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Parametrization of equations of state: definition of a methodology applicable to SAFT models for pure species (with and without association term) and evaluation of their influence on model performances

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Nicolás Ramírez-Vélez. Parametrization of equations of state: definition of a methodology applicable to SAFT models for pure species (with and without association term) and evaluation of their influence on model performances. Chemical and Process Engineering. Université de Lorraine, 2022. English. NNT: 2022LORR0020 . tel-03769078

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THESE

Présentée par

Nicolás RAMÍREZ-VÉLEZ

Ingénieur de Université Pontificale Bolivarienne

pour l'obtention du grade de

DOCTEUR DE L'UNIVERSITÉ DE LORRAINE

Spécialité : Génie des Procédés, des Produits et des Molécules

Parametrization of equations of state: definition of a methodology applicable to SAFT models for pure species (with and without association term) and evaluation of their influence on model performances.

Paramétrage des équations d'état : définition d'une méthodologie applicable aux modèles SAFT pour les corps purs (avec et sans terme d'association) et évaluation de leur influence sur les performances des modèles.

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Contents

List of Figures	5
List of Tables.....	9
ACKNOWLEDGEMENTS.....	13
INTRODUCTION (ENGLISH)	15
Context	16
Outline.....	19
INTRODUCTION (FRANÇAIS).....	21
Contexte	22
Plan de la thèse	25
Chapter 1 : Industrialization of equations of state: status of the statistically associating fluid theory (SAFT) framework.....	27
1.1. The phase equilibrium problem	28
1.2. The virial equation of state	32
1.3. Cubic equations of state.....	32
1.3.1. Influence of a consistent alpha function and a volume translation on CEoS.....	37
1.4. Multiparametric equations of state	38
1.5. Statistical associating fluid theory equations of state	39
1.5.1. The SAFT description of pure fluids.....	39
1.5.2. The original SAFT and the CK-SAFT EoS	41
1.5.3. The SAFT-VR EoS	43
1.5.4. The soft-SAFT EoS	45
1.5.5. The PC-SAFT EoS	46
1.6. SAFT models and the industrialization problem.....	56
Chapter 2 : Parametrization of the PC-SAFT equation of state for non-associating pure compounds.	66
2.1. Introduction	68
What experimental properties should be used to parametrize an EoS?	68
Parametrization of CEoS.....	69
Parametrization of SAFT-type EoS.....	70
2.2. Literature review: parametrization procedures for SAFT-type EoS	71
SAFT-VR EoS.....	71
Soft-SAFT EoS	79

PC-SAFT EoS	79
2.3. Identification of the safe and optimal methods, to fit the parameters of pure-component SAFT-type EoS	81
The global methodology.....	81
Component selection and data collection.....	83
Evaluation of the fitting procedure.....	84
Selection of optimal weight factors for each of the 12 OF considered.....	84
Implementation of the optimization procedure.....	87
Results and Discussion.....	88
2.6. Conclusion.....	94
Chapter 3 : Associating terms in equations of state: are they essential to describe self-associating compounds?.....	96
3.1. The hydrogen bond.....	98
3.2. Associating character of a pure compound.....	100
3.3. Determining the associating character for a pure compound from the COSMO-RS model	102
3.4. Construction of a PC-SAFT and I-PC-SAFT pure-compound parameter database for 1800 pure compounds	111
3.4.1. Construction of a PC-SAFT and I-PC-SAFT molecular parameter database for a large number of non-associating pure compounds obtained from an optimal fitting procedure.....	111
3.4.2. Extension of the molecular parameter PC-SAFT and I-PC-SAFT databases to include self-associating compounds.....	111
3.5. Performance of non-associating SAFT models in reproducing self-associating pure compounds	112
3.5.1. Introduction.....	113
3.5.2. Brief overview of the studied molecular-based EoS.....	117
3.5.2.1. PC-SAFT EoS.....	117
3.5.2.2. I-PC-SAFT EOS	117
3.5.3. Assessing the accuracy of the PC-SAFT and I-PC-SAFT EoS: results and discussion	118
3.5.3.1. Influence of the associating character of components.....	120
3.5.4. Conclusion	132
Chapter 4 : Parametrization of SAFT EoS for associating compounds – overview of the association schemes and parametrization trends	134
4.1. The Association schemes.....	135
4.2. Association Scheme Selection: literature review and trends.....	156

4.3. Parametrization of SAFT EoS for associating compounds: literature review and trends	164
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Chapter 5 : On the effect of the associating term on the performance of the PC-SAFT EOS
..... 168

5.1. Introduction	169
5.2. Methodology.....	170
5.2.1. Chemical family and compound selection	170
5.2.2. Parametrization of the PC-SAFT EoS.....	173
5.3. Results and discussion	178
5.4. Conclusions	190

Chapter 6 Development of a database of reference binary system data to evaluate the performance of equations of state..... 191

6.1. Introduction	193
6.2. Criterion to build a benchmark database	194
6.2.1. Literature review	194
6.2.2. Which thermophysical properties should be included?.....	195
6.2.3. Which binary systems should be included?	196
6.2.4. How many systems and how many data should be included?	204
6.2.5. The built database.....	205
6.3. Grading of a thermodynamic model by means of the proposed database in order to assess its accuracy	216
6.3.1. Evaluation of the deviations between model predictions and experimental data	216
6.3.2. Treatment of "out of model" data points	218
6.3.3. Grading of a thermodynamic model.....	219
6.4. Illustration: grading and discussion around the accuracy of the Peng-Robinson EoS with classical mixing rules and a temperature-dependent BIP.....	224
6.4.1. The model.....	224
6.4.2. The fitting procedure	225
6.4.3. System-by-system results of the fitting procedure	228
6.4.4. Grading of the model: {PR EoS + classical mixing rules with a T-dependent k_{ij} }.	229
6.5. Conclusion	233

Chapter 7 : Evaluation of the Universal Mixing Rule Peng-Robinson EoS with UNIFAC-type model using a benchmark database for thermodynamic models 235

7.1 Introduction	236
7.2. UMR-PRU model.....	237

7.3.	PSRK model	240
7.4.	tc-PR-UNIQUAC model	240
7.5.	Benchmark database	240
7.6.	Grading procedure	241
7.7.	Simulis thermodynamics	246
7.8.	Results and Discussion	250
7.9.	Conclusions	277
CONCLUSIONS AND PERSPECTIVES (ENGLISH).....		279
CONCLUSIONS ET PERSPECTIVES (FRANÇAIS).....		283
Appendix		288
	Appendix A1 - Parameter dependency of properties predicted from the non-associating version of the PC-SAFT model.....	289
	Appendix A2 - Pure component selection.....	290
	Appendix A3 – Determination of the associating character of a pure component.....	292
	Appendix A4 – Initial value selection for the three PC-SAFT molecular parameters...	293
	Appendix A5 – Temperature range selected for regression of pure-compound parameters and MAPE estimation	294
	Appendix A7 – Compound-by-compound results for the 2 investigated SAFT-type EoS described in Chapters 2 and 3.	374
	Appendix A8 – Numerical values of the experimental data included in the benchmark database with the corresponding references and experimental data visualization.	520
	Appendix A9 – 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.....	522
	Appendix A10 – System-by-system analysis of the {PR EoS + classical mixing rules with a I-dependent k_{ij} } performances to correlate the data included in the proposed database.	522
Bibliography		523
Résumé		604
	Résumé	605
	Abstract	605

List of Figures

Figure 1.1. Diagram of a two-phase multicomponent system.....	28
Figure 1.2. Illustration of the volumetric translation concept. Taken from Jaubert & Privat ²⁴	37
Figure 1.3. Schematics of a molecule formation for the SAFT framework. Left image represents Process I, as described by Chapman et al ⁶ . Right image represents process II as described by Gross & Sadowski ¹² . Adapted from: https://www.itt.uni-stuttgart.de/en/research/	40
Figure 1.4. Illustration of an association interaction through hydrogen bonding for two secondary amines.	50
Figure 1.5. Illustration of an association interaction through hydrogen bonding for a secondary amine and a 1-alkanol.	51
Figure 1.6. Graphical representation of the universal m functions of the acentric factor, critical temperature and critical pressure for $m < 10$. Taken from Privat et al. ⁹⁴	62
Figure 3.1. Example of a hydrogen bond between an alcohol and a sulfonated compound. The green molecules R and R' are carbon chains of any length. The black dots represent electron pairs. The solid lines are covalent bonds while the dashed line represents the HB.	99
Figure 3.2. Cross-association between acetaldehyde (left) and dichloromethane (right). Solid lines represent covalent bonds. Dotted lines represent hydrogen bonds.	101
Figure 3.3. Associating sites of a water molecule. HA sites are presented in red, while HD sites are presented in blue. A HB formed between two water molecules is shown in the purple circle.	103
Figure 3.4. Sigma-profile for different compounds. On top: water and chloroform. On the bottom: 2-hexanone and benzene. The two red vertical lines indicate the threshold for HD or HA characteristics of a molecule, which are set to the value suggested by Khan et al ¹²¹	104
Figure 3.5. Molecular representation of 2-hexanone. The red circles correspond to HA sites for the molecule.	105
Figure 3.6. Molecular representation of chloroform. The blue circle corresponds to the HD site for the molecule.....	106
Figure 3.7. Sigma-profile and molecular structure for acetyl chloride The cutoff value for HB is the one proposed by Klamt et al ¹²⁰	107
Figure 3.8. Probability of hydrogen bonding (P(HB)) versus enthalpy of hydrogen bonding.	110
Figure 3.9. Ratio of well and badly modeled molecules by the PC-SAFT EoS classified into non-self-associating (NSA) and self-associating (SA) fluids. Green: Well-modeled molecules. Red: Badly-modeled molecules.	126
Figure 3.10. Ratio of well and badly modeled molecules by the I-PC-SAFT EoS classified into non-self-associating (NSA) and self-associating (SA) fluids. Green: Well-modeled molecules. Red: Badly-modeled molecules.	126
Figure 3.11. Ratio of well and badly modeled molecules by the tc-PR EoS classified into non-self-associating (NSA) and self-associating (SA) fluids. Green: Well-modeled molecules. Red: Badly-modeled molecules.	126
Figure 3.12. Hydrogen bond enthalpy vs. (MAPE on P^{sat} + MAPE on v_{liq}^{sat}) for the 548 SA compounds modeled with the PC-SAFT EoS. ○: 311 well-modeled components. ●: 237 badly-	

modeled components. The vertical line is an approximate border between the region where the fluids are well-modeled (WM) and badly-modeled (BM).	128
Figure 3.13. Hydrogen bond enthalpy vs. (MAPE on P^{sat} + MAPE on v_{liq}^{sat}) for the 548 SA compounds modeled with the I-PC-SAFT EoS. ○: 377 well-modeled components. ●: 171 badly-modeled components. The vertical line is an approximate border between the region where the fluids are well-modeled (WM) and badly-modeled (BM).	129
Figure 3.14. Hydrogen bond enthalpy vs. (MAPE on P^{sat} + MAPE on v_{liq}^{sat}) for the 548 SA compounds modeled with the tc-PR EoS. ○: 366 well-modeled components. ●: 182 badly-modeled components. The vertical line is an approximate border between the region where the fluids are well-modeled (WM) and badly-modeled (BM).	130
Figure 4.1. (left) Saturated liquid and vapor densities for methanol, 1-pentanol and 1-nonanol. Comparison of PC-SAFT (solid) and SAFT (dashed) to experimental data; (right) Isobaric vapor-liquid equilibrium and liquid-liquid equilibria for methanol at P = 1.013 bar. Comparison of experimental data to PC-SAFT ($k_{ij} = 0.051$) and SAFT ($k_{ij} = 0.044$)	158
Figure 4.2. Comparison of the predictions of various models and schemes for the monomer fraction of pure water.	159
Figure 4.3. Distribution of HB number per molecule of methanol at 300K.	160
Figure 4.4. Monomer fraction for the first eight 1-alkanols from Monte Carlo simulations (square symbols), the 3B scheme (solid lines) and 2B scheme (dashed lines)	162
Figure 4.5. AAD (%) for P^{sat} of Methanol for various association schemes as reported by several authors.	163
Figure 4.6. Single parameter sensitivity analysis for pure MEG density and vapor pressure using the 4C scheme. Taken from Kruger et al. ¹³⁸	165
Figure 5.1. Strategy for the calculation of the associating parameter mesh, where n is the current pair of associating parameters and j is the total number of associating parameter pairs.	177
Figure 5.2. Contour plot of the associating parameter mesh (black dots) constructed for a) The sum of the global MAPE (global means that the MAPE is calculated by averaging the MAPEs of the 11 alcohols) on vapor pressure and liquid density, b) the global MAPE on vapor pressure and c) the global MAPE on liquid density. All MAPE values are in percentage (%).	179
Figure 5.3. MAPE on liquid density vs. MAPE on vapor pressure obtained for every combination of associating parameters for 1-pentanol.	186
Figure 5.4. Sum of the average MAPE of P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$ and as a function of the number of alcohols included in the OF. The purple line represents OF1 which only includes and in the minimization objective. The red line represents OF2 in which all four target properties are included in the minimization objective. Dots represent the value of the OF at a given number of alcohols.	188
Figure 6.1. (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..	197
Figure 6.2. Procedure followed to build the proposed database.	202
Figure 6.3. Notation used in the files database.xlsx and BACi_with visualization of the data.xlsx (i=1 to 9) when the experimental pressure is not mentioned.	218
Figure 6.4. Illustration of all the cases in which out of model data points can appear. For such exp. data points, the MAPE cannot be evaluated. (a): experimentally 2-phase data points that	

are found to be 1-phase by the model. (b) An azeotropic system is predicted as a zeotropic system so that the homogeneous azeotrope is declared out of model. In addition, for small mole fractions, $y_{1,exp} > x_{1,exp}$ whereas the model predicts the opposite. (c) A homogeneous azeotrope is predicted as heterogeneous. (d) A 3-phase line is not predicted by the model. (e) 2 critical points that are not predicted by the model are experimentally observed. (f) The model predicts 2 critical points whereas only one is experimentally observed. 219

Figure 6.5 . Overview of the accuracy of the model: {PR EoS + classical mixing rules with a T-dependent k_{ij} } by plotting the marks in ten properties for the four categories of binary systems based on the type of association they exhibit. 231

Figure 6.6. Marks in 10 properties calculated for five categories of binary systems based on how they deviate from ideality (marks on VLE data are not shown due to a lack of information for some categories of binary systems). 233

Figure 7.1. Overview of the marks obtained by the UMR-PRU model for each property over the four categories of binary systems of the benchmark database. 256

Figure 7.2. Overview of the final marks obtained for the tc-PR-Wilson, tc-PR-UNIQUAC, tc-PR-NRTL, PR-van Laar, PC-SAFT-vdW1f, PSRK and UMR-PRU. 257

Figure 7.3. Mark obtained by the tc-PR-UNIQUAC, PSRK and UMR-PRU for the four categories of binary mixtures. In parenthesis, besides each of the model's name, we find the final mark obtained by each one. 259

Figure 7.4. Marks obtained by the tc-PR-UNIQUAC, PSRK and UMR-PRU for each property for the first category of binary mixtures (mixtures with no association). In parenthesis, besides the name of each model we find the mark obtained by each one for this category. 261

Figure 7.5. VLE diagram for A) nitrogen-methane @T =142.89 K with the UMR-PRU ; B) nitrogen-methane @ T =142.89 K with the PSRK; C) CO2-ethane @ T= 250 K with the UMR-PRU; D) CO2-ethane @ T = 250 K with the PSRK. Blue colors symbolize liquid phases, while red colors symbolize vapor phases. Solid lines represent calculated VLE data. Asterisks represent experimental VLE data. Solid diamonds and triangles represent experimental critical and azeotropic data respectively. Hollow diamonds and triangles represent calculated critical and azeotropic data. Diagrams A and B belong to BAC 1 while diagrams C and D belong to BAC 2. 263

Figure 7.6. VLE diagram for E) chloroform-n-hexane @T =298.15 K with the UMR-PRU; F) chloroform-n-hexane @T =298.15 K with the PSRK; G) CO2-ethyl acetate @ T= 313.15 K with the UMR-PRU; G) CO2-ethyl acetate @ T= 313.15 K with the PSRK. Blue colors symbolize liquid phases, while red colors symbolize vapor phases. Solid lines represent calculated VLE data. Asterisks represent experimental VLE data. Diagrams E and D belong to BAC 3 while diagrams G and H belong to BAC 4. 264

Figure 7.7. Marks obtained by the tc-PR-UNIQUAC, PSRK and UMR-PRU for each property for the second category of binary mixtures (mixtures where self-association tends to be broken). In parenthesis, besides the name of each model we find the mark obtained by each one for this category 266

Figure 7.8. VLE diagram for I) methanol-benzene @T =318.15 K with the UMR-PRU; J) methanol-benzene @T =318.15 K with the PSRK. Blue colors symbolize liquid phases, while red colors symbolize vapor phases. Solid lines represent calculated VLE data. Asterisks represent experimental VLE data. Both diagrams belong to BAC5. 268

Figure 7.9. Marks obtained by the tc-PR-UNIQUAC, PSRK and UMR-PRU for each property for the third category of binary mixtures (mixtures where only cross-association takes place).

In parenthesis, besides the name of each model we find the mark obtained by each one for this category. 270

Figure 7.10. VLE diagram for K) chloroform-acetone @T =323.15 K with the UMR-PRU; L) chloroform-acetone @T =323.15 K with the PSRK;. Blue colors symbolize liquid phases, while red colors symbolize vapor phases. Solid lines represent calculated VLE data. Asterisks represent experimental VLE data. Solid triangles represent experimental azeotropic data. Hollow triangles represent calculated azeotropic data. Diagrams K and L belong to BAC 6. 272

Figure 7.11. Marks obtained by the tc-PR-UNIQUAC, PSRK and UMR-PRU for each property for the fourth category of binary mixtures (mixtures with cross and self-association). In parenthesis, besides the name of each model we find the mark obtained by each one for this category. 274

Figure 7.12. VLE diagram for M) 2-butanol-trichloroethylene @P = 1.0 bar with the UMR-PRU; N) 2-butanol-trichloroethylene @P = 1.0 bar with the PSRK; O) methanol-diisopropyl ether @ T = 325.15 K with the UMR-PRU; P) methanol-diisopropyl ether @ T = 325.15 K with the PSRK; Q) methanol-1-propanol @ T= 333.17 K with the UMR-PRU and R) methanol-1-propanol @ T= 333.17 K with the PSRK .Blue colors symbolize liquid phases, while red colors symbolize vapor phases. Solid lines represent calculated VLE data. Asterisks represent experimental VLE data. Solid triangles represent experimental azeotropic data. Hollow triangles represent calculated azeotropic data. Diagrams K and L belong to BAC 6. 276

List of Tables

Table 1.1. Summary of the van der Waals, Soave-Redlich-Kwong and Peng-Robinson cubic equations of state with their internal expressions and the value of the critical compressibility factor. u and w taken from Pina-Martinez et al. ³¹	33
Table 1.2. Alpha-function expressions and consistency conditions as tested and shown by Le Guennec et al. ³⁵	35
Table 1.3. Effect of using a consistent alpha-function and volume translation on the mean average percent error (MAPE) on the PR EoS ⁴³	38
Table 1.4. Association scheme for the secondary amine illustrated in Figure 1.4 . Y means that an interaction can form. N means that the two sites cannot interact.	51
Table 1.5. Association scheme for the secondary amine-1-alkanol system illustrated in Figure 5. Y means that an interaction can form. N means the two sites cannot interact. The orange quadrant is the self-association scheme for the amine and the red quadrant is the self-association scheme for the alcohol.....	52
Table 1.6. Associating schemes as proposed by Huang & Radosz, with examples of chemical species that may present them. The circles represent the association sites. The red circles represent a hydrogen acceptor site, the blue circles represent a hydrogen donor site and the black circle represents a binary site in which the former two sites are combined into one.	53
Table 1.7. Non-bonded site fractions X^A for different association scheme types.....	54
Table 2.1. Overview of the various parametrization strategies used with the SAFT-VR, soft-SAFT and PC-SAFT EoS.....	73
Table 2.2. List of the 15 property data combinations of $\{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}\}$ usable for fitting SAFT parameters.....	82
Table 2.3. Variable set of each VLE property of interest for the present study	83
Table 2.4. Illustration on an arbitrary molecule of the procedure aimed at selecting the weight factor $\omega_{energetic\ prop}$	87
Table 2.5. Average MAPEs on $\{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}\}$ and related standard deviations calculated over 656 non-associating species, when the PC-SAFT parameters are fitted to $P^{sat} + \rho_{liq}^{sat} + \Delta_{vap}H + c_{P,liq}^{sat}$ (refer to OF 1 in Table 2).	88
Table 2.6. Average values of the MAPEs on $\{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}\}$, and the critical temperature, pressure and molar volume $\{T_c, P_c, v_c\}$ calculated over 544 non-associating pure species, corresponding each to a different combination of property data on which the PC-SAFT parameters were adjusted.	90
Table 3.1. Overview of the data available in the database proposed by Piña-Martinez et al. ¹²⁷	114
Table 3.2. List of the chemical families and corresponding distribution of the 1 800 pure compounds available in the database proposed by Piña-Martinez et al. ¹²⁷	115
Table 3.3. MAPE on $P^{sat}, v_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}, T_c, P_c$ and v_c as predicted by the PC-SAFT, I-PC-SFAT and tc-PR EoS.....	119

Table 3.4. MAPE on P^{sat} , v_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$, T_c , P_c and v_c depending on the associating character (NSA or SA) of the fluids as predicted by the PC-SAFT, I-PC-SFAT and tc-PR EoS.	121
Table 3.5. MAPE on P^{sat} , v_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$, T_c , P_c and v_c as predicted by the PC-SAFT EoS for the 20 chemical families defined in Table 3.2	122
Table 3.6. MAPE on P^{sat} , v_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$, T_c , P_c and v_c as predicted by the I- PC-SAFT EoS for the 20 chemical families defined in Table 3.2	123
Table 3.7. Average MAPE on P^{sat} and v_{liq}^{sat} as predicted by the PC-SAFT and I-PC-SAFT for the 1252 NSA compounds and corresponding standard deviations (SD).	124
Table 3.8. Distribution of well-modeled compounds across different chemical families for the PC-SAFT, I-PC-SAFT and tc-PR EoS.....	131
Table 4.1. Association schemes and their structural representation. Red circles correspond to HA sites, blue circles to HD sites and black circles to binary sites.	152
Table 4.2. Associating scheme types, associating strength apporximations, unbonded monomer fraction approximations and expressions.	154
Table 5.1. List of selected n-alcohols with their PC-SAFT non-associating parameters and MAPE on vapor pressure, liquid density, enthalpy of vaporization and liquid heat capacity and their modeling classification. WM means well-modeled and BM means badly-modeled....	172
Table 5.2. Average values of the MAPEs on $\{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}\}$, calculated over 152 self-associating pure species, corresponding each to a different combination of property data on which the PC-SAFT parameters were adjusted.....	175
Table 5.3. PC-SAFT parameters including association and MAPE for P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$ for the 11 studied n-alcohols. The associating parameters are chosen so that the vapor pressure and the liquid density are minimized.	181
Table 5.4. PC-SAFT parameters including association and MAPE for P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$ for the 11 studied n-alcohols. The associating parameters are chosen so that the all four target properties are minimized.....	183
Table 5.5. PC-SAFT parameters including association and MAPE for P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$ for the 11 studied n-alcohols. The associating parameters are assumed component-dependent and chosen so that the four properties are minimized.....	185
Table 6.1. Definition of the ten families of binary systems and their corresponding BAC (binary association code).	199
Table 6.2. 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 (the abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”).	203
Table 6.3. 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 (the abbreviations used for the associating character of a pure compound are: NA for “Non-	

Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”).	206
Table 6.4. List of the 26 binary systems for which the binary association code is: BAC=1 (NA-NA). Such a BAC corresponds to a binary system involving a “Non-Associating” (NA) molecule + another “Non-Associating” (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.	207
Table 6.5. List of the 24 binary systems for which the binary association code is: BAC=2 (HA-NA). Such a BAC corresponds to a binary system involving a “Hydrogen-Acceptor” (HA) molecule + a “Non-Associating” (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.	208
Table 6.6. List of the 20 binary systems for which the binary association code is: BAC=3 (HD-NA). Such a BAC corresponds to a binary system involving a “Hydrogen-Donor” (HD) molecule + a “Non-Associating” (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.	209
Table 6.7. List of the 22 binary systems for which the binary association code is: BAC=4 (HA-HA or HD-HD). 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.	210
Table 6.8. List of the 18 binary systems for which the binary association code is: BAC=5 (SA-NA). Such a BAC corresponds to a binary system involving a “Self-Associating” (SA) molecule + a “Non-Associating” (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.	211
Table 6.9. List of the 25 binary systems for which the binary association code is: BAC=6 (HD-HA). 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.	212
Table 6.10. List of the 16 binary systems for which the binary association code is: BAC=7 (SA-HD). Such a BAC corresponds to a binary system involving a “Self-Associating” (SA) molecule + a “Hydrogen-Donor” (HD) 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.	213
Table 6.11. List of the 26 binary systems for which the binary association code is: BAC=8 (SA-HA). 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.	214
Table 6.12. List of the 23 binary systems for which the binary association code is: BAC=9 (SA-SA). 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.	215

Table 6.13. Specified and calculated variables for the different binary-system properties involved in the database.	217
Table 6.14. 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 9 binary association codes (BACs). The abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”.	229
Table 6.15. Rating of the 9 binary association codes in order to finally grade the model: {PR EoS + classical mixing rules with a T-dependent k_{ij} }. The abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”.	230
Table 7.1. Definition of the ten families of binary systems and their corresponding BAC (binary association code).	241
Table 7.2. Summary of the 18 compounds that cannot be decomposed with the available groups defined in the UNIFAC- UMR-PRU model, the associated binary systems to be excluded from the benchmarking and their respective BACs.	247
Table 7.3 List of 13 binary mixtures for which no UMR-PRU group-interaction parameters are available and their respective BACs.	248
Table 7.4. Summary of number of systems removed in each BAC.	249
Table 7.5. Overview of the MAPE between experimental data and values calculated with the UMR-PRU model for the 152 binary systems included in the proposed database that are classified in nine binary association codes (BACs). The abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”.	251
Table 7.6. Overview of the Success Ratio (SR) between experimental data and values calculated with the UMR-PRU model for the 152 binary systems included in the proposed database that are classified in nine binary association codes (BACs). The abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”.	252
Table 7.7. Rating of the nine binary association codes in order to finally grade the UMR-PRU model. The abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”.	253

ACKNOWLEDGEMENTS

This dissertation was done at the Laboratoire Réactions et Génie des Procédés (LRGP) at the Ecole Nationale Supérieure des Industries Chimiques (ENSIC) at Nancy, France.

I have to express my deepest gratitude to professors Romain Privat and Jean-Noël Jaubert, my thesis directors. I cannot express enough gratitude towards them for believing in me and trusting such an important project on my shoulders. Their kindness, patience and disposition, as well as their constant strive for scientific excellence have not only made this entire work possible, but have left in me the most profound lessons for both my professional and personal life. I could not have asked for better mentors on this doctoral journey.

I want to thank professors Jean-Charles De Hemptinne and Patrice Paricaud for accepting to evaluate my thesis as thesis reporters. It was a complete honor to have both of them as members of my jury and I thank them for taking the time to come personally to the defense.

I would also like to thank madame Céline Houriez for accepting to participate on my thesis jury as a reviewer and for taking the time to travel to the event.

I would like to extend my deepest gratitude to TotalEnergies, for their financial support throughout the entire development of my thesis. In particular, I would like to thank Laurent Avauillée for taking the time to be present in my thesis defence as a jury and for his valuable insights during the discussion that followed.

I would like to thank Xiaochun Xu for also participating as a member of my jury and for the work and exchanges we had during my time in Nancy. Our discussions and the projects we worked on were both enjoyable and enriching and his kindness will be always remembered and appreciated.

I would like to thank my colleagues and friends Andres Piña Martínez and Thomas Di Pietro. Their kindness and disposition even in some of the most difficult parts of my journey have left me with the deepest appreciation for them and I wish them both the best on whatever they do.

I want to thank professors Silvia Lasala and Fabrice Mutelet which have made me feel a part of the team from the moment I met them. The scientific exchanges and their perspectives in subjects different than mine have helped construct a deeper view of the research scopes for me and for the team and were much appreciated.

I want to mention my fellow Ph.D students Aghilas Dehlouz, Fransisco Paes, Aya Barakat, Michel Molière and Luis Pinilla. Their camaraderie and some of our discussions have been both refreshing and delightful. I wish them all the greatest success.

In general, I want to thank the ThermE team for making me feel at home at the laboratory. Their kindness and hospitality will never be forgotten.

I want to extend my gratitude to all of the people from the ENSIC and the LRGP that I did not mention but that in one way or another made all of this possible.

Finally, I want to thank my family, without which I would not be here in the first place.

My sister Sofia, which has become one of my closest partners during this time and which always finds a way to make me laugh even in the most difficult times.

To my parents, Angela and Jaime, whose love and support have gone above and beyond all barriers and limits and who made the tremendous effort to be present in my defense. I cannot thank them enough for all their love and sacrifices even before my doctoral thesis. Words fall short for gratitude I have for you two.

Finally, to my loving wife, Daniela. This work is entirely dedicated to you. I cannot even begin to describe how big of an impact you have had on this dissertation, let alone on my life. You have pushed me into becoming not only a better scientist, but a better human being altogether. This success goes all to you for all the love, support patience and sacrifices you have made for me and for us. Thank you from the bottom of my heart. I love you.

Nancy, le 5 avril 2022.

Nicolas Ramirez Velez

INTRODUCTION (ENGLISH)

Context

Modern day process engineering and design requires the aid of specialized tools such as process simulators (Aspen, ProSim, PRO/II, etc. REFS). Indeed, the accuracy of the simulations is closely tied to the thermodynamic models available in the chosen software. Furthermore, phase equilibria for multicomponent mixtures for which no available data is available is often required, in addition to energetic properties (such as enthalpy, entropy or heat capacities) for calculation of energy and entropy balances to perform exergy analysis. Evidently, these properties can be measured. However, measurements, although necessary, are often time consuming, thus highlighting the necessity of thermodynamic models which can simultaneously:

- Predict equilibrium properties without the need of previous use of experimental data,
- Yield accurate results in the subcritical I and supercritical regions.
- Calculate with acceptable accuracy, energy, entropy and exergy balances.

This presents a highly challenging task for any thermodynamic model. Furthermore, as pointed out by the Working Party on Thermodynamics and Transport Properties (WP-TTP)¹ thermodynamic models still face major challenges in the eyes of the industrial community^{2,3}. As pointed out by Hendricks et al.², the wide variety of models presents a major concern as their usability is not often transparent or available in the working environments. Furthermore, on the follow-up study of the WP-TTP, Kontogeorgis et al.³ pointed out several comments in their survey that:

“A model that only exists in a journal article does not provide much use to industry”.

Or,

“Clean up with the zoo of variants and subvariants of equations of state and property models. Transform existing models with empirical parameters to models with theoretically based (and calculable) parameters with a physical meaning”.

In general, some of the main concerns regarding thermodynamic models lie in several points:

- The model should be validated and implemented on an available environment (usually software simulators such as AspenPlus or ProSim). Chemical and process engineers who use these environments are often tied to the models available to them, even if there exists a better choice in the open literature. Alternatively, the model should be presented in such a way that its in-house implementation is possible.
- Parameter estimation and validation, especially for physically based models, needs further improvement and transparency in order to guarantee reliable results with the parameters as well as the ability of regressing new parameters when needed.
- Advanced models, based on physical theories, should be further developed and extended to more species and mixtures. In addition, they should be able to reproduce secondary properties such as heat capacities and transport properties such as viscosities.

Both surveys mention that the industry has high interest in the Statistical Associating Fluid Theory (SAFT) framework of equations of state (EoS), which come from the doctoral work of Walter Chapman⁴⁻⁷. This family of thermodynamic models offers a solid theoretical

background, which takes into account strong intermolecular forces, such as hydrogen bonding, often present in associating and polar compounds. This has been one of the main features of this family of EoS. However, they raise several questions as well. One of the main concerns lies on the number of different variants of the model (SAFT-VR⁸, soft SAFT⁹, GC-SAFT^{10,11}, etc.), which is deemed as a negative aspect. Two versions were of particular interest: the perturbed chain SAFT (PC-SAFT)^{12,13} and the SAFT- γ Mie¹⁴ which have seen increased use in the industrial setting. The SAFT- γ Mie which is parametrized through a group-contribution method has had positive remarks due to the notion that “*EoS-based group contribution models are inherently more useful than activity coefficient models such as UNIFAC since they are applicable to both pure compounds and mixtures*”³

Regarding the PC-SAFT, although it has seen increased use on an industrial level, many of the original challenges presented by Hendricks et al.² for the SAFT family remain. These ones include:

- The necessity to dispose of characterization methods for complex mixtures, such as petroleum oils.
- The calculation speed must be improved for routine applications.
- The lack of pure component and mixture parameter databases that are validated and easily available.
- The highlight of the strengths of the SAFT family over other well-known models, especially cubic EoS.
- The extension of the EoS class to electrolyte and polymer thermodynamics.
- The standardization of the SAFT framework.

Furthermore, as pointed out by Kontogeorgis et al.³, some companies are still cautious about molecular-based models, especially those including association such as the PC-SAFT. The issue goes into two directions: first the implementation and documentation of the model in the current process simulation tools is lacking. Some companies pointed out that “PC-SAFT slows down the Aspen Plus simulations so much that it cannot be used in practice yet” and “PC-SAFT has been greatly improved but the usability remains poor”. Although there exist several open source projects such as Clapeyron¹⁵ (implemented in Julia) or the Python PC-SAFT library¹⁶ which address the calculation speed, it is often the case that including these options is not viable due to the lack of technical know-how in programming languages or due to the simulation software simply being more convenient. It is well acknowledged that the main feature of the SAFT family of EoS, the associating contribution to the Helmholtz energy, introduces a high mathematical complexity and an increase in parameters to be estimated, thus affecting the computational time when compared to simpler (yet still powerful) models such as cubic EoS.

