1896.
(370) 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* **1946**, *23*, 177−182.
(371) Kojima, K.; Tochigi, K.; Kurihara, K.; Nakamichi, M. Isobaric Vapor-Liquid Equilibria for Acetone + Chloroform + Benzene and the Three Constituent Binary Systems. *J. Chem. Eng. Data* **1991**, *36*, 343−345.
(372) Akamatsu, Y.; Ogawa, H.; Murakami, S. Molar Excess Enthalpies, Molar Excess Volumes and Molar Isentropic Compressions of Mixtures of 2-Propanone with Heptane, Benzene and Trichloromethane at 298.15 K. *Thermochim. Acta* **1987**, *113*, 141−150.
(373) Möbius, H.-H. Mischungsenthalpien Und Mischbarkeit von Aceton, Benzol Und Wasser. *J. Prakt. Chem.* **1955**, *2*, 95−104.
(374) Yamanaka, K.; Ogawa, H.; Murakami, S. Excess Molar Isobaric Heat Capacities of Mixtures of 2-Propanone with Heptane, Benzene, and Trichloromethane at 298.15 K. *Thermochim. Acta* **1990**, *169*, 193−201.
(375) Lebedeva, E. S.; Khodeeva, S. M. Phase Equilibrium and Volume Relations in the System Methylene Chloride-Ethylene. *Tr., Gos. Nauchno-Issled. Proektn. Inst. Azotn. Prom-sti. Prod. Org. Sint.* **1963**, *13*, 79−90.
(376) Wang, X.; Wang, Y.; Shi, J.; Lu, B. C. Y. Isothermal Vapor-Liquid Equilibria at Elevated Pressures for the Systems Containing Nitrogen, Carbon Dioxide, and Chlorodifluoromethane. *J. Chem. Eng. Data* **1991**, *36*, 436−439.
(377) Nohka, J.; Sarashina, E.; Arai, Y.; Saito, S. Correlation of Vapor-Liquid Equilibria for Systems Containing a Polar Component by the BWR Equation. *J. Chem. Eng. Jpn.* **1973**, *6*, 10−17.

(378) Wang, X.; Wang, Y. S. Vapor-Liquid Equilibria for Nitrogen-Carbon Dioxide-Chlorodifluoromethane at Moderate Pressure. *Nanjing Huagong Xueyuan Xuebao* **1991**, *13*, 35−44.
(379) Maslennikova, V. Y.; Goryunova, N. P.; Tsiklis, D. S. Phase Equilibriums in the Nitrogen-Freon 12 and Nitrogen-Freon 22 Systems. *Russ. J. Phys. Chem. CC.* **1967**, *41*, 383−385.
(380) 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* **1995**, *11*, 87−92.
(381) Nagata, I. Vapor-Liquid Equilibrium at Atmospheric Pressure for the Ternary System, Methyl Acetate-Chloroform-Benzene. *J. Chem. Eng. Data* **1962**, *7*, 360−366.
(382) Chen, G.-H.; Wang, Q.; Ma, Z.-M.; Yan, X.-H.; Han, S.-J. Phase Equilibria at Superatmospheric Pressures for Systems Containing Halohydrocarbon, Aromatic Hydrocarbon, and Alcohol. *J. Chem. Eng. Data* **1995**, *40*, 361−366.
(383) Hirobe, H. Thermochemical Studies. *J. Fac. Sci., Univ. Tokyo, Sect. 1* **1926**, *1*, 155−222.
(384) Nagata, I.; Tamura, K.; Tokuriki, S. Excess Enthalpies and Complex Formation of Acetonitrile with Acetone, Chloroform, and Benzene. *Thermochim. Acta* **1981**, *47*, 315−331.
(385) Rastogi, R. P.; Nath, J.; Misra, R. R. Thermodynamics of Weak Interactions in Liquid Mixtures of Chloroform and Aromatic Hydrocarbons. *J. Chem. Thermodyn.* **1971**, *3*, 307−317.
(386) Grolier, J.-P. E.; Roux-Desgranges, G.; Kooner, Z. S.; Smith, J. F.; Hepler, L. G. Thermal and Volumetric Properties of Chloroform +benzene Mixtures and the Ideal Associated Solution Model of Complex Formation. *J. Solution Chem.* **1987**, *16*, 745−752.
(387) Paul, H. I. *Experimentelle Untersuchung Der Flüssigkeits -Dampf-Phasengleichgewichte Und Volumetrischen Eigenschaften Binärer Und Ternärer Mischungen*; Fortschritt-Berichte VDI Reihe 3, Verfahrenstechnik; VDI-Verlag: Düsseldorf, 1987.
(388) 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 Equilib.* **1999**, *166*, 91−100.
(389) 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* **1990**, *1990*, 59−78.
(390) Góral, M.; Oracz, P.; Warycha, S. Vapour—Liquid Equilibria. IV. The Ternary System Carbon Tetrachloride—Methanol—Chloroform at 293.15 K. *Fluid Phase Equilib.* **1988**, *44*, 77−93.
(391) 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. *J. Prakt. Chem.* **1968**, *37*, 122−136.
(392) Krauze, R.; Serwinski, M. Liquid-Vapor Equilibrium in He System Chloroform-Carbon Tetrachloride. *Zesz. Nauk. − Politech. Lodz., Chem.* **1973**, *24*, 53−63.
(393) Siddiqi, M. A.; Lucas, K. Excess Enthalpy of the System Chloroform + Carbon Tetrachloride and a Thermodynamic Evaluation of Its State Dependence. *Fluid Phase Equilib.* **1984**, *16*, 87−98.
(394) Hu, P.; Chen, L.-X.; Chen, Z.-S. 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 Equilib.* **2013**, *360*, 293−297.
(395) Dong, X.; Gong, M.; Zhang, Y.; Wu, J. Vapor−Liquid Equilibria of the Fluoroethane (R161) + 1,1,1,2-Tetrafluoroethane (R134a) System at Various Temperatures from (253.15 to 292.92) K. *J. Chem. Eng. Data* **2008**, *53*, 2193−2196.
(396) Kleiber, M. Vapor-Liquid Equilibria of Binary Refrigerant Mixtures Containing Propylene or R134a. *Fluid Phase Equilib.* **1994**, *92*, 149−194.
(397) Bobbo, S.; Fedele, L.; Camporese, R.; Stryjek, R. VLE Measurements and Modeling for the Strongly Positive Azeotropic R32+propane System. *Fluid Phase Equilib.* **2002**, *199*, 175−183.
(398) Kim, J. H.; Kim, M. S.; Kim, Y. Vapor−Liquid Equilibria for Pentafluoroethane + Propane and Difluoromethane + Propane Systems over a Temperature Range from 253.15 to 323.15 K. *Fluid Phase Equilib.* **2003**, *211*, 273−287.
(399) Coquelet, C.; Chareton, A.; Valtz, A.; Baba-Ahmed, A.; Richon, D. 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. *J. Chem. Eng. Data* **2003**, *48*, 317−323.
(400) Van Poolen, L. J.; Holcomb, C. D.; Rainwater, J. C. Isoplethic Method to Estimate Critical Lines for Binary Fluid Mixtures from Subcritical Vapor−Liquid Equilibrium: Application to the Azeotropic Mixtures R32 + C3H8 and R125 + C3H8. *Ind. Eng. Chem. Res.* **2001**, *40*, 4610−4614.
(401) Higashi, Y. Experimental Determination of the Critical Locus for the Difluoromethane (R32) and Propane (R290) System. *Fluid Phase Equilib.* **2004**, *219*, 99−103.
(402) Zhang, Y.; Gong, M.; Zhu, H.; Wu, J. Vapor−Liquid Equilibrium Data for the Ethane + Trifluoromethane System at Temperatures from (188.31 to 243.76) K. *J. Chem. Eng. Data* **2006**, *51*, 1411−1414.
(403) Kordikowski, A.; Poliakoff, M. Acoustic Probing of Phase Equilibria in Near-Critical Fluids. *Fluid Phase Equilib.* **1998**, *150−151*, 493−499.
(404) Baginskii, V. A.; Zakharov, N. D.; Lapardin, N. I. Study and Calculation of the Liquid-Vapor Phase Equilibrium of Mixtures of Refrigerants. *Sb. Issled. Teplofiz. Svoistva Rab. Veshchestv Protsessov. Teploobmen Kholod. Tekh.* **1989**, *9*, 9−15.
(405) 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.* **1985**, *22*, 10−18.
(406) Hou, S.-X.; Duan, Y.-Y. Isothermal Vapor−Liquid Equilibria for the Pentafluoroethane+propane and Pentafluoroethane +1,1,1,2,3,3,3-Heptafluoropropane Systems. *Fluid Phase Equilib.* **2010**, *290*, 121−126.
(407) Bobbo, S.; Fedele, L.; Camporese, R.; Stryjek, R. Hydrogen-Bonding of HFCs with Dimethyl Ether: Evaluation by Isothermal VLE Measurements. *Fluid Phase Equilib.* **2002**, *199*, 153−160.
(408) Lim, J. S.; Park, J. Y.; Lee, K.-S.; Kim, J.-D.; Lee, B. G. Measurement of Vapor−Liquid Equilibria for the Binary Mixture of Pentafluoroethane (HFC-125) + Propane (R-290). *J. Chem. Eng. Data* **2004**, *49*, 750−755.
(409) Kubic, W. L.; Stein, F. P. An Experimental and Correlative Study of the Vapor-Liquid Equilibria of the Tetrafluoromethane-Chlorotrifluoromethane System. *Fluid Phase Equilib.* **1981**, *5*, 289−304.
(410) Madani, H.; Valtz, A.; Coquelet, C.; Meniai, A. H.; Richon, D. 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 Equilib.* **2008**, *268*, 68−73.
(411) Madani, H.; Valtz, A.; Coquelet, C. Isothermal Vapor−Liquid Equilibrium Data for the Decafluorobutane (R3110)+1,1,1,3,3-Pentafluorobutane (R365mfc) System at Temperatures from 333K to 441K. *Fluid Phase Equilib.* **2013**, *354*, 109−113.
(412) Kriebel, M. Liquid-Vapor Phase Equilibriums of the Binary System Difluoromonochloromethane (R 22)-Difluorodichloromethane (R 12). *Kaeltetechnik* **1967**, *19*, 8−14.
(413) 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* **1985**, *19*, 58−67.
(414) Nishiumi, H.; Kohmatsu, S.; Yokoyama, T.; Konda, A. Phase Behavior of the Binary Refrigerant Mixtures HCF22 - CFC12 and HCF22 - HCFC123. *Fluid Phase Equilib.* **1995**, *104*, 131−143.
(415) Geller, Z. I.; Chaikovskii, V. F.; Egorov, A. V. Heats of Mixing of Freons. *Teplofiz. Svoistva Zhidk.* **1973**, 148−152.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(416) Geller, Z. I.; Chaikovskii, V. F.; Egorov, A. V. Heats of Mixing of Freons 112 and 115 with Freon 22. *Kholod. Tekh.* **1971**, *48*, 29−30.
(417) 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* **1984**, *29*, 31−36.
(418) Siddiqi, M. A.; Lucas, K. The Excess Enthalpy of (Tetrachloromethane + Carbon Disulphide) and (Tetrachloromethane + Dichloromethane) over a Range of Temperatures and Pressures. *J. Chem. Thermodyn.* **1983**, *15*, 1181−1187.
(419) 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. *J. Chem. Thermodyn.* **1975**, *7*, 131−136.
(420) Kudryavtseva, L. S.; Susarev, M. P. Liquid-Vapor Equilibrium in Systems Chloroform-Hexane and Acetone-Chloroform. *J. Appl. Chem. USSR* **1963**, *36*, 1231−1237.
(421) Brzostowski, W.; Verhoeye, L. Thermodynamic Properties of Mixtures of Hexane and Chloroform. *Rocz. Chem.* **1968**, *42*, 507−515.
(422) Ortega, J.; Placido, J. Excess Enthalpies of Trichloromethane + N-Alkanes. Measurement and Comparison with the DISQUAC Model. *ELDATA: Int. Electron. J. Phys.-Chem. Data* **1995**, *1*, 59−68.
(423) 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. *J. Chem. Thermodyn.* **1971**, *3*, 393−399.
(424) Sharma, B. R.; Pundeer, G. S.; Singh, P. P. Thermodynamics of Weak Interactions: Excess Enthalpies and Excess Gibbs Free Energies of Mixing. *Thermochim. Acta* **1975**, *11*, 105−114.
(425) 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* **1995**, *1*, 217−237.
(426) 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.* **1973**, *70*, 1355−1359.
(427) Shatas, J. P.; Abbott, M. M.; Van Ness, H. C. Excess Thermodynamic Functions for Ternary Systems. II. Chloroform-Ethanol-n-Heptane at 50°C. *J. Chem. Eng. Data* **1975**, *20*, 406−409.
(428) Zurita, J. L.; De Soria, M. L. G.; Postigo, M. A.; Katz, M. Vapor-Liquid Equilibrium for the n-Pentane-Dichloromethane System at 298.15 K. *J. Chem. Eng. Data* **1986**, *31*, 389−390.
(429) Tenn, F. G.; Missen, R. W. A Study of the Condensation of Binary Vapors of Miscible Liquids: Part I: The Equilibrium Relations. *Can. J. Chem. Eng.* **1963**, *41*, 12−14.
(430) Postigo, M. A.; Zurita, J. L.; Soria, M. L. G. D.; Katz, M. Excess Thermodynamic Properties of N-Pentane + Dichloromethane System at 298.15 K. *Can. J. Chem.* **1986**, *64*, 1966−1968.
(431) Tsang, C. Y.; Streett, W. B. Vapor-Liquid Equilibrium in the System Carbon Dioxide/Dimethyl Ether. *J. Chem. Eng. Data* **1981**, *26*, 155−159.
(432) Jonasson, A.; Persson, O.; Fredenslund, A. High Pressure Solubility of Carbon Dioxide and Carbon Monoxide in Dimethyl Ether. *J. Chem. Eng. Data* **1995**, *40*, 296−300.
(433) Laursen, T.; Rasmussen, P.; Andersen, S. I. VLE and VLLE Measurements of Dimethyl Ether Containing Systems. *J. Chem. Eng. Data* **2002**, *47*, 198−202.
(434) Ferrell, J. K.; Rousseau, R. W.; Bass, D. G. *The Solubility of Acid Gases in Methanol*, Interagency Energy/Environmental R&D Program Report; EPA, 1979; pp 1−40.
(435) Chapoy, A.; Coquelet, C.; Liu, H.; Valtz, A.; Tohidi, B. Vapour−Liquid Equilibrium Data for the Hydrogen Sulphide (H2S)+carbon Dioxide (CO2) System at Temperatures from 258 to 313K. *Fluid Phase Equilib.* **2013**, *356*, 223−228.
(436) Sobocinski, D. P.; Kurata, F. Heterogeneous Phase Equilibria of the Hydrogen Sulfide−Carbon Dioxide System. *AIChE J.* **1959**, *5*, 545−551.
(437) Bierlein, J. A.; Kay, W. B. Phase-Equilibrium Properties of System Carbon Dioxide-Hydrogen Sulfide. *Ind. Eng. Chem.* **1953**, *45*, 618−624.
(438) Wagner, Z.; Pavlíček, J. Vapour-Liquid Equilibrium in the Carbon Dioxide—Ethyl Acetate System at High Pressure. *Fluid Phase Equilib.* **1994**, *97*, 119−126.
(439) Chrisochoou, A.; Schaber, K.; Bolz, U. Phase Equilibria for Enzyme-Catalyzed Reactions in Supercritical Carbon Dioxide. *Fluid Phase Equilib.* **1995**, *108*, 1−14.
(440) Zahran, F.; Pando, C.; Renuncio, J. A. R.; Cabañas, A. Excess Molar Enthalpies for Mixtures of Supercritical CO2 and Ethyl Acetate and Their Role in Supercritical Fluid Applications. *J. Chem. Thermodyn.* **2012**, *51*, 59−64.
(441) Byun, H.-S.; Choi, M.-Y.; Lim, J.-S. High-Pressure Phase Behavior and Modeling of Binary Mixtures for Alkyl Acetate in Supercritical Carbon Dioxide. *J. Supercrit. Fluids* **2006**, *37*, 323−332.
(442) Juntarachat, N.; Privat, R.; Coniglio, L.; Jaubert, J.-N. Development of a Predictive Equation of State for CO2 + Ethyl Ester Mixtures Based on Critical Points Measurements. *J. Chem. Eng. Data* **2014**, *59*, 3205−3219.
(443) Reiff, W.-E.; Roth, H.; Lucas, K. Phase Equilibria in the Binary System Carbon Disulfide-Carbon Dioxide. *Fluid Phase Equilib.* **1992**, *73*, 323−338.
(444) 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 Equilib.* **2003**, *204*, 303−308.
(445) Lee, M. H.; Yim, J.-H.; Kang, J. W.; Lim, J. S. Measurement of VLE Data of Carbon Dioxide+dimethyl Carbonate System for the Direct Synthesis of Dimethyl Carbonate Using Supercritical CO2 and Methanol. *Fluid Phase Equilib.* **2012**, *318*, 77−82.
(446) Im, J.; Kim, M.; Lee, J.; Kim, H. Vapor−Liquid Equilibria of Binary Carbon Dioxide + Alkyl Carbonate Mixture Systems. *J. Chem. Eng. Data* **2004**, *49*, 243−245.
(447) 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* **2013**, *29*, 11−16.
(448) Matsuda, H.; Yoshii, S.; Nagashima, A.; Kurihara, K.; Ochi, K. 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. *J. Chem. Eng. Data* **2005**, *50*, 1419−1424.