The second issue with the PC-SAFT (and generally of the SAFT family) is the lack of standardization: Kontogeorgis et al.³ noted the common feeling that there are many variants of the SAFT model and it is not often clear which one to choose. Additionally, as noted before by Hendricks et al.², it can happen that different results are obtained with equivalent models (such as the different SAFT versions). This linked to the fact that the parameter estimation routines are not often clear for these models or that the parameters are fit to a very specific case study with particular conditions in mind. Polishuk¹⁷ and Moine et al.¹⁸ described the standardization

issue of SAFT models as a lack of industrialization. They defined an EoS as industrialized when:

- The method to obtain compound-specific parameters follows a transparent and universal methodology. This means that the parameter estimation must be systematic and clearly laid out in order to achieve reproducible and reliable results for any compound each time the model's parameters are derived.
- The numerical inputs are easily available whether it be in validated databases or through predictive correlations. This means that the requirements to parametrize the model for a given compound or mixture (experimental property data, molar mass, etc.) should be of easy access regardless of the chemical species treated.

SAFT-type EoS are not regarded as industrialized. The reason behind this is that the input parameters, which are component dependent molecular parameters, are obtained through fitting experimental data in most cases. However, the fitting procedure is not standardized: some authors may include different types of experimental data with different number of data points and temperature/pressure ranges. Furthermore, since not all SAFT variants use the same number of parameters, the actual number of inputs required for each member of the SAFT family is different, and the impact of such divergence is not often considered. As a consequence, the input parameter sets and correlations found in the literature differ from one author to another, even when working with the same SAFT version. This lack of standardization is what leaves the SAFT models outside of the industrialized definition and thus raising the concerns of chemical and process engineers in the industrial, the software and the academic communities altogether.

The first objective of this dissertation was to develop a fully standardized parameter estimation methodology in which reliable results are obtained through fitting SAFT molecular parameters systematically over easily available experimental data for the largest number possible of pure compounds. This will allow to have a universal and transparent protocol for any member of the SAFT family allowing for it to be more accessible to the industrial and academic audiences. The second objective, which comes as a consequence of the first objective, is to propose a database of SAFT molecular parameters that is easily available and that guarantee reliable and reproducible results for a large number of chemical species of different associating natures.

The third goal of this work is to evaluate the associating contribution of the SAFT family of EoS, by testing the performance of the model with and without taking association into account.

Achieving these three goals will give answer to the industrial needs mentioned here for the SAFT family of EoS, with a standardized parameter estimation methodology, reliable parameter databases and exploring the capabilities of the physical background of the SAFT framework. To do so, the study first begins by analyzing a SAFT EoS' capabilities of reproducing compounds where no association is present (e.g. n-alkanes) and which properties to include in the optimization objective. Next, the parametrization routine is used to obtain pure compound parameters for associating compounds (e.g. alcohols) without taking association into account: This would lead to a large database of pure compound parameters which are reliable and easily accessible. Finally, the influence of the associating term is studied to understand the need for it when dealing with associating compounds:

Thus, this thesis addressed the following research questions:

- I. How to parametrize SAFT models in a standardized and universal manner so that non-associating compounds can be described reliably? Which properties are needed to guarantee that the minimization objective is safe?
- II. How does a non-associating EoS perform for associating compounds using a standardized parametrization protocol?
- III. What is the impact of the associating term on self-associating pure compounds within the SAFT framework?

Finally, this dissertation will study the performance of a predictive thermodynamic model, the Peng-Robinson EoS with Universal Mixing Rules and a UNIFAC type model (UMR-PRU)^{19,20}, in reproducing a benchmark database of high-quality thermodynamic experimental data for 200 binary mixtures²¹.

Outline

This dissertation consists of seven chapters, presenting a background on thermodynamic models, in particular equations of state and a detailed description of the methodologies and results used in order to answer the research questions. The thesis is divided into two parts: chapters 1 through 5 deal with the SAFT parametrization for non-associating and self-associating compounds, while chapters 6-7 present the benchmark database for comparing thermodynamic models and the benchmarking of the UMR-PRU EoS. The chapters are presented as follows:

- **Chapter 1:** presents a brief description of the phase equilibrium problem, equations of state with particular emphasis in the SAFT family of models, as well as a more detailed description of the SAFT industrialization problem.
- **Chapter 2:** presents the research work devoted to developing a standardized parametrization methodology for SAFT EoS including the analysis of the experimental properties to be included in the fitting objectives and the results obtained when applying the procedure to non-associating compounds.
- **Chapter 3:** presents a description of chemical association, including the definition of hydrogen bonding. Then it presents the methodology to determine the associating character of a pure compound, followed by the application of the new parametrization methodology using a non-associating SAFT EoS for associating compounds. This includes the construction of a pure-compound parameter database for 1800 pure compounds, including non-associating and self-associating species. The chapter is closed by an analysis on the performance of the SAFT-type EoS for all the compounds in the database mentioned previously.
- **Chapter 4:** presents a detailed description of associating schemes in the SAFT context, as well as a literature review in scheme selection and parametrization tendencies for self-associating compounds using associating EoS.

- **Chapter 5:** presents the analysis and discussion of the impact of the associating term of the SAFT framework in reproducing pure compound properties by extending the parametrization methodology proposed in Chapter 2.
- **Chapter 6:** presents the work done in developing a benchmark database to compare thermodynamic models in the form of presenting the published article.
- **Chapter 7:** presents the results and analysis of the benchmarking of the UMR-PRU EoS as well as contrasting it with other models that have already been benchmarked by using the high-quality experimental database of binary mixtures.

Finally, the manuscript closes with general conclusions and perspectives regarding the future work on SAFT EoS regarding the associating term, the associating schemes and extension to mixtures.

INTRODUCTION (FRANÇAIS)

Contexte

L'ingénierie et la conception de procédés modernes nécessitent l'utilisation d'outils spécialisés tels que les simulateurs de procédés (Aspen, ProSim, PRO/II, etc.). En effet, la précision des simulations est fortement liée aux modèles thermodynamiques disponibles au sein du logiciel choisi. De plus, les équilibres de phase pour les mélanges multiconstituants pour lesquels aucune donnée n'est disponible sont souvent nécessaires, ainsi que les propriétés énergétiques (telles que l'enthalpie, l'entropie ou les capacités calorifiques) pour le calcul des bilans d'énergie et d'entropie afin de réaliser une analyse exergetique. Ces propriétés peuvent, bien entendu, être mesurées. Cependant, les mesures, bien que nécessaires, prennent souvent beaucoup de temps, ce qui met en évidence la nécessité de modèles thermodynamiques qui peuvent simultanément :

- Prédire les propriétés d'équilibre sans avoir besoin d'utiliser préalablement des données expérimentales,
- Donner des résultats précis dans les régions subcritiques et supercritiques.
- Calculer avec une précision acceptable les bilans énergétiques, entropiques et exergetiques.

Il s'agit d'une tâche très difficile pour tout modèle thermodynamique. En outre, comme l'a souligné le groupe de travail sur la thermodynamique et les propriétés de transport (WP-TTP)¹, les modèles thermodynamiques sont toujours confrontés à des défis majeurs aux yeux de la communauté industrielle^{2,3}. Comme l'ont souligné Hendricks et al.², la grande variété de modèles constitue une préoccupation majeure car le domaine dans lequel ils s'appliquent n'est pas souvent transparent ou renseigné dans les environnements de travail. En outre, dans le cadre de la suite de l'étude du groupe de travail européen WP-TTP, Kontogeorgis et al.³ ont relevé plusieurs commentaires dans leur enquête selon lesquels :

“A model that only exists in a journal article does not provide much use to industry”.

Ou,

“Clean up with the zoo of variants and subvariants of equations of state and property models. Transform existing models with empirical parameters to models with theoretically based (and calculable) parameters with a physical meaning”.

En général, les principales préoccupations concernant les modèles thermodynamiques résident dans plusieurs points :

- Le modèle doit être validé et mis en œuvre sur un environnement disponible (généralement des simulateurs logiciels tels que AspenPlus ou ProSim). Les ingénieurs en chimie et en procédés qui utilisent ces environnements sont souvent attachés aux modèles qui sont disponibles au sein de leurs outils logiciels, même s'il existe un meilleur choix dans la littérature ouverte. Sinon, le modèle doit être présenté de manière à ce que sa mise en œuvre en interne soit possible.
- L'estimation et la validation des paramètres, en particulier pour les modèles théoriques reposant sur des concepts physiques, doivent encore être améliorées et transparentes afin de garantir des résultats fiables avec les paramètres ainsi que la capacité de régresser de nouveaux paramètres si nécessaire.

- Les modèles avancés, reposant sur des théories physiques, doivent être développés et étendus à davantage d'espèces et de mélanges. En outre, ils devraient être capables de reproduire les propriétés dérivées telles que les capacités thermiques ainsi que les propriétés de transport telles que les viscosités.

Les deux enquêtes mentionnent que l'industrie porte un grand intérêt aux équations d'état (EoS) de la théorie statistique des fluides associés (SAFT), qui provient des travaux de doctorat de Walter Chapman⁴⁻⁷. Cette famille de modèles thermodynamiques offre une base théorique solide, qui tient compte des forces intermoléculaires fortes, telles que la liaison hydrogène, souvent présentes dans les composés associés et polaires. C'est l'une des principales caractéristiques de cette famille de EoS. Cependant, ils soulèvent également plusieurs questions. L'une des principales préoccupations réside dans le nombre de variantes différentes du modèle (SAFT-VR⁸, soft SAFT⁹, GC-SAFT^{10,11}, etc.), ce qui est considéré comme un aspect négatif. Deux versions présentent un intérêt particulier : le modèle SAFT reposant sur la théorie de la perturbation (PC-SAFT)^{12,13} et le modèle SAFT- γ Mie¹⁴ qui ont connu une utilisation accrue dans le cadre industriel. Le modèle SAFT- γ Mie, dans le paramétrage utilise une méthode de contribution de groupes, a fait l'objet de commentaires positifs car *"les modèles d'EoS s'appuyant sur des contribution de groupes sont intrinsèquement plus utiles que les modèles de coefficient d'activité tels que UNIFAC, car ils sont applicables à la fois aux composés purs et aux mélanges"*³.

En ce qui concerne le modèle PC-SAFT, bien qu'il ait connu une utilisation accrue au niveau industriel, bon nombre des défis initiaux présentés par Hendricks et al.² pour la famille SAFT persistent. Ceux-ci incluent :

- La nécessité de disposer de méthodes de caractérisation pour les mélanges complexes, tels que les huiles pétrolières.
- La vitesse de calcul doit être améliorée pour les applications de routine.
- Le manque de bases de données de paramètres de composants purs et de mélanges validées et facilement disponibles.
- La mise en évidence des points forts de la famille SAFT par rapport à d'autres modèles bien connus, notamment les équations cubiques.
- L'extension de ces modèles à la thermodynamique des électrolytes et des polymères.
- La standardisation des modèles SAFT.

En outre, comme l'ont souligné Kontogeorgis et al.³, certaines entreprises restent prudentes vis-à-vis des modèles moléculaires, et en particulier, de ceux qui incluent un terme d'association tel le modèle PC-SAFT. Le problème est double : premièrement, l'implémentation et la documentation du modèle dans les outils actuels de simulation de procédés font défaut. Certaines entreprises ont fait remarquer que "PC-SAFT ralentit tellement les simulations d'Aspen Plus qu'il n'est pas envisageable de l'utiliser en pratique" et que "le modèle PC-SAFT a été grandement amélioré mais sa simplicité d'utilisation reste faible". Bien qu'il existe plusieurs projets open source tels que Clapeyron¹⁵ (implémenté en Julia) ou la bibliothèque PC-SAFT en Python¹⁶ qui adressent le problème de la vitesse de calcul, il arrive souvent que ces outils ne soit pas pris en compte en raison du manque de savoir-faire technique dans les langages de programmation ou parce que le logiciel de simulation est tout simplement plus pratique. Il est bien connu que la principale caractéristique de la famille d'équations SAFT, le terme d'association, introduit une grande complexité mathématique et une augmentation des

paramètres à estimer, ce qui affecte le temps de calcul par rapport à des modèles plus simples (mais néanmoins puissants) tels que les équations d'état cubiques.

Le deuxième problème avec le modèle PC-SAFT (et plus généralement, la famille SAFT) est le manque de standardisation : Kontogeorgis et al.³ ont relevé le sentiment partagé qu'il existe de nombreuses variantes du modèle SAFT et qu'il n'est pas toujours évident de savoir laquelle choisir. De plus, comme l'ont déjà noté Hendricks et al.², il peut arriver que des résultats différents soient obtenus avec des modèles équivalents (comme les différentes versions de SAFT). Ceci est lié au fait que les méthodes d'estimation des paramètres ne sont pas beaucoup explicitées pour ces modèles ou que les paramètres sont adaptés à une étude de cas très spécifique ; applicables à des conditions particulières. Polishuk¹⁷ et Moine et al.¹⁸ ont décrit le problème de normalisation des modèles SAFT comme un manque d'industrialisation. Ils ont défini un modèle comme industrialisé lorsque :

- La méthode pour obtenir les paramètres spécifiques au composé suit une méthodologie transparente et universelle. Cela signifie que l'estimation des paramètres doit être systématique et clairement exposée afin d'obtenir des résultats reproductibles et fiables pour tout composé, à chaque fois que les paramètres du modèle sont estimés.
- Les données numériques sont facilement disponibles, que ce soit dans des bases de données validées ou par le biais de corrélations prédictives. Cela signifie que les exigences pour paramétrer le modèle pour un composé ou un mélange donné (données de propriétés expérimentales, masse molaire, etc.) doivent être facilement accessibles quelle que soit l'espèce chimique traitée.

Les équations de type SAFT ne sont pas considérées comme industrialisées. La raison en est que les paramètres d'entrée, qui sont des paramètres moléculaires spécifiques aux constituants, sont obtenus par ajustement sur des données expérimentales dans la plupart des cas. Cependant, la procédure d'ajustement n'est pas standardisée : certains auteurs peuvent inclure différents types de données expérimentales avec un nombre différent de points de données et des plages de température/pression variables. De plus, comme toutes les variantes de SAFT n'utilisent pas le même nombre de paramètres, le nombre réel d'entrées requises pour chaque membre de la famille SAFT est différent, et l'impact de cette divergence n'est pas souvent pris en compte. En conséquence, les jeux de paramètres d'entrée et les corrélations trouvés dans la littérature diffèrent d'un auteur à l'autre, même lorsqu'ils travaillent avec la même version de SAFT. Ce manque de standardisation est ce qui éloigne les modèles SAFT de l'industrialisation et pose souvent question aux ingénieurs du génie des procédés dans les communautés industrielles et universitaires.

Le premier objectif de cette thèse était de développer une méthodologie d'estimation des paramètres entièrement standardisée dans laquelle des résultats fiables sont obtenus par l'ajustement systématique des paramètres moléculaires SAFT sur des données expérimentales facilement disponibles pour le plus grand nombre possible de composés purs. Cela permettra d'avoir un protocole universel et transparent pour n'importe quel membre de la famille SAFT, ce qui la rendra plus accessible aux industriels et aux universitaires. Le second objectif, qui découle du premier, est de proposer une base de données des paramètres moléculaires SAFT facilement accessible et garantissant des résultats fiables et reproductibles pour un grand nombre d'espèces chimiques associées de différentes natures.

Le troisième objectif de ce travail est d'évaluer le terme d'association de la famille d'équations d'état SAFT, en testant les performances du modèle avec et sans prise en compte de l'association.

La réalisation de ces trois objectifs permettra de répondre aux besoins industriels mentionnés ici pour la famille SAFT d'EoS, avec une méthodologie standardisée d'estimation des paramètres, des bases de données de paramètres fiables et l'exploration des capacités de l'arrière-plan physique du cadre SAFT. Pour ce faire, l'étude commence d'abord par analyser les capacités d'une EoS SAFT à reproduire des composés où aucune association n'est présente (par exemple, les n-alcanes) et quelles propriétés inclure dans l'objectif d'optimisation. Ensuite, la routine de paramétrage est utilisée pour obtenir des paramètres de composés purs pour les composés associés (par exemple, les alcools) sans tenir compte de l'association : Cela permettrait d'obtenir une grande base de données de paramètres de composés purs, fiables et facilement accessibles. Enfin, l'influence du terme associatif est étudiée afin de comprendre sa nécessité dans le cas de composés associés :

Ainsi, cette thèse a abordé les problématiques suivantes :

- I. Comment paramétrer les modèles SAFT de manière standardisée et universelle afin que les composés non-associés puissent être décrits de manière fiable ? Quelles propriétés sont nécessaires pour garantir que l'objectif de minimisation est atteint ?
- II. Comment se comporte un modèle sans terme d'association lorsqu'il est appliqué à des composés associés utilisant un protocole de paramétrage standardisé ?
- III. Quel est l'impact du terme d'association sur les composés purs auto-associés dans le cadre des modèles SAFT ?

Enfin, cette thèse étudiera la capacité d'un modèle thermodynamique prédictif, l'équation de Peng-Robinson munie règles de mélange universelles et combinée à un modèle de type UNIFAC (UMR-PRU)^{19,20}, à reproduire une base de données thermodynamiques expérimentales de référence pour 200 mélanges binaires²¹.

Plan de la thèse

Cette thèse se compose de sept chapitres, présentant, en premier lieu, le contexte général des modèles thermodynamiques, et en particulier celui des équations d'état, et se poursuivant par une description détaillée des méthodologies et des résultats utilisés afin d'apporter des réponses aux problématiques abordées. La thèse est divisée en deux parties : les chapitres 1 à 5 traitent du paramétrage des modèles de type SAFT pour les composés non-associés et auto-associés, tandis que les chapitres 6-7 présentent la base de données de référence pour la comparaison des modèles thermodynamiques et l'évaluation des performances du modèle UMR-PRU. Les chapitres sont organisés comme suit :

- **Chapitre 1:** il propose une brève description du problème de l'équilibre de phases, des différents types d'équations d'état existantes et s'intéresse en particulier) la famille des équations d'état de type SAFT. Il se conclut par une description plus détaillée du problème de l'industrialisation des modèles SAFT.

- **Chapitre 2**: il présente le travail de recherche consacré au développement d'une méthodologie standardisée de paramétrage pour les équations d'état SAFT, y compris l'analyse des propriétés expérimentales à inclure dans les procédures d'ajustement et les résultats obtenus lors de l'application de la procédure à des composés non-associés.
- **Chapitre 3**: il présente une description de l'association chimique, incluant la définition de la liaison hydrogène. Il décrit ensuite la méthodologie utilisée pour déterminer le caractère associé d'un composé pur ; la nouvelle méthodologie de paramétrage des modèles SAFT sans terme d'association est ensuite appliquée à des composés associés. Ce travail induit la construction préalable d'une base de données de paramètres SAFT pour 1800 composés purs incluant à la fois les espèces non-associées et auto-associées. Le chapitre se conclut par une analyse de la performance de l'équation PC-SAFT pour tous les composés de la base de données mentionnée précédemment.
- **Chapitre 4** : il présente une description détaillée des schémas d'association utilisés dans les modèles SAFT, ainsi qu'une revue de la littérature sur la sélection des schémas et les méthodes de paramétrage pour les composés auto-associés.
- **Chapitre 5** : il présente l'analyse de l'impact du terme d'association des modèles SAFT sur la reproduction des propriétés des composés purs en étendant la méthodologie de paramétrage proposée au chapitre 2.
- **Chapitre 6** : présente le travail effectué dans le cadre du développement d'une base de données de référence pour comparer les modèles thermodynamiques. Il est donné sous la forme d'une présentation de l'article publié.
- **Chapitre 7** : présente les résultats et l'analyse du benchmarking de l'équation UMR-PRU ainsi que sa comparaison avec d'autres modèles qui ont déjà été évalués en utilisant la base de données expérimentale des mélanges binaires décrite au chapitre 6.

Enfin, le manuscrit se termine par des conclusions générales et des perspectives concernant les travaux futurs sur les modèles SAFT en ce qui concerne le terme d'association, les schémas d'association et l'extension aux mélanges.

**Chapter 1 : Industrialization of equations of state:
status of the statistically associating fluid theory
(SAFT) framework**

Most chemical engineering applications must deal with the phase equilibrium problem, particularly separation processes (such as distillation, adsorption, absorption, evaporation, etc.) where two or more phases are in contact and reach a state of equilibrium in which the net transfer of matter, heat and work is null between them. These processes usually involve multicomponent systems, which add another layer of complexity to them. Chemical engineers are in need then of a method to describe the conditions in which these applications are carried out, including the pressure, temperature and composition of each chemical species in each phase present in their application at hand. It is therefore necessary to obtain models that can deal with the phase equilibrium problem on a wide range of conditions and a large set of chemical species in order to describe accurately the conditions or states of their applications. In addition, thermodynamic models enable to estimate the energy flow of single or multicomponent systems in chemical processes. They are the essential tool to calculate energy, entropy, and exergy balances independently of the number of phases present in the process. Therefore, they become a powerful tool when describing systems either in phase equilibrium or outside of it, which in turn allows chemical engineers to modify, optimize and control any of the number of operations mentioned.

1.1. The phase equilibrium problem

The phase equilibrium problem has been well-described in the past and a thorough discussion can be found in the respective publications^{22,23}. Consider a system in which two phases are in contact as shown in **Figure 1.1**.

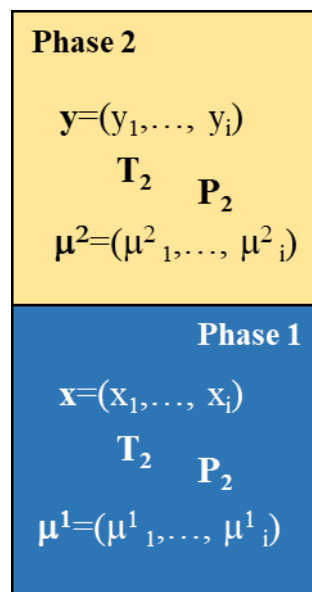


Figure 1.1.Diagram of a two-phase multicomponent system.

In order to completely characterize the intensive state of the system phases, a number of independent and intensive phase properties must be specified according to Gibbs phase rule

$$N^\circ \text{ of independent properties} = N^\circ \text{ of components} + 2 - N^\circ \text{ of phases in equilibrium} \quad (1.1)$$

For the system shown previously (a particular case of a binary system in 2-phase equilibrium), the number of intensive phase properties that must be specified is two. Thus either pair of combination from x_i, y_i, T and P must be specified in order to find the other two and fully describe the system. The phases of a system are considered in equilibrium if three conditions are met:

- There must not be heat transfer between the phases. Consequently, all phases must have the same temperature. This is the **thermal equilibrium condition**.
- There must not be transfer of mechanical work between the phases. In consequence, the pressure must be the same in all phases. This is the **mechanical equilibrium condition**.
- There must not be matter transfer between the phases; therefore, the chemical potential (the partial molar Gibbs energy) of each species must remain the same in all phases. This is the **diffusive equilibrium condition**.

In order to solve the phase equilibrium problem through the framework of thermodynamics we must have a mathematical framework that allows us to describe the phases in equilibrium. It should be noted that one of the most common phase equilibrium problem faced by process engineers is the vapor-liquid equilibrium (VLE), meaning that a liquid and a gaseous phase will be at equilibrium for a given system.

There are two approaches that can be used to solve the phase equilibrium problem for a system at VLE. The first one is known as the **gamma-phi approach** ($\gamma - \phi$), in which an **activity coefficient model** is used to describe the properties of the liquid phase while an **equation of state** is used to describe the gas phase properties. This approach is useful when working below the critical region (i.e. the temperature is below the lowest vapor-liquid critical temperature of each component of the mixture and the pressure is below the lowest vapor-liquid critical pressure of each component in of the mixture). It can be used to describe mixtures containing any type of compounds, including polar (e.g. ketones), non-polar/non-associating (e.g. alkanes) or associating (e.g. alcohols) species.

The second method is known as the **phi-phi approach** ($\phi - \phi$) in which the properties of both liquid and gas phases are described by using the same **pressure-explicit** equation of state. This approach is useful for describing subcritical and supercritical fluid states. It is often said that the weakness of this approach is that most equations of state are limited to barely polar (e.g. ethers) and non-associating compounds (e.g. alkanes). However, some equations of state are said to have high capacity of describing polar and associating pure compounds and mixtures. One family of said equations is the **Statistical Associating Fluid Theory (SAFT) family** of equations of state, which will be described in upcoming sections.

According to these approaches, the two-phase equilibrium relation is described by using any of the following expressions, resulting from equating the expressions of chemical potential of component i in the two phases at equilibrium:

$$\text{Phi-phi approach: } x_i \phi_{i,\alpha}(T, P, \mathbf{x}) = y_i \phi_{i,\beta}(T, P, \mathbf{y}) \quad (1.2)$$

$$\text{Gamma-phi approach: } P_i^{sat}(T) x_i \gamma_{i,liq}(T, P, \mathbf{x}) = P y_i C_i(T, P, \mathbf{y}) \quad (1.3)$$

In Eq. (1.2), \mathbf{x} and \mathbf{y} are the mole fraction vectors in the α and β phases respectively (e.g., liquid and vapor phase or two liquid phases in equilibrium), $\varphi_{i,\alpha}$ and $\varphi_{i,\beta}$ are the fugacity coefficients in the α and β phases for component i . This expression is commonly referred to as the phase equilibrium condition through the φ - φ approach.

For Eq.(1.3), assuming that the two phases in equilibrium are liquid and vapor, $\gamma_{i,liq}$ is the activity coefficient of component i in the liquid phase. The function C_i is given by:

$$C_i(T, P, \mathbf{y}) = \frac{\varphi_{i,vap}(T, P, \mathbf{y})}{\varphi_{i,vap}^*(T, P_i^{sat})} \exp\left(\frac{1}{RT} \int_P^{P_i^{sat}} v_{i,liq}^*(T, P) dP\right) \quad (1.4)$$

Where $\varphi_{i,vap}$ is the fugacity coefficient for component i in the gas phase, $\varphi_{i,vap}^*$ is the fugacity coefficient of pure component i in a saturated-gas phase at T (and thus, at $P_i^{sat}(T)$), $v_{i,liq}^*$ is the pure-liquid molar volume of component i which can be estimated through the use of correlations. The exponential part of Eq. (1.4) is known as the **Poynting factor**²⁴. Eq. (1.3) is commonly referred to as the vapor-liquid equilibrium condition through the γ - φ approach.

For the γ - φ approach, a family of thermodynamic models known as **activity coefficient models** or **excess Gibbs energy models** are used to describe the liquid phase while another family of thermodynamic models known as **equations of state (EoS)** are used for the gas phase. For the φ - φ approach, **EoS** are used to describe both phases. This dissertation will be focusing on the latter, as it is the core of the work presented here, thus the reader is referred to the literature^{25,26} for a deeper look into activity coefficient models and their expressions.

In chemical engineering thermodynamics, an **EoS** is a mathematical equation that relates a **state variable** or **state property** to some others (e.g. $P(T, v)$ or $U(T, P)$) which allows, at least, to estimate the change of different **state functions**. An EoS relating the variables **pressure** (P), **temperature** (T) and **volume** (V) of a pure component is referred to as a **volumetric EoS**²⁴.

There are two main categories of volumetric EoS: **pressure-explicit EoS** and **volume-explicit EoS**.

Pressure-explicit EoS are those in which the pressure is related to the temperature, the molar volume and the composition (described, e.g., by \mathbf{z} , the vector of component mole fractions) of a given phase, as $P = f(T, v, \mathbf{z})$. They can be used to describe gas or liquid phases or diphasic vapor-liquid equilibrium. These EoS include:

- The **virial expansion** of the pressure, used for gases (in particular the truncated version of the virial EoS, where the EoS is truncated at the first or second order, enabling it to describe gas phases),
- **Cubic Equations of State (CEoS)**, applicable to liquid or gas phases or systems in vapor-liquid equilibrium,
- The **Statistical Associating Fluid Theory (SAFT)** EoS, applicable to liquid or gas phases or systems in vapor-liquid equilibrium and
- Compound-specific EoS such as the Span-Wagner²⁷ or the GERG equations^{28,29} which are applicable to liquid or gas phases or systems in vapor-liquid equilibrium.

Volume-explicit EoS are those in which the molar volume is related to the temperature, the pressure and the composition in the form $v = f(T, P, z)$. They are limited to describe single-phase states (exclusively gas phases) and cannot predict phase equilibrium because at a given T and P they can only predict a single molar volume.

Coming back to Eq. (1.2), a relation must be established in order to calculate the fugacity coefficients of each component. To attain them two equivalent expressions may be used:

$$\ln \varphi_i = \frac{1}{RT} \int_0^P \left[\left(\frac{\partial V}{\partial n_i} \right)_{T, P, n_{j \neq i}} - \frac{RT}{P} \right] dP \quad (1.5)$$

$$\ln \varphi_i = \frac{1}{RT} \int_V^\infty \left[\left(\frac{\partial P}{\partial n_i} \right)_{T, V, n_{j \neq i}} - \frac{RT}{V} \right] dV - \ln \left(\frac{PV}{nRT} \right) \quad (1.6)$$

Eq. (1.5) is best suited for calculating the fugacity coefficient for volume-explicit EoS. In turn, Eq. (1.6) is best adapted for pressure-explicit EoS. In these equations n_i is the number of moles for a given component i , in a phase, V is the total volume of a phase, R is the universal gas constant and z is the molar compressibility factor, which can be written as a function of T and P or as a function of T and v , depending on whether a pressure-explicit or volume-explicit EoS is used:

$$\text{For a volume-explicit EoS: } z \equiv \frac{P \cdot v(T, P)}{RT} = F_p(T, P) \quad (1.7)$$

$$\text{For a pressure-explicit EoS: } z \equiv \frac{P(T, v) \cdot v}{RT} = F_v(T, v) \quad (1.8)$$

In the γ - φ approach, the gas phase can be described using either a volume-explicit or a pressure-explicit EoS. On the contrary, the φ - φ approach requires the use of a pressure-explicit EoS. The choice of an EoS depends mainly on the temperature and pressure regions studied and the chemical nature of the components of the mixture.

The discussion will proceed to present some of the most popular EoS used in both literature and industry. Among these EoS, the SAFT family of EoS, which are the focal point of this dissertation, will be explained with more detail.

1.2. The virial equation of state

The virial equation of state is a polynomial series of the molar compressibility factor (denoted z) in pressure or inverse molar volume $\rho = 1/v$ that have temperature-dependent coefficients for a given pure fluid. The expressions for both forms for the initial terms are:

$$z(T, P) = 1 + B(T) \cdot \left(\frac{P}{RT} \right) + [C(T) - [B(T)]^2] \left(\frac{P}{RT} \right)^2 + \dots \quad (1.9)$$

$$z(T, v \text{ or } \rho) = 1 + \frac{B(T)}{v} + \frac{C(T)}{v^2} + \dots = 1 + B(T) \cdot \rho + C(T) \cdot \rho^2 + \dots \quad (1.10)$$

Where B is the second virial coefficient, C is the third virial coefficient and so on and so forth. According to Eq.(1.10), the second virial coefficient is defined as:

$$B = \lim_{\rho \rightarrow 0} \left(\frac{\partial z}{\partial \rho} \right)_T \quad (1.11)$$

In the same fashion, the third virial coefficient can be defined as:

$$C = \lim_{\rho \rightarrow 0} \frac{1}{2!} \left(\frac{\partial^2 z}{\partial \rho^2} \right)_T \quad (1.12)$$

1.3. Cubic equations of state

Cubic equations of state (CEoS) are the most widespread used analytical pressure-explicit EoS. They receive the adjective *cubic* because at a given T , P , the molar volume is found as a solution to a third-degree polynomial equation. They are derived from Van der Waals theory³⁰ and have been studied for over a century and a half. For a pure fluid the general form for CEoS can be expressed as:

$$P = \frac{RT}{v-b} - \frac{a(T)}{v^2 + uv + wb^2} \quad (1.13)$$

Where the parameter a is a measure of the attractive forces between molecules; b is the covolume parameter, which aims to correct the perfect-gas law to the fact that molecules have a non-zero effective volume; the constants u and w are either universal real numbers or compound-dependent variables³¹.

The temperature dependent $a(T)$ is often written as:

$$a(T) = a_c \alpha(T) \quad (1.14)$$

Which is the product of the value of the attractive term of the EoS at the critical temperature (a_c) and the temperature-dependent alpha function ($\alpha(T)$). The form of Eq. (1.14) allows the

determination of a_c , b and the critical molar volume (v_c) by applying the so-called critical constraints³²:

$$\begin{cases} P(T_{c,exp}, v_{c,EoS}) = P_{c,exp} \\ \left(\frac{\partial P}{\partial v} \right)_{T=T_{c,exp}, v=v_{c,EoS}} = 0 \\ \left(\frac{\partial^2 P}{\partial v^2} \right)_{T=T_{c,exp}, v=v_{c,EoS}} = 0 \end{cases} \quad (1.15)$$

Where $T_{c,exp}$ and $P_{c,exp}$ are the experimental critical temperature and pressure and $v_{c,EoS}$ is the critical molar volume calculated by the CEoS at the critical temperature and pressure. The values for the critical attractive energy parameter and the covolume are then expressed in terms of the **universal constants** Ω_a and Ω_b :

$$\begin{cases} a_c = \Omega_a \frac{R^2 T_{c,exp}^2}{P_{c,exp}} \\ b = \Omega_b \frac{RT_{c,exp}}{P_{c,exp}} \end{cases} \quad (1.16)$$

The values of Ω_a and Ω_b depend on the version of the CEoS used, as they depend on the value of u and w . Another consequence of this equation-dependency is the value of the critical molar compressibility factor (z_c). An overview of these differences is highlighted in **Table 1.1**, which includes the most popular versions of the CEoS.

Table 1.1. Summary of the van der Waals, Soave-Redlich-Kwong and Peng-Robinson cubic equations of state with their internal expressions and the value of the critical compressibility factor. u and w taken from Pina-Martinez et al.³¹

EOS	FORM	INTERNAL EXPRESSIONS
Van der Waals (vdW) EoS ³⁰	$P = \frac{RT}{v-b} - \frac{a_c}{v^2}$	$u = w = 0$
		$a_c = \frac{27 R^2 T_{c,exp}^2}{64 P_{c,exp}}$
		$b = \frac{1 RT_{c,exp}}{8 P_{c,exp}}$
		With:
		$z_c = \frac{3}{8}$
Soave-Redlich-Kwong (SRK) EoS ³³	$P = \frac{RT}{v-b} - \frac{a(T)}{v(v-b)}$	$u = 1$
		$w = 0$
		$a(T) = \text{Eq.}(1.14)$

EOS	FORM	INTERNAL EXPRESSIONS
		$\alpha(T) = \left[1 + m \left(1 - \sqrt{T/T_c} \right) \right]^2$ $m = 0.480 + 1.574\omega_{exp} - 0.176\omega_{exp}^2$ $\begin{cases} a_c \\ b \end{cases} = \text{Eq. (1.16)}$ $\Omega_a = \frac{1}{9(\sqrt[3]{2} - 1)} \approx 0.42748$ $\Omega_b = \frac{\sqrt[3]{2} - 1}{3} \approx 0.08664$ <p style="text-align: center;">With:</p> $z_c = \frac{1}{3}$
		$u = 2$ $w = -1$ $a(T) = \text{Eq. (1.14)}$ $\alpha(T) = \left[1 + m \left(1 - \sqrt{T/T_c} \right) \right]^2$ $m = 0.437464 + 1.54226\omega_{exp} - 0.26992\omega_{exp}^2$ $\begin{cases} a_c \\ b \end{cases} = \text{Eq. (1.16)}$ $\Omega_a = \frac{8(5X + 1)}{49 - 37X} \approx 0.45724$ $\Omega_b = \frac{X}{X + 3} \approx 0.0778$ $X = \left[1 + \sqrt[3]{4 - 2\sqrt{2}} + \sqrt[3]{4 + 2\sqrt{2}} \right]^{-1} \approx 0.25308$ <p style="text-align: center;">With:</p> $z_c = \frac{1}{X + 3} \approx 0.3074$
Peng-Robinson (PR) EoS³⁴	$P = \frac{RT}{v - b} - \frac{a(T)}{v(v + b) + b(v - b)}$	

It is well-acknowledged that the alpha function has great influence on the prediction of vapor-liquid equilibrium (VLE) properties such as the vapor pressure, the enthalpy of vaporization or the saturated liquid heat capacity³¹. Furthermore, Le Guennec et al.³⁵ stressed on the importance of the alpha function not only in the VLE region, but also on the pure-compound supercritical properties.

For this reason, a careful selection of the alpha function is crucial to have accurate results with any CEoS. Le Guennec et al.³⁵ developed a consistency test to evaluate alpha functions which guarantees safe extrapolation to the supercritical region without the need of adding any further parameters or constraints to the regression procedure. They showed in their work that a proper alpha function must simultaneously satisfy the following constraints:

$$\text{For all } T : \begin{cases} \alpha \geq 0 \text{ and } \alpha(T) \text{ continuous} \\ \frac{d\alpha}{dT_r} \leq 0 \text{ and } \frac{d\alpha}{dT_r} \text{ continuous} \\ \frac{d^2\alpha}{dT_r^2} \geq 0 \text{ and } \frac{d^2\alpha}{dT_r^2} \text{ continuous} \\ \frac{d^3\alpha}{dT_r^3} \leq 0 \end{cases} \quad (1.17)$$

In brief, an alpha function must be positive and continuous at any temperature value (line 1 of Eq. (1.17)); the first derivative with respect to temperature must exist and be continuous and the alpha function must decrease monotonically ($\frac{d\alpha}{dT_r} \leq 0$) at any temperature value (line 2 of Eq. (1.17)); the second of the alpha function derivative with respect to temperature must also exist and be continuous and the alpha function must be convex ($\frac{d^2\alpha}{dT_r^2} \geq 0$) at any temperature value (line 3 of Eq. (1.17)) and the third derivative with respect to temperature must be negative or zero at any temperature value (line 4 of Eq. (1.17)). Any CEoS that utilizes an alpha function which meets all the conditions of Eq. (1.17) can guarantee accurate and physically meaningful descriptions of pure compounds and mixtures at both the subcritical and supercritical regions. **Table 1.2** shows four alpha functions tested by Le Guennec et al.³⁵ in their work and the conditions to make them consistent.

Table 1.2. Alpha-function expressions and consistency conditions as tested and shown by Le Guennec et al.³⁵

α -FUNCTION	EXPRESSION	CONSISTENCY CONDITIONS
Trebble-Bishnoi ³⁶	$\alpha(T) = \exp[L(1 - T/T_c)]$	$L \geq 0$
Melhem-Saini-Goodwin ³⁷	$\alpha(T) = \exp[m(1 - T/T_c) + n(1 - \sqrt{T/T_c})^2]$	$m \geq n \geq 0$
Twu (1988) ³⁸	$\alpha(T) = (T/T_c)^{2(M-1)} \exp[L(1 - (T/T_c)^{2M})]$	$LM \geq 0$ $M \leq 0.8909$
Twu(1991) ³⁹	$\alpha(T) = (T/T_c)^\delta \exp[L(1 - (T/T_c)^\gamma)]$	$\begin{cases} \delta \leq 0 \\ L\gamma \geq 0 \text{ or} \\ \gamma \leq 1 - \delta \end{cases}$ $\begin{cases} \delta \leq 0 \\ L\gamma \geq 0 \\ \gamma \leq 1 - 2\delta + 2\sqrt{\delta(\delta - 1)} \\ 4Y^3 + 4ZX^3 + 27Z^2 - 18XYZ - X^2Y^2 \geq 0 \end{cases}$ Where

α -FUNCTION	EXPRESSION	CONSISTENCY CONDITIONS
		$\begin{cases} X = -3(\gamma + \delta - 1) \\ Y = \gamma^2 + 3\delta\gamma - 3\gamma + 3\delta^2 - 6\delta + 2 \\ Z = -\delta(\delta^2 - 3\delta + 2) \\ \delta = N(M - 1) \\ \gamma = MN \end{cases}$

One notable weakness of CEoS lies on their ability to reproduce volumetric properties, such as the molar liquid density at saturation (ρ_{liq}^{sat}) as pointed out in the past by several authors^{24,40,41}. For instance, the SRK and the PR EoS predict ρ_{liq}^{sat} with an average deviation of 16% and 8% respectively⁴¹. Given the importance of this property for industry applications as pipeline design or in the calculation of transport properties such as viscosity or surface tension, which require the liquid phase density, an accurate description of the volumetric properties is required.

To this end, a method for correcting the volumetric properties calculated by CEoS was proposed by Peneloux et al.⁴² (although it was later implemented in other EoS such as the PC-SAFT as done in the work of Moine et al.¹⁸) by applying the concept of **volume translation**. The idea is to correct or *translate* the calculated molar volumes (therefore densities) by a constant quantity often referred to as **volume correction parameter** or **volume translation parameter**, symbolized by c . This correction significantly improves the performance of CEoS calculating liquid densities as long as the reduced temperature is below 0.9³². For a CEoS with molar volume v and covolume b , the translated volume v_{trans} and covolume b_{trans} are:

$$\begin{cases} v_{trans} = v - c \\ b_{trans} = b - c \end{cases} \quad (1.18)$$

For the PR CEoS, in which $u = 2$ and $w = -1$ in Eq. (1.13), the translated EoS, when including Eq. (1.18), becomes:

$$P = \frac{RT}{v_{trans} - b_{trans}} - \frac{a(T)}{(v_{trans} + c)^2 + 2[b_{trans}v_{trans} + b_{trans}c + v_{trans}c + c^2] - (b_{trans} + c)^2} \quad (1.19)$$

Figure 1.2 illustrates the effect of including Eq. (1.18) into Eq. (1.13).

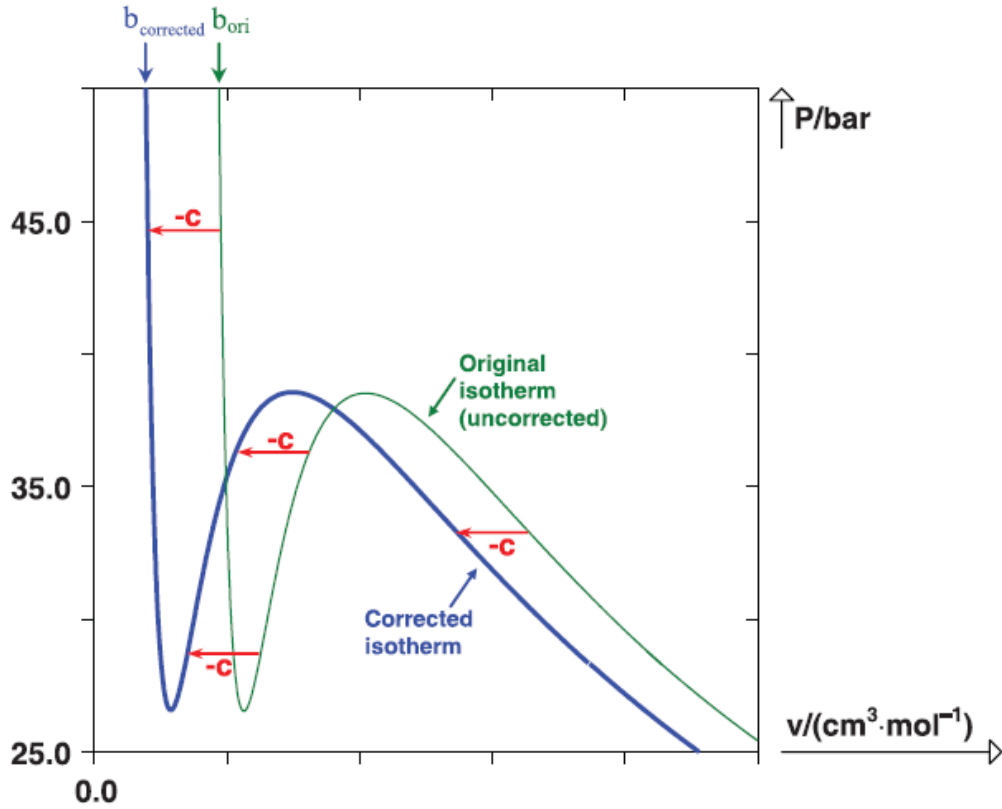


Figure 1.2. Illustration of the volumetric translation concept. Taken from Jaubert & Privat²⁴ ISBN: 978-1-78548-209-0.

It is important to note that c must be temperature-independent to avoid certain non-physical phenomena to be calculated by the CEoS, such as crossing isotherms in the pressure-volume diagram or negative heat capacities as pointed out by Jaubert & Privat²⁴.

A second important remark regarding c is that it is not universal, meaning that it must be estimated for each component studied with the chosen EoS. For any given compound, c is calculated to reproduce exactly an experimental saturated liquid molar volume at a reference temperature (T_{ref}):

$$c = v_{liq,EoS}^{sat}(T_{ref}) - v_{liq,exp}^{sat}(T_{ref}) \quad (1.20)$$

Where $v_{liq,EoS}^{sat}(T_{ref})$ is the molar volume calculated by the EoS at the reference temperature.

1.3.1. Influence of a consistent alpha function and a volume translation on CEoS

One interesting observation found out by several authors^{32,41} about the volumetric translation is the fact that the accuracy of phase equilibrium properties (vapor pressure, enthalpy of vaporization, heat capacities at saturation, etc.) do not change at all because these properties are not affected by volume translation.

From this point of view, it would seem desirable to add volume translation to a CEoS to make up for its weakness in the molar volume department, while a consistent alpha function should be included to guarantee safe and physically sound results. **Table 1.3** shows the influence of selecting a Twu91 alpha function³⁹ as suggested by Le Guennec et al.³² and performing a volume translation where c is calculated to a reference reduced temperature of 0.8 over the PR EoS. The original version of the PR is included for the sake of comparison.

Table 1.3. Effect of using a consistent alpha-function and volume translation on the mean average percent error (MAPE) on the PR EoS⁴³.

CEoS	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat} ($T_r < 0.9$)	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$
PR ³⁴	2.8%	8.8%	3.1%	7.3%
<i>tc</i>-PR³²	1.0%	2.1%	1.9%	2.5%

$$MAPE_{property} = \frac{100}{N_T} \sum_{i=1}^{N_T} \left| \frac{Property_{i,calc} - Property_{i,exp}}{Property_{i,exp}} \right|$$

It is seen from these results that the vapor pressure, enthalpy of vaporization and liquid heat capacity are greatly improved with the choice of a better alpha function, in this case the Twu91 over the Soave function. On the other hand, and as stated before, the volume translation done to the EoS improves on its capacity of describing liquid molar densities.

We can conclude that CEoS shine due to their simple yet powerful mathematical model. They perform well on phase equilibrium properties and can be further improved by using a consistent alpha function. On the other hand, these EoS struggle to reproduce accurately liquid densities, but one can overcome this fact by using the volume translation method presented here with a temperature-independent volume translation parameter.

1.4. Multiparametric equations of state

Another family of EoS are those tailored to reproduce specific pure compounds (e.g. CO₂) or mixtures (e.g. natural gas mixtures). They offer a very high degree of accuracy for their respective targets, by giving up on the flexibility of species that can be modeled. They usually include a large number of component parameters (generally, more than 40 for describing a pure species), thus giving place to the name **Multiparametric equations of state** (MEoS).

REFPROP⁴⁴ is a software developed by the National Institute of Standards and Technology (NIST) which supports MEoS for 147 pure compounds. Some notable members of this family of EoS include:

- The GERG-2008²⁹ EoS developed for natural gases.
- The Span-Wagner²⁷ EoS used for CO₂.
- The Benedict-Webb-Rubin (BWR) EoS, developed for light hydrocarbons such as methane and ethane.

It is worth noting again that the practical use of these EoS is hindered by the lack of flexibility they possess. In reality, an EoS should not trade off its robustness when it comes to the number of species it can describe, as the impact of its predictions will be severely limited by this factor.

1.5. Statistical associating fluid theory equations of state

The Statistical Associating Fluid Theory (SAFT) family of EoS are a group of non-analytical EoS which follows the works of Chapman et al.^{5,6} and Huang & Radosz^{45,46} in the late 1980s and early 1990s, which proposed their model based upon Wertheim's⁴⁷⁻⁴⁹ Thermodynamic Perturbation Theory (TPT). Since then, for the last three decades, the SAFT family of EoS has gained a lot of popularity. It is often said that one of their strengths is their capability of accurately representing the liquid phase for both associating and non-associating compounds, as well as for a wide variety of systems, including polar systems, polymeric systems and electrolytic systems.

The following section will be dedicated to explaining in detail the SAFT EoS, including its conceptual basis, mathematical expressions and parameters as well as presenting the most popular versions that are currently in use. A special section will be dedicated to one of these versions, the Perturbed Chain SAFT (PC-SAFT) which is the main focus for this work.

1.5.1. The SAFT description of pure fluids

The SAFT model describes pure fluids as a group of hard-spheres that occupy an effective volume and interact with each other whether it is attracting or repulsing. This process is described in two different ways^{6,12,26}, depending on the SAFT version being used:

Process I:

- a) The fluid is assumed to consist of equal sized **hard spheres**.
- b) A **dispersive potential** is added to take into account **attraction** between these spheres (e.g. a square-well or Lennard-Jones potential).
- c) Each sphere is given two or more spots that allow for **chain formation** and thus allowing for chains of hard spheres.
- d) Specific interaction sites are added to particular parts of the chain that account for **highly directional attractive interactions**, such as the **hydrogen bond**, that allow chains to associate through these interactions. In the case of the hydrogen bond, the energy is often taken as a square-well potential.

Process II:

- a) The fluid is assumed to consist of equal sized **hard spheres**.
- b) **Chain formation** is allowed by adding chain sites and forming **hard-sphere chains**.
- c) A **dispersive potential** is added to account **attraction** between the hard-sphere chains.
- d) Specific interaction sites are added to particular parts of the hard-sphere chain to account for **highly directional attractive interactions**, like **hydrogen bonds**.

Figure 1.3 presents an illustration of Process I and Process II, for the sake of conceptual clarity.

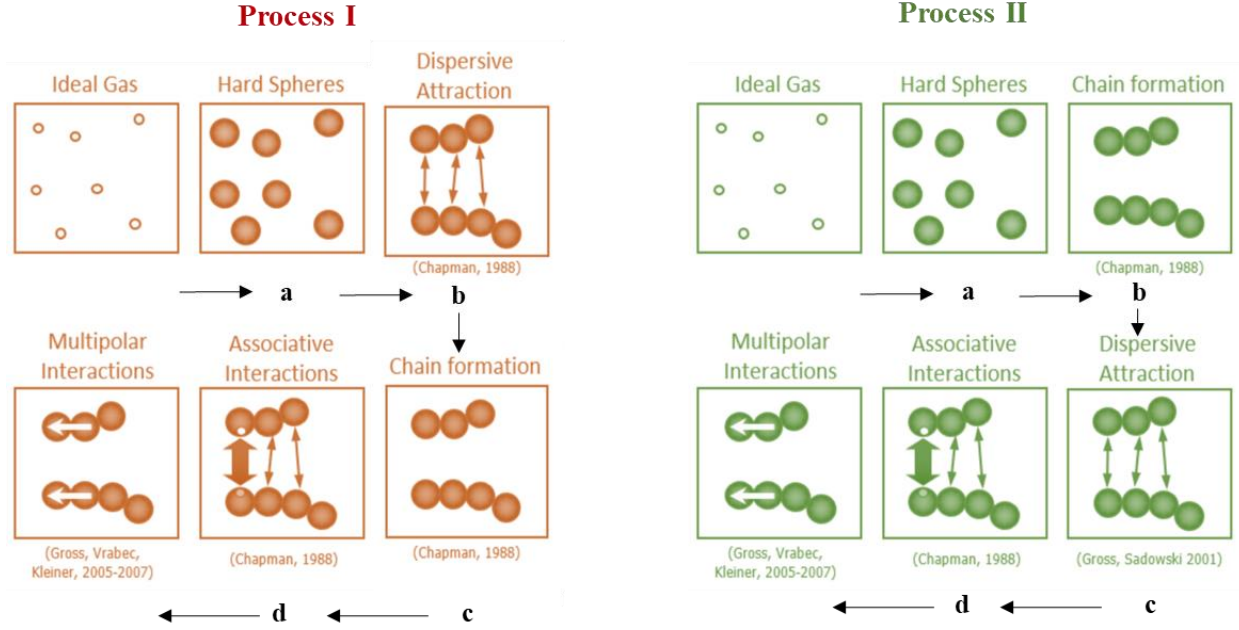


Figure 1.3. Schematics of a molecule formation for the SAFT framework. Left image represents Process I, as described by Chapman et al⁶. Right image represents process II as described by Gross & Sadowski¹². Adapted from: <https://www.itt.uni-stuttgart.de/en/research/>

All the steps mentioned above contribute to the residual Helmholtz energy of the fluid on an additive way. In general, the **residual Helmholtz energy** (a^{res}) can be written as:

$$a^{res} = \underbrace{a^{hs} + a^{disp-hs}}_{\substack{\text{real-segment reference} \\ \text{denoted } a^{seg}}} + a^{chain-rs} + a^{assoc} \quad \text{for Process I} \quad (1.21)$$

$$a^{res} = \underbrace{a^{hs} + a^{chain-hs}}_{\text{hard-chain reference}} + a^{disp-chain} + a^{assoc} \quad \text{for Process II}$$

For Process I, a^{hs} is the **hard-sphere contribution**; $a^{disp-hs}$ is the **dispersive force contribution for the hard spheres**; $a^{chain-rs}$ is the **chain formation contribution of real segments of hard-spheres**. For Process II, the hard-sphere term is the same as Process I; $a^{chain-hs}$ is the **hard-sphere chain formation contribution**; $a^{disp-chain}$ is the **dispersive force contribution for the hard-sphere chains**. For both cases, a^{assoc} is the **contribution coming from associating interactions**.

The main difference across the SAFT EoS that use Process I is found in the dispersive force term, which will be discussed in the following sections. Once the residual Helmholtz energy is calculated, the compressibility factor in Eq. (1.8) is then calculated as a function of a density derivative of a^{res} and thus allowing for the calculations of any of the other thermodynamic properties.

The discussion will proceed by showing the main characteristics of each SAFT version, including the original version^{6,45}, which will include mostly the chain and dispersive terms,

where the associating term will be discussed in general for all SAFT EoS, as the same equations are used regardless of the version, as mentioned before.

1.5.2. The original SAFT and the CK-SAFT EoS

These SAFT EoS consider non-associating fluids as chains of real segments; their formation is described by Process I, mentioned above. Most EoS of the SAFT family use the original chain and associating terms of, albeit with some minor difference in some cases. Given that, the chain formation is the base for the SAFT model, it will be discussed first.

The **chain term** for the original SAFT EoS is given by:

$$\frac{a^{chain-rs}}{RT} = \sum_i x_i (1 - m_i) \ln [g_{ii}(d_{ii})^{hs}] \quad (1.22)$$

Where m_i is the **segment number parameter** for component i ; $g_{ii}(d_{ii})^{hs}$ is the **hard sphere radial distribution function** and d_{ii} is the **hard sphere diameter**, which can be temperature dependent or independent, which varies from one version to another. For the original SAFT, the temperature-dependent diameter is given by:

$$d = \sigma f\left(\frac{k_B T}{\varepsilon}, m\right) \quad (1.23)$$

With

$$f\left(\frac{k_B T}{\varepsilon}, m\right) = \frac{1 + 0.2977\left(\frac{k_B T}{\varepsilon}\right)}{1 + 0.33163\left(\frac{k_B T}{\varepsilon}\right) + f(m)\left(\frac{k_B T}{\varepsilon}\right)^2} \quad (1.24)$$

And

$$f(m) = 0.0010477 + 0.025337\left(\frac{m-1}{m}\right) \quad (1.25)$$

Where σ is the **temperature-independent segment diameter** (or equivalently, the **segment diameter at T = 0 K**), ε is the **characteristic segment dispersive energy** and k_B is the **Boltzmann constant**. It is important to note that in order to perform any sort of calculation with any of the SAFT-type EoS these three parameters must be determined for each **pure compound**, (in general, some versions add one or more parameters to be estimated). They are thus considered the inputs of the SAFT family models.

These three parameters are not defined inherently by the model and thus a value must be assigned to them for each new compound to be able to use any of the SAFT EoS. The process of estimating pure component parameters for an EoS is referred to as **parametrization**. This process has been well-studied for CEoS but has not seen as much attention for the SAFT EoS.

This issue will be addressed in a further section while a deeper look into parametrization of the PC-SAFT for non-associating molecules will be the object of Chapter 2.

The radial distribution function is another commonly shared feature among SAFT versions. The expression for a mixture of hard spheres for $g_{ii}(d_{ii})^{hs}$ is derived from the Carnahan-Starling^{26,50,51} EoS using the expressions proposed by Boublík^{12,52} and Mansoori et al.^{12,53}

$$g_{ii}(d_{ii})^{hs} = \frac{1}{1-\zeta_3} + \left(\frac{d_i d_j}{d_i + d_j} \right) \frac{3\zeta_2}{(1-\zeta_3)^2} + \left(\frac{d_i d_j}{d_i + d_j} \right)^2 \frac{2\zeta_2^2}{(1-\zeta_3)^3} \quad (1.26)$$

Where:

$$\zeta_k = \frac{\pi N_{AV}}{6} \rho \sum_i x_i m_i d_{ii}^k; \quad (1.27)$$

$$k = 0, 1, 2, 3$$

The **segment term** presented in Eq. (1.21) is more precisely written as:

$$a^{seg} = a_0^{seg} \sum_i x_i m_i \quad (1.28)$$

Where the zero subscript indicates a non-chained segment. a_0^{seg} is given by:

$$a_0^{seg} = a_0^{hs} + a_0^{disp} \quad (1.29)$$

The **hard-sphere term** is given by the Carnahan-Starling⁵⁰ equation:

$$\frac{a_0^{hs}}{RT} = \frac{4\eta - 3\eta^2}{(1-\eta)^2} \quad (1.30)$$

Where η is the **reduced density** which corresponds to Eq. (1.27) for $k = 3$.

The **dispersion term** used by Chapman et al.⁶ was estimated by using a reference EoS for argon on different compounds. This term is given by:

$$a_0^{disp} = \frac{\varepsilon R}{k_B} \left(a_{01}^{disp} + \frac{a_{02}^{disp-hs}}{T_R} \right) \quad (1.31)$$

There is another SAFT version also referred to as “the original SAFT”, which is the one proposed by Huang & Radosz⁴⁵, which follows the original work done by Chapman et al.⁶. In this version, two differences are present in both the hard-sphere and dispersive contributions. For the hard-sphere term, the full Carnahan-Starling equation for the hard-sphere mixture reference system is employed:

$$\frac{a_0^{hs}}{RT} = \frac{1}{\zeta_0} \left[\frac{3\zeta_1 \zeta_2}{1-\zeta_3} + \frac{\zeta_2^3}{\zeta_3(1-\zeta_3)^2} + \left(\frac{\zeta_2^3}{\zeta_3^2} - \zeta_0 \right) \ln(1-\zeta_3) \right] \quad (1.32)$$

The dispersion term, is based on simulation data for square-well fluids:

$$\frac{a_0^{disp-hs}}{RT} = \sum_i \sum_j D_{ij} \left(\frac{u}{k_B T} \right)^i \left(\frac{\eta}{\tau} \right)^j \quad (1.33)$$

Where D_{ij} are universal constants and u is the **temperature-dependent energy parameter** (which is used instead of the segment energy parameter). Another slight difference is that the segment size parameter is replaced by a **volume parameter** v^∞ defined as

$$v^\infty = \frac{\pi N_{AV} \sigma^3}{6\tau} \quad (1.34)$$

Where τ is the highest possible packing fraction for a system comprised of pure hard spheres. This SAFT is often referred to as CK-SAFT due to the use of the universal constants D_{ij} and the volume parameter which were both proposed by Chen & Kreglewski⁵⁴.

1.5.3. The SAFT-VR EoS

This SAFT EoS considers non-associating fluids as chains of real segments; their formation is described by Process I, mentioned above.

Gil-Villegas et al.⁸ used the CK-SAFT as their base for their model but proposed a modified dispersive contribution based on a **square-well potential**. This change introduced a new pure compound parameter: the **width** of the square well (λ). The range of attraction of a chain segment changes with λ , thus constructing an EoS which accounts for attraction at different ranges in the potential. Thus, they introduced their SAFT for chain molecules with attractive potentials of variable range EoS, commonly referred to as Variable Range SAFT or SAFT-VR. This additional parameter offered the SAFT EoS greater flexibility for describing pure components.

The **dispersive contribution** to a^{res} is given by the expression:

$$a^{disp-hs} = \frac{a_1}{k_B T} + \frac{a_2}{(k_B T)^2} \quad (1.35)$$

The coefficient a_1 is given by:

$$a_1 = -\rho \sum_i \sum_j x_{s,i} x_{s,j} \alpha_{ij}^{VDW} g^{HS} [\sigma_k; \zeta_k^{eff}] \quad (1.36)$$

Where the subscript s refers to **segment properties**. The **Van der Waals attractive constant** α_{ij}^{VDW} is given by:

$$\alpha_{ij}^{VDW} = \frac{2\pi \epsilon_{ij} \sigma_{ij}^3 (\lambda_{ij}^3 - 1)}{3} \quad (1.37)$$

g^{HS} corresponds to the **radial distribution function** presented in Eq. (1.26) but with the following modified arguments:

$$\zeta_k^{eff} = c_1 \zeta_k + c_2 \zeta_k^2 + c_3 \zeta_k^3 \quad (1.38)$$

$$\sigma_x^3 = \sum_i \sum_j x_{s,i} x_{s,j} \sigma_{ij}^3 \quad (1.39)$$

$$\zeta_k = \frac{\pi}{6} \rho_s \sigma_k^3 \quad (1.40)$$

The c_i constants are a functions of λ and their values can be found in the original publication⁸. The second order term a_2 obtained by deriving the first order a_1 with respect to the segment density:

$$a_2 = \sum_i \sum_j x_{s,i} x_{s,j} \frac{1}{2} K_{HS} \varepsilon_{ij} \rho_s \frac{\partial a_1}{\partial \rho_s} \quad (1.41)$$

Where K_{HS} is the **hard-sphere isothermal compressibility** given by:

$$K_{HS} = \frac{\zeta_0 (1 - \zeta_3)^4}{\zeta_0 (1 - \zeta_3)^2 + 6\zeta_1 \zeta_2 (1 - \zeta_3) + 9\zeta_2^3} \quad (1.42)$$

A follow-up version of the SAFT-VR was later introduced by Lafitte et al.⁵⁵ by changing the square-well potential to a **Mie potential** (generalized Lennard-Jones Potential). This change introduces two parameters instead of one: the attractive (λ^a) and repulsive (λ^r) exponents of the Mie potential, which is given by:

$$u^{Mie}(r) = C \varepsilon \left[\left(\frac{\sigma}{r} \right)^{\lambda^r} - \left(\frac{\sigma}{r} \right)^{\lambda^a} \right] \quad (1.43)$$

$$C = \frac{\lambda^r}{\lambda^r - \lambda^a} \left(\frac{\lambda^r}{\lambda^a} \right)^{\frac{\lambda^r}{\lambda^r - \lambda^a}}$$

Introducing this new potential changes the expressions of the first and second order perturbation terms presented in Eqs. (1.36) and (1.41). The first order term a_1 becomes:

$$a_1^{Mie} = C \left[-a_1^S(\eta_{eff}, \lambda_2) + a_1^S(\eta_{eff}, \lambda_1) \right] \quad (1.44)$$

Where a_1^S is the mean attractive energy for a Sunderland- λ system evaluated for the effective packing fraction η_{eff} given by

$$\left\{ \begin{array}{l} a_1^S(\eta_{BH}, \lambda) = a_1^{vDW}(\eta_{BH}, \lambda) g^{hs}(1, \eta_{eff}(\eta_{BH})) \\ a_1^{vDW}(\eta_{BH}, \lambda) = -4\eta_{BH} \varepsilon \left(\frac{3}{\lambda - 3} \right) \\ g^{hs}(1, \eta_{eff}(\eta_{BH})) = \frac{1 - 0.5\eta_{eff}(\eta_{BH})}{(1 - \eta_{eff}(\eta_{BH}))^3} \end{array} \right. \quad \text{for } 3 < \lambda \leq 12 \quad (1.45)$$

Where the effective packing fraction is given by:

$$\left\{ \begin{array}{l} \eta_{eff}(\eta, \lambda) = c_1 \eta_{BH} + c_2 \eta_{BH}^2 \\ \eta_{BH} = \pi \sigma_{BH}^3 \rho_s / 6 \\ \sigma_{BH}(T) = \int_0^r \left[1 - \exp\left(\frac{-u^{Mie}}{k_B T}\right) \right] dr \end{array} \right. \quad (1.46)$$

The subscript *BH* denotes that the term is described by the Barker and Henderson perturbation theory⁵⁶. The second order term a_2 for a system with the Mie potential is given by:

$$\left\{ \begin{array}{l} a_2^{Mie} = \frac{C}{2} \varepsilon K_{HS} \eta_{BH} \frac{\partial a_1^S(\eta_{BH}, \lambda)}{\partial \eta_{BH}} \\ K_{HS} = \frac{(1 - \eta_{BH})^4}{1 + 4\eta_{BH} + 4\eta_{BH}^2} \end{array} \right. \quad \text{for } \lambda_2 > 6 \quad (1.47)$$

The dispersive contribution to the Helmholtz energy through the SAFT-VR-Mie is obtained by combining Eqs. (1.45) and (1.47) with Eq. (1.35), yielding:

$$a^{disp-hs} = \frac{a_1^{Mie}}{k_B T} + \frac{a_2^{Mie}}{(k_B T)^2} \quad (1.48)$$

1.5.4. The soft-SAFT EoS

This SAFT EoS considers non-associating fluids as chains of real segments; their formation is described by Process I, mentioned above.

Blas & Vega⁹ presented two major changes to the original SAFT formulation by:

- (i) replacing the real-segment term a^{seg} (i.e., hard-sphere segment + dispersive-segment terms) of Eq. (1.21) by a Lennard-Jones term
- (ii) and by adapting the **chain term** for a mixture of **Lennard-Jones spheres**.

Note that the overall process I scheme presented in **Figure 1.3** remains unchanged. The soft-SAFT is presented as:

$$\frac{a}{RT} = \frac{a^{ideal}}{RT} + \frac{a^{res}}{RT} = \frac{a^{ideal}}{RT} + \frac{a^{ref}}{RT} + \frac{a^{assoc}}{RT} \quad (1.49)$$

The ideal (i.e., perfect-gas) contribution to Helmholtz energy is:

$$\frac{a^{ideal}}{RT} = \sum_i \left[x_i \ln(\rho_m^{(i)} \Lambda_i^3) \right] - 1 \quad (1.50)$$

Where x_i is the mole fraction for component i and n the total mole number of the system; $\rho_m^{(i)}$ is the molecular density for the same component and Λ_i is the thermal de Broglie wavelength.

The new reference term for the soft-SAFT is expressed by:

$$\frac{a^{ref}}{RT} = \frac{a^{LJ}}{RT} + \frac{a^{chain-rs}}{RT} \quad (1.51)$$

Where a^{LJ} is the **Helmholtz energy for a mixture of LJ segments**. This contribution is given by a modified **Benedict-Webb-Rubin** EoS⁵⁷ (MBWR) fitted to simulation data for a LJ fluid, which is expressed as:

$$\frac{a^{LJ}}{RT} = \sum_{i=1}^8 \frac{a_i \eta}{i} + \sum_{i=1}^6 b_i G_i \quad (1.52)$$

Where the coefficients a_i and b_i are temperature-dependent functions. The G_i functions contain exponentials of the density and a non-linear adjustable parameter γ . In Eq. (1.52), the reduced density η is equal to

$$\eta = \rho_m^{(i)} \sigma^3 \quad (1.53)$$

Where σ is the **LJ diameter**. The contribution for the **LJ chain** formation becomes:

$$\frac{a^{chain-rs}}{RT} = \sum_i x_i (1 - m_i) \ln(y_R^{ii}(\sigma_{ii})) \quad (1.54)$$

With $y_R^{ii}(\sigma_{ii})$ being the **contact value of the cavity correlation function** for spherical segments of component i in the reference LJ fluid. This function is related to **the LJ radial distribution function** and becomes equal to it at the contact value due to the fact that the LJ potential vanishes at this point.