(449) Sun, Y.; Li, Y.; Zhou, J.; Zhu, R.; Tian, Y. Experimental Determination and Calculation of the Critical Curves for the Binary Systems of CO2 Containing Ketone, Alkane, Ester and Alcohol, Respectively. *Fluid Phase Equilib.* **2011**, *307*, 72−77.
(450) Hou, Y.; Chen, X.; Ren, S.; Song, Z.; Wu, W. Phase Behavior, Densities, and Isothermal Compressibility of (Carbon Dioxide + Dimethyl Carbonate). *J. Chem. Eng. Data* **2010**, *55*, 1580−1587.
(451) Huamin, S. Solubility Of Carbon Monoxide In Methanol And Carbon Dioxide Under High Pressure. *Huaxue Gongcheng* **1991**, *19*, 61−69.
(452) Kaminishi, G.-I.; Arai, Y.; Saito, S.; Maeda, S. Vapor-Liquid Equilibria For Binary And Ternary Systems Containing Carbon Dioxide. *J. Chem. Eng. Jpn.* **1968**, *1*, 109−116.
(453) Christiansen, L. J.; Fredenslund, A.; Gardner, N. Gas-Liquid Equilibria of the CO_2−CO and CO_2−CH_4−CO Systems. In *Advances in Cryogenic Engineering*; Timmerhaus, K. D., Ed.; Springer: Boston, MA, 1995; pp 309−319.
(454) Fredenslund, A.; Sather, G. A. Gas-Liquid Equilibrium of the Oxygen-Carbon Dioxide System. *J. Chem. Eng. Data* **1970**, *15*, 17−22.
(455) Chueh, P. L.; Muirbrook, N. K.; Prausnitz, J. M. Multicomponent Vapor-Liquid Equilibria at High Pressures: Part II. Thermodynamic Analysis. *AIChE J.* **1965**, *11*, 1097−1102.
(456) 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 J.* **1965**, *11*, 1092−1096.
(457) Booth, H. S.; Carter, J. M. The Critical Constants of Carbon Dioxide-Oxygen Mixtures. *J. Phys. Chem. E.* **1930**, *34*, 2801−2825.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(458) Kim, C. N.; Park, Y. M. Vapor−Liquid Equilibrium of HFC-32/134a And HFC-125/134a Systems. *Int. J. Thermophys.* **1999**, *20*, 519−530.
(459) Kobayashi, M.; Nishiumi, H. Vapor−Liquid Equilibria for the Pure, Binary and Ternary Systems Containing HFC32, HFC125 and HFC134a. *Fluid Phase Equilib.* **1998**, *144*, 191−202.
(460) Nishiumi, H.; Ohno, T. High Pressure Vapor-Liquid Equilibria and Critical Loci for the HFC125-HFC134a System. *Korean J. Chem. Eng.* **2000**, *17*, 668−671.
(461) Kato, R.; Nishiumi, H. Vapor−Liquid Equilibria and Critical Loci of Binary and Ternary Systems Composed of CH2F2, C2HF5 and C2H2F4. *Fluid Phase Equilib.* **2006**, *249*, 140−146.
(462) Nagel, M.; Bier, K. Vapor-Liquid Equilibriums of New Refrigerant Mixtures as Alternatives to R 22 and R 502. *DKV-Tagungsberichte* **1993**, *20/2.1*, 39−59.
(463) Arita, K.; Tomizawa, T.; Nagakawa, Y.; Yoshida, Y. Vapour—Liquid Equilibrium of the Non-Azeotropic Refrigerant Mixture Formed by Chlorofluoromethane and 1,1,1,2-Tetrafluoroethane. *Fluid Phase Equilib.* **1991**, *63*, 151−156.
(464) Nishiumi, H.; Komatsu, M.; Yokoyama, T.; Kohmatsu, S. Two- and Three-Phase Equilibria and Critical Locus for the System of HCFC22-HFC134a. *Fluid Phase Equilib.* **1993**, *83*, 109−117.
(465) Chung, E.-Y.; Kim, M. S. Vapor−Liquid Equilibria for the Difluoromethane (HFC-32) + 1,1,1,2-Tetrafluoroethane (HFC-134a) System. *J. Chem. Eng. Data* **1997**, *42*, 1126−1128.
(466) Cui, X.; Chen, G.; Li, C.; Han, X. Vapor−Liquid Equilibrium of Difluoromethane +1,1,1,2-Tetrafluoroethane Systems over a Temperature Range from 258.15 to 343.15K. *Fluid Phase Equilib.* **2006**, *249*, 97−103.
(467) 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.* **2002**, *23*, 801−808.
(468) 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. *Int. J. Thermophys.* **1996**, *17*, 873−888.
(469) Kordikowski, A.; Robertson, D. G.; Poliakoff, M.; DiNoia, T. D.; McHugh, M.; Aguiar-Ricardo, A. Acoustic Determination of the Critical Surfaces in the Ternary Systems CO2 + CH2F2 + CF3CH2F and CO + C2H4 + CH3CHCH2 and in Their Binary Subsystems. *J. Phys. Chem. B* **1997**, *101*, 5853−5862.
(470) 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* **1995**, *21*, 613−618.
(471) 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)}. *J. Chem. Thermodyn.* **1993**, *25*, 1419−1441.
(472) Engelmann, K.; Bittrich, H. J. Estimation of Isothermal Mixing Functions from Isobaric Liquid-Vapor Equilibriums. *Wiss. Z. Tech. Hochsch. Chem. "Carl Schorlemmer" Leuna-Merseburg* **1969**, *11*, 213−218.
(473) 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. "Carl Schorlemmer" Leuna-Merseburg* **1966**, *8*, 289−291.
(474) 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. "Carl Schorlemmer" Leuna-Merseburg* **1966**, *8*, 148−153.
(475) Comelli, F.; Francesconi, R.; Ottani, S. Isothermal Vapor−Liquid Equilibria of Dimethyl Carbonate + Diethyl Carbonate in the Range (313.15 to 353.15) K. *J. Chem. Eng. Data* **1996**, *41*, 534−536.
(476) Luo, H.-P.; Xiao, W.-D.; Zhu, K.-H. Isobaric Vapor−Liquid Equilibria of Alkyl Carbonates with Alcohols. *Fluid Phase Equilib.* **2000**, *175*, 91−105.
(477) Francesconi, R.; Comelli, F. Excess Molar Enthalpies, Densities, and Excess Molar Volumes of Binary Mixtures Containing Esters of Carbonic Acid at 298.15 and 313.15 K. *J. Chem. Eng. Data* **1995**, *40*, 811−814.
(478) Francesconi, R.; Comelli, F. 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. *J. Chem. Eng. Data* **1996**, *41*, 736−740.
(479) 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.* **1966**, *17*, 297−309.
(480) Noles, J. R.; Zollweg, J. A. Isothermal Vapor-Liquid Equilibrium for Dimethyl Ether + Sulfur Dioxide. *Fluid Phase Equilib.* **1991**, *66*, 275−289.
(481) 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. *Bull. Acad. Pol. Sci., Ser. Sci. Chim.* **1970**, *18*, 555−560.
(482) Feng Yaosheng, Li. C.; Shou, Z. Vapor-Liquid Equilibrium for Trifluoromethane and Chlorodifluoromethane. *Huaxue Gongcheng* **1984**, *12*, 41−47.
(483) 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 Equilib.* **1992**, *73*, 147−166.
(484) 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**, *7*, 162−173.
(485) Sameshima, J. On The System Acetone—Ethyl Ether. *J. Am. Chem. Soc.* **1918**, *40*, 1482−1503.
(486) Litvinov, N. D. Isothermal Equilibrium of Vapor and Liquid in Systems of Three Fully Miscible Liquids. *Zh. Fiz. Khim.* **1952**, *26*, 1405−1412.
(487) von Zawidzki, J.. Über Die Dampfdrücke Binärer Flüssigkeitsgemische. *Z. Phys. Chem.* **1900**, *35U*, 129−203.
(488) Loiseleur, H.; Merlin, J.-C.; Paris, R. A. Diagrammes d'ébullition-Rosée (Sous 740 Mm) Des Systèmes Acétone-Sulfure de Carbone, Acétone-Tétrachloréthylène et Cycopentanone-Sulfure de Carbone. *J. Chim. Phys.* **1964**, *61*, 1231−1233.
(489) Bittrich, H. J.; Rodrigues, L. F. T. G. Dampf-Flüssigkeit-Gleichgewichte Der Mischungen von Triethylamin Mit Tetrahydrofuran Und 1,4-Dioxan. *Z. Phys. Chem.* **1988**, *269O*, 879−887.
(490) Grolier, J.-P. E.; Roux-Desgranges, G.; Berkane, M.; Wilhelm, E. Heat Capacities and Densities of Mixtures of Very Polar Substances. 3. Mixtures Containing Either Trichloromethane or 1,4-Dioxane or Diisopropylether. *J. Solution Chem.* **1994**, *23*, 153−166.
(491) Ahlers, S. Systematische Messung Thermodynamischer Daten Für Das System Thiophen - Sulfolan Zur Erweiterung Der Gruppenbeitragsmethode Modified UNIFAC (Dortmund). Bachelorarbeit Thesis, Universität Oldenburg, 2009.
(492) 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. *Z. Phys. Chem.* **1979**, *260O*, 705−718.
(493) Conti, G.; Gianni, P.; Matteoli, E. Excess Enthalpies and Excess Heat Capacities of (N,N-Dimethylformamide + Tetrahydrofuran + Cyclohexane) at the Temperature 298.15 K. *J. Chem. Thermodyn.* **1994**, *26*, 1249−1257.
(494) Shealy, G. S.; Sandler, S. I. Vapor-Liquid Equilibrium for Four Mixtures Containing N,N-Dimethylformamide. *J. Chem. Eng. Data* **1985**, *30*, 455−459.
(495) 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. *J. Chem. Eng. Data* **2000**, *45*, 515−517.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(496) Reamer, H. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. n-Butane-Water System in the Two-Phase Region. *Ind. Eng. Chem.* **1952**, *44*, 609−615.
(497) Danneil, A.; Tödheide, K.; Franck, E. U. Verdampfungsgleichgewichte Und Kritische Kurven in Den Systemen Äthan/Wasser Und n-Butan/Wasser Bei Hohen Drücken. *Chem. Ing. Tech.* **1967**, *39*, 816−822.
(498) 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). *J. Chem. Thermodyn.* **1986**, *18*, 545−550.
(499) Tian, Y.; Zhao, X.; Chen, L.; Zhu, H.; Fu, H. High Pressure Phase Equilibria and Critical Phenomena of Water + Iso-Butane and Water + n-Butane Systems to 695 K and 306 MPa. *J. Supercrit. Fluids* **2004**, *30*, 145−153.
(500) 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. *Ind. Eng. Chem.* **1944**, *36*, 381−383.
(501) Bader, M. S. H.; Gasem, K. A. M. Determination of Infinite Dilution Activity Coefficients for Organic-Aqueous Systems Using a Dilute Vapor-Liquid Equilibrium Method. *Chem. Eng. Commun.* **1995**, *140*, 41−72.
(502) Tu, M.; Lai, G.; Fei, D. Phase Equilibrium for the System of Phosphoric Acid-Water-Benzene. *J. Chengdu Univ. Sci. Technol.* **1982**, *3*, 65−70.
(503) Thompson, W. H.; Snyder, J. R. Mutual Solubilities of Benzene and Water. Equilibria in the Two Phase Liquid - Liquid Region. *J. Chem. Eng. Data* **1964**, *9*, 516−520.
(504) 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). *J. Chem. Soc., Faraday Trans.* **1997**, *93*, 1921−1926.
(505) 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. *J. Chem. Thermodyn.* **1996**, *28*, 627−636.
(506) Jiménez-Gallegos, R.; Galicia-Luna, L. A.; Bouchot, C.; Camacho-Camacho, L. E.; Elizalde-Solis, O. Experimental Determination and Correlation of Phase Equilibria for the Ethane + 1-Propanol and Propane + 1-Propanol Systems. *J. Chem. Eng. Data* **2006**, *51*, 1629−1633.
(507) Suzuki, K.; Sue, H.; Itou, M.; Smith, R. L.; Inomata, H.; Arai, K.; Saito, S. 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. *J. Chem. Eng. Data* **1990**, *35*, 63−66.
(508) McFall, T. A.; Post, M. E.; Christensen, J. J.; Izatt, R. M. The Excess Enthalpies of Eight (Ethane + Alcohol) Mixtures at 298.15 K. *J. Chem. Thermodyn.* **1981**, *13*, 441−446.
(509) 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. *J. Chem. Thermodyn.* **1995**, *27*, 1033−1045.
(510) Kodama, D.; Tanaka, H.; Kato, M. High Pressure Phase Equilibrium for Ethane + 1-Propanol at 314.15 K. *J. Chem. Eng. Data* **2001**, *46*, 1280−1282.
(511) Lam, D. H.; Jangkamolkulchai, A.; Luks, K. D. Liquid-Liquid-Vapor Phase Equilibrium Behavior of Certain Binary Ethane + n-Alkanol Mixtures. *Fluid Phase Equilib.* **1990**, *59*, 263−277.
(512) Reamer, H. H.; Sage, B. H. Phase Behavior in the Nitrogen-Ammonia System. *J. Chem. Eng. Data* **1959**, *4*, 303−305.
(513) Lindroos, A. E.; Dodge, B. F. Phase-Equilibria at High Pressures; the System Nitrogen-Ammonia at Pressures above 1000 Atmospheres. *Chem. Eng. Prog., Symp. Ser.* **1952**, *48*, 10−17.
(514) Naumowicz-Węglińska, E.; Wóycicki, W. Excess Enthalpies of Gaseous Mixtures Containing Ammonia 2. (Ammonia + Nitrogen) and (Ammonia + Methane). *J. Chem. Thermodyn.* **1986**, *18*, 1047−1052.
(515) Folas, G. K.; Froyna, E. W.; Lovland, J.; Kontogeorgis, G. M.; Solbraa, E. Data and Prediction of Water Content of High Pressure Nitrogen, Methane and Natural Gas. *Fluid Phase Equilib.* **2007**, *252*, 162−174.
(516) Goodman, J. B.; Krase, N. W. Solubility of Nitrogen in Water at High Pressures and Temperatures. *Ind. Eng. Chem.* **1931**, *23*, 401−404.
(517) Rigby, M.; Prausnitz, J. M. Solubility of Water in Compressed Nitrogen, Argon, and Methane. *J. Phys. Chem. F.* **1968**, *72*, 330−334.
(518) Maslennikova, V. Y.; Vdovina, N. A.; Tsiklis, D. S. Solubility of Water in Compressed Nitrogen. *Russ. J. Phys. Chem. DD.* **1971**, *45*, 1354.
(519) Wiebe, R.; Gaddy, V. L.; Heinss, C. Solubility of Nitrogen in Water at 25°C from 25 to 1000 Atmospheres. *Ind. Eng. Chem.* **1932**, *24*, 927.
(520) Gillespie, P. C.; Wilson, G. M. *Vapor−Liquid Equilibrium Data on Water-Substitute Gas Components: N_2−H_2O, H_2−H_2O, CO−H_2O, H_2−CO−H_2O, and H_2S−H_2O*, GPA Research Report; Gas Processors Association, 1980; pp 1−34.
(521) Wiebe, R.; Gaddy, V. L.; Heins, C. The Solubility of Nitrogen in Water at 50, 75 and 100° from 25 to 1000 Atmospheres. *J. Am. Chem. Soc.* **1933**, *55*, 947−953.
(522) Maslennikova, V. Y. Solubility of Nitrogen in Water. *Tr. Gos. Nauchno-Issled. Proektn. Inst. Azotn. Prom-sti. Prod. Org. Sint.* **1971**, *12*, 82−87.
(523) Richards, P.; Wormald, C. J.; Yerlett, T. K. The Excess Enthalpy of (Water + Nitrogen) Vapour and (Water + n-Heptane) Vapour. *J. Chem. Thermodyn.* **1981**, *13*, 623−628.
(524) Wormald, C. J.; Colling, C. N. Excess Enthalpies for (Water + Nitrogen)(g) up to 698.2 K and 12.6 MPa. *J. Chem. Thermodyn.* **1983**, *15*, 725−737.
(525) Prokhorova, V. M.; Tsiklis, D. S. Vapor− Vapor Equilibrium in the System Nitrogen−Water. *Zh. Fiz. Khim.* **1970**, *44*, 2069−2070.
(526) Siedler, R.; Grote, L.; Kauert, E.; Werner, U.; Bittrich, H. J. Zur Thermodynamik Der Binären Systeme von Benzol Mit Diäthylamin Und Triäthylamin. *Z. Phys. Chem.* **1969**, *241O*, 203−216.
(527) Velasco, I.; Otin, S.; Gutierrez Losa, C. Excess Enthalpies of Some Aliphatic Amine (C3 - C8) + Benzene Mixtures. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1981**, 60−64.
(528) Dehmelt, C.; Finke, M.; Bittrich, H. J. Untersuchungen Zur Zwischenmolekularen Wechselwirkung in Systemen von Diäthylamin Mit Aromatischen Komponenten. *Z. Phys. Chem.* **1974**, *255O*, 251−260.
(529) Ruffine, L. Équilibres de Phases à Basse Température de Systèmes Complexes CO_2—Hydrocarbures Légers—Méthanol—Eau: Mesures et Modélisation. New Ph.D. Thesis, Université Claude Bernard, 2005.
(530) Ruffine, L.; Barreau, A.; Brunella, I.; Mougin, P.; Jose, J. New Apparatus for Low-Temperature Investigations: Measurements of the Multiphase Equilibrium of Mixtures Containing Methane, Ethane, Propane, Butane, Methanol, and Carbon Dioxide. *Ind. Eng. Chem. Res.* **2005**, *44*, 8387−8392.