1.5.5. The PC-SAFT EoS

This SAFT EoS considers non-associating fluids as chains of real segments; their formation is described by Process II, mentioned above.

As mentioned in the previous section, a special section will be dedicated to the **Perturbed Chain SAFT EoS** (PC-SAFT) as it is the predominant model studied for this dissertation. This model was first presented in the papers by Gross & Sadowski^{12,13} in the early 2000s. It applies Barker & Henderson's **perturbation theory**⁵⁶ to a reference fluid with hard repulsion and a temperature-dependent segment diameter, which is known as a **hard-chain fluid** with an effective collision diameter of each of the chain's segments.

In this work, the PC-SAFT EoS will be divided into the **non-associating term** and the **associating term**, studying each one independently in the following chapters.

1.5.5.1. The non-associating term

Previously we mentioned that the PC-SAFT changes the reference term from a mixture of hard spheres to a mixture of hard-chain fluids. This change can be thought of as a shift in the order in which the SAFT framework describes a fluid. Instead of going through the steps of Process I as shown in **Figure 3** for all the SAFT versions presented thus far, the PC-SAFT framework first forms hard-sphere chains, then adds a chain dispersion term and then proceeds with the remaining interactions, effectively changing to Process II in **Figure 1.3**.

The general form of the SAFT EoS, when changing the reference term to a **hard-chain fluid** becomes:

$$a^{res} = a^{hc} + a^{disp-chain} + a^{assoc} \quad (1.55)$$

Where a^{hc} takes into account the hard-sphere contribution and the chain-formation contribution.

In this section, the PC-SAFT where only the first two terms appear, the hard-chain and dispersive contributions respectively, will be described and presented as the **non-associating term** of the PC-SAFT.

The **hard-chain reference term** proposed by Gross & Sadowski¹² is given by:

$$\frac{a^{hc}}{RT} = \bar{m} \frac{a_0^{hs}}{RT} - \sum_i x_i (m_i - 1) \ln(g_{ii}^{hs}(\sigma_{ii})) \quad (1.56)$$

Where the mean segment number is $\bar{m} = \sum_i x_i m_i$. The **radial distribution function** of the

hard spheres $g_{ii}^{hs}(\sigma_{ii})$ is given by Eq. (1.26) and the ζ_k functions are defined by Eq.(1.27). The hard sphere Helmholtz energy remains the same as Eq.(1.32). The non-associating PC-SAFT uses a **temperature-dependent segment diameter**, which is the effective collision diameter of the chain segments mentioned before. This quantity is expressed as:

$$d(T) = \int_0^\sigma \left[1 - \exp\left(\frac{u(r)}{k_B T}\right) \right] dr \quad (1.57)$$

Where r is the radial distance between two segments and $u(r)$ is the pair potential. The one used in the PC-SAFT is the same as the one used in the CK-SAFT⁵⁴, given by:

$$u(r) = \begin{cases} \infty & r < (\sigma - s_1) \\ 3\varepsilon & (\sigma - s_1) \leq r < \sigma \\ -\varepsilon & \sigma \leq r < \lambda\sigma \\ 0 & r \geq \lambda\sigma \end{cases} \quad (1.58)$$

Where $s_1 = 0.12\sigma$ and λ is the reduced well width. For this potential, function integrating Eq.(1.57) yields the final expression for the **temperature-dependent diameter**:

$$d_i(T) = \sigma_i \left[1 - 0.12 \exp\left(-\frac{3\varepsilon_i}{k_B T}\right) \right] \quad (1.59)$$

The **dispersion contribution** of the hard chain fluids is given by

$$\frac{a^{disp}}{Nk_B T} = -2\pi\rho I_1(\eta, \bar{m}) \overline{m^2 \varepsilon \sigma^3} - \pi\rho \bar{m} C_1 I_2(\eta, \bar{m}) \overline{m^2 \varepsilon^2 \sigma^3} \quad (1.60)$$

Where $I_1(\eta, \bar{m})$ and $I_2(\eta, \bar{m})$ are the integrals of the perturbation theory, which are substituted by a power series in density:

$$I_1(\eta, \bar{m}) = \sum_{i=0}^6 a_i(\bar{m}) \eta^i \quad (1.61)$$

$$I_2(\eta, \bar{m}) = \sum_{i=0}^6 b_i(\bar{m}) \eta^i \quad (1.62)$$

Where the coefficients a_i and b_i depend on the chain length:

$$a_i(\bar{m}) = a_{0,i} + \frac{\bar{m}-1}{\bar{m}} a_{1,i} + \frac{\bar{m}-1}{\bar{m}} \frac{\bar{m}-2}{\bar{m}} a_{2,i} \quad (1.63)$$

$$b_i(\bar{m}) = b_{0,i} + \frac{\bar{m}-1}{\bar{m}} b_{1,i} + \frac{\bar{m}-1}{\bar{m}} \frac{\bar{m}-2}{\bar{m}} b_{2,i} \quad (1.64)$$

The $a_{k,i}$ and $b_{k,i}$ constants are universal and are given in Table1 of the original paper by Gross & Sadowski¹². C_1 is an abbreviation for the compressibility term:

$$C_1 = \left(1 + Z^{hc} + \rho \frac{\partial Z^{hc}}{\partial \rho} \right)^{-1} \quad (1.65)$$

$$= \left(1 + \bar{m} \frac{8\eta - 2\eta^2}{(1-\eta)^4} + (1-\bar{m}) \frac{20\eta - 27\eta^2 + 12\eta^3 - 2\eta^4}{[(1-\eta)(2-\eta)]^2} \right)^{-1}$$

$\overline{m^2 \varepsilon \sigma^3}$ and $\overline{m^2 \varepsilon^2 \sigma^3}$ are abbreviations of the following expressions:

$$\overline{m^2 \varepsilon \sigma^3} = \sum_i \sum_j x_i x_j m_i m_j \left(\frac{\varepsilon_{ij}}{k_B T} \right) \sigma_{ij}^3 \quad (1.66)$$

$$\overline{m^2 \varepsilon^2 \sigma^3} = \sum_i \sum_j x_i x_j m_i m_j \left(\frac{\varepsilon_{ij}}{k_B T} \right)^2 \sigma_{ij}^3 \quad (1.67)$$

For a pair of unlike segments; conventional combinatory rules are used to estimate ε_{ij} and σ_{ij}

$$\sigma_{ij} = \frac{I}{2} (\sigma_i + \sigma_j) \quad (1.68)$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j} (1 - k_{ij}) \quad (1.69)$$

Where k_{ij} is a binary interaction parameter.

1.5.5.2. The association term

As mentioned previously and as presented by Gross & Sadowski^{12,13}, the contribution of associating interactions for the PC-SAFT EoS is obtained when adding the **association term** to Eq. (1.55). It is worth noting that the association term is essentially the same as the one presented in the original SAFT⁶ (although some slight modifications are introduced for the soft-SAFT EoS⁹). The original SAFT and the underlying Wertheim theory⁴⁷⁻⁴⁹ beneath it, was conceived to account for the short, strong and highly directional intermolecular forces between molecules. These forces appear when a molecule has sites in which a strong Coulombic interaction between the two molecules occurs. This interaction is stronger than the dispersive attractive forces but not quite as a covalent bond. The most common of these interactions is the hydrogen-bond (HB) and they will be described in more detail in Chapter 3. For now, the main remark is that, given a molecule which possesses a site within its structure that can participate in such interactions (e.g., hydrogen-bonding) it is said that it can associate.

For an associating molecule, the associating contribution to the Helmholtz energy is given by:

$$\frac{a^{assoc}}{N k_B T} = \sum_i x_i \left[\sum_{A_i} \left(\ln(X^{A_i}) - \frac{X^{A_i}}{2} \right) + \frac{1}{2} M_i \right] \quad (1.70)$$

Where M_i is the **number of association sites** of molecule and X^{A_i} is the **fraction of molecules i not bonded to site A** and i which is given by:

$$X^{A_i} = \left[1 + \sum_j \sum_{B_j} \rho x_j X^{B_j} \Delta^{A_i B_j} \right]^{-1} \quad (1.71)$$

Where x_j is the mole fraction of j and $\Delta^{A_i B_j}$ is the **association strength** between two sites A and B belonging to two different molecules i and j which is expressed as:

$$\Delta^{A_i B_j} = d_{ij}^3 g_{ij}^{hs}(\sigma_{ij}) \kappa^{AB} \left[\exp\left(\frac{\varepsilon^{AB}}{k_B T}\right) - 1 \right] \quad (1.72)$$

As an addition to the pure-compound parameters involved in the non-associating mode, the association term adds two more parameters per site to account for associating interactions:

- The **association energy** ε^{AB} (which is usually expressed as ε^{AB}/k_B in Kelvin).
- The **association volume** κ^{AB} (made dimensionless).

Thus, the PC-SAFT requires at least five parameters per compound to describe the thermodynamic properties for pure associating components and related mixtures. This presents a challenge as the number of parameters coupled with the mathematical complexity of the PC-SAFT EoS can lead to highly demanding computational power and time, which can be a minor issue if one works with a few pure components or binary systems. However, it is often the case in chemical engineering applications, such as petroleum distillation columns, where both associating and non-associating compounds are mixed in different proportions, elevating the computational demand exponentially. This issue will be addressed throughout the remainder of this dissertation.

One should note that the monomer fraction term presented in the associating term equations is not generally explicit in X^{A_i} , meaning that an analytical form of the equation cannot be given. This stems from the fact that a molecule can have multiple association sites and can thus participate in an associating interaction in multiple ways. Assuming that two molecules have two sites A and B each, the association may occur in such a way that likewise sites form the interaction (AA or BB) or that unlike sites form it (AB). The map of all possible configurations of an associating interaction is known as an **association scheme**. Let us consider a simple example using two molecules of the same secondary amine illustrated in **Figure 1.4**.

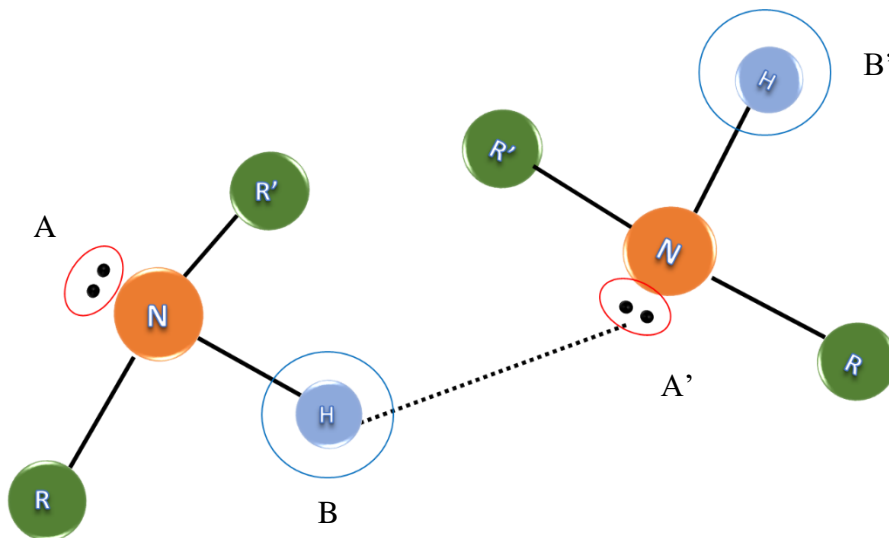


Figure 1.4. Illustration of an association interaction through hydrogen bonding for two secondary amines.

As shown in the figure, both molecules have two sites where the interaction may happen (in this case the interaction corresponds to forming a hydrogen bond). Site A is located at the

nitrogen's pair of electrons (red circles) and site B is located at the labile hydrogen atom (blue circles). We will denote them A and B for molecule 1 and A' and B' for molecule 2 for the sake of clarity, since they are effectively the same type of site. We can see that site A cannot interact with site A' as they are similar and a repulsive interaction would occur rather than an attractive one. The same is true for sites B and B'. However, site A may interact with site B' and form a hydrogen bond through Coulombic and slightly covalent (due to charge transfer) interactions. Site A' would behave in the same way with site B. All possible interactions for these two molecules are then A-B' and A'-B. It is evident that this amine can associate with itself, a phenomenon known as **self-association**, which will be discussed with detail in later chapters. **Table 1.4** presents the association scheme for the **self-association** of this amine.

Table 1.4. Association scheme for the secondary amine illustrated in **Figure 1.4**. Y means that an interaction can form. N means that the two sites cannot interact.

SITES	A'	B'
A	N	Y
B	Y	N

It is worth noting that this scheme will be symmetrical for a pure compound regardless of the number of association sites. Furthermore, for mixtures, the association configuration will also be symmetrical in cases where the association occurs between two different molecules with sites that only allow for unlike interactions. We will illustrate this by changing one of the amine molecules of our previous example to a linear 1-alkanol. This time the alcohol molecule will have three association sites: C and D, which are electron pair sites, and E, which is a labile hydrogen site. **Figure 1.5** shows the association sites for this molecule.

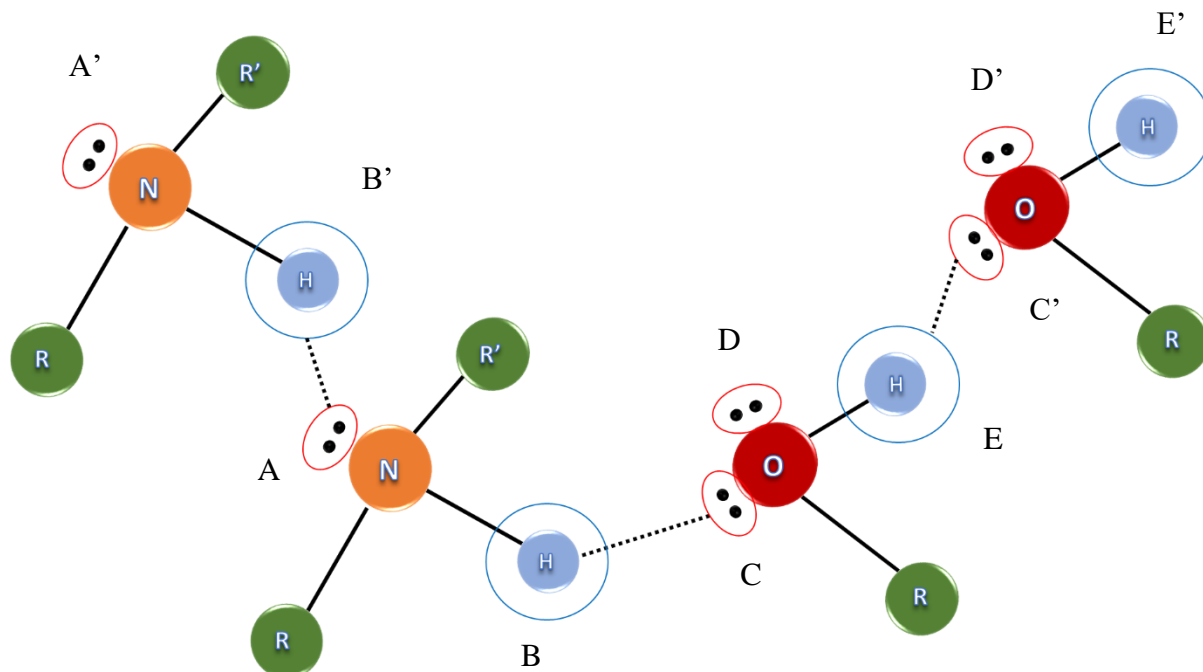


Figure 1.5. Illustration of an association interaction through hydrogen bonding for a secondary amine and a 1-alkanol.

In this case, sites A, C and D can only interact with sites B and E. This configuration is shown in **Table 1.5**. The interaction may occur from any combination of the unlike sites, i.e. AB', AE,

CB, BD, CE' or DE' are the possible hydrogen bonds that can be formed for this system. Associating interactions between two sites of different molecules (i.e. a BC interaction) is known as **cross-association**. In a binary mixture, both self-association (i.e. AB' or CE' interactions) and cross-association (i.e. BC or AE) interactions may occur.

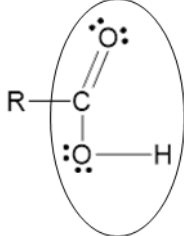
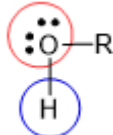
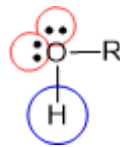
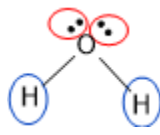
Table 1.5. Association scheme for the secondary amine-1-alkanol system illustrated in Figure 5. Y means that an interaction can form. N means the two sites cannot interact. The orange quadrant is the self-association scheme for the amine and the red quadrant is the self-association scheme for the alcohol.

SITES	A	B	C	D	E
A	N	Y	N	N	Y
B	Y	N	Y	Y	N
C	N	Y	N	N	Y
D	N	Y	N	N	Y
E	Y	N	Y	Y	N

As seen in the table the symmetry is conserved both in the pure compound quadrants (orange for the amine and red for the alcohol) of the table, as well as in the overall mixture and we can expect only unlike sites to participate in association phenomena. This is due to the fact that, in reality, molecules that have similar association sites will not be able to form site-site interactions (e.g. an A-C interaction). We will denote this as a **rigorous scheme** because it considers all possible association interactions among the available sites and will consider each site as a different individual associating locus.

We observe that the use of rigorous schemes gives more light to the issue that the association term introduces in the associating mode of the PC-SAFT. Each pair of sites will have a pair of parameters ε^{AB} and κ^{AB} which introduces a large number of parameters the more pairs of possible association sites are involved. However, Huang & Radosz⁴⁵ proposed a series of **approximations** based on the nature of the associating compound to be parametrized. They presented a series of suppositions on the associating strength that allows for X^{A_i} to be analytically calculated. This approximations will referred as **approximated associated schemes**. **Table 1.6** presents the original associating schemes presented by Huang & Radosz, which are still widely used to this day and they are often referred to in the literature simply as association schemes.

Table 1.6. Associating schemes as proposed by Huang & Radosz, with examples of chemical species that may present them. The circles represent the association sites. The red circles represent a hydrogen acceptor site, the blue circles represent a hydrogen donor site and the black circle represents a binary site in which the former two sites are combined into one.

Scheme type	Chemical species	Structural representation
1A	Acids	
	Nitriles	
	Tertiary amines	
	NO ₂ , NO	
2B	Alcohols	
	Secondary Amines	
	DES	
3B	Alcohols	
Primary amines		
4C	Water	
	Glycols	

As seen in the table, depending on the chemical group involved in the molecule, the associating site number changes and each of these possibilities is given a type of scheme. In the case of hydrogen bonding molecules, a site can either be a hydrogen acceptor site (HA) or a hydrogen donor site (HD). A detailed explanation on each on the nature of hydrogen bonding will be given out in **Chapter 3** while the discussion related to associating schemes, their notation and recent extensions will be discussed in **Chapter 4**.

Each of these types of schemes defines the form X^{A_i} will take. Following the original associating schemes from Huang & Radosz **Table 1.7** shows the X^{A_i} expressions for each of the associating bonding types. It should be noted that these expressions are only valid for estimating the unbonded fraction for pure compounds, meaning that they are only taken into account if the molecule is self-associating.

Table 1.7. Non-bonded site fractions X^{A_i} for different association scheme types.

Scheme type	Δ approximation	X^A approximation	X^A
1A	$\Delta^{AA} \neq 0$	-	$\frac{-1 + \sqrt{1 + 4\rho\Delta^{A_i A_i}}}{2\rho\Delta^{A_i A_i}}$
2B	$\Delta^{AA} = \Delta^{BB} = 0$ $\Delta^{AB} \neq 0$	$X^A = X^B$	$\frac{-1 + \sqrt{1 + 4\rho\Delta^{A_i B_i}}}{2\rho\Delta^{A_i B_i}}$
3B	$\Delta^{AA} = \Delta^{BB} = \Delta^{CC} = \Delta^{AB} = 0$ $\Delta^{AC} = \Delta^{BC} \neq 0$	$X^A = X^B$ $X^C = 2X^A - 1$	$\frac{-(1 - \rho\Delta^{A_i C_i}) + \sqrt{(1 + \rho\Delta^{A_i C_i})^2 + 4\rho\Delta^{A_i C_i}}}{4\rho\Delta^{A_i C_i}}$
4C	$\Delta^{AA} = \Delta^{BB} = \Delta^{CC} = \Delta^{DD} = \Delta^{AB} = \Delta^{CD} = 0$ $\Delta^{AC} = \Delta^{BC} = \Delta^{AD} = \Delta^{BD} \neq 0$	$X^A = X^B = X^C = X^D$	$\frac{-1 + \sqrt{1 + 8\rho\Delta^{A_i C_i}}}{4\rho\Delta^{A_i C_i}}$

These approximations allow for X^{A_i} to be analytically calculated and thus reducing the complexity of the associating term. This however implies that one knows a priori the structure and functional groups of the working molecule set. A deeper look into the associating schemes, their selection and use will be presented in **Chapter 4**.

Similar to the CK-SAFT, several versions of the PC-SAFT have been developed throughout the years by different groups. One of the most notable versions of the PC-SAFT is the **simplified** PC-SAFT proposed by von Solms et al.⁵⁸ in which all segments are assumed to have the same diameter, with $\eta \equiv \zeta_3$ where $\eta = \pi d^3 / 6$. The average diameter is expressed as:

$$d = \left(\frac{\sum_i x_i m_i d_i^3}{\sum_i x_i m_i} \right)^{1/3} \quad (1.73)$$

The first consequence of this modification is a simplification of the radial distribution function $g_{ii}(d_{ii})^{hs}$ which is now written as:

$$g_{ii}(d)^{hs} = \frac{1 - 0.5\eta}{(1 - \eta)^3} \quad (1.74)$$

The second consequence of using the average diameter of Eq. (1.73) is that the hard-sphere contribution to the Helmholtz energy is also simplified:

$$\frac{a^{hs}}{RT} = \frac{4\eta - 3\eta^2}{(1 - \eta)^2} \quad (1.75)$$

These two changes simplify the hard-chain term for the non-associating mode and the associating strength in the associating mode:

$$\Delta^{A_i B_j} = \sigma_{ij}^3 g_{ij}^{hs}(\eta) \kappa^{AB} \left[\exp\left(\frac{\varepsilon^{AB}}{k_B T}\right) - 1 \right] \quad (1.76)$$

Another version of the PC-SAFT is the PC-SAFT with the **standardized critical point based solution** or CP-PC-SAFT, proposed by Polishuk.¹⁷ This version estimates the pure-component parameters by numerically solving the following set of equations:

$$\begin{cases} \left(\frac{\partial P}{\partial v} \right)_{T_c} = \left(\frac{\partial^2 P}{\partial v^2} \right)_{T_c} = 0 \Big|_{v_c, EoS = \delta v_c} \\ P_{c, EoS} = P_c \\ \rho_{liq, EoS} = \rho_{liq, exp} \Big|_{T_{TP}} \end{cases} \quad (1.77)$$

Where δ is the critical volume displacement between the experimental values and those calculated by the EoS and T_{TP} is the triple point temperature.

Other versions of the PC-SAFT come from extending the associating mode to take into account other types of interactions between molecules. Although these extensions will not be considered in this dissertation, they are worth mentioning.

The first notable extension is the **polar** version of the PC-SAFT in which in addition to the PC-SAFT association mode, contributions to the Helmholtz energy due to dipole-dipole and quadrupolar interactions, $\frac{a^{DD}}{RT}$ and $\frac{a^{QQ}}{RT}$ respectively, are added to account for these polar interactions. The dipole and quadrupole moments are necessary in order to calculate this contribution and each type of polar interaction adds a component dependent parameter: x^{DD} and x^{QQ} which are the fraction of dipole and quadrupole segments in the chain respectively. The PC-SAFT with an extended polar term is usually referred to as Polar-PC-SAFT^{59,60}.

The second notable extension is the electrostatic or **ionic** contribution to the Helmholtz energy, $\frac{a^{ion}}{RT}$. This contribution aims to account for Columbic forces present in a fluid with electrostatic charges or, in other words, ions by applying the Debye-Huckel theory^{61,62}. This extension is often used when modeling aqueous systems or even systems that contain ionic liquids (IL). No additional parameter is added as the only component-dependent information needed is the charge of the modeled ion, which is given by its valence. This PC-SAFT extension is usually referred to as e-PC-SAFT.

Other versions of PC-SAFT include coupling the EoS with group-contribution (GC) methods in order to estimate pure compound and mixture parameters. These methods are known as additive methods in where molecules are broken down and any property is estimated through the sum of the contribution of each group that represents a given molecule⁶³. The GC-PC-SAFT couples the GC method proposed by Tamouza et al.⁶⁴ with the PC-SAFT EoS. The pure compound parameters m is estimated through the sum of the number of groups and their contribution; σ is calculated through an arithmetic average of the segment diameter of each group and ε is calculated as the geometrical mean of the segment energy of each group. The associating parameters were fitted to experimental data for the first ten 1-alcohols and kept constant for the remaining alcohols used in their study. This approach was later extended by Tamouza et al.⁶⁵ by using Lorentz-Berthelot combining rules for the non-associating

parameters. Once obtained with the GC method the parameters are used to perform the remaining calculations for the PC-SAFT as proposed by its original authors¹².

The PC-SAFT is mainly used by including the association term in spite of its added complexity. Some of the better known commercial process simulation software such as PRO/II⁶⁶ or ASPEN Plus⁶⁷. However, their use is limited to the availability of the pure compound parameters (both associating and non-associating). In the case of both mentioned software the parameters are linked to those originally proposed by Gross & Sadowski in their original works^{12,13}, in particular for the associating parameters. This practice is common throughout the SAFT academic literature regardless of the version.

Other commercial software that uses PC-SAFT with association is ProSim Plus⁶⁷. This software uses a group contribution version of the polar-PC-SAFT, namely the GC-PPC-SAFT⁶⁸ in which, additionally to the pure compound parameters found using the GC method a pseudo-ionization energy parameter J is found for each compound in similar fashion to the segment energy, by a geometrical mean. This parameter is later used to determine binary interaction parameters (k_{ij}) for mixtures including polar compounds.

The use of parameter databases in commercial software and academic research is justified when considering the highly demanding task of parametrizing all five parameters for the PC-SAFT EoS (using the association mode only). Using already fitted parameters as input data is simpler and allows to use the robustness of the PC-SAFT (or SAFT models in general) on a “plug and play” fashion, meaning that you can perform calculations and process simulations with the EoS by importing the stored parameters. This, however, brings two limitations to both the process engineer and the software developer:

- a) The simulation is restricted to only those compounds for which PC-SAFT parameters are available. This is specially the case with associating parameters.
- b) Perhaps most important, the parameters are not standardized, meaning that the parameter database may differ if it was gathered from different sources, e.g. one user may take the PC-SAFT parameters for methanol proposed by Gross & Sadowski¹³ ($m = 1.5255, \sigma = 3.23\text{\AA}, \varepsilon/k_B = 188.9K, \varepsilon^{AB}/k_B = 2899.5K, \kappa^{AB} = 0.0352$) or the methanol parameters proposed by Lafitte et al.⁶⁹ ($m = 3.236, \sigma = 2.4825\text{\AA}, \varepsilon/k_B = 161.36K, \varepsilon^{AB}/k_B = 2054.5K, \kappa^{AB} = 0.1074$) for their calculations. Furthermore, different parameter sets are obtained at different temperature ranges with varying amounts of data points (sometimes linked to the availability of the data), which makes the use of these EoS far more convoluted for anyone unaware of these issues. This will evidently affect the quality of the results and the domain of use one can have with the PC-SAFT EoS.

The following section will address these two issues with more detail.

1.6.SAFT models and the industrialization problem

So far, a discussion of the underlying theories and mathematical structures that make up the SAFT family of EoS has been presented. These models have a solid physical background that

allows them to yield accurate predictions for pure compounds and mixtures alike, with special accuracy for the liquid density. Furthermore, the existence of the associating term for the SAFT family allows it to describe complex systems with associating phenomena like systems containing water or alcohols due to Wertheim's theory explicitly accounting for this interaction.

Nonetheless, the SAFT family is rather young when compared to the CEoS family, where the latter has been studied for almost a century and a half while the former has been around for only 30 years. This knowledge gap is seemingly not apparent in the academic world, where the SAFT is well acknowledged, and it is being pushed forward by current research. On the hind side, the industrial world is not as eager to incorporate SAFT models in their practices as it is with other models, such as CEoS.

Hendricks et al.² pointed out in 2010 that the industrial community has still many concerns regarding SAFT models. They summarized these concerns in six major points:

- A lack of methods to characterize complex mixtures such as oils and asphaltenes.
- Computational speed.
- Pure component and binary mixture parameters are not collected and available.
- Proof of the improvement in performance (if any) over CEoS, as there are not many studies that show this contrast.
- Applications on polymer and electrolyte thermodynamics.
- Standardization of the SAFT models.

This dissertation is aimed to answer the second, third, fourth and sixth point recollected by Hendricks et al.², as these are the key to have an industrialized version of any SAFT EoS. By industrialization we follow the concept presented by the studies of Moine et al.¹⁸ which also follows those of Postnikov et al.⁷⁰ in which a model for pure species is deemed industrialized when:

- The method used to derive the component-specific parameters follows a universal and transparent protocol and
- The numerical inputs for each pure compound can be easily attained in databases or estimated from predictive correlations.

These two concepts define an industrialized model and also sum up the issue of lack of standardization and recollection of pure compound. Note that EoS versions for mixtures are deemed as industrialized when, in addition to pure-component parameters, (binary) interaction parameters can be estimated from transparent and robust methods and can be easily attained. Moine et al.¹⁸ go into further detail by explaining that SAFT models obtain their parameters by fitting to vapor pressure and liquid density data (which is easily available for a large number of molecules), however, the parameter estimation routines, the temperature ranges, number of data points and performances of the parameter estimation are rarely discussed, save for some exceptions⁷⁰⁻⁷³. The lack of standardization of the different SAFT versions leads to varying degrees of industrialization, thus raising the concerns of the industrial community. A summary of the state of industrialization for each SAFT version presented will be discussed.

The CK-SAFT has seen efforts lately regarding the parameter estimation methods. In particular, Pakravesch et al.⁷⁴ recently presented the PpT parametrization strategy, using pressure, temperature and density data, which introduces explicit data selection and validation steps and

two optimization methods based on the Differential Evolution Algorithm and the Levenberg-Marquardt algorithm. They applied this to 60 non-associating and self-associating compounds for over 93.000 data points, including fitting and validation data. They compared this new methodology against the traditional parametrization for the CK-SAFT and observed an overall improvement, especially in second derivative properties such as speed of sound and isothermal compressibility.

The SAFT-VR has seen most of the research efforts devoted to modifications of the EoS itself (which is the most common practice for all the other SAFT versions presented thus far). Some examples found in the literature include:

- McCabe & Kiselev⁷⁵, who introduced a crossover treatment to the original SAFT-VR EoS which scales the predictions in the critical region, while falling back to the original formulation away from it;
- Eriksen et al.⁷⁶ who included two additional contributions, a Born contribution and a Columbic (ionic) contribution to the Helmholtz energy, using a mean-spherical approximation framework for modeling electrolytes;
- Müller & Mejía⁷⁷ who introduced a ring-formation contribution to the Helmholtz energy to the SAFT-VR Mie EoS in order to better predict thermodynamic properties of molecules with ring-like structures;
- Cripwell et al.⁷⁸ who introduced the polar contribution of Gross & Vrabec to the SAFT-VR Mie to achieve a predictive model for polar compounds and their mixtures.
- Other notable efforts for the SAFT-VR shift towards the implementation of group contribution methods, most notably, derived from the SAFT- γ proposed by Lympiradis et al.⁷⁹ which extends the SAFT-VR with a predictive group contribution method.

In general, most authors have not explored deeply the parametrization side of the SAFT-VR sub-family, with some exceptions being Dufal et al.⁷¹ which goes into deeper insight regarding the properties and parametrization strategies and Perdomo-Hurtado et al.⁸⁰ in which the parameter estimation is coupled with a discrete potential theory to obtain a generalized version of the EoS, able to predict thermodynamic properties from molecular liquids to complex colloidal systems. The evidence, however, suggests that the SAFT-VR is not yet on an industrialized state and further studies need to be performed in this area.

The case of the soft SAFT EoS is very similar to that of the SAFT-VR, where many studies have been devoted to modifying the EoS to account for new interactions, such as the polar soft SAFT presented in the work of Alkhatib et al.⁸¹ using the approach of Jog and Chapman to extend the model to polar species. Other approaches include the use of a crossover treatment with a renormalization group as shown in the works of Llovel et al.⁸² and Dias et al.⁸³. Several studies have touched on the parametrization issue for the soft SAFT EoS: Pamies & Vega⁸⁴ introduced correlations developed from optimized n-alkane parameters to estimate the molecular parameters of heavier members of the homologous series (from n-nonane onwards) by relating the molecular parameters to the molecular weight of their respective compound:

$$\begin{cases} m = 0.0255M_w + 0.628 \\ m\sigma^3 = 1.73M_w + 22.8 \\ m\varepsilon/k_B = 7.89M_w + 38.0 \end{cases} \quad (1.78)$$

Dias et al. 95 used a similar approach for perfluorinated alkanes, but relating the molecular parameters as function of the carbon number:

$$\begin{cases} m = 0.358C_n + 0.6794 \\ m\sigma^3 = 35.53C_n + 42.27 \\ m\varepsilon/k_B = 96.42C_n + 92.25 \end{cases} \quad (1.79)$$

Where C_n is the carbon number of the molecule. Castro-Marcano et al.⁸⁵ implemented a critical-point based parametrization of the soft SAFT EoS by adjusting the non-associating parameters to reproduce exactly the experimental critical temperature, critical pressure and acentric factor through the following polynomial expressions:

$$\begin{cases} m = \sum_{i=0}^3 p_i \omega^i \\ \varepsilon/k_B = T_c \sum_{i=0}^6 q_i m^i \\ \sigma^3 = \frac{k_B T_c}{P_c} \sum_{i=0}^6 s_i m^i \end{cases} \quad (1.80)$$

Where p , q and s are coefficients adjusted for values of the acentric factor below 1.3. Oliveira et al.⁸⁶ discussed in detail the effects of including additional properties to the parameter estimation routines for non-associating compounds, reaching the conclusion that for the soft SAFT, vapor pressure and liquid density data with corresponding weights of 0.8 and 0.2 are enough to obtain optimal and balanced results.

Although some attention has been given to the parametrization side of the soft SAFT EoS, it has not yet reached its industrialized version, as some of the parametrization methods are rather family specific (correlations based on homologous series rather than universal ones) or have not been explored and standardized enough to be considered fully industrialized.

The PC-SAFT EoS has also seen efforts in modifications of the model in order to account for different interactions, such as the polar PC-SAFT introduced in the work of Tumakaka et al.⁶⁰, the e-PC-SAFT proposed by Cameretti et al.⁶² with an electrolyte contribution to the Helmholtz energy or the group contribution approach introduced in the works of Tamouza et al.^{64,65}.

However, many efforts have been devoted to the parametrization of the PC-SAFT: Castro-Marcano et al.⁸⁵ used the same set of equations as with the soft SAFT, with a parameter set adjusted specifically for the PC-SAFT; Ferrando et al.⁸⁷ used Monte Carlo simulations to determine:

- The association schemes as the maximum number of independent association sites that can participate in hydrogen bonding for a given molecule finding the distribution of hydrogen bonds in methanol at 300K and by relating the monomer fraction and the free-hydrogen fractions.
- The associating parameters by rewriting Eq. (1.72) as a linear function in which ε^{AB}/k_B is the slope and $\ln(\kappa^{AB})$ is the intercept:

$$\ln\left(\frac{\Delta^{AB}}{d(T)^3 g^{hs}(T)}\right) = \frac{\varepsilon^{AB}}{k_B T} + \ln(\kappa^{AB}) \quad (1.81)$$

For a given set of non-associating parameters, they estimated the denominator of the left-hand side of Eq.(1.81), followed by a linear regression to determine the corresponding associating parameters, then verifying that their objective function, that included vapor pressure and liquid molar volumes, was minimized, using the polar PC-SAFT for 1-alkanols, with fixed polar parameters. Even though their paper focuses on 1-alkanols, the authors claim that their methodology can be easily extended to other associating families; Other authors such as Fuenzalida et al.⁸⁸ used an a priori sensitivity analysis coupled with a multi-objective variable cost function in order to improve parameter estimation for alcohols and amines and their binary and ternary mixtures; Jaber et al.⁸⁹ used a neighborhood-correction for the segment number for branched alkanes coupled with the GC-PC-SAFT, which slightly improves the predictions for these compounds and allows to identify different isomers; Matsukawa et al.⁹⁰ introduced an artificial neural network (ANN) approach as an alternative to group contribution methods for the PC-SAFT. Their approach provides improved results for vapor pressure, liquid densities and critical properties as well as estimating properties for compounds without group contribution parameters reported. These approaches, although addressing the issues of parametrization of PC-SAFT, do not go directly into the industrialization issue. Nevertheless, some authors have done this analysis for the PC-SAFT. Anoune et al.⁹¹ for example, recently proposed a method in which the three non-associating parameters are obtained by reproducing the critical pressure and temperature for 94 pure non-associating compounds as indicated by the following expressions:

$$\begin{cases} P(T_{c,\text{exp}}, \eta_c) - P_{c,\text{exp}} = 0 \\ \left(\frac{\partial P}{\partial \eta}\right)_{T_{c,\text{exp}}, \eta_c} = 0 \\ \left(\frac{\partial^2 P}{\partial \eta^2}\right)_{T_{c,\text{exp}}, \eta_c} = 0 \end{cases} \quad (1.82)$$

They begin with an initial value for the critical reduced density (η_c) and solve Eq. (1.82) through a Newton-Raphson method to obtain the non-associating parameter vector. Next, they calculate an objective function including vapor pressure and liquid density for the current η_c and minimize it using a dichotomic method. They use the new η_c value to repeat the entire process until they reach their convergence criterion for both the parameter set and the critical reduced density. They later extended their approach by introducing correlations that relate the molecular parameters of the PC-SAFT to the critical properties and the acentric factor:

$$\begin{cases} m = 0.43344\omega^2 + 7.84968\omega + 0.92734 \\ \sigma^3 \frac{P_c}{T_c} = -0.06388m^{-2} + 1.28018m^{-1} - 0.3879 \\ \varepsilon/k_B \frac{1}{T_c} = -0.15924m^{-2} + 0.70433m^{-1} + 0.54264 \end{cases} \quad (1.83)$$

This approach improves on the critical properties and vapor pressure while it struggles describing the liquid densities for both pure compounds and the binary mixtures studied in their paper.

Polishuk¹⁷ introduced an approach which presents an industrialized version of the PC-SAFT: the Standardized Critical-point based PC-SAFT (often referred to as CP-PC-SAFT) in which the molecular parameters of the EoS are obtained through the knowledge of the critical point and the triple-point liquid density:

$$\begin{cases} \left(\frac{\partial P}{\partial v} \right)_{T_c} = \left(\frac{\partial^2 P}{\partial v^2} \right)_{T_c} = 0 \Big|_{v_c, EoS = \delta v_{c, \text{exp}}} \\ P_{c, EoS} = P_{c, \text{exp}} \\ \rho_{\text{liq}, EoS} = \rho_{\text{liq}, \text{exp}} \Big|_{\text{triple point}} \end{cases} \quad (1.84)$$

This approach avoids fitting parameters altogether and improves on the predictions of the PC-SAFT, avoiding some mathematical issues inherent to the model^{92,93}. A major drawback of this approach is its inaccuracy of describing vapor pressures for heavy compounds away from the critical point.

Moine et al.¹⁸ proposed a second industrialized version of the PC-SAFT EoS, in which the three non-associating parameters of the PC-SAFT EoS are obtained through exact reproduction of the experimental critical temperature, critical pressure and acentric factor. They used the approach of Privat et al.⁹⁴, whom established universal relationships between the segment parameter, m and the three aforementioned experimental properties by:

$$\begin{cases} T_c^* = f(m) \\ P_c^* = f(m) \\ \omega = f(m) \end{cases} \quad (1.85)$$

Where:

$$\begin{cases} T_c^* = \frac{T_{c, \text{exp}}}{\varepsilon/k_B} \\ P_c^* = \frac{P_{c, \text{exp}} \sigma^3}{k_B (\varepsilon/k_B)} \end{cases} \quad (1.86)$$

Which are dimensionless expressions for the critical temperature and pressure.

Figure 1.6 shows a graphical representation of these universal relations.

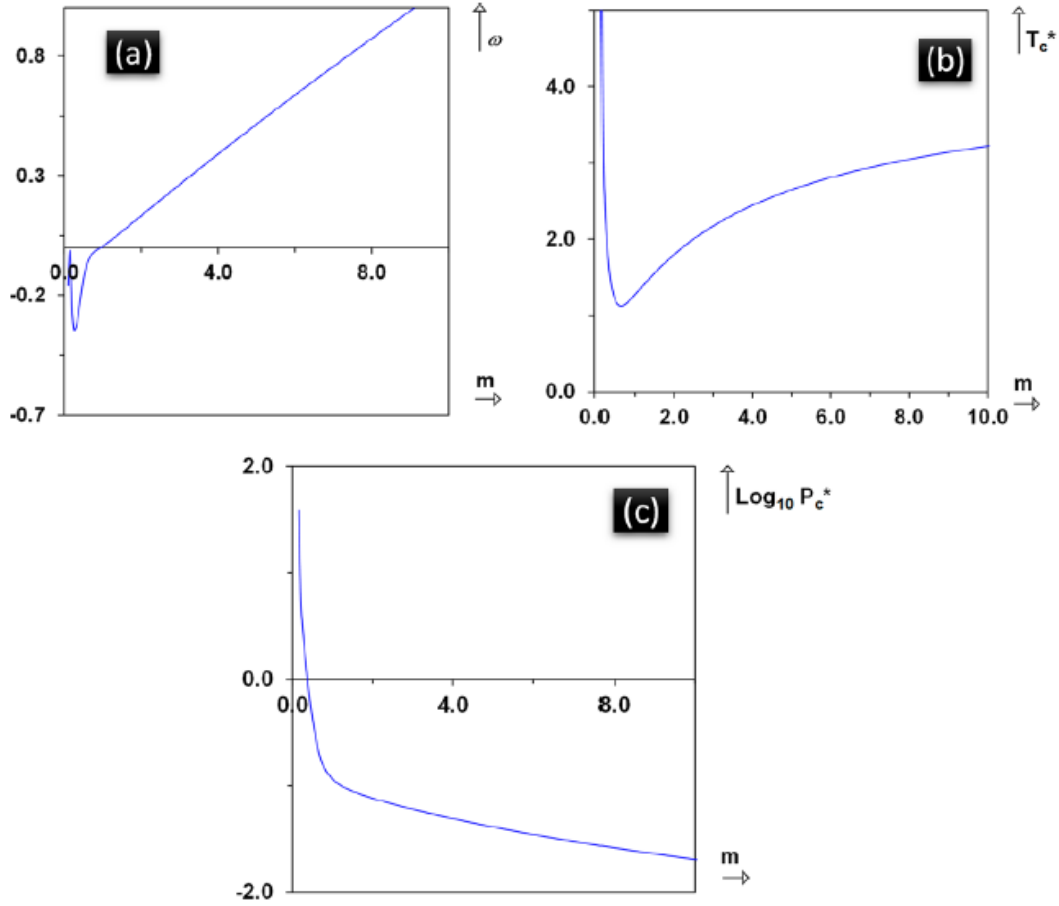


Figure 1.6. Graphical representation of the universal m functions of the acentric factor, critical temperature and critical pressure for $m < 10$. Taken from Privat et al.⁹⁴. DOI: 10.1021/acs.iecr.8b06083.

Privat et al.⁹⁴ also showed that the following correlations can be used for estimating T_c^* , P_c^* and ω from m :

$$\begin{cases} \omega(m) \approx -8.5775 \cdot 10^{-4} m^2 + 0.13079m - 0.12138 \\ T_c^*(m) \approx 4.7968 \cdot 10^{-6} m^5 - 3.0895 \cdot 10^{-4} m^4 + 7.8649 \cdot 10^{-3} m^3 - 0.10215m^2 + 0.75358m + 0.63659 \\ P_c^*(m) \approx 1.6345 \cdot 10^{-7} m^6 - 1.1346 \cdot 10^{-5} m^5 + 3.1389 \cdot 10^{-4} m^4 - 4.4618 \cdot 10^{-3} m^3 + 3.6282 \cdot 10^{-2} m^2 - 0.22498m - 0.77655 \end{cases} \quad (1.87)$$

With the idea of finding the three non-associating parameters from the experimental critical point and acentric factor, the following constraints were applied:

$$\begin{cases} \omega_{\text{exp}} = \omega_{EoS} = \omega(m) \\ T_{c,\text{exp}} = T_{c,EoS} = T_c^*(m) \cdot \varepsilon / k_B \\ P_{c,\text{exp}} = P_{c,EoS} = P_c^*(m) \cdot \varepsilon / \sigma^3 \end{cases} \quad (1.88)$$

With the knowledge of ω_{exp} , **Figure 1.6a** gives the m parameter univocally. With m known, **Figure 1.6b** provides the value of T_c^* , which in combination with Eq. (1.88) gives the ε_i/k parameter:

$$\varepsilon/k = \frac{T_{c,\text{exp}}}{T_c^*(m)} \quad (1.89)$$

With m and ε_i/k the segment diameter can be obtained from Eq. (1.88):

$$\sigma = \left[\frac{\varepsilon}{k_B} \left(\frac{k_B P_c^*(m)}{P_{c,\text{exp}}} \right) \right]^{1/3} \quad (1.90)$$

Moine et al.¹⁸ later introduced the following practical correlations, based in Eqs 1.81-1.81:

$$\begin{cases} m_i \approx 0.5959\omega_{i,\text{exp}}^2 + 7.5437\omega_{i,\text{exp}} + 0.9729 \\ \varepsilon_i/k \approx T_{c,i,\text{exp}} / \left(4.7968 \cdot 10^{-6} m_i^5 - 3.0895 \cdot 10^{-4} m_i^4 + 7.8649 \cdot 10^{-3} m_i^3 - 0.10215 m_i^2 + 0.75358 m_i + 0.63659 \right) \\ \sigma_i \approx \left[\varepsilon_i/k \cdot \frac{k}{P_{c,i,\text{exp}}} 10^{\left(1.6345 \cdot 10^{-7} m_i^6 - 1.1346 \cdot 10^{-5} m_i^5 + 3.1389 \cdot 10^{-4} m_i^4 - 4.4618 \cdot 10^{-3} m_i^3 + 3.6282 \cdot 10^{-2} m_i^2 - 0.22498 m_i - 0.77655 \right)} \right]^{1/3} \end{cases} \quad (1.91)$$

However, they showed that using this approach sacrificed accuracy on the description of liquid densities for the PC-SAFT. For this reason, they added an additional parameter to the model: a **volume translation parameter** (c) in which an experimental saturated liquid molar volume data point at a reduced temperature equal to 0.8 is exactly reproduced. This parameter is expressed as:

$$c = v_{\text{liq,calc}}^{\text{sat}}(T_r = 0.8) - v_{\text{liq,exp}}^{\text{sat}}(T_r = 0.8) \quad (1.92)$$

This volume-translated PC-SAFT, parametrized to exactly reproduce the experimental critical temperature, pressure and acentric factor was labeled the Industrialized PC-SAFT or I-PC-SAFT.

This approach presented by Moine et al.¹⁸ tackles the industrialization problem by having critical point and acentric factor data of each compound and using predictive correlations to produce a standardized, ready-to-use industrial PC-SAFT EoS version for pure species. Its performance when paired up against a “traditionally” fitted PC-SAFT will be the object of the following chapters.

In this work, an approach using easily available data such as vapor pressure or liquid density and estimating the pure-component parameters by fitting will be taken and described in Chapter 2. The goal is to propose an entirely transparent and safe parameter estimation routine for a SAFT EoS. The procedure will evaluate all the possible property combinations to be included in the fitting from four key properties: vapor pressure, saturated liquid density data, heat of vaporization and saturated liquid heat capacity. This guarantees that the methodology will be applicable to any SAFT EoS. This will also include standardizing the number of experimental data points as well as the temperature ranges for each property in order have an even field regardless of the molecule. In this dissertation, the focus will be the PC-SAFT EoS but

reiterating our point mentioned above, the procedure would be applicable to any SAFT EoS, even if the final fitting functions use different properties. With this we aim to answer the SAFT standardization issue raised by Hendricks et al.².

Following up, with the best fitting procedure defined, a large database of parameters will be constructed for all compounds for which we can gather the data for the key properties included in the fitting. It should be noted that, in principle the non-associating parameters per compound will make up this database. The case for the associating parameters will be studied in terms of their necessity and how to estimate them on a systematic way as the non-associating parameters. This database creation procedure will be replicated for the I-PC-SAFT EoS. The goal of this step is to address the third SAFT issue (pure component parameters collected and made available) raised by Hendricks et al.²

A comparison between the two PC-SAFT EoS and well-known high-performing CEoS such as the *tc*-PR introduced in previous sections will be done in order to truly assess the strengths and weaknesses of each model when predicting pure compound properties for non-associating and associating species. This study will be done over 300.000 experimental data points including the four key properties mentioned, as well as the critical properties. With this, we address the fourth (proof of improvement, if any, over CEoS) SAFT issue raised by Hendricks et al.²

Coming back to the associating parameters, it is well known that they add increased complexity both mathematically and computationally to the PC-SAFT EoS and SAFT EoS in general if they are included in the parameter estimation. However, taking inspiration from conclusions reached by Postnikov et al.⁷⁰ in which the effects of association seem to be “diluted” as the molecule chain grows for 1-alcohols, this dissertation will investigate the influence of the associating term of the SAFT EoS in Chapter 3 and study if it is really necessary for every compound that can associate. Furthermore, the need for the associating parameters to be compound-dependent (as described by the original SAFT⁶) or if it can be treated as a chemical family feature (similar as to how the GC-SAFT⁶⁴ uses the associating parameters) will be analyzed. The proper estimation of these variables will also be discussed. The aim of this is to have a PC-SAFT version that can be computationally more efficient in estimating parameters and properties due to the fact that molecules that participate in complex interactions such as hydrogen bonding may not need a sophisticated associating term added and thus leaving behind a big computational load for process simulators or in-house SAFT software used by researchers or process engineers. This aims to address the second issue (computational speed) raised by Hendricks et al.².

This dissertation will not address the first (lack of methods to characterize oils and asphaltenes) and fifth issues (applications on polymer and electrolyte thermodynamics) of the SAFT standardization problem. The extension to mixtures is, of course, the natural follow up for this thesis and this coupled with characterization of complex mixtures such as asphaltenes can be an entire dissertation on its own. The same can be said for polymer and electrolyte systems modeled with SAFT models, although the latter can be even more complex because of the fact that solid-state thermodynamics must be used. These issues will have to remain unanswered here but they are the next two challenges in order to have a fully standardized PC-SAFT EoS. We hope, nonetheless, that with this work at least the partially-standardized PC-SAFT can be adopted by both industrial and academic communities to have a powerful and easy-to-use tool

at their disposal to perform chemical engineering thermodynamics, not meant to replace any existing model but to complement the pane of options for process engineers and researchers.

**Chapter 2 : Parametrization of the PC-SAFT
equation of state for non-associating pure
compounds.**

In this chapter, the study presenting the parameter estimation methodology that will be used from this point forward for the PC-SAFT EoS was extracted from Ramirez-Velez et al.⁹⁵ published in the Journal of Chemical & Engineering Data in August of 2020.

“Parameterization of SAFT models: analysis of different parameter estimation strategies and application to the development of a comprehensive database of PC-SAFT molecular parameters” (DOI: 10.1021/acs.jced.0c00792.)”

In **Chapter 2**, the SAFT standardization problem is addressed as we seek to propose an entirely transparent and universal methodology to obtain pure compound parameters for the non-associating mode of the PC-SAFT EoS.

The main highlights for this chapter include:

- The proposition of a safe, transparent, and universal parameter estimation routine based on available pure compound data such as vapor pressure, liquid density, enthalpy of vaporization and liquid heat capacity.
- Evaluation of the impact of setting different objectives for the parameter estimation routines to select the safest and most accurate possible parameter estimation.

The following chapter will discuss the first two points mentioned above, while giving a quick context on the parametrization tendencies for non-associating compounds amongst SAFT developers and users.

For a thorough comparison between SAFT EoS and CEoS, as well as the access to the databases for the pure compound parameters for the non-associating compounds studied in this chapter, the reader is referred to the following chapter.

2.1. Introduction

Equations of state (EoS) derived from the three-parameter corresponding-state law⁹⁴ are one of the most important tools for chemical and energy industries due to their ability to reproduce and predict thermodynamic properties of pure compounds and mixtures with the knowledge of few inputs to perform such calculations. Two of the most popular families of EoS in the industry are:

- (1) the Cubic EoS (CEoS), derived from the original Van der Waals model which include the reference EoS by Peng and Robinson³⁴ or Soave³³,
- (2) the SAFT-type EoS (SAFT stands for Statistical Associating Fluid Theory⁶) which include, among others, the well-known SOFT SAFT⁹, SAFT-VR⁸ and the PC-SAFT¹² models.

To make their model accepted by the scientific community, EoS developers must guarantee not only a sound theoretical background but also a correct parametrization strategy in order to obtain reliable values for the various thermodynamic properties of interest^{18,94}. By *parametrization*, it is here meant the methodology used to assign values to model parameters that are not fixed by the theory. Well-calibrated procedures deducing parameter values from experimental input data are then required. In this paper, we address the key issue of EoS parametrization and more particularly, of EoS parameter fitting.

What experimental properties should be used to parametrize an EoS?

An EoS has not the capacity to reproduce all thermodynamic properties with an infinite accuracy. The adjustable EoS parameters must be determined in order to reproduce preferentially a series of properties considered as priority³¹ (called *target properties* thereafter).

Of course, there is formally no universal definition of the target properties to be used for the parametrization of a SAFT-type or CEoS, as it essentially depends on the application field of the EoS. Nevertheless, it is observed in practice that most of cubic and SAFT-type EoS users (and users from industry, more specifically) agree on the following ordered list of pure-component target properties:

- EoS are expected to predict VLE transitions in the pressure-temperature domain with a high accuracy. For this reason, vapor pressure P^{sat} is certainly the most prominent property,
- Saturated-liquid densities ρ_{liq}^{sat} (that are used for many applications and sizing issues of a number of unit operations in particular),
- In order to guaranty the accuracy of energy and exergy balances, temperature-derived properties are deemed as essential. In that respect, enthalpy of vaporization $\Delta_{vap}H$ and liquid heat capacity $c_{P,liq}^{sat}$ are often considered.

To sum up, it will be assumed in the present study that the goal of a parametrization procedure for CEoS or SAFT-type EoS is to reproduce these four properties according to the following pecking order:

$$P^{sat} \geq \rho_{liq}^{sat} > \Delta_{vap}H \text{ and } c_{P,liq}^{sat} \quad (2.1)$$

Once identified the target properties and their relative importance, the work is not finished yet. In order to meet the above goal, i.e., a satisfactory reproduction of all 4 target properties, it is not always necessary to include all of them in the fitting procedure (this is especially true if we notice that some of them have a marginal impact on the result of the fitting procedure).

One needs thus to specify which property data have to be included necessarily in the regression procedure to meet safely our objective. In addition, the mathematical method used to relate EoS parameters and these data and the precise weight of the various properties remain pending issues. All these aspects must be clarified in order to get a transparent and universal parametrization procedure.

Parametrization of CEoS

For this class of EoS, parametrization strategies fall back on more than a century of expertise. In a previous work, Piña-Martinez et al.⁹⁶ summarized well-known safe practices and identified a series of new ones for parametrizing CEoS involving an α -function with component-specific parameters. Working on volume-translated versions of the Peng-Robinson (PR) and Redlich-Kwong (RK)³² CEoS combined to a consistent^{35,97} 3-parameter Twu alpha function³⁹, they investigated which parametrization strategy yields a proper description of the three target properties: P^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$. To do so, they selected 783 pure components present in a reference database reporting experimental data for each of the 3 target properties and each compound. Then, for each of the 783 components, they tested out all the possible combinations of property data among P^{sat} , $\Delta_{vap}H$ and $c_{P,liq}$ against which the three Twu parameters could be adjusted. They thus determined the sets of Twu parameters over:

- individual properties (P^{sat} or $\Delta_{vap}H$ or $c_{P,liq}^{sat}$) followed by,
- all possible combinations of two of the three properties (e.g., P^{sat} and $\Delta_{vap}H$, P^{sat} and $c_{P,liq}^{sat}$ etc.) and finally,
- all three properties (P^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$)

Eventually, each of the tested combinations was either validated or rejected depending on the average deviation over the 3 target properties (P^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$) returned by the EoS and the 783 species. They found that including P^{sat} data in the fitting procedure was absolutely necessary, while fitting parameters using only $c_{P,liq}^{sat}$ data led to high deviations across all target properties and should be avoided. On the basis of these results, they developed a database of Twu parameters for 1721 molecules for which the availability of at least experimental P^{sat} data enabled the implementation of a safe parametrization.

Péneloux's volume-translation shift does not affect^{41,42} P^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$ so that it was determined for each component in a second step in order to exactly reproduce the liquid density at a reduced temperature of 0.8.

Parametrization of SAFT-type EoS

This class of model is more recent than CEoS and parametrization procedures are therefore in a less-advanced stage. Furthermore, as SAFT EoS developers are continuously searching for improving their models, most of the focus goes into discussing the theory behind them while little attention is given to the way that the component-dependent parameters of each model are being obtained. This little interest to parametrization issues could be highly prejudicial to the industrialization of this class of models. In 2010, a college of researchers from academy and industry pointed out the “lack of standardization, reference data, and correct and transparent implementations, especially in commercially available simulation programs”. These observations led them to assert that if “the use of new methods, such as SAFT, is increasing, they are not yet in position to replace traditional methods such as cubic EoS”². As pointed out by Polishuk¹⁷ and Moine et al.¹⁸ “the classical parameterization method for SAFT EoS is far from being standardized and is sometimes vague, explaining why there is currently no industrialized version of this family of EoS”. Indeed, the experimental properties used to fit the parameters, the corresponding temperature ranges and the resulting performance are usually not discussed thoroughly and remain very much attached to the data availability and the developer's habits.

SAFT EoS models usually have 3 component-dependent parameters for describing pure non-associating compounds (e.g., n-alkanes), namely: segment number (m), segment diameter (σ) and an energy parameter (ε/k)¹². These parameters are present in every iteration of the SAFT family of EoS and they are usually fitted to experimental data. Traditionally, SAFT developers and users have not departed very far from the original SAFT⁶ parametrization relying on the use of P^{sat} and saturated-liquid density (ρ_{liq}^{sat}) experimental data.

The main objective of this work is to identify the list of property data that are absolutely necessary for a safe estimation of component-dependent SAFT-type EoS parameters (enabling to minimize the deviations on P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$). With this goal in mind and following the strategy developed by Piña-Martinez et al.⁹⁶ on CEoS, we will test all the possible combinations of property data (among P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$) to fit the PC-SAFT parameters. To do so, the largest possible database of molecules containing experimental data related to the four target properties P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ will be considered. Eventually, following recommendations from European experts^{2,18}, a totally transparent and universal parametrization protocol will be proposed and a new and comprehensive database for pure-component PC-SAFT parameters will be built.

In this work, only non-associating compounds are considered and described using three EoS parameters (m , σ , ε/k). The case of associating species will be discussed in a next study.

2.2. Literature review: parametrization procedures for SAFT-type EoS

As mentioned in the introduction, SAFT users and developers essentially determine pure-component EoS parameters by minimizing an OF formed from mean average deviations over P^{sat} and ρ_{liq}^{sat} experimental data. There is however no clear evidence that it is the best strategy. While the first paper introducing explicitly the SAFT EoS⁷ ignores completely parametrization issues (EoS parameters for real molecules are even not provided), the subsequent papers mention the use of P^{sat} and ρ_{liq}^{sat} experimental data but do not provide much detail about the fitting procedure^{6,45}. In the following versions of SAFT EoS, this practice is frequent but not systematic. In addition, the number and distribution of experimental data for each property, the corresponding temperature ranges or the expression of the OF can be disparate from one author to another.

Table 2.1 illustrates the various methodologies reported in the open literature for the main versions of SAFT-type EoS. It is by no means comprehensive but provides a general overview of parametrization practices employed by SAFT-EoS users and developers.

SAFT-VR EoS

The SAFT with attractive potentials of variable range (SAFT-VR) EoS⁸ proposed by the team at the Imperial College of London is one of the most popular versions of the SAFT family of EoS. When a square-well, a Sutherland or a Yukawa intermolecular potential is used to describe the monomer-monomer interactions, one extra adjustable parameter (denoted λ) is added to account for the interaction range, regardless of the associative nature of the modeled compound. The SAFT-VR version using Mie potentials (SAFT-VR-Mie) offers the possibility to add two additional parameters to the original three, namely λ_r and λ_a , which refer to variable repulsive and attractive exponents, respectively. **Table 2.1** shows several strategies used with the SAFT-VR EoS to parametrize non-associating compounds. It can be observed that the earliest studies dealing with the SAFT-VR EoS pay very little attention to parametrization issues and solely mention the nature of the properties used to fit pure-component parameters. It appears that the SAFT-VR developers have then gradually increased their interest in parametrization issues. In 2006, Lafitte et al.⁵⁵ have highlighted the necessity to add speed-of-sound data (or an equivalent property) in the set of properties used to determine pure-species parameter for improving the description of derivative properties (isothermal compressibility, isobaric thermal expansivity, heat capacity). For this reason, in most of papers posterior to the study by Lafitte et al.⁵⁵, the speed of sound was considered as one of the target properties. In 2015, the SAFT-VR developers devote a complete paper to the parametrization of their model⁷¹ in which they partially change of opinion regarding the necessity to include speed of sound data in the parametrization procedure. They justify this late interest for the topic of parametrization as follows: “*although excellent models for real fluids were developed, a detailed examination of the model parameter space was not conducted and, accordingly, it remained to gain the insight necessary to be able to best exploit the enhanced capability of the new theory in terms of developing models to represent real fluids*”. In this thorough study, authors show that:

- the use of 3 adjustable parameters ($m, \sigma, \varepsilon/k$) with $\lambda_r = 12$ and $\lambda_a = 6$ to describe a non-associating species is inadequate except for the simplest fluids (e.g., argon or methane),
- the use of 5 adjustable parameters ($m, \sigma, \varepsilon/k, \lambda_r, \lambda_a$) is excessive and leads to a high degree of correlation between these parameters,
- The use of 4 adjustable parameters ($m, \sigma, \varepsilon/k, \lambda_r$) with $\lambda_a = 6$ is reasonable as it enables to describe accurately any real non-associating compound.

They reach the conclusion that if the parametrization methodology is well-calibrated, target properties can be limited to saturation properties ($P^{sat}, \rho_{liq}^{sat}$). They observe that the resulting performance in terms of other thermodynamic properties “*is nevertheless excellent*”⁷¹.