(531) Ohgaki, K.; Sano, F.; Katayama, T. Isothermal Vapor-Liquid Equilibrium Data for Binary Systems Containing Ethane at High Pressures. *J. Chem. Eng. Data* **1976**, *21*, 55−58.
(532) Ishihara, K.; Tanaka, H.; Kato, M. Phase Equilibrium Properties of Ethane+methanol System at 298.15 K. *Fluid Phase Equilib.* **1998**, *144*, 131−136.
(533) Ma, Y. H.; Kohn, J. P. Multiphase and Volumetric Equilibria of the Ethane-Methanol System at Temperatures between -40° and 100°C. *J. Chem. Eng. Data* **1964**, *9*, 3−5.
(534) 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. *J. Chem. Thermodyn.* **1989**, *21*, 1085−1093.
(535) Lev, A.-D.; Robinson, D. B.; Chung, S. Y.-K.; Chen, C.-J. The Equilibrium Phase Properties of the Propane-Methanol and n-Butane-Methanol Binary Systems. *Can. J. Chem. Eng.* **1992**, *70*, 330−334.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(536) Galivel-Solastiouk, F.; Laugier, S.; Richon, D. Vapor-Liquid Equilibrium Data for the Propane-Methanol and Propane-Methanol-Carbon Dioxide System. *Fluid Phase Equilib.* **1986**, *28*, 73−85.
(537) Joung, S. N.; Shin, H. Y.; Kim, H. S.; Yoo, K.-P. High-Pressure Vapor−Liquid Equilibrium Data and Modeling of Propane + Methanol and Propane + Ethanol Systems. *J. Chem. Eng. Data* **2004**, *49*, 426−429.
(538) 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). *J. Chem. Thermodyn.* **1993**, *25*, 999−1004.
(539) 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. *J. Chem. Thermodyn.* **1991**, *23*, 551−559.
(540) 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.* **1972**, *15*, 1654−1658.
(541) Brown, I.; Smith, F. Liquid-Vapour Equilibria. IX. The Systems n-Propanol + Benzene and n-Butanol + Benzene at 45°C. *Aust. J. Chem.* **1959**, *12*, 407.
(542) Strubl, K.; Svoboda, V.; Holub, R.; Pick, J. Liquid-Vapour Equilibrium in the Benzene-n-Propanol System. *Collect. Czech. Chem. Commun.* **1975**, *40*, 1647−1656.
(543) Hiaki, T.; Tochigi, K.; Kojima, K. Measurement of Vapor-Liquid Equilibria and Determination of Azeotropic Point. *Fluid Phase Equilib.* **1986**, *26*, 83−102.
(544) Wang, S.; Zao, C. VLE Data for Benzene-n-Propanol-Lithium Chloride System. *Huaxue Gongcheng* **1991**, *19*, 72−76.
(545) Cen, P.; Zhu, Z. The Measurement of Mixing Heat and the Prediction of Vapor-Liquid Equilibrium Data for Hydrocarbon - Alcohol Systems. *Huagong Xuebao* **1984**, *35*, 51−65.
(546) 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. *Thermochim. Acta* **1988**, *123*, 285−291.
(547) 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.* **1968**, *16*, 549−552.
(548) Skaates, J. M.; Kay, W. B. The Phase Relations of Binary Systems That Form Azeotropes. *Chem. Eng. Sci.* **1964**, *19*, 431−444.
(549) Iguchi, A. Vapor-Liquid Equilibriums at 25°C for Binary Systems between Alcohols and Hydrocarbons. *Kagaku Sochi* **1978**, *20*, 66−68.
(550) Smith, V. C.; Robinson, R. L. Vapor-Liquid Equilibria at 25°C in the Binary Mixtures Formed by Hexane, Benzene, and Ethanol. *J. Chem. Eng. Data* **1970**, *15*, 391−395.
(551) Tamir, A.; Apelblat, A.; Wagner, M. A New Device for Measuring Isothermal Vapor - Liquid Equilibria. *Fluid Phase Equilib.* **1981**, *6*, 237−259.
(552) 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.* **1963**, *36*, 2397−2402.
(553) Udovenko, V. V.; Fatkulina, L. G. Vapor Pressure of Three-Component Systems. I. The System Ethyl Alcohol-1,2-Dichloroethane-Benzene. *Zh. Fiz. Khim.* **1952**, *26*, 719−730.
(554) Stokes, R. H.; Burfitt, C. Enthalpies of Dilution and Transfer of Ethanol in Non-Polar Solvents. *J. Chem. Thermodyn.* **1973**, *5*, 623−631.
(555) 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* **1986**, *2*, 141−145.
(556) Missopolinou, D.; Tsivintzelis, I.; Panayiotou, C. Excess Enthalpies of Binary Mixtures of 2-Ethoxyethanol with Four Hydrocarbons at 298.15, 308.15, and 318.15K. *Fluid Phase Equilib.* **2006**, *245*, 89−101.
(557) Perrakis, N. The Physical Properties of Liquid Double Mixtures in the Neighborhood of the Critical State of Miscibility. *J Chim Phys* **1925**, *22*, 280−305.
(558) Tanaka, R.; Toyama, S. 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. *J. Chem. Eng. Data* **1997**, *42*, 871−874.
(559) Neau, E.; Blanc, C.; Bares, D. Les Fonctions Thermodynamiques d'excès Du Binaire 2 Propanol-Isooctane. *J. Chim. Phys.* **1973**, *70*, 843−849.
(560) Pavlíček, J.; Wichterle, I. Isothermal (Vapour+liquid) Equilibria in the Binary and Ternary Systems Composed of 2-Propanol, 2,2,4-Trimethylpentane, and 2,4-Dimethyl-3-Pentanone. *J. Chem. Thermodyn.* **2012**, *45*, 83−89.
(561) 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* **1999**, *5*, 179−189.
(562) Lin, D.-Y.; Tu, C.-H. (Vapour+liquid) Equilibria for Binary and Ternary Mixtures of 2-Propanol, Tetrahydropyran, and 2,2,4-Trimethylpentane at P=101.3kPa. *J. Chem. Thermodyn.* **2012**, *47*, 260−266.
(563) Hiaki, T.; Takahashi, K.; Tsuji, T.; Hongo, M.; Kojima, K. Vapor-Liquid Equilibria of 1-Propanol or 2-Propanol with 2,2,4-Trimethylpentane at 101.3 KPa. *J. Chem. Eng. Data* **1994**, *39*, 602−604.
(564) Huang, T.-T.; Tu, C.-H. Vapor−Liquid Equilibria for Binary and Ternary Mixtures of 1,3-Dioxolane, 2-Propanol, and 2,2,4-Trimethylpentane at 101.3 KPa. *J. Chem. Eng. Data* **2010**, *55*, 513−518.
(565) Heintz, A. The Pressure Dependence of the Excess Enthalpy of Mixtures of Isopropanol with Heptane and Isooctane up to 553 Bar. *Ber. Bunsenges. Phys. Chem.* **1981**, *85*, 632−635.
(566) Zhang, L.; Han, J.; Wang, R.; Qiu, X.; Ji, J. 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. *J. Chem. Eng. Data* **2007**, *52*, 1401−1407.
(567) Belabbaci, A.; Villamañán, R. M.; Negadi, L.; Martín, M. C. Vapor−Liquid Equilibria of Binary Mixtures Containing 2-Butanol and Hydrocarbons at 313.15 K. *J. Chem. Eng. Data* **2012**, *57*, 982−987.
(568) 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. *J. Chem. Thermodyn.* **1993**, *25*, 1295−1299.
(569) 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. *Phys. Chem. Liq.* **2003**, *41*, 1−13.
(570) Feng, L.-C.; Chou, C.-H.; Tang, M.; Chen, Y.-P. Vapor−Liquid Equilibria of Binary Mixtures 2-Butanol + Butyl Acetate, Hexane + Butyl Acetate, and Cyclohexane + 2-Butanol at 101.3 KPa. *J. Chem. Eng. Data* **1998**, *43*, 658−661.
(571) French, H. T. Thermodynamic Functions for the Systems 1-Butanol, 2-Butanol, Andt-Butanol + Cyclohexane. *J. Solution Chem.* **1983**, *12*, 869−887.
(572) Veselý, F.; Dohnal, V.; Valentová, M.; Pick, J. Concentration and Temperature Dependence of Heats of Mixing of 1-Butanol, 2-Butanol, and 2-Methyl-2-Propanol with Cyclohexane. *Collect. Czech. Chem. Commun.* **1983**, *48*, 3482−3494.
(573) 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**, *66*, 747−755.
(574) Maciel, M. R. 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. *J. Chem. Thermodyn.* **1988**, *20*, 539−544.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(575) Oh, B. C.; Kim, Y.; Shin, H. Y.; Kim, H. Vapor−Liquid Equilibria for the System 1-Propanol+n-Hexane near the Critical Region. *Fluid Phase Equilib.* **2004**, *220*, 41−46.
(576) Gmehling, J.; Meents, B. Excess Enthalpy. 1-Propanol - Hexane System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1992**, 158.
(577) 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. *J. Therm. Anal. Calorim.* **2005**, *80*, 303−309.
(578) Brown, I.; Fock, W.; Smith, F. Heats of Mixing. V. Systems of n-Alcohols with n-Hexane. *Aust. J. Chem.* **1964**, *17*, 1106.
(579) Gil, L.; Blanco, S. T.; Rivas, C.; Laga, E.; Fernández, J.; Artal, M.; Velasco, I. 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. *J. Supercrit. Fluids* **2012**, *71*, 26−44.
(580) Berro, C.; Rogalski, M.; Péneloux, A. A New Ebulliometric Technique. Vapour-Liquid Equilibria in the Binary Systems Ethanol-n-Heptane and Ethanol-n-Nonane. *Fluid Phase Equilib.* **1982**, *8*, 55−73.
(581) Ratcliff, G. A.; Chao, K. C. Prediction of Thermodynamic Properties of Polar Mixtures by a Group Solution Model. *Can. J. Chem. Eng.* **1969**, *47*, 148−153.
(582) Diaz Pena, M.; Rodriguez Cheda, D. R. Liquid-Vapor Equilibrium. II. Ethanol-n-Heptane System at 40 and 60.Deg. *An. Quim.* **1970**, *66*, 737−745.
(583) Seo, J.; Lee, J.; Kim, H. Measurement and Correlation of Vapor−Liquid Equilibria for the 2-Propanol + n-Hexane System near the Critical Region. *J. Chem. Eng. Data* **2003**, *48*, 856−859.
(584) Van Ness, H. C.; Soczek, C. A.; Kochar, N. K. Thermodynamic Excess Properties for Ethanol-n-Heptane. *J. Chem. Eng. Data* **1967**, *12*, 346−351.
(585) Kao, C.-P. C.; Miller, R. N.; Sturgis, J. F. Double Azeotropy in Binary Mixtures 1,1,1,2,3,4,4,5,5,5-Decafluoropentane + Tetrahydrofuran. *J. Chem. Eng. Data* **2001**, *46*, 229−233.
(586) Lietzmann, A.; Loewen, B.; Schulz, S. 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. *J. Chem. Eng. Data* **1994**, *39*, 785−788.
(587) Grosse-Wortmann, H.; Jost, W.; Wagner, H. Gg. Kalorimetrische Messungen Am System Äthanol - Cyclohexan - n-Heptan. *Z. Phys. Chem.* **1966**, *49*, 74−93.
(588) van Ness, H. C.; Abbott, M. M. Excess Enthalpy. Ethanol (Ethyl Alcohol)-n-Hexane System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1976**, *1976*, 11.
(589) 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). *Ber. Bunsenges. Phys. Chem.* **1995**, *99*, 1123−1130.
(590) Tanaka, R.; Toyama, S.; Murakami, S. Heat Capacities of {xCnH2n+1OH + (1 − x)C7H16} for n = 1 to 6 at 298.15 K. *J. Chem. Thermodyn.* **1986**, *18*, 63−73.
(591) Iguchi, A. Excess Molal Specific Heat of Nonelectrolyte Solutions. *Kagaku Sochi* **1977**, *19*, 64−65.
(592) 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. *J. Chem. Thermodyn.* **1994**, *26*, 1323−1334.
(593) Fortier, J.-L.; Benson, G. C. Excess Heat Capacities of Binary Liquid Mixtures Determined with a Picker Flow Calorimeter. *J. Chem. Thermodyn.* **1976**, *8*, 411−423.
(594) Klesper, I. Messung Der Spezifischen Wärmen Binärer Flüssigkeitsgemische. *Z. Phys. Chem.* **1966**, *51*, 1−12.
(595) Soo, C.-B.; Théveneau, P.; Coquelet, C.; Ramjugernath, D.; Richon, D. Determination of Critical Properties of Pure and Multi-Component Mixtures Using a "Dynamic−Synthetic" Apparatus. *J. Supercrit. Fluids* **2010**, *55*, 545−553.
(596) Wang, L.; Han, K.; Xia, S.; Ma, P.; Yan, F. Measurement and Correlation of Critical Properties for Binary Mixtures and Ternary Mixtures Containing Gasoline Additives. *J. Chem. Thermodyn.* **2014**, *74*, 161−168.
(597) Scheller, M.; Schuberth, H.; Könnecke, H. G. Ergebnisse von Dampf-Flüssigkeits-Phasengleichgewichtsuntersuchungen Am System n-Hexan/Methylcyclohexan/Methanol Bei 60 °C. *J. Prakt. Chem.* **1969**, *311*, 974−982.
(598) Blanco, A. M.; Ortega, J. Experimental Study of Miscibility, Density and Isobaric Vapor-Liquid Equilibrium Values for Mixtures of Methanol in Hydrocarbons (C5, C6). *Fluid Phase Equilib.* **1996**, *122*, 207−222.
(599) Kurihara, K.; Iguchi, T.; Banaka, T.; Ochi, K.; Kojima, K. Measurement and Correlation of Excess Molar Enthalpies for the Partially Miscible Systems 2-Butanone+water and Methanol+hexane. *Fluid Phase Equilib.* **2001**, *180*, 59−69.
(600) Andreoli-Ball, L.; Patterson, D.; Costas, M.; Cáceres-Alonso, M. Heat Capacity and Corresponding States in Alkan-1-Ol−n-Alkane Systems. *J. Chem. Soc., Faraday Trans. 1* **1988**, *84*, 3991.
(601) Costas, M.; Patterson, D. Self-Association of Alcohols in Inert Solvents. Apparent Heat Capacities and Volumes of Linear Alcohols in Hydrocarbons. *J. Chem. Soc., Faraday Trans. 1* **1985**, *81*, 635.
(602) Gao, L.; Hou, Z.; Zhang, H.; He, J.; Liu, Z.; Zhang, X.; Han, B. Critical Parameters of Hexane + Carbon Monoxide + Hydrogen and Hexane + Methanol + Carbon Monoxide + Hydrogen Mixtures in the Hexane-Rich Region. *J. Chem. Eng. Data* **2001**, *46*, 1635−1637.
(603) de Loos, T. W.; Poot, W.; de Swaan Arons, J. Vapour-Liquid Equilibria and Critical Phenomena in Methanol + n-Alkane Systems. *Fluid Phase Equilib.* **1988**, *42*, 209−227.
(604) Liu, J.; Qin, Z.; Wang, G.; Hou, X.; Wang, J. Critical Properties of Binary and Ternary Mixtures of Hexane + Methanol, Hexane + Carbon Dioxide, Methanol + Carbon Dioxide, and Hexane + Carbon Dioxide + Methanol. *J. Chem. Eng. Data* **2003**, *48*, 1610−1613.
(605) Zawisza, A. 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}. *J. Chem. Thermodyn.* **1985**, *17*, 941−947.
(606) Toghiani, H.; Toghiani, R. K.; Viswanath, D. S. Vapor-Liquid Equilibria for the Methanol-Benzene and Methanol-Thiophene Systems. *J. Chem. Eng. Data* **1994**, *39*, 63−67.
(607) Strubl, K.; Svoboda, V.; Holub, R. Liquid-Vapour Equilibrium. LV. The System Methanol-Benzene. *Collect. Czech. Chem. Commun.* **1972**, *37*, 3522−3531.
(608) Scatchard, G.; Wood, S. E.; Mochel, J. M. Vapor-Liquid Equilibrium. VI. Benzene-Methanol Mixtures. *J. Am. Chem. Soc.* **1946**, *68*, 1957−1960.
(609) Butcher, K. L.; Medani, M. S. Thermodynamic Properties of Methanol-Benzene Mixtures at Elevated Temperatures. *J. Appl. Chem.* **2007**, *18*, 100−107.
(610) Battler, J. R.; Rowley, R. L. Excess Enthalpies between 293 and 323 K for Constituent Binaries of Ternary Mixtures Exhibiting Partial Miscibility. *J. Chem. Thermodyn.* **1985**, *17*, 719−732.
(611) Veselý, F.; Hynek, V.; Svoboda, V.; Holub, R. Isothermal Calorimeter for Measuring Endothermic Heats of Mixing. *Collect. Czech. Chem. Commun.* **1974**, *39*, 355−365.
(612) Williamson, A. G.; Scott, R. L. Heats of Mixing of Non-Electrolyte Solutions. I. Ethanol + Benzene and Methanol + Benzene. *J. Phys. Chem. G.* **1960**, *64*, 440−442.
(613) Hudson, J. W.; Van Winkle, M. Multicomponent Vapor-Liquid Equilibriums in Systems of Mixed Positive and Negative Deviations. *J. Chem. Eng. Data* **1969**, *14*, 310−318.
(614) Triday, J.; Andrade, A.; Aguirre Ode, F. Isobaric Study of the Binary Systems Formed by Thiophene or Benzene with Light Alcohols. *Scientia* **1978**, *43*, 1−24.