Table 2.1. Overview of the various parametrization strategies used with the SAFT-VR, soft-SAFT and PC-SAFT EoS

Model	Non-associating compounds	Parameters fitted	Properties considered for parametrization	Temperature range	Objective function expression	References
SAFT-VR with a square-well potential (SW)	C ₁ -C ₂₀ , C ₂₄ , C ₂₈ , C ₃₂ , C ₃₆ n-alkanes, perfluoroalkanes	$m, \sigma, \varepsilon/k, \lambda$	$P^{sat}, \rho_{liq}^{sat}$	from the triple-point (T_{triple}) to the critical temperature (T_c)	Unknown	8,98
SAFT-VR (SW)	C ₁₂ -C ₁₄ n-alkanes, CO ₂	$m, \sigma, \varepsilon/k, \lambda$	First, $m, \sigma, \varepsilon/k, \lambda$ are fitted to P^{sat} and ρ_{liq}^{sat} data; σ and ε/k are then rescaled to T_c and the critical pressure (P_c)	Unknown	Unknown. The rescaling procedure allows for an exact reproduction of the critical coordinates which are ordinarily overshoot when fitting uniquely P^{sat} and ρ_{liq}^{sat} data.	99

Model	Non-associating compounds	Parameters fitted	Properties considered for parametrization	Temperature range	Objective function expression	References
SAFT-VR (SW)	C ₁ -C ₁₀ n-alkanes, n-C ₁₂ , CO ₂ , benzene, H ₂ S	$m, \sigma, \varepsilon/k, \lambda$	$P^{sat}, \rho_{liq}^{sat}$	From T_{triple} to T_c	$F_{ob} = \sum_{i=1}^{N_{exp,psat}} \left(\frac{P_i^{sat,calc} - P_i^{sat,exp}}{P_i^{sat,exp}} \right)^2$ $+ \sum_{i=1}^{N_{exp,\rho_{liq}^{sat}}} \left(\frac{\rho_{liq,i}^{sat,calc} - \rho_{liq,i}^{sat,exp}}{\rho_{liq,i}^{sat,exp}} \right)^2$	100
SAFT-VR Mie	C ₁ -C ₂₀ , C ₂₂ , C ₂₃ , C ₂₄ , C ₂₈ , C ₃₆ n-alkanes	$m, \sigma, \varepsilon/k, \lambda_r$	$P^{sat}, \rho_{liq}^{sat}, \rho_{liq}$ (non-saturated liquid density), u_{liq} (speed of sound) $\lambda_a = 6$	For saturated properties: $T_r \in [0.45; 0.9]$; for liquid properties, T_r and P_r ranges are component dependent	$F_{ob} = \frac{1}{N_{exp,P^{sat}}} \sum_{i=1}^{N_{exp,psat}} \left(\frac{P_i^{sat,calc} - P_i^{sat,exp}}{P_i^{sat,exp}} \right)^2$ $+ \frac{1}{N_{exp,\rho_{liq}^{sat}}} \sum_{i=1}^{N_{exp,\rho_{liq}^{sat}}} \left(\frac{\rho_{liq,i}^{sat,calc} - \rho_{liq,i}^{sat,exp}}{\rho_{liq,i}^{sat,exp}} \right)^2$ $+ \frac{0.5}{N_{exp,\rho_{liq}}} \sum_{i=1}^{N_{exp,\rho_{liq}}} \left(\frac{\rho_{liq,i}^{calc} - \rho_{liq,i}^{exp}}{\rho_{liq,i}^{exp}} \right)^2$ $+ \frac{0.5}{N_{exp,u_{liq}}} \sum_{i=1}^{N_{exp,\rho_{liq}}} \left(\frac{u_{liq,i}^{calc} - u_{liq,i}^{exp}}{u_{liq,i}^{exp}} \right)^2$	55

Model	Non-associating compounds	Parameters fitted	Properties considered for parametrization	Temperature range	Objective function expression	References
SAFT-VR-Mie	C ₁ -C ₁₀ , C ₁₂ , C ₁₅ , C ₂₀ , perfluoroalkanes, F ₂ , CO ₂ , benzene, toluene	$m, \sigma, \varepsilon/k, \lambda_r$ (λ_a was adjusted for perfluoromethane, perfluoroethane and CO ₂)	$P^{sat}, \rho_{liq}^{sat}, \rho_{liq}$ (non-saturated liquid density), u_{liq} (speed of sound) $\lambda_a = 6$ (except for CO ₂ and perfluoroalkanes)	Component dependent	$F_{ob} = \frac{1}{N_{exp, P^{sat}}} \sum_{i=1}^{N_{exp, P^{sat}}} \left(\frac{P_i^{sat, calc} - P_i^{sat, exp}}{P_i^{sat, exp}} \right)^2$ $+ \frac{1}{N_{exp, \rho_{liq}^{sat}}} \sum_{i=1}^{N_{exp, \rho_{liq}^{sat}}} \left(\frac{\rho_{liq, i}^{sat, calc} - \rho_{liq, i}^{sat, exp}}{\rho_{liq, i}^{sat, exp}} \right)^2$ $+ \frac{1}{N_{exp, \rho_{liq}}} \sum_{i=1}^{N_{exp, \rho_{liq}}} \left(\frac{\rho_{liq, i}^{calc} - \rho_{liq, i}^{exp}}{\rho_{liq, i}^{exp}} \right)^2$ $+ \frac{0.25}{N_{exp, u_{liq}}} \sum_{i=1}^{N_{exp, u_{liq}}} \left(\frac{u_{liq, i}^{calc} - u_{liq, i}^{exp}}{u_{liq, i}^{exp}} \right)^2$	14
Soft-SAFT	C ₁ -C ₈ n-alkanes, perfluoroalkanes, O ₂ , Xe, CF ₄	$m, \sigma, \varepsilon/k$	$P^{sat}, \rho_{liq}^{sat}$	Unknown	$F_{ob} = \sum_{i=1}^{N_{exp}} \left\{ \begin{aligned} & \left[\rho_{liq}^{calc}(T_i^{exp}, P_i^{sat, exp}) - \rho_{liq, i}^{sat, exp} \right]^2 \\ & + \left[\mu_{liq}^{calc}(T_i^{exp}, P_i^{sat, exp}) - \mu_{gaz}^{calc}(T_i^{exp}, P_i^{sat, exp}) \right]^2 \end{aligned} \right\}$	84,101

Model	Non-associating compounds	Parameters fitted	Properties considered for parametrization	Temperature range	Objective function expression	References
Crossover Soft-SAFT	Perfluoroalkanes	$m, \sigma, \varepsilon/k$ and 2 additional parameters involved in crossover terms: L, ϕ	$P^{sat}, \rho_{liq}^{sat}$	Unknown	$F_{ob} = \sum_{i=1}^{N_{exp}} \left\{ \begin{aligned} & \left[\rho_{liq}^{calc}(T_i^{exp}, P_i^{sat,exp}) - \rho_{liq,i}^{sat,exp} \right]^2 \\ & + \left[\mu_{liq}^{calc}(T_i^{exp}, P_i^{sat,exp}) - \mu_{gaz}^{calc}(T_i^{exp}, P_i^{sat,exp}) \right]^2 \end{aligned} \right\}$	82,83
Soft-SAFT	Ionic liquids	$m, \sigma, \varepsilon/k$ (association parameters were not fitted; they were set to alkanol parameter values)	ρ_{liq}^{sat}	Unknown	Unknown	102

Model	Non-associating compounds	Parameters fitted	Properties considered for parametrization	Temperature range	Objective function expression	References
Soft-SAFT	n-alkanes and perfluoroalkanes	$m, \sigma, \varepsilon / k$	$P^{sat}, \rho_{liq}^{sat}$, residual heat capacities (C_P^{res}, C_V^{res}), thermal expansivity (α_P), isothermal compressibility (k_T), speed of sound (u)	Unknown	$F_{ob} = \frac{\delta}{N_{exp,VLE}} \left[\begin{aligned} &0.20 \sum_{i=1}^{N_{exp,VLE}} \left(\frac{P_i^{sat,calc} - P_i^{sat,exp}}{P_i^{sat,exp}} \right)^2 \\ &+ 0.80 \sum_{i=1}^{N_{exp,VLE}} \left(\frac{\rho_{liq,i}^{sat,calc} - \rho_{liq,i}^{sat,exp}}{\rho_{liq,i}^{sat,exp}} \right)^2 \end{aligned} \right]$ $+ \frac{1-\delta}{N_{exp,DER}} \sum_{i=1}^{N_{exp,DER}} \left(\frac{X_{liq,i}^{calc} - X_{liq,i}^{exp}}{X_{liq,i}^{exp}} \right)^2$ <p>with: $X \in \{C_P^{res}, C_V^{res}, \alpha_P, k_T, u\}$, $\delta \in [0; 1]$</p>	86
PC-SAFT	n-, branched and cyclo alkanes, alkenes, aromatics, permanent gases, halogenated compounds, ethers, esters	$m, \sigma, \varepsilon / k$	P^{sat} , saturated-liquid volume (v_{liq}^{sat})	Component dependent	$F_{ob} = \sum_{i=1}^{N_{exp,P^{sat}}} \left(\frac{P_i^{sat,calc} - P_i^{sat,exp}}{P_i^{sat,exp}} \right)^2$ $+ \sum_{i=1}^{N_{exp,v_{liq}^{sat}}} \left(\frac{v_{liq,i}^{sat,calc} - v_{liq,i}^{sat,exp}}{v_{liq,i}^{sat,exp}} \right)^2$	12

Model	Non-associating compounds	Parameters fitted	Properties considered for parametrization	Temperature range	Objective function expression	References
PC-SAFT	n-hexane	$m, \sigma, \varepsilon / k$	10 sets of 2 or 3 properties chosen among: $P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{v,liq}^{sat}$ and u_{liq}^{sat}	$T_r \in [0.5; 0.9]$	$F_{ob} = \sum_{\text{properties } X} \sum_{i=1}^{30} \left(\frac{X_i^{calc} - X_i^{exp}}{X_i^{exp}} \right)^2$	103
PC-SAFT	Hexafluoropropylene, hexafluoropropylene oxide	$m, \sigma, \varepsilon / k$	$P^{sat}, \rho_{liq}^{sat}$	HFP - [231.39 - 359.20 K] HFPO - [253.26 - 358.76]	$F_{ob} = 0.5 \left[\frac{100}{N_1} \sum_{i=1}^{N_1} \left(\frac{P_i^{sat,calc} - P_i^{sat,exp}}{P_i^{sat,exp}} \right)^2 + \frac{100}{N_2} \sum_{i=1}^{N_2} \left(\frac{\rho_{liq,i}^{sat,calc} - \rho_{liq,i}^{sat,exp}}{\rho_{liq,i}^{sat,exp}} \right)^2 \right]$	104

Soft-SAFT EoS

The soft-SAFT EoS⁹ uses a Lennard-Jones fluid as the reference fluid. This iteration of the SAFT EoS also includes the same parameters as those present in the original SAFT development ($m, \sigma, \varepsilon/k$) for describing non-associating species.

In passing, note that in order to account for density fluctuations near the critical region, a crossover treatment was frequently applied to the soft-SAFT EoS⁸². Although parametrization issues in relation with the crossover technique are beyond the scope of this article, let us mention however, that crossover parameters are generally fitted to the same properties as other parameters.

As illustrated in **Table 2.1**, one can observe that most of soft-SAFT developers perform the parametrization for the pure components by fitting to P^{sat} and ρ_{liq}^{sat} data (both below and near the critical point when a crossover treatment is applied). As previously observed with the SAFT-VR EoS, it is noticeable that the interest of soft-SAFT developers for parametrization issues has gradually increased through the years. Although the mathematical formulation of the optimization problem they used for estimating the EoS parameters is different from the formulations used by other SAFT EoS developers, the principle of the fitting procedure remains very similar: in all cases: the goal is to reproduce P^{sat} and ρ_{liq}^{sat} data with the highest accuracy.

For heavy molecules like ionic liquids, for which vapor pressures are so low under ambient conditions that they cannot be measured (or, with difficulty), SAFT parameters are solely fitted to liquid-density data.

As a key point, a more recent study done by Oliveira et al.⁸⁶ tested the performance of the parametrization for the soft-SAFT EoS when adding derivative properties (speed of sound, isobaric and isochoric heat capacities, thermal expansivity, isothermal compressibility) to the OF. By considering some n-alkanes and n-perfluoroalkanes as non-associating compounds, they reached the following conclusion: *“for non-associating families, accurate vapor-liquid equilibria are sufficient to obtain transferable parameters for other properties, provided that care has been taken in the fitting procedure and the physical meaning of them”* (note that the word *transferable* means here that the same parameter set can be used to describe different properties). Let us highlight that this conclusion is essentially similar to the one reached by Dufal et al.⁷¹, working on the SAFT-VR EoS.

It can also be noticed that the OF included the sum of the relative differences between VLE data (P^{sat} and ρ_{liq}), with a previously tested weight of 0.80 for the vapor pressure and 0.20 for the liquid density (see of OF expression in **Table 2.1**). These weights *“were found to provide the most balanced and optimal results”*⁸⁶.

PC-SAFT EoS

The Perturbed Chain SAFT EoS¹² relies on the perturbation theory of Barker and Henderson⁵⁶ applied to a hard-chain reference fluid. This model is amongst the most popular choices for SAFT-type users. The original PC-SAFT publication¹² deals exclusively with the modelling of non-associating pure components. PC-SAFT parameters are reported for 85 compounds

including normal, branched and cyclic alkanes, alkenes, aromatic compounds; chlorinated hydrocarbons; permanent gases; ethers and esters. In this paper, Gross and Sadowski¹² performed a classical fitting of the three molecular parameters (m , σ , ε/k) for non-associating pure compounds by minimizing a least squares OF summing relative deviations over P^{sat} and ρ_{liq} experimental data. As observed in the original papers from other developers, emphasis is given to model foundations while the selection of properties involved in the OF and their respective weights are not much discussed.

De Villiers et al.¹⁰³ performed a very interesting study aimed at establishing against which properties EoS parameters should be regressed for a good description of VLE and derivative properties. In particular, for the PC-SAFT EoS, they considered different combinations of 2 or 3 properties chosen among P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$, $c_{v,liq}^{sat}$ and u_{liq}^{sat} to fit the 3 molecular parameters of n-hexane (for each property, 30 data points were considered, in the range $0.5 < T_r < 0.9$). Although based on a single compound, they reported the following important conclusions:

- “only marginal improvements could be obtained by including different properties in the regression in addition to P^{sat} and ρ_{liq}^{sat} ”,
- “model parameters of PC-SAFT can be marginally optimized for non-associating components by including the $\Delta_{vap}H$ in the regression routine, although the improvement is not really significant”,
- “properties that primarily depend on the first-order volume derivative (P^{sat} , ρ_{liq}^{sat}) and second-order volume derivative (u_{liq}^{sat}) cannot be accurately described simultaneously”.

Moine et al.¹⁸ studied the influence of parametrization on cubic and PC-SAFT EoS. They presented three methodologies:

- Exact reproduction of $P_{c,exp}$, $T_{c,exp}$ and ω_{exp} (traditional CEoS parametrization)
- Fitting to P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ (traditional SAFT parametrization with addition of two target properties in the OF)
- Determination of the 3 molecular parameters (m , σ , ε/k) and a fourth parameter, c , called *volume-translation parameter* in order to exactly reproduce 4 properties: $P_{c,exp}$, $T_{c,exp}$, ω_{exp} and $v_{liq,exp}^{sat}(T_r = 0.8)$.

Using the first two, they showed that, when parametrized in the same way, both models have similar strengths and weaknesses, but when adding a volume translation these weaknesses can be mitigated. For PC-SAFT specifically, using the traditional CEoS parametrization yielded acceptable results for P^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ (deviations below 4%) while having high deviations for the liquid volume (17%). However, using the volume-translation to parametrize the PC-SAFT EoS, they showed that much lower deviations could be obtained for the volume without sacrificing much regarding the rest of the properties (deviations lowered from 17% to 4.1%). They named this translated PC-SAFT version: industrialized PC-SAFT (I-PC-SAFT) EoS. Although the alternative parametrization could lead to substantial advances, the traditional

parametrization method for SAFT EoS remains quasi-unanimously used today and is the starting point for obtaining pure component parameters of most complex SAFT versions involving associating, polar and electrolytic contributions. For this reason, this parametrization method is the focus of the present study.

As a conclusion of this overview of the main parametrization habits for SAFT EoS, let us hammer home that although the underlying theory plays a key role on the performance of SAFT-type and EoS in general, the parametrization also comes in as a key aspect to this performance, as shown recently by several author. Nevertheless, parametrization, as shown by the other examples given in **Table 2.1.**, has not seen a deep enough exploration as the theoretical side of SAFT-type EoS.

2.3. Identification of the safe and optimal methods, to fit the parameters of pure-component SAFT-type EoS

As discussed in the introduction, the first step of the present study lies in identifying the safe ways to parametrize a SAFT-type EoS by fitting parameters over experimental data. Note that the methodology we have adopted is straightforwardly inspired from Piña-Martinez et al.⁹⁶. Although various different properties could be included in this screening, we have decided to limit our investigation to the four most-available pure-component properties: the vapor pressure (P^{sat}), the liquid density (ρ_{liq}^{sat}), the enthalpy of vaporization ($\Delta_{vap}H$) and the liquid heat capacity ($c_{P,liq}^{sat}$). The PC-SAFT EoS was chosen as reference SAFT EoS for performing our calculations. The questions we have attempted to answer in this part are:

- a) Which property data should be included necessarily in the parametrization procedure in order to reproduce optimally vapor pressure, liquid density and energetic property data?
Obviously, including the 4 property data in the OF to be minimized enables to immediately meet this objective. However, having in mind that some of these 4 property data can have a negligible impact on the result of the fitting procedure or are not systematically available for any compound, we will investigate whether a safe parametrization remains possible when less experimental property data are used.
- b) Is the classical procedure - involving the use of P^{sat} and ρ_{liq}^{sat} properties in the fitting - safe? Can it be considered as optimal?
- c) How should one weight the properties involved in the OF?

The global methodology.

To answer the previous questions, it has been decided to consider a large number of pure species (several hundreds - in order to reach general and undisputable conclusions), and for each of them, to fit the 3 SAFT parameters to different property data (denoted X). As discussed in the

introduction, the safeness of a parametrization procedure is evaluated with respect to its ability to reproduce the following four properties according to this pecking order of accuracy: $P^{sat} > \rho_{liq}^{sat} > \Delta_{vap}H$ and $c_{P,liq}^{sat}$ (the vapor pressure data being associated with the highest expected accuracy).

For a given pure component j and a given property X ($X \in \{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}\}$), the relative mean square deviation is evaluated according to Eq. (2.2) as the average of the square deviations between experimental and calculated properties over the N_T temperature points.

$$F_{j,X} = \frac{1}{N_T} \sum_{i=1}^{N_T} \left[\frac{X_{j,calc}(T_i) - X_{j,exp}(T_i)}{X_{j,exp}(T_i)} \right]^2 \quad (2.2)$$

$X_{j,calc}(T_i)$ and $X_{j,exp}(T_i)$ correspond to the calculated and experimental values of the component j 's property X , at temperature T_i . In the present study, $N_T = 50$. The temperature ranges for each property are provided in the supporting information (**Table S1**). The OF is obtained by summing the square deviations of each property weighted by property-specific factors ω_X :

$$OF_{component\ j} = \sum_{property\ X} \omega_X F_{j,X} \quad (2.3)$$

To identify the sets of property data enabling to fit safe SAFT parameters, we have decided to test all possible combinations of the four properties $\{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}\}$ giving rise to 15 possibilities and thus to 15 objective functions (OF) to be minimized, as shown in **Table 2.2**.

Table 2.2. List of the 15 property data combinations of $\{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}\}$ usable for fitting SAFT parameters.

OF index	Property data involved in the OF
1	$(P^{sat} + \rho_{liq}^{sat} + \Delta_{vap}H + c_{P,liq}^{sat})$
2	(P^{sat})
3	(ρ_{liq}^{sat})
4	$(\Delta_{vap}H)$
5	$(c_{P,liq}^{sat})$
6	$(P^{sat} + \rho_{liq}^{sat})$

OF index	Property data involved in the OF
7	$(P^{sat} + \Delta_{vap}H)$
8	$(P^{sat} + c_{P,liq}^{sat})$
9	$(\rho_{liq}^{sat} + \Delta_{vap}H)$
10	$(\rho_{liq}^{sat} + c_{P,liq}^{sat})$
11	$(\Delta_{vap}H + c_{P,liq}^{sat})$
12	$(P^{sat} + \rho_{liq}^{sat} + \Delta_{vap}H)$
13	$(P^{sat} + \rho_{liq}^{sat} + c_{P,liq}^{sat})$
14	$(P^{sat} + \Delta_{vap}H + c_{P,liq}^{sat})$
15	$(\rho_{liq}^{sat} + \Delta_{vap}H + c_{P,liq}^{sat})$

However, as explained in **Appendix A1** and highlighted in **Table 2.3**, both the enthalpy of vaporization and the liquid heat capacity are σ independent. Consequently, fitting the three molecular parameters ($m, \sigma, \varepsilon/k$) for OF 4, OF 5 and OF 11 which include either enthalpy of vaporization data alone or liquid heat capacity data alone or both of them is senseless and thus, these three functions must be disregarded, leaving the remaining 12 to be studied.

Table 2.3. Variable set of each VLE property of interest for the present study

Property	Variables on which the property depends
P^{sat}	$(T, m, \sigma, \frac{\varepsilon}{k})$
$\Delta_{vap}H$	$(T, m, \frac{\varepsilon}{k})$ Note that $\Delta_{vap}H$ is σ independent
$c_{P,liq}^{sat}$	$(T, m, \frac{\varepsilon}{k})$ Note that $c_{P,liq}^{sat}$ is σ independent
ρ_{liq}^{sat}	$(T, m, \sigma, \frac{\varepsilon}{k})$

Component selection and data collection.

Keeping the spirit of the work done by Pina-Martinez et al. ⁹⁶, the studied OFs were tested to the largest possible number of compounds for which pseudo-experimental data for the four target properties are available. **Appendix A2** gives a brief explanation on the selection of the pure components from the DIPPR databank, based on the simultaneous availability of the four properties of interest $\{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}\}$ with a reasonable level of accuracy. This procedure yielded a working set made of 808 associating and non-associating pure components.

Among these, we have only kept the non-associating ones. The associating character of each species was quantified following a methodology explained in **Appendix A3**. In short, the screening charge density distribution (sigma profile) of each compound was generated and analyzed to determine its tendency to associate. After this step, the working set contained 656 non-associating molecules.

Evaluation of the fitting procedure.

The quality of each of the 12 fitting procedures (a fitting procedure is defined by the OF definition including the list of involved properties and the corresponding weight factors as well) is assessed from the mean average percentage errors (MAPEs) on each of the four properties $\{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}\}$. Eq. (2.4) shows the expression used to calculate the MAPE on a given property X :

$$MAPE_X = \frac{100}{N_T} \sum_{i=1}^{N_T} \left| \frac{X_{i,calc} - X_{i,exp}}{X_{i,exp}} \right| \quad (2.4)$$

Selection of optimal weight factors for each of the 12 OF considered.

Depending on the values assigned to the weight factors ω_X (see Eq.(2.3)), a multiplicity of different parameter sets ($m, \sigma, \varepsilon / k$) can be obtained for a given OF, leading to different model qualities (evaluated in terms of MAPEs). Consequently, it is necessary to define carefully the expected objectives in terms of MAPE and then, to identify the weight factors ω_X leading as close as possible to these objectives.

In the present case, considering that SAFT users expect high accuracy on the reproduction of both vapor pressure and liquid density we aim to have the MAPEs between these two properties as close to equal as possible. In addition, we aim for $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ to have their MAPEs as close to equal as possible between each other. This led us to define the first objective as:

$$\text{Objective 1: } \begin{cases} MAPE_{P^{sat}} \approx MAPE_{\rho_{liq}^{sat}} \\ MAPE_{\Delta_{vap}H} \approx MAPE_{c_{P,liq}^{sat}} \end{cases} \quad (2.5)$$

We have searched empirically the weight factors reaching systematically this objective and found that the vapor-pressure weight must be half-higher than the liquid-density weight while the weights of the energetic properties must be chosen equal. We have thus arbitrarily set:

$$\text{Weight factors enabling the satisfaction of objective 1: } \begin{cases} \omega_{P^{sat}} = 3 \\ \omega_{\rho_{liq}^{sat}} = 2 \\ \omega_{\Delta_{vap}H} \approx \omega_{c_{P,liq}^{sat}} \end{cases} \quad (2.6)$$

Secondly, we seek to find a value for the relative weight between energetic properties on one side and (P^{sat} and ρ_{liq}^{sat}) on the other side. Given that the energetic properties act as secondary properties and the hierarchy of importance we defined for the four properties (P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}$), higher deviations are allowed for them with respect to P^{sat} and ρ_{liq}^{sat} .

To characterize the second objective, a global energetic MAPE was defined as:

$$MAPE_{energetic\ prop} = \begin{cases} MAPE_{\Delta_{vap}H} + MAPE_{c_{P,liq}^{sat}} & \text{if both } \Delta_{vap}H \text{ and } c_{P,liq}^{sat} \text{ are} \\ & \text{present in the OF definition} \\ MAPE_{\Delta_{vap}H} & \text{if only } \Delta_{vap}H \text{ is present in the OF definition} \\ MAPE_{c_{P,liq}^{sat}} & \text{if only } c_{P,liq}^{sat} \text{ is present in the OF definition} \end{cases} \quad (2.7)$$

As second objective, it was decided to impose the EoS to predict P^{sat} and ρ_{liq}^{sat} properties with an error twice lower than the error on energetic properties; we used then the criterion:

$$\text{Objective 2 - a : } MAPE_{energetic\ prop} \gg 2 \times MAPE_{VLE}$$

$$\text{with } MAPE_{VLE} = \begin{cases} MAPE_{P^{sat}} + MAPE_{\rho_{liq}^{sat}} & \text{if both } P^{sat} \text{ and } \rho_{liq}^{sat} \text{ are} \\ & \text{present in the OF definition} \\ MAPE_{P^{sat}} & \text{if only } P^{sat} \text{ is present in the OF definition} \\ MAPE_{\rho_{liq}^{sat}} & \text{if only } \rho_{liq}^{sat} \text{ is present in the OF definition} \end{cases} \quad (2.8)$$

The corresponding weight factor $\omega_{energetic\ prop}$ was thus determined in order to satisfy objective 2-a. To do so, 10 discrete values of $\omega_{energetic\ prop}$ ranging between 0.15 and 1.5 (step = 0.15) were tested for each OF expression (except OF 2, 3 and 6 which do not involve energetic properties) and the one approaching best the objective 2-a was selected. However, in some cases, we noticed that by slightly deteriorating objective 2-a, it was possible to significantly lower the sum over all MAPEs (see Eq.(2.9)) which was thus used as second objective:

$$\text{Objective 2 - b : } \min_{\omega_{\text{energetic prop}}} \{MAPE_{\text{energetic prop}} + MAPE_{VLE}\} \quad (2.9)$$

It was decided finally to switch from the weight factor $\omega_{\text{energetic prop}}$ that better satisfies objective 2-a to the one that better satisfies objective 2-b each time the quantity $(MAPE_{VLE})_{\text{approaching objective 2-a}}$ was significantly higher than the quantity $(MAPE_{VLE})_{\text{approaching objective 2-b}}$.

Therefore, we used as second objective:

$$\text{Objective 2} = \begin{cases} \text{Objective 2 - a if } \frac{(MAPE_{VLE})_{\text{approaching objective 2-a}}}{(MAPE_{VLE})_{\text{approaching objective 2-b}}} \leq 1.5 \\ \text{Objective 2 - b, otherwise.} \end{cases} \quad (2.10)$$

To illustrate this procedure, let us consider an example. For a given molecule, selecting $\omega_{\text{energetic prop}}$ in order to satisfy either objective 2-a or objective 2-b leads to the values reported in **Table 2.4**.

Table 2.4. Illustration on an arbitrary molecule of the procedure aimed at selecting the weight factor $\omega_{\text{energetic prop}}$.

MAPEs	$\omega_{\text{energetic prop}}$ was selected in order to satisfy objective 2-a	$\omega_{\text{energetic prop}}$ was selected in order to satisfy objective 2-b
$MAPE_{p^{sat}}$	1.8%	0.7%
$MAPE_{\rho_{liq}^{sat}}$	2.1%	0.7%
$MAPE_{\text{energetic prop}}$	7.8%	6.6%
$MAPE_{VLE}$	3.9%	1.4%
$\frac{MAPE_{\text{energetic prop}}}{MAPE_{VLE}}$	2.0	4.7
Total MAPE	11.7%	8.0%
$(MAPE_{VLE} + MAPE_{\text{energetic prop}})$		

It appears that it is possible to decrease notably both the quantity $MAPE_{VLE}$ (from 3.9% to 1.4%) and the total MAPE (from 11.7% to 8.0%), by allowing the ratio $\frac{MAPE_{\text{energetic prop}}}{MAPE_{VLE}}$ to be higher than 2. In such a case, the value finally considered for $\omega_{\text{energetic prop}}$ is the one associated with objective 2-b.

Implementation of the optimization procedure.

The minimization of each OF was performed using the classical Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm belonging to the quasi-Newton class of optimization methods. Depending on the initial parameter set value, the solution returned by this type of iterative procedure may converge either to a local or to the global minimum. One way to circumvent this issue (i.e., to ensure that the algorithm found the global minimum) is to run multiple optimizations, each characterized by a specific initial parameter set, and to select as final parameter set, the one associated with the lowest OF value.

In order to estimate safely the molecular parameters for the 12 OFs, different sets of initial values to m , σ and ε/k were generated and used with each OF expression, thus ensuring a solid starting point to the parametrization routine. **Appendix A4** give the reader an extended explanation on the selection of initial values.

Results and Discussion

Table 2.5 presents the average results and the average standard deviation obtained for the PC-SAFT parametrization using OF 1 (the one in which the PC-SAFT parameters are fitted to all four properties $\{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}\}$), for the 656 non-associating pure compounds.

Table 2.5. Average MAPEs on $\{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}\}$ and related standard deviations calculated over 656 non-associating species, when the PC-SAFT parameters are fitted to $P^{sat} + \rho_{liq}^{sat} + \Delta_{vap}H + c_{P,liq}^{sat}$ (refer to OF 1 in Table 2).

Property	Average MAPE (%)	Standard deviation (%)
P^{sat}	0.94	0.71
ρ_{liq}^{sat}	0.96	0.69
$\Delta_{vap}H$	2.76	1.52
$c_{P,liq}^{sat}$	2.91	2.96
Sum of the 4 MAPEs	7.57	4.28

As a first highlight, we observe that the average MAPEs for P^{sat} and ρ_{liq}^{sat} are very close to equal with 0.94% and 0.96%, respectively. Similarly, the average MAPEs on $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ are also very close to equal. The first objective for the parametrization routine (see Eq.(2.5)) is thus perfectly met. The second highlight is that the ratio $\frac{MAPE_{\text{energetic prop}}}{MAPE_{VLE}}$ is close to 3

indicating that objective 2-b was satisfied instead of objective 2-a for many species (see Eqs.(2.8) - (2.10)). However, after a deeper look into each individual compound, we observed that the sum of the MAPEs for the four properties for 104 compounds is greater than the sum of the average MAPE for all four properties (7.57%) plus 1 standard deviation (4.28%), meaning that these compounds have a sum of the four MAPEs above 11.84%. We considered that these molecules cannot be properly modeled and we therefore removed them from the studied set. Furthermore, we observed that 36 additional molecules had a MAPE on the vapor pressure, which was higher than the average MAPE for this property plus 1 standard deviation (0.71%), meaning the MAPE for P^{sat} was above 1.65%. Since we consider P^{sat} as the most important property for any EoS, we concluded that these 34 molecules could not be modeled neither. Taking out these 136 molecules from the original dataset of 656, we ended up with a curated dataset of 544 non-associating species. The main reason for the removal of these 136 molecules is simply to avoid that they introduce a bias in the parametrization procedure definition. **Table 2.6** presents the average results obtained for the PC-SAFT parametrization

using the 12 OF for the newly obtained 544 non-associating pure compounds for which all target properties have experimental data available.

It is worth recalling that our unique objective is a simultaneous accurate description of both VLE and energetic properties explaining why the sum of the 4 MAPEs on P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ that we wish to minimize (see Eq. (2.11)) is given in the last column of **Table 2.6**.

$$Objective = minimize \left\{ \begin{array}{l} MAPE \text{ on } P^{sat} + MAPE \text{ on } \rho_{liq}^{sat} + \\ MAPE \text{ on } \Delta_{vap}H + MAPE \text{ on } c_{P,liq}^{sat} \end{array} \right\} \quad (2.11)$$

In order to better highlight our objective recalled in Eq. (2.11) the results in **Table 2.6** are ranked by increasing values of the 4 MAPEs sum.

Table 2.6. Average values of the MAPEs on $\{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, C_{P,liq}^{sat}\}$, and the critical temperature, pressure and molar volume $\{T_c, P_c, v_c\}$ calculated over 544 non-associating pure species, corresponding each to a different combination of property data on which the PC-SAFT parameters were adjusted.

OF index	Property data included in the parameter fitting procedure	Average value of MAPE calculated over 544 species							Sum of the 4
		P^{sat}	ρ_{liq}^{sat}	$\Delta_{vap}H$	$C_{P,liq}^{sat}$	T_c	P_c	v_c	MAPEs on P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$, $C_{P,liq}^{sat}$
		(%)	(%)	(%)	(%)	(%)	(%)	(%)	
1	$(P^{sat} + \rho_{liq}^{sat} + \Delta_{vap}H + C_{P,liq}^{sat})$	0.72	0.82	2.41	2.24	2.08	15.9	3.19	6.2%
13	$(P^{sat} + \rho_{liq}^{sat} + C_{P,liq}^{sat})$	0.72	0.69	2.57	2.20	2.19	16.3	3.05	6.2%
6	$(P^{sat} + \rho_{liq}^{sat})$	0.60	0.67	2.57	2.42	2.22	16.4	3.05	6.3%
12	$(P^{sat} + \rho_{liq}^{sat} + \Delta_{vap}H)$	0.74	0.89	2.34	2.31	2.05	15.8	3.28	6.3%
14	$(P^{sat} + \Delta_{vap}H + C_{P,liq}^{sat})$	0.70	7.57	1.41	2.16	1.24	8.9	8.87	11.8%
7	$(P^{sat} + \Delta_{vap}H)$	0.65	7.56	1.34	2.37	1.23	8.8	9.31	11.9%
15	$(\rho_{liq}^{sat} + \Delta_{vap}H + C_{P,liq}^{sat})$	8.82	0.51	1.58	1.87	1.18	15.8	2.80	12.8%
9	$(\rho_{liq}^{sat} + \Delta_{vap}H)$	8.75	0.49	1.30	2.45	1.20	15.9	2.80	13.0%
8	$(P^{sat} + C_{P,liq}^{sat})$	0.57	16.8	4.29	1.58	3.00	20.7	11.02	23.2%
2	(P^{sat})	0.46	15.5	4.99	3.18	3.91	29.1	10.89	24.1%

OF index	Property data included in the parameter fitting procedure	Average value of MAPE calculated over 544 species							Sum of the 4 MAPESs on P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$, $C_{P,liq}^{sat}$
		P^{sat} (%)	ρ_{liq}^{sat} (%)	$\Delta_{vap}H$ (%)	$C_{P,liq}^{sat}$ (%)	T_c (%)	P_c (%)	v_c (%)	
10	$(\rho_{liq}^{sat} + C_{P,liq}^{sat})$	18.4	0.37	6.14	1.24	1.68	15.9	3.43	26.2%
3	(ρ_{liq}^{sat})	22.5	0.42	7.77	3.85	2.00	16.3	3.39	34.5%

We immediately notice that 4 fitting procedures (1, 13, 6, 12) among the 12 tested lead to extremely similar results. For these for cases, the sum of the 4 MAPEs on P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ is as small as 6.2% (the MAPEs on P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ are 0.7%, 0.8%, 2.5% and 2.3% respectively). Common to all these 4 regression procedures is the inclusion of experimental P^{sat} and ρ_{liq}^{sat} data in the fitting procedure. At this point, it is thus possible to immediately conclude that:

1. PC-SAFT parameters have to be absolutely fitted to both vapor pressure and liquid density data.
2. Only extremely marginal improvements can be obtained on energetic properties by including $\Delta_{vap}H$ and/or $c_{P,liq}^{sat}$ in the regression procedure demonstrating that this inclusion is not advised because not necessary.

Table 6 also shows that for the 8 other fitting procedures (14, 7, 15, 9, 8, 2, 10, 3) the sum of the 4 MAPEs on P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ is from twice to five times higher than the one obtained previously (with the fitting procedures that include P^{sat} and ρ_{liq}^{sat} data). These 8 fitting procedures must thus be disregarded.

From **Table 2.6**, it is also possible to conclude that by regressing PC-SAFT parameters against P^{sat} or ρ_{liq}^{sat} data only (OF 2 and 3 respectively), extremely high deviations on the MAPE of the missing VLE property is observed. Regressing the parameters on P^{sat} only (see OF 2) yields a MAPE of 0.46 % for the vapor pressure but a MAPE of 15.51 % on the liquid density. Likewise, regressing the parameters on ρ_{liq}^{sat} only (refer to OF 3) yields a MAPE of 0.42 % for liquid density but a MAPE of 22.46 % for the vapor pressure. The enthalpy of vaporization is notably high for these two fitting procedures with 4.99 % and 7.77% for OF 2 and OF3 respectively. Including $\Delta_{vap}H$ (see OF 7 and OF 9) improves the MAPE on the missing VLE property but still not to a satisfactory level. For instance, OF 7 for which the parameters are regressed on P^{sat} and $\Delta_{vap}H$ increases the deviations on the vapor pressure (from 0.49 % to 0.65 %) but improves the MAPEs on the enthalpy (from 4.99 % to 1.34 %) and on the liquid density (from 15.5 % to 7.56 %). Nevertheless, the latter still does not meet any of the goals set up for the parametrization and has a rather high deviation. A similar behavior is observed between OF 3 and OF 9 in which deviations on ρ_{liq}^{sat} increase (from 0.42 % to 0.49 %) while improving the MAPE on $\Delta_{vap}H$ (from 7.77 % to 1.30 %) and on P^{sat} (from 22.46 % to 8.75 %) with the latter still outside of acceptable deviations. Adding $c_{P,liq}^{sat}$ instead of $\Delta_{vap}H$ (refer to OF 8 and 10) leads to the same conclusions. Moreover, one reaches the same conclusion having both energetic properties and only one of the VLE properties (refer to OF 14 and 15).