(615) Strubl, K.; Voňka, P.; Svoboda, V.; Holub, R. Liquid-Vapour Equilibrium LVI. Correlation of the Benzene-Methanol Systems. *Collect. Czech. Chem. Commun.* **1973**, *38*, 468−476.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(616) Krichevskii, I. R.; Khazanova, N. E.; Linshits, L. R. The Liquid-Vapor Equilibrium in the Benzene-Methanol System at High Pressures. *Zh. Fiz. Khim.* **1957**, *31*, 2711−2716.
(617) Lee, J. M.; Lee, B.-C.; Cho, C.-H. Measurement of Bubble Point Pressures and Critical Points of Carbon Dioxide and Chlorodifluoromethane Mixtures Using the Variable-Volume View Cell Apparatus. *Korean J. Chem. Eng.* **2000**, *17*, 510−515.
(618) 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. *J. Chem. Eng. Data* **2002**, *47*, 59−61.
(619) 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 Equilib.* **2002**, *199*, 213−222.
(620) Lim, J. S.; Jin, J. M.; Yoo, K.-P. VLE Measurement for Binary Systems of CO2+1,1,1,2-Tetrafluoroethane (HFC-134a) at High Pressures. *J. Supercrit. Fluids* **2008**, *44*, 279−283.
(621) Uchida, Y.; Yasumoto, M.; Yamada, Y.; Ochi, K.; Furuya, T.; Otake, K. 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). *J. Chem. Eng. Data* **2004**, *49*, 1615−1621.
(622) 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 Equilib.* **2003**, *207*, 53−67.
(623) Kim, S. A.; Lim, J. S.; Kang, J. W. Isothermal Vapor−Liquid Equilibria for the Binary System of Carbon Dioxide (CO2) + 1,1,1,2,3,3,3-Heptafluoropropane (R-227ea). *J. Chem. Eng. Data* **2010**, *55*, 4999−5003.
(624) Chevalier, J. L. Systèmes Binaires Chloroforme-Éthers Aliphatiques - III. — Équilibres Liquide-Vapeur. *J. Chim. Phys. Phys.-Chim. Biol.* **1969**, *66*, 1457−1466.
(625) Becker, F.; Kiefer, M. Heat of Mixing and Formation of Compounds in Binary Liquid Systems. III. Ether-Chloroform Systems. *Z. Naturforsch., A: Astrophys., Phys. Phys. Chem.* **1971**, *26*, 1040−1046.
(626) Im, J.; Lee, G.; Lee, J.; Kim, H. Vapor−Liquid Equilibria of the 1,1,1-Trifluoroethane (HFC-143a)+dimethyl Ether (DME) System. *Fluid Phase Equilib.* **2007**, *251*, 59−62.
(627) Chevalier, J.-L.; Bares, D. Systèmes Binaires Chloroforme-Éthers Aliphatiques - I. — Chaleurs de Mélange à 25 °C. *J. Chim. Phys.* **1969**, *66*, 1448−1452.
(628) Stein, F. P.; Adams, R. A. Vapor-Liquid Equilibriums for Carbon Dioxide-Difluoromethane System. *J. Chem. Eng. Data* **1971**, *16*, 146−149.
(629) 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 Equilib.* **2004**, *218*, 95−101.
(630) Diefenbacher, A.; Türk, M. (Vapour+liquid) Equilibria of Binary Mixtures of CO2, CH2F2, CHF3, and SF6. *J. Chem. Thermodyn.* **2002**, *34*, 1361−1375.
(631) 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* **2005**, *50*, 128−132.
(632) Coquelet, C.; Valtz, A.; Richon, D. 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 Equilib.* **2005**, *232*, 44−49.
(633) Im, J.; Lee, G.; Kim, H. Vapor−Liquid Equilibria of the Difluoromethane + Dimethyl Ether and 1,1,1,2-Tetrafluoroethane + Dimethyl Ether Systems. *J. Chem. Eng. Data* **2006**, *51*, 1126−1129.
(634) 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. *Int. J. Thermophys.* **2004**, *25*, 1695−1711.
(635) Rao, M. R.; Rao, K. V. K.; Rao, C. V. Vapour-Liquid Equilibria of Ethyl Acetate-Trichloroethylene System. *J. Appl. Chem.* **1957**, *7*, 666−671.
(636) 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 Equilib.* **2004**, *220*, 77−83.
(637) Noles, J. R.; Zollweg, J. A. Vapor-Liquid Equilibrium for Chlorodifluoromethane + Dimethyl Ether from 283 to 395 K at Pressures to 5.0 MPa. *J. Chem. Eng. Data* **1992**, *37*, 306−310.
(638) Im, J.; Lee, G.; Lee, J.; Kim, H. (Vapour+liquid) Equilibria of the {pentafluoroethane (HFC-125)+dimethyl Ether (DME)} System. *J. Chem. Thermodyn.* **2006**, *38*, 1510−1514.
(639) Teodorescu, M.; Aim, K.; Wichterle, I. 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 Equilib.* **1998**, *147*, 215−228.
(640) Bobbo, S.; Fedele, L.; Camporese, R.; Stryjek, R. 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 Equilib.* **2000**, *174*, 3−12.
(641) Bobbo, S.; Camporese, R.; Stryjek, R. (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. *J. Chem. Thermodyn.* **1998**, *30*, 1041−1046.
(642) 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* **1968**, *41*, 2764−2766.
(643) 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 Equilib.* **1985**, *20*, 297−304.
(644) Röck, H.; Schröder, W. Dampf-Flüssigkeits-Gleichgewichtsmessungen Im System Azeton-Chloroform. *Z. Phys. Chem.* **1957**, *11*, 41−55.
(645) 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**, *48*, 1109−1113.
(646) Beckmann, E.; Faust, O. Die Dampfspannung Der Aceton-Chloroformgemische in Abhängigkeit von Der Temperatur. *Z. Phys. Chem.* **1914**, *89U*, 235.
(647) Segura, H.; Mejía, A.; Reich, R.; Wisniak, J.; Loras, S. Isobaric Vapor-Liquid Equilibria and Densities for the Binary Systems Oxolane + Ethyl 1,1-Dimethylethyl Ether, Oxolane + 2-Propanol and Propan-2-One + Trichloromethane. *Phys. Chem. Liq.* **2003**, *41*, 283−301.
(648) 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**, *10*, 34−38.
(649) Kulanek, M.; Bittrich, H. J. Heat of Solution of the System Acetone-Chloroform. *Wiss. Z. Tech. Hochsch. Chem. "Carl Schorlemmer" Leuna-Merseburg* **1962**, *4*, 139−141.
(650) Morris, J. W.; Mulvey, P. J.; Abbott, M. M.; Van Ness, H. C. Excess Thermodynamic Functions for Ternary Systems. I. Acetone-Chloroform-Methanol at 50.Deg. *J. Chem. Eng. Data* **1975**, *20*, 403−405.
(651) Jaubert, J.-N.; Privat, R.; Juntarachat, N. General Reflection on Critical Negative Azeotropy and Upgrade of the Bancroft's Rule with Application to the Acetone+chloroform Binary System. *J. Supercrit. Fluids* **2014**, *94*, 17−29.
(652) Ohta, T.; Asano, H.; Nagata, I. Thermodynamic Study of Complex Formation in Four Binary Liquid Mixtures Containing Chloroform. *Fluid Phase Equilib.* **1980**, *4*, 105−114.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(653) Nagata, I. Isobaric Vapor-Liquid Equilibria for the Ternary System Chloroform-Methanol-Ethyl Acetate. *J. Chem. Eng. Data* **1962**, *7*, 367−373.
(654) Ortega, J. Excess Enthalpy. Trichloromethane-Ethyl Methanoate System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1993**, *21*, 40.
(655) Fang, W.; Yu, Q.; Lin, R.; Zong, H. Vapor Heat Capacities of Some Polar−Polar Binary Systems. *Thermochim. Acta* **2000**, *352*−*353*, 19−23.
(656) Haase, R.; Tillmann, W. Negative Values of the Entropy of Mixing. *Z. Phys. Chem.* **1992**, *175*, 209−216.
(657) Suri, S. K.; Maheshwari, R. C. Molar Excess Enthalpies of Arsenic Tribromide + Benzene, +cyclohexane, and +tetrachloromethane at 313.15 K. *J. Chem. Thermodyn.* **1980**, *12*, 1191−1192.
(658) van Ness, H. C.; Abbott, M. M. Excess Enthalpy. Trichloromethane (Chloroform)-Oxolane (Tetrahydrofuran) System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1974**, *1974*, 67.
(659) Inglese, A.; Castagnolo, M.; Dell'atti, A.; de Giglio, A. Excess Heat Capacities and Excess Volumes of Binary Liquid Mixtures of Chloroform with Cyclic Ethers at 298.15 K. *Thermochim. Acta* **1981**, *44*, 77−87.
(660) Beath, L. A.; Williamson, A. G. Thermodynamics of Ether Solutions I. Enthalpies of Mixing of Ethers with Carbon Tetrachloride and with Chloroform. *J. Chem. Thermodyn.* **1969**, *1*, 51−57.
(661) Becker, F.; Kiefer, M. Kontinuierliche Bestimmung von Mischungswärmen Durch Isotherme Enthalpietitration. *Z. Naturforschung A* **1969**, *24*, 7−17.
(662) Nagata, I.; Hayashida, H. Vapor-Liquid Equilibrium Data For The Ternary Systems: Methyl Acetate-2-Propanol-Benzene And Methyl Acetate-Chloroform-Benzene. *J. Chem. Eng. Jpn.* **1970**, *3*, 161−166.
(663) 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* **1996**, *2*, 85−96.
(664) Teodorescu, M.; Barhala, A.; Dragoescu, D. 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. *J. Chem. Thermodyn.* **2006**, *38*, 1432−1437.
(665) Pathak, G.; Tripathi, A. D.; Phalgune, U. D.; Pradhan, S. D. Enthalpies of Mixing of Tetrachloroethane with Furan, Methylfuran, Tetrahydrofuran, Cyclopentanone and 1,4-Dioxane. *Thermochim. Acta* **1995**, *258*, 109−115.
(666) Chadha, R.; Tripathi, A. 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. *J. Chem. Eng. Data* **1995**, *40*, 645−646.
(667) Farkova, J.; Wichterle, I. Vapor-Liquid Equilibria of 1, 1, 2, 2-Tetrachloroethane + Some n-Alkyl n-Alkanoates. *ELDATA: Int. Electron. J. Phys.-Chem. Data* **1995**, *1*, 13−22.
(668) Ortega, J. Excess Enthalpy. 1,1,2,2-Tetrachloroethane - Ethyl Ethanoate System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1991**, *4*, 249.
(669) Chao, J.-P.; Zhang, F.-Q.; Dai, M. Studies of Thermodynamic Properties of Binary Mixtures Containing an Alcohol XVIII. Excess Molar Enthalpies of Each of (One of the Four Butanols + Trichloromethane or 1,2-Dichloroethane). *J. Chem. Thermodyn.* **1992**, *24*, 823−827.
(670) Nagata, I.; Kawamura, Y.; Asano, H.; Fujiwara, K.; Ogasawara, Y. Excess Enthalpies for Binary Mixtures of Chloroform with Alcohols. *Z. Phys. Chem.* **1978**, *259*, 1109−1116.
(671) Aucejo, A.; Gonzalez-Alfaro, V.; Monton, J. B.; Vazquez, M. I. Isobaric Vapor-Liquid Equilibria of Trichloroethylene with 1-Propanol and 2-Propanol at 20 and 100 KPa. *J. Chem. Eng. Data* **1995**, *40*, 332−335.
(672) Iloukhani, H. Excess Molar Enthalpies for Binary Mixtures with Trichloroethylene + Alkan-1-Ols (C3−C8) at 298.15 K. *J. Chem. Eng. Data* **1997**, *42*, 802−804.
(673) Dejoz, A.; González-Alfaro, V.; Miguel, P. J.; Vázquez, M. I. Isobaric Vapor−Liquid Equilibria of Trichloroethylene with 1-Butanol and 2-Butanol at 20 and 100 KPa. *J. Chem. Eng. Data* **1996**, *41*, 89−92.
(674) Iloukhani, H.; Parsa, J. B. Excess Molar Enthalpies of Binary Mixtures of Trichloroethylene with Six 2-Alkanols at 25°C. *J. Solution Chem.* **2001**, *30*, 425−433.
(675) Harris, H. G. Vapor-Liquid Equilibria in Binary Hydrocarbon - Polar Solvent Systems. Ph.D. Thesis, University of California, Berkeley, 1968.
(676) Desplanches, H.; Chevalier, J.-L.; Llinas, R. Étude Thermodynamique de Solutions d'acétonitrile et d'hydrocarbures Acétyléniques. *J. Chim. Phys.* **1977**, *74*, 259−265.
(677) Nagata, I. Vapor-Liquid Equilibria for the Ternary System 2-Propanol-Chloroform-Benzene at 50 °C. *J. Chem. Eng. Data* **1985**, *30*, 80−82.
(678) Hanumantharao, G.; Subbarao, B. V. Isobaric Vapor-Liquid-Equilibria-Chloroform-Isopropanol, Tertiary Butanol-Toluene and Tertiary Butanol-trichloroethylene Systems. *Indian J. Technol.* **1974**, *12*, 292−295.
(679) Zudkevitch, D.; Lindrud, M.; Chu, Y.-Z. Vapor−Liquid Equilibria for Ethanol + Hept-1-Yne and Butyric Acid + Butyric Anhydride. *J. Chem. Eng. Data* **1999**, *44*, 393−397.
(680) Letcher, T. M.; Schoonbaert, F. E. Z.; Bean, B. The Molar Excess Enthalpies and Volumes of 1-Alkyne + Methanol and + Ethanol Mixtures at 298.15 K. *Fluid Phase Equilib.* **1990**, *61*, 111−119.
(681) Scatchard, G.; Raymond, C. L. Vapor—Liquid Equilibrium. II. Chloroform—Ethanol Mixtures at 35, 45 and 55°. *J. Am. Chem. Soc.* **1938**, *60*, 1278−1287.
(682) Roeck, H.; Schroeder, W. Beitrag Zur Kenntnis Des Konzentrationsverlaufs Thermodynamischer Mischungsfunktionen. *Z. Phys. Chem.* **1956**, *9*, 277−284.
(683) Bourrelly, V.; Chevalier, J.-L. Appareil Pour La Détermination Rapide Des Équilibres Isothermes Liquide-Vapeur. *J. Chim. Phys.* **1968**, *65*, 1561−1564.
(684) 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**, *47*, 1423−1427.
(685) Orchillés, A. V.; Miguel, P. J.; Vercher, E.; Martínez-Andreu, A. Isobaric Vapor−Liquid and Liquid−Liquid Equilibria for Chloroform + Ethanol + 1-Ethyl-3-Methylimidazolium Trifluoromethanesulfonate at 100 KPa. *J. Chem. Eng. Data* **2008**, *53*, 2642−2648.
(686) Roach, M.; Van Ness, H. C. Excess Thermodynamic Functions for Ternary Systems. 10. HE and SE for Ethanol/Chloroform/1,4-Dioxane at 50°C. *J. Chem. Eng. Data* **1984**, *29*, 181−183.
(687) 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. *Can. J. Chem.* **1963**, *41*, 407−429.
(688) Conti, J. J.; Othmer, D. F.; Gilmont, R. Composition of Vapors from Boiling Binary Solutions. Systems Containing Formic Acid, Acetic Acid, Water, and Chloroform. *J. Chem. Eng. Data* **1960**, *5*, 301−307.
(689) 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. *Can. J. Chem.* **1964**, *42*, 186−189.
(690) 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.* **1972**, *22*, 26−32.
(691) Ratkovics, F. Adiabatic Calorimeter for Determining Heats of Mixing. *Magy. Kem. Foly.* **1971**, *77*, 499−502.
(692) Gmehling, J.; Onken, U.; Schulte, H. W. Vapor-Liquid Equilibriums for the Binary Systems Diethyl Ether-Halothane (1,1,1-Trifluoro-2-Bromo-2-Chloroethane), Halothane-Methanol, and Diethyl Ether-Methanol. *J. Chem. Eng. Data* **1980**, *25*, 29−32.
(693) Fenclova, D.; Dohnal, V. Excess Gibbs Energy. Bromochloro-1,1,1-Trifluoroethane - Methanol System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1993**, *21*, 100.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(694) Costas, M. Excess Heat Capacity. Bromochloro-1,1,1-Trifluoroethane - Methanol System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1993**, *21*, 158.
(695) Jonasson, A.; Savoia, M.; Persson, O.; Fredenslund, A. Isothermal Vapor-Liquid Equilibrium Data for Ether + Glycol, Chloroalkene + Glycol, Epoxy Ether + Alkane, Epoxy Ether + Alkene, and Epoxy Ether + Chloroalkane Systems. *J. Chem. Eng. Data* **1994**, *39*, 134−139.
(696) Venkatesulu, D.; Rao, M. V. P.; Veeranna, D. Excess Enthalpies of 2-Alkoxyethanols with Trichloroethylene and Tetrachloroethylene at 298.15 K. *Thermochim. Acta* **1994**, *242*, 33−39.
(697) Lazarte, M.; Gómez Marigliano, A. C.; Sólimo, H. 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. *J. Solution Chem.* **2004**, *33*, 1549−1563.
(698) Nagata, I.; Kawamura, Y. Excess Thermodynamic Functions and Complex Formation in Binary Liquid Mixtures Containing Acetonitrile. *Fluid Phase Equilib.* **1979**, *3*, 1−11.
(699) Mato, F.; Sanchez, M. Liquid-Vapor Equilibriums of Binary Mixtures of Acetonitrile. *An. R. Soc. Esp. Fis. Quim., Ser. B* **1967**, *63*, 1−11.