Table 6 also shows that the critical temperature is well represented, although higher deviations can be found if only the vapor pressure is included (3.18 % with OF 2). Including one VLE property (P^{sat} or ρ_{liq}^{sat}) and either one or both energetic properties ($\Delta_{vap}H$ and $c_{P,liq}^{sat}$) shows the lowest deviations for the critical temperatures with a MAPE around 1.2 % for all four possible cases (OF 7, OF 9, OF 14 and OF15) . For the critical pressure, as expected with the PC-SAFT EoS, poor representation of this property was achieved, with all deviations above 8.8%.The OFs which include de vapor pressure and either one ($\Delta_{vap}H$) or both energetic properties (OF 7 and OF 14 respectively) have the lowest MAPE for the critical pressure. On the other hand, OF 2, which includes only the vapor pressure, has the highest deviation for the critical pressure with 29.1 %. A similar behavior is observed for the critical molar volume, where the OFs that include the liquid density plus one ($\Delta_{vap}H$) or both of the energetic properties (OF 9 and OF 15 respectively) have the lowest deviations with 2.80 % for both. OF 8 (P^{sat} and $c_{P,liq}^{sat}$) and OF 2 (P^{sat}) have the highest deviations for the critical molar volume with MAPES around 11 %.

It is worth noting that commonly treated compounds, such as the ones found in the chemical families present in this work, have a common objective, shared by most model users, which is to represent the VLE and the energetic properties to the best of the model's ability. For heavy molecules, such as ionic liquids (ILs) or deep eutectic solvents (DES), the objectives are different, especially because of the lack of (or the very negligible) vapor pressure. In such cases the selection of the OF used for PC-SAFT may vary depending on the user's objective: are they looking for the absolute or the relative deviation for this property. The user must be aware that selecting an OF which does not include P^{sat} data leads to high deviations on this property. This is then left to the user's choice as their objectives might not be the same as the ones established in the present work. Furthermore, a deeper look into the behavior of these heavy molecules requires a proper study in itself, which is beyond the scope of the present work.

2.6. Conclusion

In this paper, 12 combinations of property data (among P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$) that could be used to fit the 3 non-associating PC-SAFT parameters were tested. Different weighting factors were assigned to each property, having fixed values of 3 and 2 for P^{sat} and ρ_{liq}^{sat} respectively, in the objective function. A weight analysis was performed on the combinations involving enthalpy and/or heat capacity data. Each time, ten different weighting factors in a range between 0.15 and 1.5 were tested. The screening included 544 non-associating compounds for which experimental data for all four properties is available in the DIPPR databank.

The study revealed that consistent molecular parameters ($m, \sigma, \varepsilon/k$) for the PC-SAFT equation of state were obtained systematically when the parameters were fitted to P^{sat} and ρ_{liq}^{sat} only (with weight factors fixed at 3 and 2 respectively). Including $\Delta_{vap}H$ and/or $c_{P,liq}^{sat}$ data in the regression procedure is not a necessity and only marginally improves the reproduction of these properties. Not including either P^{sat} or ρ_{liq}^{sat} is highly unadvised.

On a following step, a database of molecular parameters for the PC-SAFT EoS, consisting of 1252 non-associating pure compounds for which at least P^{sat} and ρ_{liq}^{sat} experimental data are available in the DIPPR databank was constructed by fitting the parameters to such data. With

these parameters, the PC-SAFT EoS leads to the following average deviations: $MAPE_{P^{sat}} = 0.97\%$, $MAPE_{\rho_{liq}^{sat}} = 0.85\%$, $MAPE_{\Delta_{vap}H} = 3.04\%$ and $MAPE_{c_{P,liq}^{sat}} = 3.35\%$.

For the same list of compounds, these results were compared to another SAFT model: the *I*-PC-SAFT and two CEoS: the *tc*-PR and generalized *tc*-PR. Overall, the PC-SAFT and *tc*-PR EoS in which the EoS parameters are fitted to experimental data show very similar accuracy. It is hard to conclude which one is superior to the other. Similarly, the predictive *I*-PC-SAFT and gen-*tc*-PR EoS, that require the knowledge of $T_{C,exp}$, $P_{C,exp}$, ω_{exp} and $v_{liq,exp}^{sat}(T_R = 0.8)$ only, show similar accuracies. If one wants to go into the details, one can claim that the PC-SAFT EoS best predicted the liquid density with the proposed parameterization method while the other properties are still in a satisfactory position in comparison with the other three models.

The cubic models perform better at predicting enthalpy of vaporization and the liquid heat capacity than the SAFT models. The vapor pressure had the highest accuracy for all studied models.

In general, all models present satisfactory results across all the target properties. The model used in this work best predicted the critical molar volume, although the critical pressure is greatly overestimated.

Both SAFT models in general have better predictions of this property than the CEoS. Both cubic models had equal deviations for the critical molar volume, while the fitted PC-SAFT EoS had

the best performance out of the SAFT models. This remark makes it possible to state that fitted models perform better over the critical molar volume in general.

**Chapter 3 : Associating terms in equations of state:
are they essential to describe self-associating
compounds?**

The previous chapter showed the process of obtaining a safe and transparent parametrization methodology for pure compounds, which was later applied to pure non-associating compounds, meaning that these molecules interact with others only via dispersion forces, such as the van der Waals interactions. However, there are molecules that can interact with forces that are, in general, stronger than dispersive interactions. These forces are known as **quasi-chemical forces**²⁶ and are responsible for the aggregation of atoms or molecules into larger units or complexes, a phenomenon known as **chemical association**¹⁰⁵.

This forces usually stand as a middle ground between dispersive forces (molar enthalpies between 8-30 kJ/mol)¹⁰⁶ and actual chemical bonds, in particular the **covalent bond** (enthalpies between 200-400 kJ/mol)¹⁰⁶. Two main chemical association interactions are of practical interest:

- $\pi - \pi$ interactions¹⁰⁶, also known as charge-transfer or Lewis acid-Lewis Base (LA-LB) interactions, which occur between aromatic-aromatic or aromatic-unsaturated structures (e.g. nitrobenzene-mesitylene), or self-associating structures and aromatic/unsaturated structures (e.g. water-benzene). These interactions have an energy (enthalpy) of 40-80 kJ/mol.
- Hydrogen bonding, which is considered the main intermolecular interaction for chemical association, in which an electronegative atom of a molecule (e.g. fluorine or oxygen atoms) interacts with labile hydrogen atoms from another molecule (regardless if it is a molecule of the same type or not). This interactions range from enthalpy values between 5-40 kJ/mol and act at further distances than $\pi - \pi$ or dispersive interactions^{26,106}.

In this chapter an introduction to the nature of hydrogen bonds as well as a discussion on how to determine whether a pure compound can be considered self-associating or not and to better understand the impact of parametrizing these types of associating species without an associating term and analyze the performance of the PC-SAFT non-associating mode of the EoS.

It is well acknowledged that compounds participating in chemical association interactions, in particular hydrogen bonding, cannot be accurately described by an EoS that does not account for the association effects^{13,107,108}. Dufal et al.¹⁰⁷ summarizes the sentiment towards the ability of non-associating EoS modeling associating compounds:

“One of the principal motivations for the development of the statistical associating fluid theory in the late 1980s was the need for a rigorous and reliable equation of state for the thermodynamic properties and phase equilibria of associating fluids; these systems could not bet described in adequate manner with the more traditional cubic EoS available at the time”.

In order to have an objective quantitative evaluation of these claims, we propose to evaluate the capacity of the PC-SAFT in the non-association mode to describe associating species. A priori, we should expect the following behavior, according to literature:

- The higher the tendency of a fluid to associate should be reflected in poor descriptions by the EoS for non-associating species. This should be evident, for example, in

homologous series such as n-alcohols, were higher deviations should be observed for lighter members of the series (i.e. methanol and ethanol) and a progressive decrease of said deviations for heavier members of the series (i.e. n-decanol and onwards)⁷⁰. There should be a **dilution effect** of the chemical association in function of the increase of molecular weight.

- The EoS in the non-associating mode should be unable to describe nearly all associating fluids inaccurately. This is because no explicit term is taking into account chemical association through hydrogen bonding.

This chapter will first present the main interaction in chemical association: the **hydrogen bond** and detail its features and characteristics. Then, the associating character for a pure compound will be described, including a methodology to categorize compounds as associating or non-associating. Finally, an article evaluating the performance of PC-SAFT in the non-associating mode when tasked to describe pure-compound properties for self-associating compounds, will conclude this chapter. Its performance will be contrasted to highly performing EoS such as the *I*-PC-SAFT EoS¹⁸ and the *tc*-PR³².

3.1. The hydrogen bond

Hydrogen bonding is a well-recognized electrostatic and chemical interaction present in all areas of chemistry, from chemical engineering to biochemistry. It is responsible for many intriguing physical phenomena such as the difference in boiling points between similar compounds like ethanol and dimethyl ether, the strength of fibers such as nylon, the hydrophobic effect in water molecules²⁶, etc. Some of the most complex systems to study and describe through the thermodynamic lenses are in one way or another involved in hydrogen bonding and thus it is key to understand this interaction to better account for it in models such as EoS.

According to the International Union of Pure and Applied Chemistry (IUPAC)¹⁰⁹ the hydrogen bond (HB) is defined as:

An attractive interaction between a hydrogen atom from a molecular fragment X-H in which X is more electronegative than H, and an atom or a group of atoms in the same or a different molecule, in which there is evidence of bond formation.

In practice, it is the electrostatic force of attraction between a hydrogen atom covalently bound to an atom X which is more electronegative than itself and another electronegative atom Y that possesses a lone pair of electrons which can be bonded to another H or a different atom Z. A typical HB comes in the form of:



The IUPAC task group also provides a list of criteria that act as evidence for HB formation in between a pair of molecules:

- The forces involved in the formation of a hydrogen bond include those of an electrostatic origin, those arising from charge transfer between the donor and acceptor leading to partial covalent bond formation between H and Y, and those from dispersion forces.
- The atom X is covalently bonded to H and the X-H bond is polarized.

- The H and the H-bonded atom are close to each other on a nearly linear angle (180°). The closer the stronger the HB.
- The X-H covalent bond is lengthened when in presence of a HB. Greater lengthening indicates stronger HB.
- The HB shown in Eq. (3.1) leads to characteristic nuclear magnetic resonance (NMR) signatures.
- The Gibbs energy of formation for the HB should be greater than the thermal energy (molar enthalpy of HB formation¹¹⁰) of the system. Typical value of Gibbs energy of HB range from -2.0 kJ/mol ¹¹¹ to -5.7 kJ/mol ¹¹² for water at 25°C .

NOTE: The hydrogen bond Gibbs energy of formation comes from modeling the HB as a equilibrium reaction in which two species bond into a more structured complex. In that sense, both the molar enthalpy and entropy of hydrogen bonding formation would be negative. Taking the example of pure water, we find that the enthalpy of formation of hydrogen bonds is approximately -21 kJ/mol . This value is lower than the Gibbs energy of HB formation shown above and thus it is possible to conclude that the molecule will tend to form HB.

Other notable characteristics and deeper justification of these criteria as sufficient evidence for HB can be found in the reports made by the IUPAC in 2011^{109,113}.

HB are characterized by having two sites in which the interaction occurs: one site is located in the molecule that possesses the H atom, otherwise known as **hydrogen donor** (HD) and another site located in the molecule that possesses the Y atom with the lone pair of electrons, otherwise known as **hydrogen acceptor** (HA). The HD site “gives away” its H atom to the HA site in order to allow for the formation of the bond itself. The following figure shows an illustration of this with an example of an alcohol molecule bonding with a chlorinated molecule.

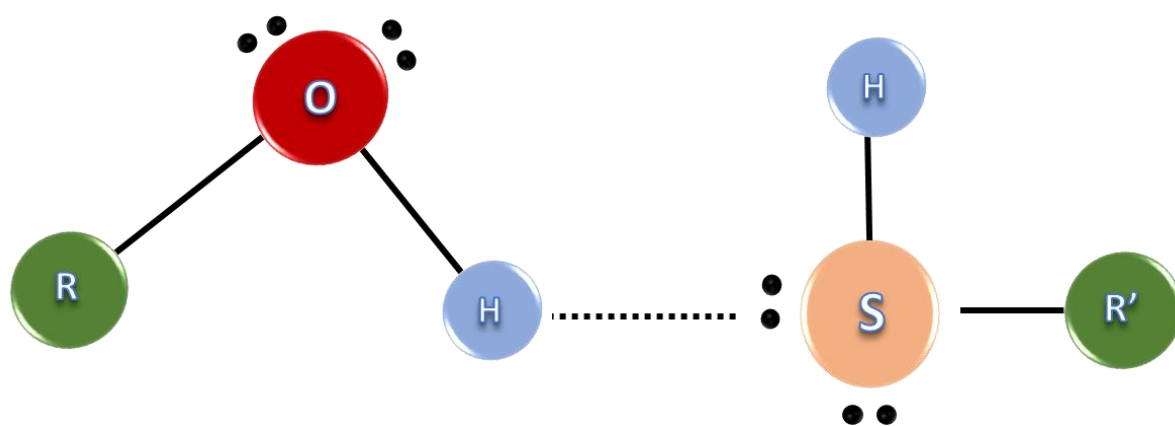


Figure 3.1. Example of a hydrogen bond between an alcohol and a sulfonated compound. The green molecules R and R' are carbon chains of any length. The black dots represent electron pairs. The solid lines are covalent bonds while the dashed line represents the HB.

From **Figure 3.1** we can show the process of formation of the HB and identify the different sites present: The oxygen atom in the alcohol polarizes the covalent bond it shares with the hydrogen, leaving an electrostatic positive charge and thus allowing its H atom to be donated. On the other hand, the highly electronegative sulfur atom does a similar thing to its covalent

bond with the carbon chain R' creating an electrostatic negative charge. The sulfur atom has two lone pair of electrons, which can form a bond with the H atom of the alcohol by accepting it through the electrostatic attraction. Thus the dashed line forms, which represents the HB.

HB are classified according to their strength of formation into three main categories¹⁰⁶:

- Weak HB, for bonds with a molar energy of formation $\Delta_{HB}H < 20$ kJ/mol.
- Intermediate or medium HB, for bonds with $\Delta_{HB}H$ between 20 and 40 kJ/mol.
- Strong HB, for bond with $\Delta_{HB}H$ above 40 kJ/mol.

The strength of the HB depends on the nature of the atom to which the H atom is bounded in the HD site and the nature of the acceptor atom in the HA site. It depends on the temperature and the medium where they occur, i.e. methanol-methanol HB is expected to have higher HB strength if it occurs in water instead of in n-hexane.

A fluid that shows H-bonding is commonly referred to as associated or associating. The following sections will discuss more in depth on this associating nature and a discussion on how to determine if it will take place.

3.2. Associating character of a pure compound

As mentioned before, an associating fluid is one that displays HB. However, there are two main types of associating fluids depending on the molecules participating in the HB:

- **Self-associating** fluids are those in which the HB takes place between molecules of the same species. Some examples of this type of association include:
 - Water-Water $\Delta_{HB}H = 21$ kJ/mol^{114,115}.
 - Methanol-Methanol $\Delta_{HB}H = 14.2$ kJ/mol^{114,115}
 - Methylamine-Methylamine $\Delta_{HB}H = 4.0$ kJ/mol^{114,115}
- **Cross-associating** or **Solvating**²⁶ fluids are those in which the HB takes place between different types of molecules. Some examples of this type of association include:
 - Water-Methanol $\Delta_{HB}H = 21$ kJ/mol¹⁰⁶.
 - Methanol-n-Butylamine $\Delta_{HB}H = 27.3$ kJ/mol¹¹⁶

It is worth noting that self-association can be intermolecular, between two molecules of the same type or intramolecular between atoms of the same molecule. This latter case will not be discussed throughout this dissertation, but it has to be mentioned nonetheless. In order for a molecule to self-associate it must have both a HD and a HA site in its structure, otherwise it will not form a HB with itself. For example, chloroform (CHCl₃) has three chlorine atoms which polarize the molecule, leaving the hydrogen atom available for being donated in a HB. It cannot receive, however, any hydrogen atoms from other molecules, in spite of having electron pairs; this is due to the fact that the larger size of chlorine atoms make them possess low electron density¹¹⁷ and thus leaving them unable, in this case, to sustain an HB as an HA. For this reason, chloroform is an HD molecule alone. On another end, we have the example of acetone (C₃H₆O), which has two pairs of free electrons capable of accepting a hydrogen atom from another molecule to form a HB. It cannot donate any of its hydrogen atoms since the carbon atoms are

not sufficiently electronegative to allow them to be available for bonding, making it a HA molecule alone. Finally, a single water molecule (H_2O) has two pairs of free electron and two hydrogens, which are available for HB participation since both of them, are bonded to the oxygen atom. This molecule is both HA and HD at the same time and thus could form HB with other water molecules. Alcohols are another example of molecules that are HD and HA at the same time.

Regarding cross-association, there are several possibilities in which the HB can form: cross-association of two self-associating compounds (e.g., water-methanol); cross-association where only one of the two compounds is self-associating (e.g., ethanol-chloroform) or cross-association where none of the involved compounds are self-associating but have one of each type of site (HA and HD) mentioned in the previous section (e.g., chloroform-acetone). **Figure 3.2** illustrates the cross association between acetaldehyde (HA) and dichloromethane (HD).

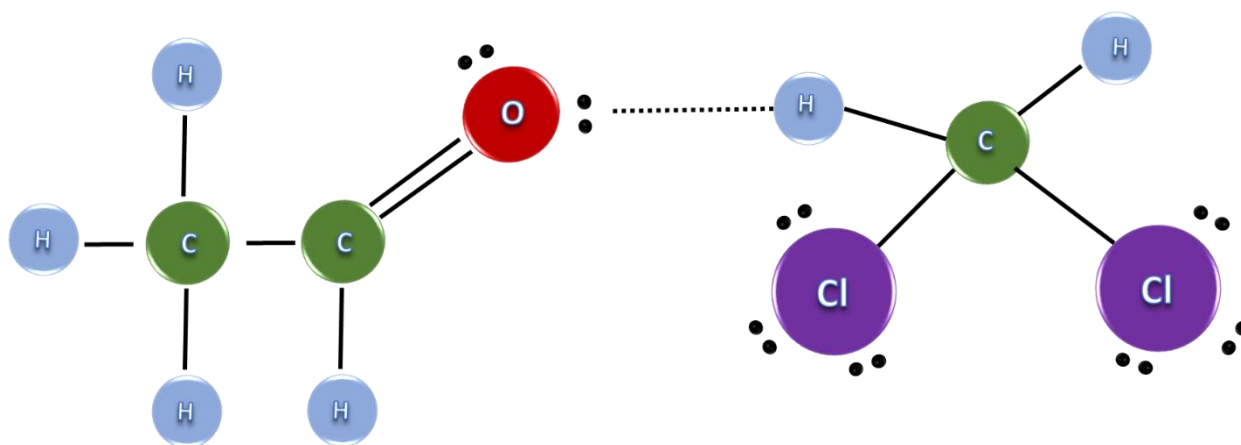


Figure 3.2. Cross-association between acetaldehyde (left) and dichloromethane (right). Solid lines represent covalent bonds. Dotted lines represent hydrogen bonds.

From the figure, we can see that a hydrogen bond can form between these two molecules but neither can participate in HB with a similar molecule: acetaldehyde can accept hydrogens from other molecules, but none of its hydrogens are available due to being bonded to carbon atoms. On the other hand, both hydrogen atoms of dichloromethane can participate in HB, but there are no regions in the molecule that can accept hydrogen atoms.

This phenomenon involves binary interactions and thus will not be studied into detail in this work. Self-association on the other hand will be treated, as it happens naturally on some pure compounds.

Although there are many pure compounds for which it is well-known that the formation of HB occurs (e.g. water, 1-alkanols or carboxylic acids are undeniably *self-associating compounds*), there are some other compounds which have highly electronegative atoms (i.e. halogen atoms like Cl and Br) for which it is not clear if they display a self-associating character and form HB with themselves. Coming back to **Figure 3.2**, one may wonder why does dichloromethane not self-associate in spite of possessing two highly electronegative chlorine atoms. In theory, if we consider two dichloromethane molecules, one of the hydrogen atoms should be able to form a HB with either chlorine atom. In reality, this is not the case. Similarly to the previous example

with chloroform, in this particular case, the size of the chlorine atoms in dichloromethane do not allow them to sustain an interaction with an hydrogen from another dichloromethane molecule, due to the low electron density¹¹⁷. This does not mean that *all* chlorinated molecules cannot self-associate (e.g. hydrogen chloride can form weak HB at very low temperatures¹¹⁷).

Furthermore, experimental evidence as suggested by the IUPAC task group^{109,113} is often difficult and time consuming to collect for a large number of compounds. For this reason, a method in order to determine automatically and without ambiguity the associating character will be shown in the next section, which will use the concepts presented in **Appendix A3** of **Chapter 2** from the COSMO-RS framework.

3.3. Determining the associating character for a pure compound from the COSMO-RS model

In order to characterize if a compound can partake in HB, we first must find a clear and systematic way to determine if a molecule has at least one of each type of site (HA and HD) that would allow for it to form HB with itself. **Figure 3.3** illustrates this with a water molecule.

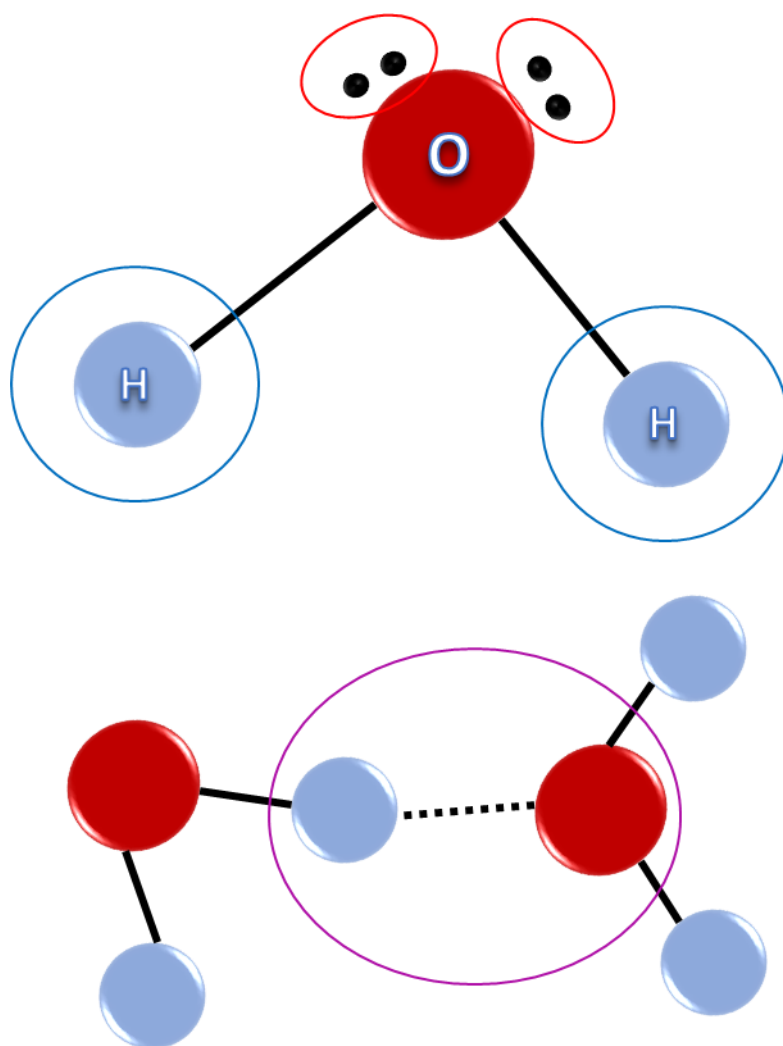


Figure 3.3. Associating sites of a water molecule. HA sites are presented in red, while HD sites are presented in blue. A HB formed between two water molecules is shown in the purple circle.

In the water molecule, both H atoms are available in donor sites, given that their bonds to the O atom are polarized by the latter. Both pair of electrons in the O atom are suitable acceptor sites. Thus, water molecules can form HB with themselves through sharing one of their H atoms with a pair of electrons from a neighboring water molecule. This self-associating display explains many of the interesting properties of water, such as the lower density of ice or its high boiling point when compared to molecules of similar size such as methane²⁶.

In order to systematically determine this self-associating (SA) character, we will introduce some concepts from the framework of another recent thermodynamic model: the COSMO-RS method.

The Conductor-like Screening Model (COSMO) is a member of the Dielectric continuum solvation models, which takes into account solvent effects in quantum chemical (QC) calculations. The extension to Real-Solvents (COSMO-RS) takes the QC calculations of COSMO and through statistical thermodynamics it obtains the interaction energy of two pairwise interacting segments^{26,118–120}.

The COSMO-RS (and all COSMO models in general) has the same input data for any given molecule: the surface-charge distribution σ_s which is the screening charge density of segment in contact with another segment of a molecule. The probability distribution of finding one of these screening charges on a typical contact segment is referred to as the sigma profile (σ -profile) which are characteristic of each chemical species. **Figure 3.4** presents the sigma profile for four different compounds.

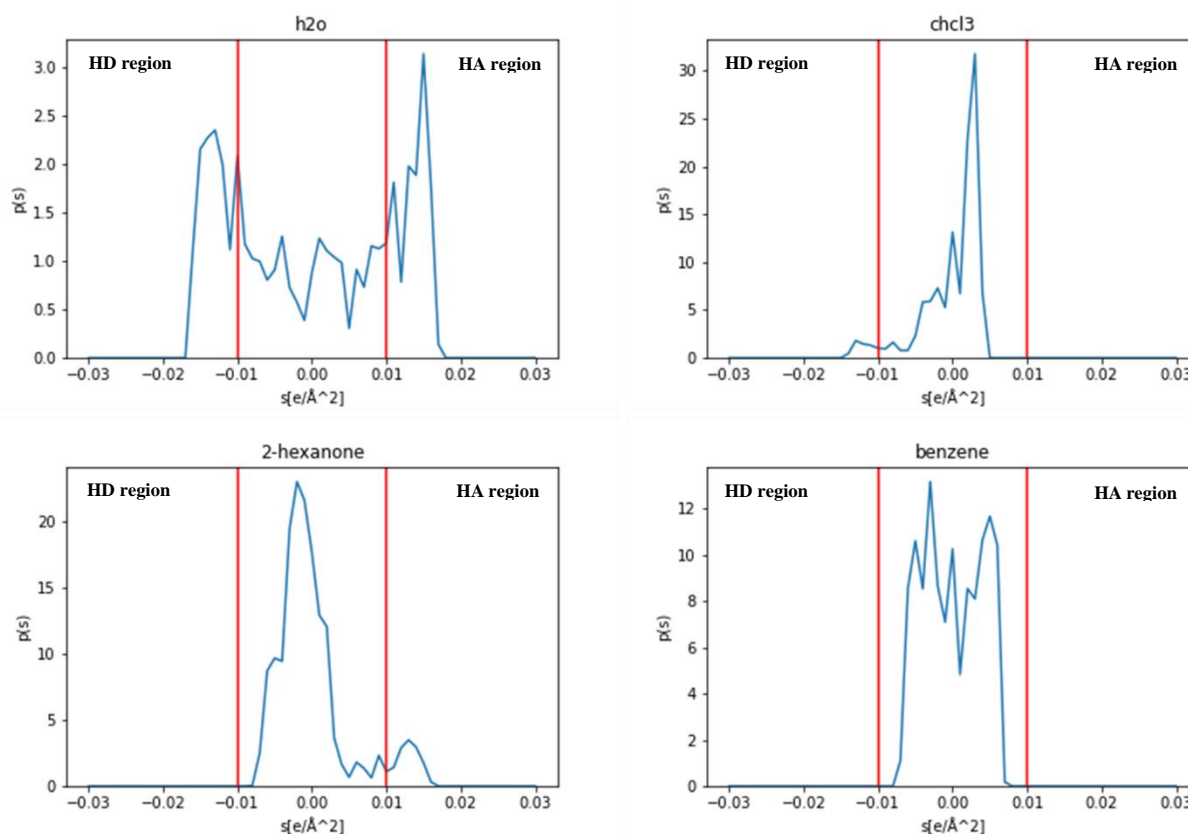


Figure 3.4. Sigma-profile for different compounds. On top: water and chloroform. On the bottom: 2-hexanone and benzene. The two red vertical lines indicate the threshold for HD or HA characteristics of a molecule, which are set to the value suggested by Khan et al¹²¹ DOI: 10.1021/jp4113552..

The x-axis for all graphs in **Figure 3.4** represent the surface-charge distribution, while the y-axis represents the σ -profile. As observed, each individual compound has a very distinct shape on its respective profile, which further corroborates the statement of how characteristic this function is for a chemical species. We also observe two red vertical solid lines on each profile which represent the HD (below left line) and HA (above right line) regions. One of the advantages of the COSMO-RS model is that it has a contribution that specifically accounts for HB interactions¹²², which occur at shorter distances than the contact distance of each segment. The COSMO-RS calculates this energy as:

$$\Delta_{HB}H \cong a_{contact} c_{hb}(T) \min(0, \sigma_s \sigma_s' - \sigma_{hb}^2) \quad (3.2)$$

Where $a_{contact}$ is the surface contact, $c_{hb}(T)$ is the temperature-dependent HB energy coefficient, $\sigma_s \sigma_s'$ is the product between two interacting segments and σ_{hb} is the minimum polarity threshold for hydrogen bond formation. Equation (3.2) corresponds to the enthalpy of hydrogen bonding^{123,124} ($\Delta_{HB}H$). This threshold can be positive or negative; peaks in the σ -profile that are lower than σ_{hb} indicate that the compound has a HD site (or sites) while a peak above $+\sigma_{hb}$ indicate that the molecule has a HA site (or sites). The region in between the HA and HD regions will be referred to as the non-polar region in which only dispersive interactions occur and no HB is formed. Klamt et al.^{123,124} have proposed an alternative form of estimating the hydrogen-bonding energy:

$$\Delta_{HB}H = 1.30 + 3.87 \left[f_{hb}^{HD}(e_{HD})(\sigma_{HD} + \sigma_{hb}^{HD}) \right] \left[f_{hb}^{HA}(e_{HA})(\sigma_{HA} - \sigma_{hb}^{HA}) \right] \quad (3.3)$$

Where f_{hb}^{HD} and f_{hb}^{HA} are HD and HA parameters for element e (in which the subscript determines if the element acts as a donor or an acceptor). σ_{hb}^{HD} and σ_{hb}^{HA} are scaling factors for each donor and acceptor element, which have been set to 0.24 and 0.65, respectively. σ_{HD} and σ_{HA} are equivalent of the interacting segments of Eq. (3.2) but at the exact interaction point where the HB occurs. The accuracy of Eq. (3.3) was tested by the authors against experimental data¹²⁴ to good success. They corroborated that the original COSMO-RS equation was useful to estimate HB energies and concluded that Eq. (3.2) is the HB energy of a molecule.

Coming back to **Figure 3.4**, we observe that benzene only has peaks in the non-polar region. Since no part of it can take place in a HB we can conclude that benzene is a non-self-associating compound (NSA) and a non-associating (NA) compound overall. For 2-hexanone, we observe once again a high peak in the middle, which is indicative of the carbon chain which is NA and a peak in the HA region. This makes sense, as the O atom has pairs of free electrons, which can accept an H atom to form a HB. However, it cannot donate any H atom, as we observe no peak in the HD region. **Figure 3.5** shows the structure of 2-hexanone highlighting the HA region of the molecule.

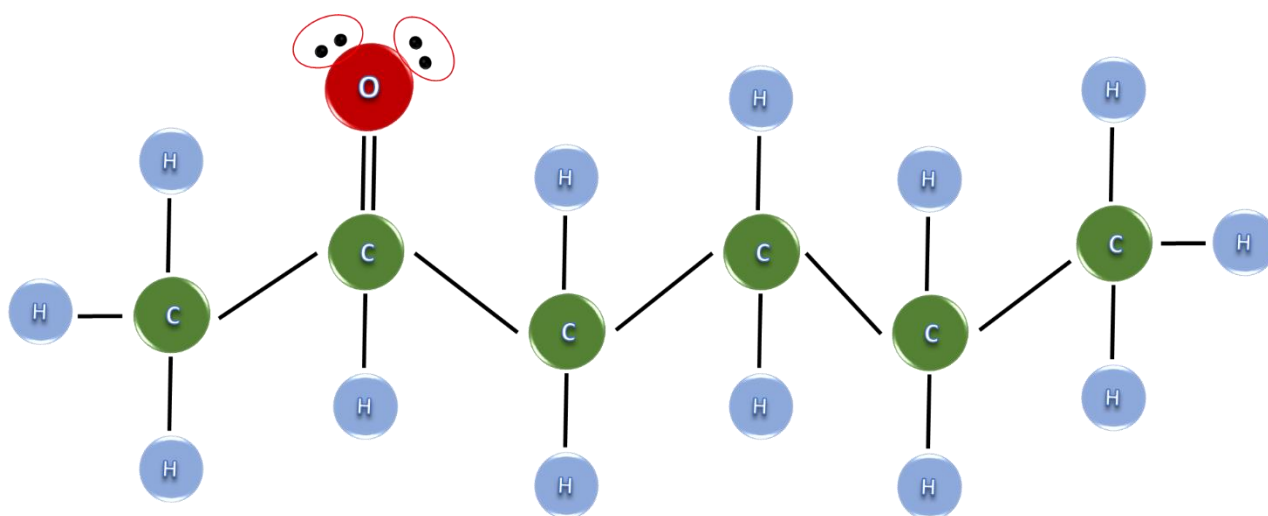


Figure 3.5. Molecular representation of 2-hexanone. The red circles correspond to HA sites for the molecule.

We can classify this molecule as NSA, but that can participate in cross-association with a HD molecule because it has a HA site, thus we classify it as a HA compound. A similar analysis can be done for chloroform but shifting the case to the HD region: chloroform has no free pair of electrons thus it cannot participate by accepting H atoms, as seen in the lack of peak in the HA region. **Figure 3.6** shows the structure of chloroform, highlighting the HD region of the molecule.