(700) Handa, Y. P.; Jones, D. E. Molar Excess Enthalpies of Acetonitrile + Chloroform and of Acetonitrile + Chloroform-D1 at 298 K. *Can. J. Chem.* **1977**, *55*, 2977−2979.
(701) Nagata, I.; Tamura, K. Excess Enthalpies of Acetonitrile + Trichloromethane, + Ethyl Acetate, and + Methyl Acetate, and of (Acetonitrile + Trichloromethane) + Ethyl Acetate and + Methyl Acetate at 308.15 K. *J. Chem. Thermodyn.* **1983**, *15*, 721−724.
(702) Zegers, H. C.; Somsen, G. Volumes and Heat Capacities of Mixtures of Dimethylformamide with Several Dialkylacetamides. *Fluid Phase Equilib.* **1984**, *18*, 299−311.
(703) Nagata, I. Isothermal (Vapour + Liquid) Equilibria of Propan-1-Ol + Acetonitrile and + Trichloromethane and of (Propan-1-Ol + Acetonitrile + Trichloromethane). *J. Chem. Thermodyn.* **1985**, *17*, 1017−1022.
(704) Wang, S.u.; Cai, S. VLE Data for Chloroform - n-Propanol and Its System Containing Salt. *Huaxue Gongcheng* **1994**, *22*, 36−40.
(705) Ortega, J. Excess Enthalpy. 1,1,2,2-Tetrachloroethane - Propyl Methanoate System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1991**, *4*, 248.
(706) Zel'venskii, Y. D. The Solubility of Carbon Dioxide in Water under Pressure. *Zh. Khim. Prom-sti.* **1937**, *14*, 1250−1257.
(707) Hou, S.-X.; Maitland, G. C.; Trusler, J. P. M. Measurement and Modeling of the Phase Behavior of the (Carbon Dioxide+water) Mixture at Temperatures from 298.15K to 448.15K. *J. Supercrit. Fluids* **2013**, *73*, 87−96.
(708) 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; Gas Processors Association, 1982; pp 1−73.
(709) Liu, Y.; Hou, M.; Ning, H.; Yang, D.; Yang, G.; Han, B. Phase Equilibria of CO2 + N2 + H2O and N2 + CO2 + H2O + NaCl + KCl + CaCl2 Systems at Different Temperatures and Pressures. *J. Chem. Eng. Data* **2012**, *57*, 1928−1932.
(710) Ferrentino, G.; Barletta, D.; Balaban, M. O.; Ferrari, G.; Poletto, M. Measurement and Prediction of CO2 Solubility in Sodium Phosphate Monobasic Solutions for Food Treatment with High Pressure Carbon Dioxide. *J. Supercrit. Fluids* **2010**, *52*, 142−150.
(711) Liu, Y.; Hou, M.; Yang, G.; Han, B. Solubility of CO2 in Aqueous Solutions of NaCl, KCl, CaCl2 and Their Mixed Salts at Different Temperatures and Pressures. *J. Supercrit. Fluids* **2011**, *56*, 125−129.
(712) King, M. B.; Mubarak, A.; Kim, J. D.; Bott, T. R. The Mutual Solubilities of Water with Supercritical and Liquid Carbon Dioxides. *J. Supercrit. Fluids* **1992**, *5*, 296−302.
(713) Zaalishvili, S. D. Solubility of Carbon Dioxide from Its Mixtures with Hydrogen and Nitrogen in Water under Pressure. *Zh. Fiz. Khim.* **1940**, *14*, 413−417.
(714) 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 Equilib.* **1993**, *83*, 149−158.
(715) D'souza, R.; Patrick, J. R.; Teja, A. S. High Pressure Phase Equilibria in the Carbon Dioxide - n-Hexadecane and Carbon Dioxide - Water Systems. *Can. J. Chem. Eng.* **1988**, *66*, 319−323.
(716) 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 Equilib.* **1987**, *36*, 235−246.
(717) 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. *J. Supercrit. Fluids* **2000**, *17*, 97−110.
(718) Pfohl, O.; Avramova, P.; Brunner, G. Two- and Three-Phase Equilibria in Systems Containing Benzene Derivatives, Carbon Dioxide, and Water at 373.15 K and 10-30 MPa. *Fluid Phase Equilib.* **1997**, *141*, 179−206.
(719) Takenouchi, S.; Kennedy, G. C. The Binary System H2O-CO2 at High Temperatures and Pressures. *Am. J. Sci.* **1964**, *262*, 1055−1074.
(720) Zawisza, A.; Malesinska, B. 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. *J. Chem. Eng. Data* **1981**, *26*, 388−391.
(721) Tödheide, K.; Franck, E. U. Das Zweiphasengebiet Und Die Kritische Kurve Im System Kohlendioxid−Wasser Bis Zu Drucken von 3500 Bar. *Z. Phys. Chem.* **1963**, *37*, 387−401.
(722) Pérez, E.; Sánchez-Vicente, Y.; Cabañas, A.; Pando, C.; Renuncio, J. A. R. Excess Molar Enthalpies for Mixtures of Supercritical Carbon Dioxide and Water+ethanol Solutions. *J. Supercrit. Fluids* **2005**, *36*, 23−30.
(723) Chen, X.; Gillespie, S. E.; Oscarson, J. L.; Izatt, R. M. Calorimetric Determination of Thermodynamic Quantities for Chemical Reactions in the System CO2-NaOH-H2O from 225 to 325°C. *J. Solut. Chem.* **1992**, *21*, 825−848.
(724) 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. *J. Chem. Thermodyn.* **1986**, *18*, 135−147.
(725) 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. *J. Chem. Eng. Data* **2010**, *55*, 476−478.
(726) Secuianu, C.; Feroiu, V.; Geană, D. Phase Behavior for Carbon Dioxide+ethanol System: Experimental Measurements and Modeling with a Cubic Equation of State. *J. Supercrit. Fluids* **2008**, *47*, 109−116.
(727) Day, C.-Y.; Chang, C. J.; Chen, C.-Y. Phase Equilibrium of Ethanol + CO2 and Acetone + CO2 at Elevated Pressures. *J. Chem. Eng. Data* **1996**, *41*, 839−843.
(728) 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* **1989**, *3*, 9−15.
(729) Tanaka, H.; Kato, M. Vapor-Liquid Equilibrium Properties of Carbon Dioxide + Ethanol Mixture at High Pressures. *J. Chem. Eng. Jpn.* **1995**, *28*, 263−266.
(730) Tochigi, K.; Namae, T.; Suga, T.; Matsuda, H.; Kurihara, K.; dos Ramos, M. C.; McCabe, C. Measurement and Prediction of High-Pressure Vapor−Liquid Equilibria for Binary Mixtures of Carbon Dioxide+n-Octane, Methanol, Ethanol, and Perfluorohexane. *J. Supercrit. Fluids* **2010**, *55*, 682−689.
(731) Joung, S. N.; Yoo, C. W.; Shin, H. Y.; Kim, S. Y.; Yoo, K.-P.; Lee, C. S.; Huh, W. S. Measurements and Correlation of High-Pressure VLE of Binary CO2−Alcohol Systems (Methanol, Ethanol, 2-Methoxyethanol and 2-Ethoxyethanol). *Fluid Phase Equilib.* **2001**, *185*, 219−230.
(732) Brandt, L. Einsatz Überkritischer Fluide Für Die Trenntechnik. Thesis, Carl von Ossietzky Universität Oldenburg, 2011.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(733) Galicia-Luna, L. 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. *J. Chem. Eng. Data* **2000**, *45*, 265−271.
(734) Tian, Y.-L.; Han, M.; Chen, L.; Feng, J.-J.; Qin, Y. Study on Vapor-Liquid Phase Equilibria for CO2-C2H5OH System. *Wuli Huaxue Xuebao* **2001**, *17*, 155−160.
(735) 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* **1999**, *5*, 157−164.
(736) Hauser, R. A.; Zhao, J. P.; Tremaine, P. R.; Mather, A. 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. *J. Chem. Thermodyn.* **1996**, *28*, 1303−1317.
(737) 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. *J. Chem. Thermodyn.* **1988**, *20*, 655−663.
(738) Sun, M.; Ye, R.; Liu, T.; Liu, H. Measurements of the Critical Temperature and Pressure of Ethylene+ Benzene+ Ethylbenzene Mixture. *Chin. J. Chem. Eng.* **2002**, *10*, 469−472.
(739) Yeo, S.-D.; Park, S.-J.; Kim, J.-W.; Kim, J.-C. Critical Properties of Carbon Dioxide + Methanol, + Ethanol, + 1-Propanol, and + 1-Butanol. *J. Chem. Eng. Data* **2000**, *45*, 932−935.
(740) Mejía, A.; Segura, H.; Cartes, M. Vapor−Liquid Equilibria and Interfacial Tensions of the System Ethanol + 2-Methoxy-2-Methylpropane. *J. Chem. Eng. Data* **2010**, *55*, 428−434.
(741) Arce, A.; Martínez-Ageitos, J.; Soto, A. VLE Measurements of Binary Mixtures of Methanol, Ethanol, 2-Methoxy-2-Methylpropane, and 2-Methoxy-2-Methylbutane at 101.32 KPa. *J. Chem. Eng. Data* **1996**, *41*, 718−723.
(742) Letcher, T. M.; Govender, P. U. Excess Molar Enthalpies of an Alkanol + a Branched Chain Ether at the Temperature 298.15 K. *J. Chem. Eng. Data* **1995**, *40*, 997−1000.
(743) 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.* **2002**, *70*, 251−254.
(744) Mato, M. M.; Illobre, M.; Verdes, P. V.; Legido, J. L.; Andrade, M. I. P. 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 Equilib.* **2010**, *296*, 37−41.
(745) 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**, *24*, 87−92.
(746) da Silva, M. V.; Barbosa, D. 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 Equilib.* **2002**, *198*, 229−237.
(747) Gutiérrez, J. E.; Bejarano, A.; de la Fuente, J. C. Measurement and Modeling of High-Pressure (Vapour+liquid) Equilibria of (CO2+alcohol) Binary Systems. *J. Chem. Thermodyn.* **2010**, *42*, 591−596.
(748) Chen, H.-I.; Chen, P.-H.; Chang, H.-Y. High-Pressure Vapor-Liquid Equilibria for CO2 + 2-Butanol, CO2 + Isobutanol, and CO2 + Tert-Butanol Systems. *J. Chem. Eng. Data* **2003**, *48*, 1407−1412.
(749) 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. EE.* **1978**, *52*, 1149−1152.
(750) Ochi, K.; Dai, W.; Wada, Y.; Hayashi, H.; Kurihara, K.; Kojima, K. Measurement and Correlation of Excess Molar Enthalpies for the Systems Containing Supercritical Carbon Dioxide and Alcohols. *Fluid Phase Equilib.* **2002**, *194−197*, 919−928.
(751) 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). *J. Chem. Thermodyn.* **1987**, *19*, 273−291.
(752) Li, N.; Ma, P.; Xia, S. Determination of Solubility of Carbon Monoxide in Methanol-Dimethyl Carbonate under High Pressure. *Shiyou Huagong* **2005**, *34*, 60−64.
(753) 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**, *9*, 317−328.
(754) Secuianu, C.; Feroiu, V.; Geană, D. Measurements and Modeling of High-Pressure Phase Behavior of the Carbon Dioxide + Pentan-1-Ol Binary System. *J. Chem. Eng. Data* **2011**, *56*, 5000−5007.
(755) Secuianu, C.; Feroiu, V.; Geană, D. High-Pressure Vapour-Liquid Equilibria of Carbon Dioxide + I-Pentanol System. Experimental Measurements and Modelling. *Rev. Chim.-Buchar.* **2007**, *58*, 1176−1181.
(756) Staby, A.; Mollerup, J. Measurement of Mutual Solubilities of 1-Pentanol and Supercritical Carbon Dioxide. *J. Supercrit. Fluids* **1993**, *6*, 15−19.
(757) Silva-Oliver, G.; Galicia-Luna, L. A.; Sandler, S. I. Vapor−Liquid Equilibria and Critical Points for the Carbon Dioxide +1-Pentanol and Carbon Dioxide +2-Pentanol Systems at Temperatures from 332 to 432 K. *Fluid Phase Equilib.* **2002**, *200*, 161−172.
(758) Bittrich, H. J.; Kauer, E. Thermodynamics of the System Diethylamine-Triethylamine. I. The Liquid-Vapor Equilibrium. *Z. Phys. Chem.* **1962**, *219*, 224−238.
(759) Bittrich, H. J.; Kulanek, M.; Duering, G. Thermodynamics of the System Diethylamine-Triethylamine. Enthalpies of Mixing at 14, 18, and 25°. *Z. Phys. Chem.* **1962**, *219*, 387−395.
(760) Ratkovics, F.; Liszi, J.; Laszlo-Parragi, M.; Szeiler, B.; Devay, J. Mixing Properties of the Ethanol-Diethylamine-Triethylamine System. *Acta Chim. Acad. Sci. Hung.* **1973**, *77*, 249−265.
(761) Kauer, E.; Grote, L.; Bittrich, H.-J. Zur Thermodynamik Des Systems Diäthylamin-Triäthylamin. IV. *Z. Für Phys. Chem.* **1966**, *232O*, 356.
(762) Fuangfoo, S.; Kersting, M.; Viswanath, D. 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. *J. Chem. Eng. Data* **1999**, *44*, 405−410.
(763) Bernatová, S.; Wichterle, I. 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 Equilib.* **2001**, *180*, 235−245.
(764) Loras, S.; Aucejo, A.; Muñoz, R. Isobaric Vapor−Liquid Equilibrium in the Systems Methyl 1,1-Dimethylethyl Ether + 2-Methyl-2-Propanol and Methyl 1,1-Dimethylethyl Ether + 2-Methylpentane + 2-Methyl-2-Propanol. *J. Chem. Eng. Data* **1999**, *44*, 1169−1174.
(765) Hiaki, T.; Tatsuhana, K.; Tsuji, T.; Hongo, M. 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 Equilib.* **1999**, *156*, 161−171.
(766) Davolio, F.; Pedrosa, G. C.; Katz, M. Vapor-Liquid Equilibrium for the p-Dioxane-Acetonitrile System at 298.15 K. *J. Chem. Eng. Data* **1981**, *26*, 26−27.
(767) Francesconi, R.; Comelli, F. Excess Thermodynamic Properties for the Binary System 1,4-Dioxane-Acetonitrile at 40.Degree.C. *J. Chem. Eng. Data* **1988**, *33*, 80−83.
(768) Grolier, J.-P. E.; Roux-Desgranges, G.; Berkane, M.; Wilhelm, E. Heat Capacities and Densities of Mixtures of Very Polar Substances 1. Mixtures Containing Acetonitrile. *J. Chem. Thermodyn.* **1991**, *23*, 421−429.
(769) Song, H. J.; Zhang, H. T.; Ying, W. Y. Study on Vapor-Liquid Equilibrium for Dimethyl Ether/Methanol Binary System. *Tianranqi Huagong* **2005**, *30*, 67−71.
(770) Pozo, M. E.; Streett, W. B. Fluid Phase Equilibria for the System Dimethyl Ether/Water from 50 to 220.Degree.C and Pressures to 50.9 MPa. *J. Chem. Eng. Data* **1984**, *29*, 324−329.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(771) Holldorff, H.; Knapp, H. Binary Vapor-Liquid-Liquid Equilibrium of Dimethyl Ether - Water and Mutual Solubilities of Methyl Chloride and Water: Experimental Results and Data Reduction. *Fluid Phase Equilib.* **1988**, *44*, 195−209.
(772) Park, S.-J.; Han, K.-J.; Gmehling, J. Isothermal Phase Equilibria and Excess Molar Enthalpies for Binary Systems with Dimethyl Ether at 323.15 K. *J. Chem. Eng. Data* **2007**, *52*, 1814−1818.
(773) Hong, J. H.; Kobayashi, R. Vapor—Liquid Equilibrium Studies for the Carbon Dioxide—Methanol System. *Fluid Phase Equilib.* **1988**, *41*, 269−276.
(774) Ohgaki, K.; Katayama, T. 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. *J. Chem. Eng. Data* **1976**, *21*, 53−55.
(775) Katayama, T.; Ohgaki, K.; Maekawa, G.; Goto, M.; Nagano, T. Isothermal Vapor-Liquid Equilibria Of Acetone-Carbon Dioxide And Methanol-Carbon Dioxide Systems At High Pressures. *J. Chem. Eng. Jpn.* **1975**, *8*, 89−92.
(776) Chang, C. J.; Day, C.-Y.; Ko, C.-M.; Chiu, K.-L. Densities and P-x-y Diagrams for Carbon Dioxide Dissolution in Methanol, Ethanol, and Acetone Mixtures. *Fluid Phase Equilib.* **1997**, *131*, 243−258.
(777) Kodama, D.; Kubota, N.; Yamaki, Y.; Tanaka, H.; Kato, M. High Pressure Vapor-Liquid Equilibria and Density Behaviors for Carbon Dioxide+Methanol System at 313.15 K. *Netsu Bussei* **1996**, *10*, 16−20.
(778) Semenova, A. I.; Emel'yanova, E. A.; Tsimmerman, S. S.; Tsiklis, D. S. Phase Equilibriums in the Methanol-Carbon Dioxide System. *Zh. Fiz. Khim.* **1979**, *53*, 2502−2505.
(779) Leu, A.-D.; Chung, S. Y.-K.; Robinson, D. B. The Equilibrium Phase Properties of (Carbon Dioxide + Methanol). *J. Chem. Thermodyn.* **1991**, *23*, 979−985.
(780) Zhu, H.-G.; Tian, Y.-L.; Chen, L.; Feng, J.-J.; Fu, H.-F. Studies on Vapor-Liquid Phase Equilibria for SCF CO2+ CH3OH and SCF CO2+ C2H5OH Systems. *Gaodeng Xuexiao Huaxue Xuebao* **2002**, *23*, 1588−1591.
(781) 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* **1999**, *44*, 161−164.
(782) Dai, W.; Ochi, K.; Kurihara, K.; Kojima, K.; Hongo, M. Measurement and Correlation of Excess Enthalpy for the System-(CO2+CH3OH) Containing Supercritical Carbon Dioxide. *Netsu Bussei* **1998**, *12*, 64−69.
(783) 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. *J. Chem. Thermodyn.* **1988**, *20*, 867−875.
(784) Staroske, J.; Figurski, G. Vapor-Liquid Equilibrium of the Ternary System Furfural - Ethyl Acetate - Methanol and Its Binary Subsystems at 298.15 K. *Chem. Tech. Leipz.* **1992**, *44*, 64−66.
(785) Murti, P.; Van Winkle, M. Vapor-Liquid Equilibria for Binary Systems of Methanol, Ethyl Alcohol, 1-Propanol, and 2-Propanol with Ethyl Acetate and 1-Propanol-Water. *Ind. Eng. Chem. Chem. Eng. Data Ser.* **1958**, *3*, 72−81.
(786) Nagata, I.; Yamada, T.; Nakagawa, S. Excess Gibbs Free Energies and Heats of Mixing for Binary Systems Ethyl Acetate with Methanol, Ethanol, 1-Propanol, and 2-Propanol. *J. Chem. Eng. Data* **1975**, *20*, 271−275.
(787) Susial, P.; Sosa-Rosario, A.; Rios-Santana, R. Vapor−Liquid Equilibria for Ethyl Acetate + Methanol at (0.1, 0.5, and 0.7) MPa. Measurements with a New Ebulliometer. *J. Chem. Eng. Data* **2010**, *55*, 5701−5706.
(788) Blanco, A. M.; Ortega, J. 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. *J. Chem. Eng. Data* **1998**, *43*, 638−645.
(789) Ortega, J. Excess Enthalpy. Ethanol-Ethyl Ethanoate System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1995**, *23*, 161.
(790) Zhang, R.; Yan, W.; Wang, X.; Lin, R. Molar Excess Enthalpies of Ethyl Acetate+alkanols at T=298.15K, P=10.0MPa. *Thermochim. Acta* **2005**, *429*, 155−161.
(791) 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. *Chem. Eng. Commun.* **1988**, *74*, 179−193.
(792) Lladosa, E.; Montón, J. B.; Burguet, M.; Muñoz, R. 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 Equilib.* **2007**, *262*, 271−279.
(793) Zhang, Z.; Yang, L.; Xing, Y.; Li, W. Vapor−Liquid Equilibrium for Ternary and Binary Mixtures of 2-Isopropoxypropane, 2-Propanol, and N,N-Dimethylacetamide at 101.3 KPa. *J. Chem. Eng. Data* **2013**, *58*, 357−363.
(794) Sieg, L.; Cruetzen, J. L.; Jost, W. Zur Thermodynamik von Mischphasen VIII. Über Das Verdampfungsgleichgewicht Methanol-n-Butylazetat. *Z. Elektrochem. Angew. Phys. Chem.* **1951**, *55*, 199−201.
(795) Park, W. K. Vapor-Liquid Equilibriums of Ester-Alcohol Systems. III. *Hwahak Konghak* **1971**, *9*, 181−190.
(796) Espiau, F.; Ortega, J.; Penco, E.; Wisniak, J. Advances in the Correlation of Thermodynamic Properties of Binary Systems Applied to Methanol Mixtures with Butyl Esters. *Ind. Eng. Chem. Res.* **2010**, *49*, 9548−9558.
(797) 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.* **1935**, *38*, 8B−12B.
(798) Gordon, A. R.; Hornibrook, E. J. Liquid-Vapor Equilibrium for the System Ethanol - Diethyl - Ether. *Can. J. Res.* **1946**, *24b*, 263−267.
(799) 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. *J. Chem. Thermodyn.* **1982**, *14*, 251−258.
(800) Kortüm, G.; Valent, V. Thermodynamische Mischungseffekte Der Systeme Wasser(1)-1,4-Dioxan(2) Und Methanol(1)-1,4-Dioxan(2); Ein Vergleich. *Ber. Bunsenges. Phys. Chem.* **1977**, *81*, 752−761.
(801) 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* **1995**, *1*, 139−166.
(802) Tamura, K.; Bhuiyan, M. M. H. Excess Molar Enthalpies of (Methanol+1-Propanol)+oxane or 1,4-Dioxane Mixtures at the Temperature 298.15 K. *J. Chem. Thermodyn.* **2003**, *35*, 1657−1669.
(803) 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.* **1991**, *61*, 2405−2410.
(804) Calvo, E.; Brocos, P.; Piñeiro, Á.; Pintos, M.; Amigo, A.; Bravo, R.; Roux, A. H.; Roux-Desgranges, G. Heat Capacities, Excess Enthalpies, and Volumes of Mixtures Containing Cyclic Ethers. 4. Binary Systems 1,4-Dioxane + 1-Alkanols. *J. Chem. Eng. Data* **1999**, *44*, 948−954.
(805) Singh, P. P.; Verma, D. V.; Arora, P. S. Thermodynamics of Binary Methanol Solutions. *Thermochim. Acta* **1976**, *15*, 267−280.
(806) Gmehling, J. VLE Data for the Design of Separation Processes. *AIChE Symp. Ser.* **1985**, *81*, 121−129.
(807) Kim, M.-G.; Park, S.-J.; Hwang, I.-C. 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 J. Chem. Eng.* **2008**, *25*, 1160−1164.
(808) Tanaka, R.; Toyama, S. 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. *J. Chem. Eng. Data* **1996**, *41*, 1455−1458.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(809) Reddy, P.; Benecke, T. P.; Ramjugernath, D. Isothermal (Vapour+liquid) Equilibria for Binary Mixtures of Diisopropyl Ether with (Methanol, or Ethanol, or 1-Butanol): Experimental Data, Correlations, and Predictions. *J. Chem. Thermodyn.* **2013**, *58*, 330−339.
(810) Fárková, J.; Linek, J.; Wichterle, I. Isothermal Vapour-Liquid Equilibria and Excess Volumes in the Methanol-Aliphatic Ether Systems. *Fluid Phase Equilib.* **1995**, *109*, 53−65.
(811) Piñeiro, Á. Excess Volumes and Isobaric Heat Capacities of Diisopropyl Ether with Several Alkanols at 298.15K. *Fluid Phase Equilib.* **2004**, *216*, 245−256.
(812) Toghiani, R. K.; Toghiani, H.; Venkateswarlu, G. Vapor-Liquid Equilibria for Methyl Tert-Butyl Ether + Methanol and Tert-Amyl Methyl Ether + Methanol. *Fluid Phase Equilib.* **1996**, *122*, 157−168.
(813) Loras, S.; Aucejo, A.; Muñoz, R.; Wisniak, J. Azeotropic Behavior in the System Methanol + Methyl 1,1-Dimethylethyl Ether. *J. Chem. Eng. Data* **1999**, *44*, 203−208.
(814) Wang, Y.; Tong, A.; Su, Y.; Yang, Z. Isobaric Vapor-Liquid Equilibrium for the System MTBE-Methanol. *Shiyou Huagong* **1989**, *18*, 442−446.
(815) Westerholt, A. Weiterentwicklung Der Gruppenbeitragszustandsgleichung VTPR Zur Beschreibung Der TAME-Synthese Und Spaltung Durch Systematische Messung Fehlender Phasengleichgewichtsdaten Und Anpassung Der Erforderlichen Parameter. Masters Thesis, Carl von Ossietzky Universität Oldenburg, 2010.
(816) Gmehling, J.; Park, S. J.; Fischer, K.; Meents, B. Excess Enthalpies of Tert-Butyl Methyl Ether, Methanol, or Ethanol+ Butane Or+ 2-Methylpropene. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1992**, *20*, 146−152.
(817) Mertl, I. Liquid-Vapour Equilibrium. IL. Phase Equilibria in the Ternary System Ethyl Acetate-Ethanol-Water. *Collect. Czech. Chem. Commun.* **1972**, *37*, 366−374.
(818) Pavlíček, J.; Bogdanić, G.; Wichterle, I. Vapour−Liquid and Chemical Equilibria in the Ethyl Ethanoate+ethanol+propyl Ethanoate+propanol System Accompanied with Transesterification Reaction. *Fluid Phase Equilib.* **2012**, *328*, 61−68.
(819) Li, Q.; Zhang, J.; Lei, Z.; Zhu, J.; Xing, F. Isobaric Vapor-Liquid Equilibrium for Ethyl Acetate + Ethanol + 1-Ethyl-3-Methylimidazolium Tetrafluoroborate. *J. Chem. Eng. Data* **2009**, *54*, 193−197.
(820) 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. *Chin. J. Chem. Eng.* **2012**, *20*, 723−730.
(821) Susial, P.; Sosa-Rosario, A.; Rodríguez-Henríquez, J. J.; Rios-Santana, R. Vapor Pressure and VLE Data Measurements on Ethyl Acetate/Ethanol Binary System at 0.1, 0.5, and 0.7 MPa. *J. Chem. Eng. Jpn.* **2011**, *44*, 155−163.
(822) Hu, J.; Tamura, K.; Murakami, S. 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 Equilib.* **1997**, *134*, 239−253.
(823) Wen-jun, F.; Qing-sen, Y.; Rui-sen, L.; Han-xing, Z. Vapor Heat Capacity of Binary and Ternary Systems. *Thermochim. Acta* **1997**, *299*, 43−47.
(824) Hu, T.; Qin, Z.; Wang, G.; Hou, X.; Wang, J. Critical Properties of the Reacting Mixture in the Esterification of Acetic Acid with Ethanol. *J. Chem. Eng. Data* **2004**, *49*, 1809−1814.
(825) Pierotti, G. J.; Deal, C. H.; Derr, E. L. Activity Coefficients and Molecular Structure. *Ind. Eng. Chem.* **1959**, *51*, 95−102.
(826) 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 Chem. Eng. Res.* **1974**, *12*, 179−187.
(827) Treiner, C.; Tzias, P. 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*; ACS Publications, 1976; Vol. *155*, pp 303−317.
(828) Lieberwirth, I.; Schuberth, H. Das Isotherme Dampf-Flüssigkeits-Phasengleichgewichtsverhalten Des Systems Aceton/Wasser Bei 35° C. *Z. Phys. Chem.* **1979**, *260O*, 669.
(829) Sokolova, E. P.; Morachevskii, A. G. Thermodynamic Properties of the Acetone-Water System. *Vestn. Leningr. Univ., Fiz. Khim.* **1967**, 110−115.
(830) Griswold, J.; Wong, S. Y. Phase-Equilibria in the Acetone-Methanol-Water System from 100° into the Critical Region. *Chem. Eng. Prog. Symp. Ser.* **1952**, *48*, 18−34.
(831) Verhoeye, L.; De Schepper, H. The Vapour-Liquid Equilibria of the Binary, Ternary and Quaternary Systems Formed by Acetone, Methanol, Propan-2-Ol, and Water. *J. Appl. Chem. Biotechnol.* **2007**, *23*, 607−619.
(832) Ochi, K.; Kojima, K. Vapor-Liquid Equilibriums for the System Acetone + Methanol + Water. *Chem. Eng.* **1971**, *35*, 583−586.
(833) Kojima, K.; Tochigi, K.; Seki, H.; Watase, K. Determination of Vapor-Liquid Equilibriums from Boiling Point Curves. *Chem. Eng.* **1968**, *32*, 149−153.
(834) Othmer, D. F.; Chudgar, M. M.; Levy, S. L. Binary and Ternary Systems of Acetone, Methyl Ethyl Ketone, and Water. *Ind. Eng. Chem.* **1952**, *44*, 1872−1881.
(835) French, H. T. Excess Enthalpies of (Acetone + Water) at 278.15, 288.15, 298.15, 308.15, 318.15, and 323.15 K. *J. Chem. Thermodyn.* **1989**, *21*, 801−809.
(836) Costas, M.; Patterson, D. Heat Capacities of Water + Organic-Solvent Mixtures. *J. Chem. Soc., Faraday Trans. 1* **1985**, *81*, 2381.
(837) Narasigadu, C.; Naidoo, P.; Coquelet, C.; Richon, D.; Ramjugernath, D. Isothermal Vapor−Liquid Equilibrium Data for the Butan-2-One + Methanol or Ethanol Systems Using a Static-Analytic Microcell. *J. Chem. Eng. Data* **2013**, *58*, 1280−1287.
(838) Martínez, N. F.; Lladosa, E.; Burguet, M.; Montón, J. 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 Equilib.* **2008**, *270*, 62−68.
(839) Wen, C.-C.; Tu, C.-H. Vapor−Liquid Equilibria for Binary and Ternary Mixtures of Ethanol, 2-Butanone, and 2,2,4-Trimethylpentane at 101.3kPa. *Fluid Phase Equilib.* **2007**, *258*, 131−139.
(840) Chao, J.-P.; Dai, M. Studies of Thermodynamic Properties of Binary Mixtures Containing an Alcohol. *Thermochim. Acta* **1991**, *179*, 257−264.
(841) Iñarrea, J.; Valero, J.; Pérez, P.; Gracia, M.; Gutiérrez Losa, C. HmE and VmE of Some (Butanone or Dipropylether + an Alkanol) Mixtures. *J. Chem. Thermodyn.* **1988**, *20*, 193−199.
(842) Nagata, I.; Ohta, T.; Nakagawa, S. Excess Gibbs Free Energies And Heats Of Mixing For Binary Alcoholic Liquid Mixtures. *J. Chem. Eng. Jpn.* **1976**, *9*, 276−281.
(843) Nagata, I.; Tago, O.; Takahashi, T. Heats of Mixing for Binary Methyl Ethyl Ketone, Methyl Acetate-Alcohol Systems. *Chem. Eng.* **1970**, *34*, 1107−1112,a1.
(844) Pikkarainen, L. Excess Enthalpies of Binary Solvent Mixtures of 2-Butanone with Aliphatic Alcohols. *Thermochim. Acta* **1987**, *114*, 239−244.
(845) Vinichenko, I. G.; Susarev, M. P. Study and Calculation of the Liquid-Vapor Equilibrium in the Acetone-Ethanol-Hexane System. *J. Appl. Chem. USSR* **1966**, *39*, 1475−1478.
(846) Lee, M.-J.; Hu, C.-H. Isothermal Vapor-Liquid Equilibria for Mixtures of Ethanol, Acetone, and Diisopropyl Ether. *Fluid Phase Equilib.* **1995**, *109*, 83−98.
(847) Campbell, S. W.; Wilsak, R. A.; Thodos, G. Vapor-Liquid Equilibrium Measurements for the Ethanol-Acetone System at 372.7, 397.7, and 422.6 K. *J. Chem. Eng. Data* **1987**, *32*, 357−362.
(848) Ku, H.-C.; Tu, C.-H. Isobaric Vapor−Liquid Equilibria for Mixtures of Acetone, Ethanol, and 2,2,4-Trimethylpentane at 101.3kPa. *Fluid Phase Equilib.* **2005**, *231*, 99−108.
(849) 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* **1990**, *4*, 1−7.
(850) Lien, P.-J.; Lin, H.; Lee, M.-J. Excess Molar Enthalpies for Binary Mixtures of Ethanol + Acetone, + Octane, + Cyclohexane and

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

1-Propanol + Acetone, + Octane, + Heptane at 323.15 K. *J. Chem. Eng. Data* **2003**, *48*, 359−361.
(851) Tamir, A.; Apelblat, A.; Wagner, M. An Evaluation of Thermodynamic Analyses of the Vapor—Liquid Equilibria in the Ternary System Acetone—Chloroform—Methanol and Its Binaries. *Fluid Phase Equilib.* **1981**, *6*, 113−139.
(852) Wilsak, R. A.; Campbell, S. W.; Thodos, G. Vapor—Liquid Equilibrium Measurements for the Methanol—Acetone System at 372.8, 397.7 and 422.6 K. *Fluid Phase Equilib.* **1986**, *28*, 13−37.
(853) Botía, D. C.; Riveros, D. C.; Ortiz, P.; Gil, I. D.; Sánchez, O. F. Vapor−Liquid Equilibrium in Extractive Distillation of the Acetone/Methanol System Using Water as Entrainer and Pressure Reduction. *Ind. Eng. Chem. Res.* **2010**, *49*, 6176−6183.
(854) Constantino, D. S. M.; Pereira, C. S. M.; Pinho, S. P.; Silva, V. M. T. M.; Rodrigues, A. E. Isobaric Vapor−Liquid Equilibrium Data for Binary System of Glycerol Ethyl Acetal and Acetonitrile at 60.0 KPa and 97.8 KPa. *J. Chem. Eng. Data* **2013**, *58*, 1717−1723.
(855) Li, W.; Sun, D.; Zhang, T.; Dai, S.; Pan, F.; Zhang, Z. Separation of Acetone and Methanol Azeotropic System Using Ionic Liquid as Entrainer. *Fluid Phase Equilib.* **2014**, *383*, 182−187.
(856) Campbell, A. N.; Kartzmark, E. M. Thermodynamic and Other Properties of Methanol + Acetone, Carbon Disulphide + Acetone, Carbon Disulphide + Methanol, and Carbon Disulphide + Methanol + Acetone. *J. Chem. Thermodyn.* **1973**, *5*, 163−172.
(857) Schmelzer, J.; Quitzsdi, K. Isobare Flüssigkeit-Dampfgleichgewichte Der Binären Systeme Benzol-Äthylendiamin Und Wasser-Äthylendiamin. *Z. Phys. Chem.* **1973**, *252O*, 280.
(858) Rivenq, F. Ebulliometry of Water-Ethylenediamine Mixtures. *Bull. Soc. Chim. Fr.* **1963**, *8−9*, 1606−1608.
(859) Ragaini, V.; Zanderighi, L.; Santi, R. The Liquid-Vapor Equilibrium of the Ethylenediamine-Water System. *Atti Soc. Peloritana Sci. Fis., Mat. Nat.* **1968**, *14*, 537−548.
(860) Bahlmann, M. Evaluation and Revision of the Modified UNIFAC (Dortmund) Approach for Alcohol Systems, M.S. Thesis, Universität Oldenburg, Germany, 2010.
(861) 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* **1984**, *10*, 181−183.
(862) Marongiu, B.; Ferino, I.; Monaci, R.; Solinas, V.; Torrazza, S. Thermodynamic Properties of Aqueous Non-Electrolyte Mixtures. Alkanols + Water Systems. *J. Mol. Liq.* **1984**, *28*, 229−247.
(863) Lee, M.-J.; Tsai, L.-H.; Hong, G.-B.; Lin, H. Multiphase Coexistence for Aqueous Systems with Amyl Alcohol and Amyl Acetate. *Ind. Eng. Chem. Res.* **2002**, *41*, 3247−3252.
(864) Polák, J.; Murakami, S.; 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. *Can. J. Chem.* **1970**, *48*, 2457−2465.
(865) Arce, A.; Martínez-Ageitos, J.; Rodil, E.; Soto, A. Phase Equilibria Involved in Extractive Distillation of 2-Methoxy-2-Methylpropane+methanol Using 1-Butanol as Entrainer. *Fluid Phase Equilib.* **2000**, *171*, 207−218.
(866) Kay, W. B.; Donham, W. E. Liquid-Vapour Equilibria in the Iso-Butanol—n-Butanol, Methanol—n-Butanol and Diethyl Ether—n-Butanol Systems. *Chem. Eng. Sci.* **1955**, *4*, 1−16.
(867) Stokes, R. H. Excess Enthalpies of (Butan-1-Ol + Methanol) at 278.15, 298.15, and 318.15 K. *J. Chem. Thermodyn.* **1988**, *20*, 1349−1352.
(868) Ogawa, H.; Murakami, S. Excess Volumes, Isentropic Compressions, and Isobaric Heat Capacities for Methanol Mixed with Other Alkanols at 25°C. *J. Solution Chem.* **1987**, *16*, 315−326.
(869) Wright, E. H. M.; Akhtar, B. A. Soluble Surface Films of Short-Chain Monocarboxylic Acids on Organic and Aqueous Substrates. *J. Chem. Soc. B* **1970**, 151.
(870) Miyamoto, S.; Nakamura, S.; Iwai, Y.; Arai, Y. Measurement of Isothermal Vapor−Liquid Equilibria for Binary and Ternary Systems Containing Monocarboxylic Acid. *J. Chem. Eng. Data* **2001**, *46*, 1225−1230.
(871) Reichl, A.; Daiminger, U.; Schmidt, A.; Davies, M.; Hoffmann, U.; Brinkmeier, C.; Reder, C.; Marquardt, W. A Non-Recycle Flow Still for the Experimental Determination of Vapor−Liquid Equilibria in Reactive Systems. *Fluid Phase Equilib.* **1998**, *153*, 113−134.
(872) Zhao, J.; Bao, J.; Hu, Y. Excess Molar Enthalpies of (an Alkanol + a Carboxylic Acid) at 298.15 K Measured with a Picker Calorimeter. *J. Chem. Thermodyn.* **1989**, *21*, 811−818.
(873) Kooner, Z.; Fenby, D. Vapour Pressure Study of the Deuterium Exchange Reaction in Methanol-Ethanol Systems: Equilibrium Constant Determination. *Aust. J. Chem.* **1980**, *33*, 1943.
(874) 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*; NTRL, 1979; pp 1−13.
(875) Oh, S.-K.; Campbell, S. W. Total Pressure Measurements for Copper(II) Chloride + Methanol + Ethanol at 303.15 K. *J. Chem. Eng. Data* **1995**, *40*, 504−508.
(876) Butcher, K. L.; Robinson, W. I. An Apparatus for Determining High-Pressure Liquid-Vapour Equilibrium Data. I. The Methanol-Ethanol System. *J. Appl. Chem.* **2007**, *16*, 289−292.
(877) Arce, A.; Martínez-Ageitos, J.; Rodil, E.; Soto, A. Measurement and Prediction of Isobaric Vapour−Liquid Equilibrium Data of the System Ethanol+methanol+2-Methoxy-2-Methylpropane. *Fluid Phase Equilib.* **1998**, *146*, 139−153.
(878) Pflug, H. D.; Pope, A. E.; Benson, G. C. Heats of Mixing of Normal Alcohols at 25.Deg. *J. Chem. Eng. Data* **1968**, *13*, 408−410.
(879) Trampe, D. M.; Eckert, C. A. Calorimetric Measurement of Partial Molar Excess Enthalpies at Infinite Dilution. *J. Chem. Eng. Data* **1991**, *36*, 112−118.
(880) Geiseler, G.; Sühnel, K.; Quitzsch, K. Exzeßeigenschaften Der Binären Mischsysteme Aus Den Isomeren Butanolen. *Z. Phys. Chem.* **1973**, *254O*, 261.
(881) 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. *J. Prakt. Chem.* **1969**, *311*, 429−437.
(882) Murakami, S.; Benson, G. C. Thermodynamic Properties of Some Isomeric Butyl Alcohol Mixtures. *Bull. Chem. Soc. Jpn.* **1973**, *46*, 74−79.
(883) Duran, J. A.; Córdoba, F. P.; Gil, I. D.; Rodríguez, G.; Orjuela, A. Vapor−Liquid Equilibrium of the Ethanol+3-Methyl-1-Butanol System at 50.66, 101.33 and 151.99kPa. *Fluid Phase Equilib.* **2013**, *338*, 128−134.
(884) Gay, L. Distillation and Rectification of Complex Mixtures. II. *Chim. Ind., Genie Chim.* **1927**, *18*, 187−203.
(885) Udovenko, V. V.; Frid, T. B. Heats of Vaporization of Binary Mixtures. II. *Zh. Fiz. Khim.* **1948**, *22*, 1135−1145.
(886) 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* **2005**, *16*, 749−754.
(887) Resa, J.; González, C.; Moradillo, B.; Ruiz, A. Isobaric Vapor-Liquid Equilibria of 3-Methyl-1-Butanol with Methanol and Vinyl Acetate at 101.3 KPa. *Fluid Phase Equilib.* **1997**, *132*, 205−213.
(888) Yamamoto, H.; Fukase, K.; Shibata, J. Vapor−Liquid Equilibria for Alcohol + Alcohol + Sodium Iodide at 298.15 K. *J. Chem. Eng. Data* **1996**, *41*, 1066−1070.
(889) Berro, C.; Deyrieux, R.; Peneloux, A. An Ebulliometer for Rapid and Precise Determination of the Vapor-Liquid Equilibrium of Solutions. The Binary System Methanol - 1-Propanol at 60.02 °C. *J. Chim. Phys. Phys. Chim. Biol.* **1975**, *72*, 1118−1123.
(890) Gultekin, N. Vapor-Liquid Equilibria at 1 Atm for Ternary and Quaternary Systems Composed of Acetone, Methanol, 2-Propanol, and 1-Propanol. *J. Chem. Eng. Data* **1990**, *35*, 132−136.
(891) Khurma, J. R.; Fenby, D. V. Thermochemical Study of Deuterium Exchange Reactions in Water-Alcohol and Alcohol-Alcohol Systems. *J. Phys. Chem. H.* **1979**, *83*, 2443−2447.
(892) Wilson, T. A. *The Total and Partial Vapor Pressures of Aqueous Ammonia Solutions*; Engineering Experiment Station, University of Illinois, 1925; Bulletin 146.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(893) 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.* **1987**, *83*, 97−127.
(894) Inomata, H.; Ikawa, N.; Arai, K.; Saito, S. Vapor-Liquid Equilibria for the Ammonia-Methanol-Water System. *J. Chem. Eng. Data* **1988**, *33*, 26−29.
(895) Clifford, I. I.; Hunter, E. The System Ammonia−Water at Temperatures up to 150°C. and at Pressures up to Twenty Atmospheres. *J. Phys. Chem. I.* **1933**, *37*, 101−118.
(896) Rizvi, S. S. H.; Heidemann, R. A. Vapor-Liquid Equilibria in the Ammonia-Water System. *J. Chem. Eng. Data* **1987**, *32*, 183−191.
(897) Chu, J. C.; Getty, R. J.; Brennecke, L. F.; Paul, R. *Distillation Equilibrium Data*; Reinhold: New York, 1950.
(898) 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**, *39*, 136−140.
(899) 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). *J. Chem. Thermodyn.* **2008**, *40*, 1527−1530.
(900) 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. *Int. J. Refrig.* **2009**, *32*, 1897−1913.
(901) 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. *J. Chem. Eng. Data* **1990**, *35*, 140−144.
(902) Tyvina, T. N.; Naumova, A. A.; Fokina, V. V. Liquid-Gas Equilibrium in an Acetonitrile-Ammonia System. *J. Appl. Chem. USSR* **1979**, *52*, 2458−2460.
(903) Ewert, M. Theory of Concentrated Solutions. XIII. Aqueous Solutions of Organic Compounds. *Bull. Soc. Chim. Belg.* **1936**, *45*, 493−515.
(904) 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: Int. Electron. J. Phys.-Chem. Data* **1996**, *2*, 1−4.
(905) Weller, R.; Schuberth, H.; Leibnitz, E. Phasengleichgewichtsmessungen. IV. Die Phasengleichgewichte Dampfförmig/Flüssig Des Systems Phenol/n-Butylacetat/Wasser Bei 44,4°C. *J. Prakt. Chem.* **1963**, *21*, 234−249.
(906) Kliment, V.; Fried, V.; Pick, J. Liquid-Vapor Equilibrium. XXXIII. The Systems Butyl Acetate-Phenol and Water-Phenol. *Collect. Czech. Chem. Commun.* **1964**, *29*, 2008−2015.
(907) 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.* **1987**, *18*, 393−399.
(908) von Erichsen, L.; Dobbert, E. The Mutual Solubility Behavior of Alkylphenols and Water. *Brennst.-Chem.* **1955**, *21*−*22*, 338−345.
(909) Schuermann, E.; Diederichs, R. Heats of Mixing of Phenol-Water Systems. *Ber. Bunsen-Ges. Phys. Chem.* **1964**, *68*, 429−434.
(910) Ferguson, J. B. The System Water-Phenol. *J. Phys. Chem. J.* **1926**, *31*, 757−763.
(911) Campbell, A. N.; Campbell, A. J. R. Concentrations, Total and Partial Vapor Pressures, Surface Tensions and Viscosities, in the Systems Phenol—Water and Phenol—Water—4% Succinic Acid. *J. Am. Chem. Soc.* **1937**, *59*, 2481−2488.
(912) Polak, J.; Lu, B. C.-Y. Excess Gibbs Free Energies and Excess Volumes of Methyl Formate + Methanol and Methyl Formate + Ethanol at 298.15 K. *J. Chem. Thermodyn.* **1972**, *4*, 469−476.
(913) Kozub, N.; Schuberth, H.; Leibnitz, E. Phasengleichgewichtsuntersuchungen Dampfförmig-Flüssig Am System Methanol/Methylformiat Unter Verwendung Einer Gaschromatographischen Analysenmethode. *J. Prakt. Chem.* **1962**, *17*, 282−292.
(914) Sundberg, A. T.; Uusi-Kyyny, P.; Pakkanen, M.; Alopaeus, V. Vapor−Liquid Equilibrium for Methoxymethane + Methyl Formate, Methoxymethane + Hexane, and Methyl Formate + Methanol. *J. Chem. Eng. Data* **2011**, *56*, 2634−2640.
(915) Zeng, J.; Fu, C.; Hu, W. L. Study on the VLE for Methyl Formate-Methanol System. *Tianranqi Huagong* **2000**, *25*, 54−56.
(916) López, M.; Fernández, J.; Sarmiento, F.; Legido, J. L.; Romani, L.; Jiménez, E.; Paz Andrade, M. I. Excess Molar Enthalpies at the Temperature 298.15 K of (an n-Alkyl Formate + an n-Alkanol) IV. {xHCO2(CH2)ICH3 + (1 − x)CjH2j+1OH} (i = 0 to 3 and j = 1 and 2). *J. Chem. Thermodyn.* **1992**, *24*, 809−814.
(917) Linek, J.; Wichterle, I.; Marsh, K. N. Vapor−Liquid Equilibria for Water + Diacetone Alcohol, Ethyl Methanoate + Water, and Ethyl Methanoate + Phenol. *J. Chem. Eng. Data* **1996**, *41*, 1219−1222.
(918) Wittig, R.; Lohmann, J.; Joh, R.; Horstmann, S.; Gmehling, J. Vapor−Liquid Equilibria and Enthalpies of Mixing in a Temperature Range from 298.15 to 413.15 K for the Further Development of Modified UNIFAC (Dortmund). *Ind. Eng. Chem. Res.* **2001**, *40*, 5831−5838.
(919) Nagata, I.; Ohta, T.; Ogura, M.; Yasuda, S. Excess Gibbs Free Energies and Heats of Mixing for Binary Systems: Ethyl Formate with Methanol, Ethanol, 1-Propanol, and 2-Propanol. *J. Chem. Eng. Data* **1976**, *21*, 310−313.
(920) Soto, A.; Hernández, P.; Ortega, J. 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 Equilib.* **1998**, *146*, 351−370.
(921) Hu, J.; Tamura, K.; Murakami, S. 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 Equilib.* **1997**, *131*, 197−212.
(922) Sazonov, V. P.; Filippov, V. V. Study of the Thermodynamic Properties of the Nitromethane-Butyl Alcohol System. *Vestn. Leningr. Univ., Ser. 4: Fiz., Khim.* **1977**, *2*, 151−153.
(923) Cerdeiriña, C. A.; Tovar, C. A.; González, D.; Carballo, E.; Romanı′, L. Thermodynamics of the Nitromethane + 1-Butanol System near the Upper Critical Point. *Fluid Phase Equilib.* **2001**, *179*, 101−115.
(924) Feng, H.; Wang, Y.; Shi, J.; Benson, G. C.; Lu, B. 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). *J. Chem. Thermodyn.* **1991**, *23*, 169−174.
(925) Rebelo, L. P. N.; Najdanovic-Visak, V.; Visak, Z. P.; Nunes da Ponte, M.; Troncoso, J.; Cerdeiriña, C. A.; Romaní, L. Two Ways of Looking at Prigogine and Defay's Equation. *Phys. Chem. Chem. Phys.* **2002**, *4*, 2251−2259.
(926) 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* **1999**, *38*, 65−69.
(927) Scatchard, G.; Wilson, G. M. Vapor-Liquid Equilibrium. XIII. The System Water-Butyl Glycol from 5 to 85°. *J. Am. Chem. Soc.* **1964**, *86*, 133−137.
(928) Chiavone-Filho, O.; Proust, P.; Rasmussen, P. Vapor-Liquid Equilibria for Glycol Ether + Water Systems. *J. Chem. Eng. Data* **1993**, *38*, 128−131.
(929) Escobedo-Alvarado, G. N.; Sandler, S. I. Vapor−Liquid Equilibrium of Two Aqueous Systems That Exhibit Liquid−Liquid Phase Separation. *J. Chem. Eng. Data* **1999**, *44*, 319−322.
(930) Aizpiri, A. G.; Monroy, F.; del Campo, C.; Rubio, R. G.; Díaz Peña, M. Range of Simple Scaling and Critical Amplitudes near a LCST. The 2-Butoxyethanol + Water System. *Chem. Phys.* **1992**, *165*, 31−39.
(931) Onken, U. Die Thermodynamischen Funktionen Des Systems Wasser/Butylglykol. *Z. Elektrochem.* **1959**, *63*, 321−327.
(932) Lim, K.-H.; Whiting, W. B.; Smith, D. H. Excess Enthalpies and Liquid-Liquid Equilibrium Phase Compositions of the Nonionic Amphiphile 2-Butoxyethanol and Water. *J. Chem. Eng. Data* **1994**, *39*, 399−403.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(933) Dobson, H. J. E. CCCXCVII.—The Partial Pressures of Aqueous Ethyl Alcohol. *J. Chem. Soc., Trans.* **1925**, *127*, 2866−2873.
(934) 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. *J. Chem. Thermodyn.* **1978**, *10*, 867−888.
(935) Vu, D. T.; Lira, C. T.; Asthana, N. S.; Kolah, A. K.; Miller, D. J. Vapor−Liquid Equilibria in the Systems Ethyl Lactate + Ethanol and Ethyl Lactate + Water. *J. Chem. Eng. Data* **2006**, *51*, 1220−1225.
(936) Kurihara, K.; Minoura, T.; Takeda, K.; Kojima, K. Isothermal Vapor-Liquid Equilibria for Methanol + Ethanol + Water, Methanol + Water, and Ethanol + Water. *J. Chem. Eng. Data* **1995**, *40*, 679−684.
(937) Niesen, V.; Palavra, A.; Kidnay, A. J.; Yesavage, V. F. An Apparatus for Vapor—Liquid Equilibrium at Elevated Temperatures and Pressures and Selected Results for the Water—Ethanol and Methanol—Ethanol Systems. *Fluid Phase Equilib.* **1986**, *31*, 283−298.
(938) Barr-David, F.; Dodge, B. F. Vapor-Liquid Equilibrium at High Pressures. The Systems Ethanol-Water and 2-Propanol-Water. *J. Chem. Eng. Data* **1959**, *4*, 107−121.
(939) Voutsas, E. C.; Pamouktsis, C.; Argyris, D.; Pappa, G. D. Measurements and Thermodynamic Modeling of the Ethanol−Water System with Emphasis to the Azeotropic Region. *Fluid Phase Equilib.* **2011**, *308*, 135−141.
(940) Jones, C. A.; Schoenborn, E. M.; Colburn, A. P. Equilibrium Still for Miscible Liquids. *Ind. Eng. Chem.* **1943**, *35*, 666−672.
(941) Hughes, H. E.; Maloney, J. O. Application of Radioactive Tracers to Diffusional Operations. Binary and Ternary Equilibrium Data. *Chem. Eng. Prog.* **1952**, *48*, 192−200.
(942) Bloom, C. H.; Clump, C. W.; Koeckert, A. H. Simultaneous Measurement of Vapor-Liquid Equilibria and Latent Heats of Vaporization. *Ind. Eng. Chem.* **1961**, *53*, 829−832.
(943) Stabnikov, V. N.; Matyushev, B. Z.; Protsyuk, T. B.; Yushchenko, N. M. Equilibrium in the Ethyl Alcohol-Water System at Atmospheric Pressure. *Pishch. Prom-st.* **1972**, *15*, 49−56.
(944) Otsuki, H.; Williams, F. C. Effect of Pressure on Vapor-Liquid Equilibria for the System Ethyl Alcohol-Water. *Chem. Eng. Prog., Symp. Ser.* **1953**, *49*, 55−67.
(945) 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 *J. Chem. Eng. Data* 1999, *444* 701 714 DOI: 10.1021/je980303x.
(946) 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. *J. Chem. Thermodyn.* **1986**, *18*, 1−12.
(947) 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. *J. Chem. Thermodyn.* **1986**, *18*, 867−875.
(948) Ott, J. B.; Stouffer, C. E.; Cornett, G. V.; Woodfield, B. F.; Guanquan, C.; 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. *J. Chem. Thermodyn.* **1987**, *19*, 337−348.
(949) Wormald, C. J.; Lloyd, M. J. Excess Enthalpies for (Water + Ethanol) AtT= 398 K ToT= 548 K Andp= 15 MPa. *J. Chem. Thermodyn.* **1996**, *28*, 615−626.
(950) Benson, G. C.; D'Arcy, P. J. Excess Isobaric Heat Capacities of Water-n-Alcohol Mixtures. *J. Chem. Eng. Data* **1982**, *27*, 439−442.
(951) Ogawa, H.; Murakami, S. Excess Isobaric Heat Capacities for Water + Alkanol Mixtures at 298.15 K. *Thermochim. Acta* **1986**, *109*, 145−154.
(952) Grolier, J.-P. E.; Wilhelm, E. Excess Volumes and Excess Heat Capacities of Water + Ethanol at 298.15 K. *Fluid Phase Equilib.* **1981**, *6*, 283−287.
(953) 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. *J. Chem. Thermodyn.* **2007**, *39*, 385−411.
(954) Vierk, A.-L. Experimentelle Untersuchungen an Den Zweistoffsystemen: Wasser-Acetonitril, Wasser-Dioxan, Äthanol-Acetonitril Und Cyclohexan-Dioxan. *Z. Anorg. Chem.* **1950**, *261*, 283−296.
(955) Park, S.-J.; Oh, H.-J.; Choi, H.-J.; Peak, S.-K.; Fischer, K.; Gmehling, J. Phase Equilibrium and Excess Molar Volume for Systems Acrylonitrile+water, Acetonitrile+water, and Acrylonitrile +acetonitrile. *Hwahak Konghak* **1997**, *35*, 678−683.
(956) Sugi, H.; Katayama, T. Ternary Liquid-Liquid And Miscible Binary Vapor-Liquid Equilibrium Data For The Two Systems n-Hexane Ethanol Acetonitrile And Water Acetonitrile-Ethyl Acetate. *J. Chem. Eng. Jpn.* **1978**, *11*, 167−172.
(957) Szydłowski, J.; Szykuła, M. Isotope Effect on Miscibility of Acetonitrile and Water. *Fluid Phase Equilib.* **1999**, *154*, 79−87.
(958) Stokes, R. H. Excess Partial Molar Enthalpies for (Acetonitrile + Water) from 278 to 318 K. *J. Chem. Thermodyn.* **1987**, *19*, 977−983.
(959) Nakamura, M.; Tamura, K.; Murakami, S. Isotope Effects on Thermodynamic Properties: Mixtures of x(D2O or H2O) + (1 − x)CH3CN at 298.15 K. *Thermochim. Acta* **1995**, *253*, 127−136.
(960) Schedemann, A. Weiterentwicklung von Thermodynamischen Vorhersagemethoden Als Grundlage Für Die Lösungsmittelauswahl Bei Der Flüssig-Flüssig-Extraktion Und Der Absorption. Hochschulschrift, BIS der Universität Oldenburg, 2013.
(961) Acosta, J.; Arce, A.; Rodil, E.; Soto, A. A Thermodynamic Study on Binary and Ternary Mixtures of Acetonitrile, Water and Butyl Acetate. *Fluid Phase Equilib.* **2002**, *203*, 83−98.
(962) De Visser, C.; Heuvelsland, W. J. M.; Dunn, L. A.; Somsen, G. Some Properties of Binary Aqueous Liquid Mixtures. Apparent Molar Volumes and Heat Capacities at 298.15 K over the Whole Mole Fraction Range. *J. Chem. Soc., Faraday Trans. 1* **1978**, *74*, 1159.
(963) Benson, G. C.; D'Arcy, P. J.; Handa, Y. P. Thermodynamics of Aqueous Mixtures of Nonelectrolytes. V. Isobaric Heat Capacities and Ultrasonic Speeds for Water + Ethanenitrile Mixtures at 25°C. *Thermochim. Acta* **1981**, *46*, 295−301.
(964) Fu, J.; Wang, K.; Hu, Y. 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* **1988**, *39*, 64−76.
(965) Maximo, G. J.; Meirelles, A. J. A.; Batista, E. A. C. Boiling Point of Aqueous D-Glucose and d-Fructose Solutions: Experimental Determination and Modeling with Group-Contribution Method. *Fluid Phase Equilib.* **2010**, *299*, 32−41.
(966) McGlashan, M. L.; Williamson, A. G. Isothermal Liquid-Vapor Equilibriums for System Methanol-Water. *J. Chem. Eng. Data* **1976**, *21*, 196−199.
(967) Yao, J.; Li, H.; Han, S. Vapor−Liquid Equilibrium Data for Methanol−Water−NaCl at 45°C. *Fluid Phase Equilib.* **1999**, *162*, 253−260.
(968) Dulitskaya, K. A. Vapor Pressure of Binary Systems. I. *Zh. Obshch. Khim.* **1945**, *15*, 9−21.
(969) Nagatani, M.; Fujino, K. Measurement of Isothermal Vapor-Liquid Equilibria for Methanol-Water System. *Fukuoka Daigaku Kogaku Shuho* **2000**, *64*, 147−152.
(970) 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* **1995**, *46*, 230−233.
(971) Schröder, W. Messungen von Siedegleichgewichten Bei Überdruck: Messungen von Siedegleichgewichten Bei Überdruck. *Chem. Ing. Tech.* **1958**, *30*, 523−525.
(972) 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.
(973) Yang, C.; Sun, F.; Ma, S.; Yin, X.; Zeng, H. Organic Salt Effect on Vapor−Liquid Equilibrium of the Methanol + Water System at Subatmospheric Pressure. *J. Chem. Eng. Data* **2012**, *57*, 2696−2701.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

(974) 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* **1970**, *43*, 1582−1586.
(975) Hirata, M.; Suda, S. Vapor-Liquid Equilibrium under Pressurized Conditions; Experimental Apparatus and Methanol-Water System. *Chem. Eng.* **1967**, *31*, 759−766.
(976) Bose, E. Remarks on Thermochemical Statement of Julius Thomsens. *Phys. Z.* **1906**, *7*, 503−505.
(977) 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 Equilib.* **1993**, *88*, 171−181.
(978) Tomaszkiewicz, I.; Randzio, S. L.; Gierycz, P. 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. *Thermochim. Acta* **1986**, *103*, 281−289.
(979) 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.* **1999**, *28*, 631−666.
(980) Benson, G. C.; D'Arcy, P. J.; Kiyohara, O. Thermodynamics of Aqueous Mixtures of Nonelectrolytes II. Isobaric Heat Capacities of Water-n-Alcohol Mixtures at 25°C. *J. Solution Chem.* **1980**, *9*, 931−938.
(981) 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. *Int. J. Thermophys.* **2004**, *25*, 805−838.
(982) Sazonov, V. P. Isothermal Liquid-Liquid-Vapor Equilibrium of Nitromethane - Isopropanol - Water. *Zh. Prikl. Khim.* **1986**, *59*, 1451−1456.
(983) Udovenko, V. V.; Mazanko, T. F. Liquid-Vapor Equilibrium in the Propan-2-Ol - Water and Propan-2-Ol - Benzene Systems. *Zh. Fiz. Khim.* **1967**, *41*, 1615−1620.
(984) Sada, E.; Morisue, T. Isothermal Vapor-Liquid Equilibrium Data of Isopropanol-water System. *J. Chem. Eng. Jpn.* **1975**, *8*, 191−195.
(985) Wu, H. S.; Hagewiesche, D.; Sandler, S. I. Vapor—Liquid Equilibria of 2-Propanol + Water + N,N-Dimethyl Formamide. *Fluid Phase Equilib.* **1988**, *43*, 77−89.
(986) Wilson, A.; Simons, E. L. Vapor-Liquid Equilibria. 2-Propanol - Water System. *Ind. Eng. Chem.* **1952**, *44*, 2214−2219.
(987) Marzal, P.; Montón, J. B.; Rodrigo, M. A. Isobaric Vapor−Liquid Equilibria of the Water + 2-Propanol System at 30, 60, and 100 KPa. *J. Chem. Eng. Data* **1996**, *41*, 608−611.
(988) Arce, A.; Arce, A.; Martínez-Ageitos, J.; Rodil, E.; Soto, A. (Vapour+liquid) Equilibrium of (DIPE+IPA+water) at 101.32kPa. *J. Chem. Thermodyn.* **2003**, *35*, 871−884.
(989) Privat, R.; Jaubert, J.-N.; Privat, Y. A Simple and Unified Algorithm to Solve Fluid Phase Equilibria Using Either the Gamma-Phi or the Phi-Phi Approach for Binary and Ternary Mixtures. *Comput. Chem. Eng.* **2013**, *50*, 139−151.
(990) Qian, J.-W.; Privat, R.; Jaubert, J.-N.; Duchet-Suchaux, P. Enthalpy and Heat Capacity Changes on Mixing: Fundamental Aspects and Prediction by Means of the PPR78 Cubic Equation of State. *Energy Fuels* **2013**, *27*, 7150−7178.
(991) Robinson, D. B.; Peng, D.-Y. *The Characterization of the Heptanes and Heavier Fractions for the GPA Peng−Robinson Programs (RR-28)*, GPA Research Report; Gas Processors Association, 1978; pp 1−36.
(992) Peng, D.-Y.; Robinson, D. B. A New Two-Constant Equation of State. *Ind. Eng. Chem. Fundam.* **1976**, *15*, 59−64.
(993) Jaubert, J.-N.; Privat, R.; Le Guennec, Y.; Coniglio, L. Note on the Properties Altered by Application of a Péneloux-Type Volume Translation to an Equation of State. *Fluid Phase Equilib.* **2016**, *419*, 88−95.
(994) Privat, R.; Jaubert, J.-N.; Le Guennec, Y. Incorporation of a Volume Translation in an Equation of State for Fluid Mixtures: Which Combining Rule? Which Effect on Properties of Mixing? *Fluid Phase Equilib.* **2016**, *427*, 414−420.
(995) Le Guennec, Y.; Lasala, S.; Privat, R.; Jaubert, J.-N. A Consistency Test for α-Functions of Cubic Equations of State. *Fluid Phase Equilib.* **2016**, *427*, 513−538.
(996) Le Guennec, Y.; Privat, R.; Jaubert, J.-N. 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 Equilib.* **2016**, *429*, 301−312.
(997) Le Guennec, Y.; Privat, R.; Lasala, S.; Jaubert, J.-N. 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 Equilib.* **2017**, *445*, 45−53.
(998) Soave, G. Equilibrium Constants from a Modified Redlich-Kwong Equation of State. *Chem. Eng. Sci.* **1972**, *27*, 1197−1203.
(999) Pina-Martinez, A.; Privat, R.; Jaubert, J.-N.; Peng, D.-Y. Updated Versions of the Generalized Soave α-Function Suitable for the Redlich-Kwong and Peng-Robinson Equations of State. *Fluid Phase Equilib.* **2019**, *485*, 264−269.
(1000) Avaullee, L.; Trassy, L.; Neau, E.; Jaubert, J. N. Thermodynamic Modeling for Petroleum Fluids I. Equation of State and Group Contribution for the Estimation of Thermodynamic Parameters of Heavy Hydrocarbons. *Fluid Phase Equilib.* **1997**, *139*, 155−170.
(1001) Kontogeorgis, G. M.; Privat, R.; Jaubert, J.-N. Taking Another Look at the van Der Waals Equation of State−Almost 150 Years Later. *J. Chem. Eng. Data* **2019**, 4619.
(1002) Jaubert, J.-N.; Mutelet, F. VLE Predictions with the Peng-Robinson Equation of State and Temperature-Dependent k_{ij} Calculated through a Group Contribution Method. *Fluid Phase Equilib.* **2004**, *224*, 285−304.
(1003) Vitu, S.; Privat, R.; Jaubert, J.-N.; Mutelet, F. Predicting the Phase Equilibria of CO^2 + Hydrocarbon Systems with the PPR[78] Model (PR EoS and k_{ij} Calculated through a Group Contribution Method). *J. Supercrit. Fluids* **2008**, *45*, 1−26.
(1004) Jaubert, J.-N.; Privat, R.; Mutelet, F. Predicting the Phase Equilibria of Synthetic Petroleum Fluids with the PPR78 Approach. *AIChE J.* **2010**, *56*, 3225−3235.
(1005) Qian, J.-W.; Jaubert, J.-N.; Privat, R. Phase Equilibria in Hydrogen-Containing Binary Systems Modeled with the Peng-Robinson Equation of State and Temperature-Dependent Binary Interaction Parameters Calculated through a Group-Contribution Method. *J. Supercrit. Fluids* **2013**, *75*, 58−71.
(1006) Xu, X.; Jaubert, J.-N.; Privat, R.; Arpentinier, P. Prediction of Thermodynamic Properties of Alkyne-Containing Mixtures with the *E*-PPR78 Model. *Ind. Eng. Chem. Res.* **2017**, *56*, 8143−8157.
(1007) Jaubert, J.-N.; Coniglio, L. The Group Contribution Concept: A Useful Tool to Correlate Binary Systems and to Predict the Phase Behavior of Multicomponent Systems Involving Supercritical CO_2 and Fatty Acids. *Ind. Eng. Chem. Res.* **1999**, *38*, 5011−5018.
(1008) Jaubert, J.-N.; Privat, R. Relationship between the Binary Interaction Parameters (k_{ij}) of the Peng−Robinson and Those of the Soave−Redlich−Kwong Equations of State: Application to the Definition of the PR2SRK Model. *Fluid Phase Equilib.* **2010**, *295*, 26−37.
(1009) Holderbaum, T.; Gmehling, J. PSRK: A Group Contribution Equation of State Based on UNIFAC. *Fluid Phase Equilib.* **1991**, *70*, 251−265.
(1010) Chen, J.; Fischer, K.; Gmehling, J. Modification of PSRK Mixing Rules and Results for Vapor−Liquid Equilibria, Enthalpy of Mixing and Activity Coefficients at Infinite Dilution. *Fluid Phase Equilib.* **2002**, *200*, 411−429.
(1011) Ahlers, J.; Gmehling, J. Development of an Universal Group Contribution Equation of State. *Fluid Phase Equilib.* **2001**, *191*, 177−188.
(1012) Ahlers, J.; Gmehling, J. Development of a Universal Group Contribution Equation of State. 2. Prediction of Vapor−liquid

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027

Equilibria for Asymmetric Systems. *Ind. Eng. Chem. Res.* **2002**, *41*, 3489−3498.
(1013) Voutsas, E.; Magoulas, K.; Tassios, D. Universal Mixing Rule for Cubic Equations of State Applicable to Symmetric and Asymmetric Systems: Results with the Peng−Robinson Equation of State. *Ind. Eng. Chem. Res.* **2004**, *43*, 6238−6246.
(1014) Voutsas, E.; Louli, V.; Boukouvalas, C.; Magoulas, K.; Tassios, D. Thermodynamic Property Calculations with the Universal Mixing Rule for EoS/G^E Models: Results with the Peng−Robinson EoS and a UNIFAC Model. *Fluid Phase Equilib.* **2006**, *241*, 216−228.
(1015) Jaubert, J.-N.; Borg, P.; Coniglio, L.; Barth, D. Phase Equilibria Measurements and Modeling of EPA and DHA Ethyl Esters in Supercritical Carbon Dioxide. *J. Supercrit. Fluids* **2001**, *20*, 145−155.
(1016) Moine, E.; Piña-Martinez, A.; Jaubert, J.-N.; Sirjean, B.; Privat, R. *I*-PC-SAFT: An *I*Ndustrialized Version of the Volume-Translated PC-SAFT Equation of State for Pure Components, Resulting from Experience Acquired All through the Years on the Parameterization of Saft-Type and Cubic Models. *Ind. Eng. Chem. Res.* **2019**, *58*, 20815−20827.

https://dx.doi.org/10.1021/acs.iecr.0c01734
Ind. Eng. Chem. Res. 2020, 59, 14981−15027