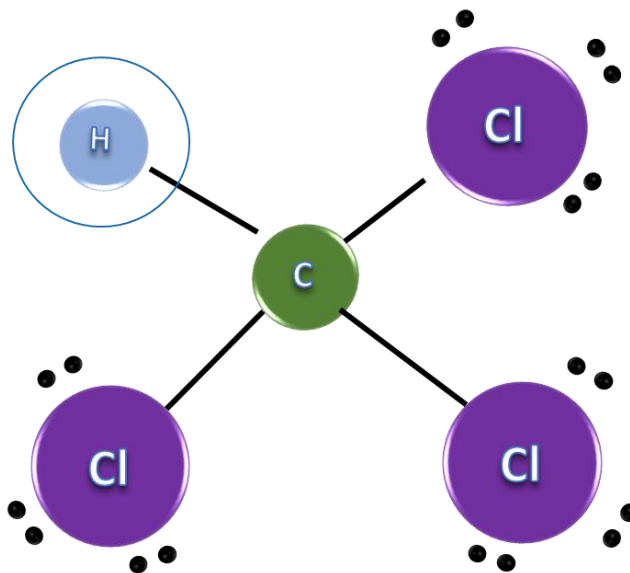


Figure 3.6. Molecular representation of chloroform. The blue circle corresponds to the HD site for the molecule.

For this reason, we can classify it as a NSA molecule that can participate in HB by donating H atoms, thus becoming a HD molecule. Finally, the water molecule is addressed. We can observe that the non-polar region has much shorter peaks than the other three. This makes sense as water is a highly polar molecule and thus interactions stronger than dispersive ones are prevalent. We can also observe that it has peaks in both HA and HD regions, which as seen previously in **Figure 3.3** is possible due to the fact that it has both labile H atoms and free electron pairs. For this reason, we can classify it as self-associating (SA).

In summary, a molecule can be classified in three categories:

- NSA, where no parts of the molecule participate in HB, thus no peaks in the HA nor HD regions of the σ - profile .
- NSA but either HD or HA when the molecule has either a labile H atom or a pair of free electrons respectively, meaning a peak in either of these regions on the σ - profile .
- SA when the molecule has both a labile H atom and a pair of free electrons, thus a peak in both HD and HA regions in the σ - profile .

The original threshold value for σ_{hb} proposed by Klamt et al.¹²⁰ is $\sigma_{hb} = \pm 0.0084 e/\text{\AA}^2$, however in **Figure 3.4** and in the remainder of this dissertation the value suggested by Khan et al.¹²¹ $\sigma_{hb} = \pm 0.01 e/\text{\AA}^2$ will be adopted, as the authors suggested that this value was accurate for defining the HA and HD regions. This approach was the one used to classify the compounds studied in **Chapter 2** and in the following chapters.

Although this approach is effective, it is heuristic in nature. This leaves room for interpretation for certain molecules in which the σ -profile and the molecular structure tell different stories, leading to possible misclassifications. **Figure 3.7** shows an example for acetyl chloride.

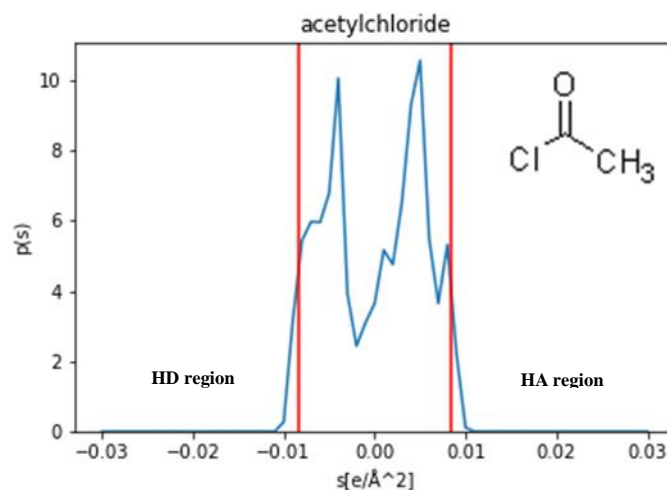


Figure 3.7. Sigma-profile and molecular structure for acetyl chloride. The cutoff value for HB is the one proposed by Klamt et al.¹²⁰ DOI: 10.1021/jp980017s..

Looking into the profile, we observe that there are two (although rather small) zones in both the HD and HA regions for acetyl chloride. This would automatically make it a SA molecule, according to our criteria thus far. However, inspecting the molecular formula, we gather two observations:

- i) The potential HA area of the molecule resides within the two highly electronegative atoms it possesses, Cl and O. However, knowing that the chlorine atom has lower chance of participating due to its lower electron density, the effect of having these two electronegative atoms may be counterbalanced.
- ii) A priori, there are no labile H atoms; all of the hydrogen atoms are involved in a methyl group, which is not bonded to any of the electronegative atoms directly (recall the chloroform example from **Figure 3.6**). It is difficult to conclude whether any of them can be donated by the molecule.
- iii) The σ -profile, as mentioned above, suggests that this molecule should have a self-associating character. Yet, both the HD and HA regions are quite small. If they effectively exist, the HD and HA characters are probably negligible (thus the SA character as well). This point highlights the need to quantify the strength of a potential HB.

The heuristic nature of this approach creates the need for a method of determining the existence of self-associating behavior in pure compounds systematically. A quantification of the existence of associating phenomena in pure fluids, i.e., HD and HA behavior simultaneously, would allow the determination of their SA character objectively and avoid any areas of uncertainty as the ones illustrated in **Figure 3.7**.

A first approach is to estimate the areas below the peaks of the σ - *profile* by simply calculating the integral below each region of the profile:

$$A_x = \int_a^b P(\sigma) d\sigma \quad (3.4)$$

Where A is the area below the σ - *profile* ($P(\sigma)$) region X . The limits of integration depend on this region:

$$\begin{cases} \text{If } X : HD & a = -\infty; b = -\sigma_{hb} \\ \text{If } X : NP & a = -\sigma_{hb}; b = \sigma_{hb} \\ \text{If } X : HA & a = \sigma_{hb}; b = +\infty \end{cases} \quad (3.5)$$

Thus the HD region takes all the negative σ values up to $\sigma_{hb} = -0.01e/\text{\AA}^2$, the non-polar (NP) region goes from the previously mentioned value up to $\sigma_{hb} = 0.01e/\text{\AA}^2$ and the HA region takes all the positive values of σ from $\sigma_{hb} = 0.01e/\text{\AA}^2$ onwards. It could be stated that a compound for which the value of A_{HD} and A_{HA} is different than zero is considered to be SA. With this we can define the **association degree** as:

$$Deg^{Assoc} = \frac{A_{HD} + A_{HA}}{A_{HD} + A_{NP} + A_{HA}} \quad (3.6)$$

Where the numerator is the **total association area** and the denominator is the **total interaction area** (associating and dispersive) for the given molecule. The association degree would then be a measure of the tendency of a molecule to self-associate. This is consistent with observable behavior for real molecules, e.g. water has a $Deg^{Assoc} = 0.556$ while ethylamine has a $Deg^{Assoc} = 0.101$. Both are SA molecules, but water can participate in more HB than ethylamine as suggested by their molecular structure and the atoms involved in the bond.

Nonetheless, this approach comes with a weakness: the associating characterization will depend on the value given to σ_{hb} because the position in which the threshold is placed will increase or reduce the total area for each region (including the NP region, making it more relevant in Eq. (3.6). Recalling **Figure 3.7**, if we change the HB threshold from the values of Klamt et al¹²⁰, $\sigma_{hb} = \pm 0.0084e/\text{\AA}^2$, to those of Khan et al.¹²¹ $\sigma_{hb} = \pm 0.01e/\text{\AA}^2$, we observe that with the latter, acetyl chloride ceases to be a SA molecule, because there are no longer peaks in either the HD and HA regions.

In the rest of the study, this approach was nonetheless adopted to estimate the HD and HA characters of the molecules of interest. The pessimistic threshold value $\sigma_{hb} = \pm 0.01e/\text{\AA}^2$ was adopted.

Note that the application of this methodology to molecules, the association character of which is obvious (alcohols, amines, water etc.) always leads to reliable results, thus reinforcing our degree of confidence in this method.

Remark 1 / 2: alternative way found in the literature to evaluate the associating character of a molecule from the sigma-profile

To avoid this issue, a modification is proposed for Eq. (3.4), following the polar¹²⁵ and apolar¹²⁶ factors proposed by Abranches et al. For the polar factors we have the general expression:

$$p_{HD} = \int_{-\infty}^{-\sigma_{hb}} P(\sigma) \cdot |\sigma| d\sigma \quad (3.7)$$

$$p_{HA} = \int_{\sigma_{hb}}^{+\infty} P(\sigma) \cdot |\sigma| d\sigma \quad (3.8)$$

For the non-polar region, the apolar factor is calculated as:

$$p_{NP} = \int_{-\sigma_{hb}}^{\sigma_{hb}} P(\sigma) \cdot (\sigma_{hb} - |\sigma|) d\sigma \quad (3.9)$$

The difference between the two approaches is that at each point of the σ -profile is weighted by the absolute charge σ at that point. With this change, the more charged a particular surface segment of a molecule the greater the contribution to the final value of either polar factor (HD or HA). With this, the importance of the cutoff value is diminished, as the region close to the polar-non-polar limit contributes less to the polar/apolar factor. This is especially relevant for charged species such as cations or anions or highly polar molecules such as ionic liquids¹²⁵.

Nevertheless, the polar factor safely predicts if a compound is HD or HA and therefore if it is SA if both factors are different from zero.

Remark 2 / 2: alternative way found in the literature to evaluate the hydrogen bonding enthalpy of a molecule from the sigma-profile

The probability of HB formation can be estimated by noting that the polar factors are weighted probability distribution. Hence, we can express the probability of HB formation as the probability of the two independent events were a molecule can donate and accept an hydrogen atom through hydrogen-bonding:

$$P(HB) = P(HD) \cdot P(HA) = p_{HD} \cdot p_{HA} \quad (3.10)$$

Through Eq. (3.10) we can state that a compound will be SA if the probability of hydrogen bonding is different from zero, which is equivalent to say that the product between the HD and HA polar factors is different from zero. Recalling the previous example of ethylamine and water, we observe that ethylamine has a $P(HB) = 1.90 \cdot 10^{-8}$, while water has a $P(HB) = 2.64 \cdot 10^{-8}$, consistently with the observable tendencies of both molecules to participate in hydrogen bonding.

Figure 3.8 shows the relationship between $P(HB)$ and the hydrogen bonding strength, represented by the energy or enthalpy of hydrogen bonding ($-\Delta_{HB}H$), obtained through expression (3.2), calculated using the COSMOthermX software¹¹⁵ for 548 self-associating compounds.

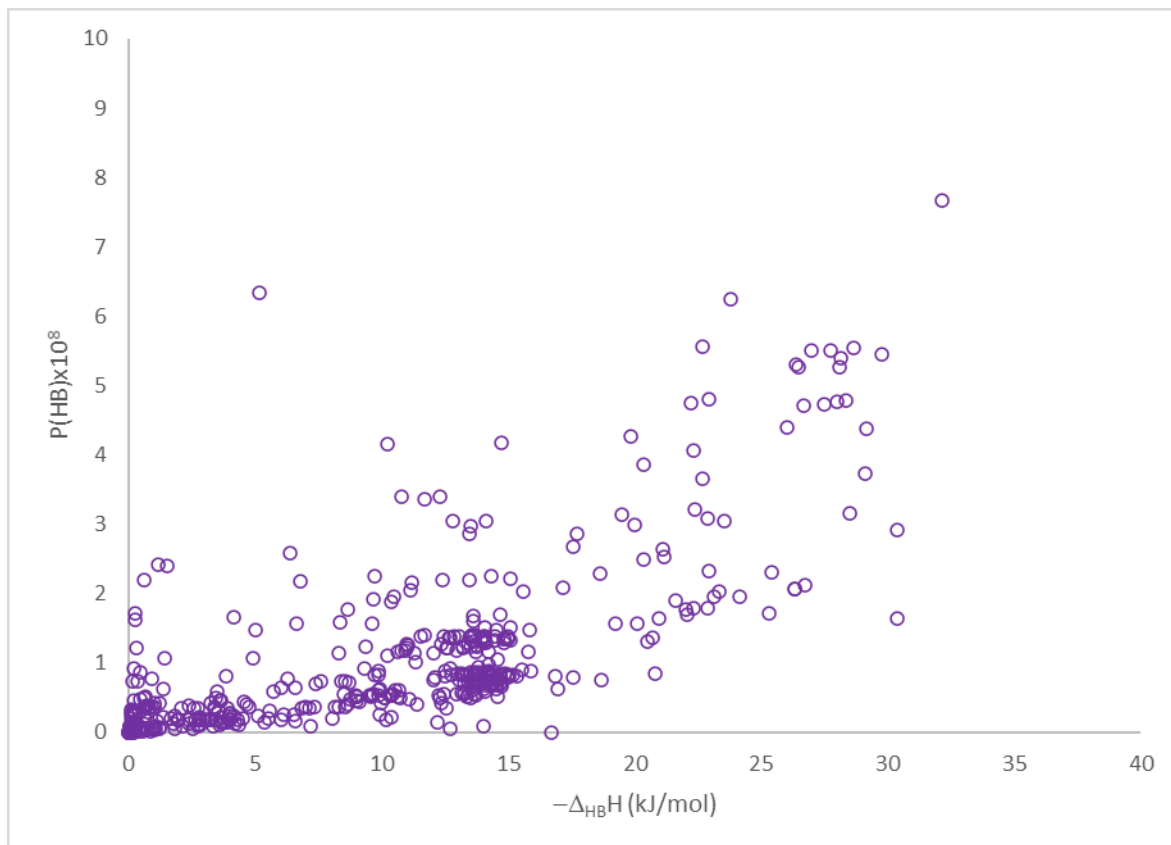


Figure 3.8. Probability of hydrogen bonding ($P(\text{HB})$) versus enthalpy of hydrogen bonding.

We observe in general that a higher energy of association yields a higher probability of hydrogen bonding. This shows the relationship between Eq. (3.10) and the hydrogen bond strength. The main advantage of this approach is its capacity to predict the associating character of a molecule as well as giving an estimate of its associating energy. However, beyond the general trend, **Figure 3.8** reveals important outliers with respect to this general trend and consequently, it was decided not to use this method and:

- To estimate the associating character of a molecule from sigma-profile area calculations, as explained below,
- To estimate HB strength from COSMO-RS calculations (Eq. (3.2))

3.4. Construction of a PC-SAFT and I-PC-SAFT pure-compound parameter database for 1800 pure compounds

This section will present the construction of the parameter database for the two SAFT EoS studied in the last two chapters. First, the construction of the parameter database for the 1252 pure NSA compounds will be presented. Afterwards, the inclusion of the 548 SA compounds will be discussed and finally the entire database for PC-SAFT and I-PC-SAFT will be given in the **Appendix** section, where **Appendix A6** will have the parameter set for both EoS for each individual pure compound and **Appendix A7** will have the compound-by-compound results for each thermodynamic property studied for each individual compound for each model.

3.4.1. Construction of a PC-SAFT and I-PC-SAFT molecular parameter database for a large number of non-associating pure compounds obtained from an optimal fitting procedure

Using the results found in **Chapter 2** as a starting point, we proceeded to gather from the DIPPR databank the largest possible non-associating pure component experimental database for which at least P^{sat} and v_{liq}^{sat} data are simultaneously available and acceptable, in order to regress the PC-SAFT parameters against both thermodynamic properties by minimizing objective function OF 6 described in **Section 2.3** in page 81.

As explained previously, weighting factors for P^{sat} and v_{liq}^{sat} were fixed to 3 and 2, respectively. Doing this, we performed the parameterization of the PC-SAFT EoS for 1252 non-associating pure compounds comprising 18 of the chemical families presented in **Table 3.2**. A detailed presentation of the results for the molecular parameters and MAPEs for the four properties for each non-associating molecule is found in the supporting information of the original publication by Ramirez-Velez et al.⁹⁵.

The same procedure is then applied to the I-PC-SAFT EoS, in which the parameters for the 1252 NSA compounds are estimated using the procedure described by Moine et al.¹⁸ The resulting molecular parameters and volume translation parameter, as well as the MAPE for each of the properties is also found in the supporting information of the work of Ramirez-Velez et al.⁹⁵.

3.4.2. Extension of the molecular parameter PC-SAFT and I-PC-SAFT databases to include self-associating compounds

Following the same philosophy as with the NSA compounds, we searched through the DIPPR databank for all SA compounds for which accurate pseudo-experimental data could be generated for P^{sat} and v_{liq}^{sat} for these molecules. In doing so, 548 compounds comprising 16 of the chemical families presented in **Table 3.2** were selected, including important groups such as alcohols, amines and organic acids.

Next, the procedure described in **Section 3.5.2.2** is applied to the 548 molecules for the PC-SAFT EoS, yielding 1644 optimal parameters, three for each compound. These parameters were added to the previous database⁹⁵ of 1252 NSA compounds, as well as the MAPE for each property as described in Section 3.5.3, leaving a database with parameters and performance indicators for 1800 pure compounds. At the moment of writing of this dissertation and as indicated in previous sections, it is believed that this is the first database published of this kind for the PC-SAFT EoS.

We then turn our attention to I-PC-SAFT, in which the procedure is repeated, but following the parametrization strategy of Moine et al.¹⁸. This procedure yields 2192 parameters, four per compound (three molecular parameters and one volume translation parameter). These parameters are then added to the previous I-PC-SAFT database⁹⁵ to end up with a database for 1800 pure compounds for this EoS. It is also believed, at the moment of writing this dissertation that this is the first database of this kind published for the I-PC-SAFT EoS.

Appendix A6 shows the parameters for the 1800 chemical species obtained for both PC-SAFT and I-PC-SAFT. **Appendix A7** shows the MAPE, compound-by-compound, for the four thermodynamic and the three critical properties studied in this chapter for the 1800 compounds, as well as showing the average MAPE of each property for both the PC-SAFT (**Table S3**) and I-PC-SAFT (**Table S4**).

3.5. Performance of non-associating SAFT models in reproducing self-associating pure compounds

In this section, a study presenting the performance of the PC-SAFT and I-PC-SAFT EoS in reproducing 1800 pure compounds for which experimental data for vapor pressure and liquid density could be gathered from the DIPPR databank. These molecules were categorized depending of their associating character, yielding 1252 NSA pure compounds and 548 SA compounds. This article is currently submitted.

The main highlights for this article include:

- Proposition of a simple method to categorize well-modeled compounds.
- Performance of the predictions of the PC-SAFT without an associating term to reproduce NSA and SA pure compound properties.
- Evaluation of the performance of both EoS per chemical families.
- Comparison on results of the PC-SAFT and the I-PC-SAFT.
- First conclusions on the need of an associating term.

The remainder of this chapter will present the study done in the aforementioned article, followed by the presentation of the entire pure compound database for both PC-SAFT and I-PC-SAFT. The reader is redirected to Piña-Martinez et al.¹²⁷ for the parameter database of the SRK, PR, *tc*-PR and *tc*-RK EoS.

3.5.1. Introduction

Equations of state (EoS) are one of the most commonly used tools in chemical and process engineering due to their capacity of predicting thermodynamic properties of pure compounds and mixtures at any given state. It is therefore clear that their performance at predicting such properties must be studied carefully and systematically to quantify their strengths and weaknesses. Recently, Jaubert et al.²¹ proposed a reference database to evaluate the accuracy of an EoS or to cross-compare two EoS when they are used to correlate the properties of binary mixtures. Their proposed database contains phase equilibrium data (VLE, LLE, VLLE), property change on mixing data (enthalpy or heat capacity)¹²⁸, azeotropic data and critical point data for 200 binary systems made up of different pair combinations of 107 non-associating and self-associating pure compounds. In addition, a complete methodology was proposed to assess the performance of EoS to correlate (or predict) binary system behaviors^{129,130}. However, it is well-known that, in order to properly correlate binary systems, an EoS must be able to accurately represent the pure-compound properties first. Regardless of the level of sophistication of any thermodynamic model or the number of parameters and form of the mixing rules employed, if the vapor pressures of each pure compound are inaccurate, the predictions of the binary system are compromised. As a convincing illustration, the reader is referred to Figure 3 in Agarwal et al.¹³¹

In this context, Piña-Martinez et al.¹²⁷ recently defined a database containing over 300 000 pseudo-experimental data points for pure components. These data come from a carefully selected portion of the DIPPR database¹³² for 1 800 different pure components representing all chemical families, and including 1252 non-self-associating (NSA) and 548 self-associating (SA) compounds. For each of the 1 800 pure components, 50 vapor pressure and 50 liquid density pseudo-experimental data points were generated from the correlations available in the DIPPR database. Among the 1 800 fluids, 1 536 also possess an accurate correlation for $\Delta_{vap}H$ and 890 for $c_{P,liq}^{sat}$ making possible to generate 50 data points for each of these properties. The critical properties (T_c , P_c and v_c) are available for the 1 800 components so that in the end, the resulting database contains 306 700 high-quality pseudo-experimental data points.

Note: It is worth noting that EoS only predict residual properties. Consequently, for estimating liquid heat capacity, it is necessary to add a perfect-gas heat capacity term ($c_{P,PG}$) to the

residual heat capacity. Therefore, an accurate correlation for the $c_{P,PG}(T)$ function is also needed when accurate $c_{P,liq}^{sat}$ data are available.

Table 3.1 summarizes the data available in such a database. For more details, and in particular the temperature range on which the data were generated, the reader is referred to the paper by Piña-Martinez et al.¹²⁷

Table 3.1. Overview of the data available in the database proposed by Piña-Martinez et al¹²⁷.

Property	Number of pure components for which the property is available	Number of data points
P^{sat}	1 800	90 000 (50 per component)
v_{liq}^{sat}	1 800	90 000 (50 per component)
$\Delta_{vap}H$	1 536	76 800 (50 per component)
$c_{P,liq}^{sat}$ (*)	890	44 500 (50 per component)
T_c	1 800	1 800
P_c	1 800	1 800
v_c	1 800	1 800
TOTAL		306 700

(*) an equivalent number of $c_{P,PG}$ data is available in order to be able to calculate $c_{P,liq}^{sat}$ from an EoS.

Table 3.2 presents a summary of the chemical families in which the 1 800 compounds are distributed. In addition, **Table 3.2** presents the distribution of NSA and SA compounds among the chemical families. As previously stated, the 1 800 pure compounds are divided into 1 252 NSA compounds and 548 SA compounds so that the molecule dataset contains 70% of NSA and 30% of SA compounds. The process used to determine the associating character (NSA or SA) of a given molecule can be found in Piña-Martinez et al.¹²⁷ In short, the screening charge density distribution, sigma-profile (σ -profile), was generated for each compound. If the σ -profile presents peaks below a hydrogen-donor sigma-cutoff value and above a hydrogen-acceptor sigma-cutoff value, it is concluded that the molecule can form hydrogen bond (HB) with another similar molecule and thus tends to self-associate.

Table 3.2. List of the chemical families and corresponding distribution of the 1 800 pure compounds available in the database proposed by Piña-Martinez et al.¹²⁷

Chemical family	Number of Compounds	Proportion of compounds (%)	Number of NSA compounds	Number of SA compounds
Alcohols	131	7.3%	4	127
Alkanes	163	9.1%	163	0
Alkenes	122	6.8%	122	0
Alkynes	18	1.0%	18	0
Amines/Amides	102	5.7%	0	102
Aromatics	158	8.8%	158	0
Epoxides	18	1.0%	16	2
Esters/Ethers	238	13.2%	203	35
Halogen Compounds	232	12.9%	197	35
Inorganic Compounds	70	3.9%	61	9
Ketones/Aldehydes	80	4.4%	78	2
Nitriles	31	1.7%	9	22
Nitrogen Compounds	99	5.5%	64	35
Organic Acids	82	4.6%	0	82
Organic Salts	13	0.7%	11	2
Other Compounds	9	0.5%	3	6
Peroxides	11	0.6%	3	8
Polyfunctional Compounds	68	3.8%	14	54
Silicon Compounds	61	3.4%	56	5
Sulfur compounds	94	5.2%	72	22
Total	1 800	100%	1 252 (70%)	548 (30%)

The above-presented database was used by Piña-Martinez et al.¹²⁷ in order to assess the accuracy of 4 cubic equations of state (CEoS): original SRK, original Peng-Robinson (PR), *tc*-RK and *tc*-PR where *tc* designates the *translated* and *consistent*^{32,35,97} versions of such EoS. In this paper, we seek to assess the performances of molecular-based EoS, in particular those belonging to the Statistical Associating Fluid Theory (SAFT)⁵⁻⁷ family. This type of EoS are far more recent than CEoS, as they have only been around for the last 30 years, while the CEoS have a century and a half long tradition. Thus, it is key to evaluate the performance of SAFT-type EoS as their powerful molecular-based theoretical background has proven to be efficient at modeling a wide array of compounds and mixtures. Their true power has however not yet been clearly assessed on thousands of pure components. In this paper, it was decided – somewhat arbitrary – to focus on the following two versions of the SAFT EoS:

- a) The Perturbed Chain SAFT (PC-SAFT) proposed by Gross and Sadowski¹², which modifies the original SAFT EoS by using a hard-chain fluid as reference and using a dispersion term based on the perturbation theory of Barker and Henderson⁵⁶ and
- b) The *Industrialized*-PC-SAFT (*I*-PC-SAFT) proposed by Moine et al.¹⁸ which is a volume-translated version of the PC-SAFT EoS in which the 3 molecular parameters ($m, \sigma, \varepsilon/k$) are constrained to exactly reproduce the experimental critical temperature and pressure and the experimental acentric factor. The volume translation^{41,133} is determined in order to exactly reproduce the liquid density at $T_r = 0.8$.

In this study, it was decided to evaluate the capabilities, strengths and weaknesses of these models in their most basic form, i.e., *without* adding an associating term. There are two main reasons for this choice: the first is that the associating contributions are usually introduced in later developments of the models. The second one, is that in many cases, users of process simulators can be led to represent self-associating compounds with a SAFT-type EoS without any association term (due to a lack of implementation of the term or a lack of available parameters for a given compound).

In summary, the performance of the PC-SAFT and the *I*-PC-SAFT EoS without an association term will be evaluated over a large number of non-associating and self-associating molecules by determining their capacity at correlating the following properties: P^{sat} , v_{liq}^{sat} , $\Delta_{vap}H$, $C_{P,liq}^{sat}$, T_c , P_c and v_c .

3.5.2. Brief overview of the studied molecular-based EoS.

3.5.2.1. PC-SAFT EoS

The PC-SAFT EoS is the first model to be evaluated in this work and all the details about its theoretical basis can be found in the original publication by Gross & Sadowski¹². The non-associating version of PC-SAFT is used in this paper, which means that all components are treated as non-associating compounds, regardless of their affiliation as SA or NSA. The PC-SAFT requires three molecular parameters, proper of each individual pure compound: m , σ and ε/k . The parametrization procedure used here is the one proposed by Ramirez-Velez et al.⁹⁵ In brief, optimal ($m, \sigma, \varepsilon/k$) parameters are obtained by minimizing an objective function (see Eq. (3.11)) that takes into account the deviations between calculated and experimental P^{sat} and ρ_{liq}^{sat} only:

$$\left\{ \begin{aligned} OF_{\text{component } j} &= \frac{1}{N_T} \left[3 \sum_{i=1}^{N_T} \left[\frac{P_{j,calc}^{sat}(T_i) - P_{j,exp}^{sat}(T_i)}{P_{j,exp}^{sat}(T_i)} \right]^2 + 2 \sum_{i=1}^{N_T} \left[\frac{\rho_{liq,j,calc}^{sat}(T_i) - \rho_{liq,j,exp}^{sat}(T_i)}{\rho_{liq,j,exp}^{sat}(T_i)} \right]^2 \right] \\ N_T &= 50 \text{ is the number of temperature points} \end{aligned} \right. \quad (3.11)$$

The key point in Eq. (3.11) is to use weighting factors for P^{sat} and ρ_{liq}^{sat} fixed at 3 and 2 respectively. Ramirez-Velez et al.⁹⁵ also concluded that including $\Delta_{vap}H$ and/or $c_{P,liq}^{sat}$ data in the regression procedure was not a necessity since it only marginally improved the reproduction of these properties and that not including either P^{sat} or ρ_{liq}^{sat} was highly unadvised. Resulting ($m, \sigma, \varepsilon/k$) parameters are reported in **Appendix A6** for the 1 800 pure components. It is believed that this paper is the first one in which molecular parameters suitable for the PC-SAFT EoS are published for 1 800 pure compounds. Such parameters can be used immediately in any commercial process simulator and complete the set of parameters previously published by Ramirez-Velez et al.⁹⁵ for 1252 NSA components.

3.5.2.2. I-PC-SAFT EOS

The *Industrialized*-PC-SAFT (*I-PC-SAFT*) EoS proposed by Moine et al.¹⁸ is a volume-translated version of the original PC-SAFT, in which, molecular parameters of pure species are

determined to exactly reproduce the experimental critical temperature, pressure and acentric factor while the volume translation is calculated in order to exactly reproduce the experimental liquid density at $T_r = 0.8$. As an advantage of the parametrization method inherent to the *I*-PC-SAFT EoS, fastidious fitting procedures to experimental data are avoided; the three molecular parameters for a pure compound, are straightforwardly obtained from the following correlations:

$$\begin{cases} m_i \approx 0.5959\omega_{i,exp}^2 + 7.5437\omega_{i,exp} + 0.9729 \\ \varepsilon_i/k \approx T_{c,i,exp} / \left(4.7968 \cdot 10^{-6} m_i^5 - 3.0895 \cdot 10^{-4} m_i^4 + 7.8649 \cdot 10^{-3} m_i^3 - 0.10215 m_i^2 + 0.75358 m_i + 0.63659 \right) \\ \sigma_i \approx \left[\varepsilon_i/k \cdot \frac{k}{P_{c,i,exp}} 10^{\left(1.6345 \cdot 10^{-7} m_i^6 - 1.1346 \cdot 10^{-5} m_i^5 + 3.1389 \cdot 10^{-4} m_i^4 - 4.4618 \cdot 10^{-3} m_i^3 + 3.6282 \cdot 10^{-2} m_i^2 - 0.22498 m_i - 0.77655 \right)} \right]^{1/3} \end{cases} \quad (3.12)$$

Resulting $(m, \sigma, \varepsilon/k)$ parameters and the corresponding volume shift (c) are reported in **Appendix A1** for the 1 800 pure components.

3.5.3. Assessing the accuracy of the PC-SAFT and *I*-PC-SAFT EoS: results and discussion

In this section, the performances of PC-SAFT and *I*-PC-SAFT are evaluated by assessing their accuracy over the 306 700 data points relative to the 1 800 pure compounds contained in the reference database proposed by Piña-Martinez et al.¹²⁷ Deviations are expressed in terms of mean absolute percentage errors (MAPEs) defined by Eq. (3.13) as the average of the absolute percentage deviations between experimental and calculated properties over N_T temperature points.

$$MAPE_X = \frac{100}{N_T} \sum_{i=1}^{N_T} \left| \frac{X_{j,exp}(T_i) - X_{j,calc}(T_i)}{X_{j,exp}(T_i)} \right| \quad (3.13)$$

$X_{j,exp}(T_i)$ and $X_{j,calc}(T_i)$ correspond to the calculated and experimental values of the component j 's property X , at temperature T_i . In the present study, $N_T = 50$.

The MAPEs on $\{P^{sat}, v_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}, T_c, P_c, v_c\}$ are reported in **Table 3.3** for the PC-SAFT and *I*-PC-SAFT EoS. The detail of deviations for each molecule are reported in **Appendix A7**. For possible comparison, the MAPEs obtained with the *tc*-PR EoS, which was found to be the most accurate of the 4 cubic equations of state evaluated against the same database in our previous article¹²⁷ are recalled.

Table 3.3. MAPE on P^{sat} , v_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$, T_c , P_c and v_c as predicted by the PC-SAFT, *I*-PC-SFAT and *tc*-PR EoS.

EoS	MAPE on P^{sat} (1800 fluids)	MAPE on v_{liq}^{sat} (1800 fluids) ($T_r < 0.9$)	MAPE on $\Delta_{vap}H$ (1536 fluids)	MAPE on $c_{P,liq}^{sat}$ (890 fluids)	MAPE on T_c (1800 fluids)	MAPE on P_c (1800 fluids)	MAPE on v_c (1800 fluids)	Global average deviation over the 306 700 available data points
PC-SAFT	1.18%	0.95%	3.25%	4.17%	2.28%	20.8%	4.38%	2.2%
<i>I</i> -PC-SAFT	2.08%	4.60%	4.00%	4.10%	0% ^(*)	0% ^(*)	12.4%	3.6%
<i>tc</i> -PR	0.98%	2.08%	1.92%	2.53%	0% ^(*)	0% ^(*)	19.6%	1.9%

(*) such MAPEs are exactly zero since the *I*-PC-SAFT and *tc*-PR EoS are parameterized in order to exactly reproduce $T_{c,exp}$ and $P_{c,exp}$.

As stated above, the parameters of the PC-SAFT EoS are fitted over experimental P^{sat} and v_{liq}^{sat} data. **Table 3.3** shows that this equation is able to reproduce such data with a deviation close to 1% which is really excellent. The deviations on $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ are higher but remain very good. The price to pay however is a huge deviation on the critical pressure.

The *I*-PC-SAFT EoS is parameterized in order to exactly reproduce the critical pressure and temperature but at the expense of a larger liquid density deviation, with an average value around 5%. Such an EoS should be particularly suitable to estimate non-volumetric properties of close-to-criticality fluids.

As discussed in one of our previous papers¹⁸, the main difference between PC-SAFT and *I*-PC-SAFT is the parameterization that modifies dramatically the model performances especially, the capability to predict v_{liq}^{sat} and P_c . From **Table 3.3**, it can be concluded that a choice has to

be made between an accurate correlation of v_{liq}^{sat} or P_c : it is indeed impossible to obtain simultaneously accurate predictions for both properties. In accordance with Moine et al.¹⁸, it is believed that the embedding of three component-dependent parameters in an EoS is not enough to describe accurately all the properties of a pure component.

The PC-SAFT and *tc*-PR EoS have similar accuracy. The PC-SAFT EoS, however predicts better liquid molar volumes, whereas the *tc*-PR EoS takes the lead for the correlation of the critical coordinates (T_c and P_c) and the energetic properties ($\Delta_{vap}H$ and $c_{P,liq}^{sat}$).

3.5.3.1. Influence of the associating character of components

As made in our previous paper devoted to CEoS, we believe interesting to investigate if the MAPEs reported in **Table 3.3** are significantly different between the NSA and SA components. Indeed, as previously stated, the evaluated SAFT-type EoS do not include an association term. MAPE on P^{sat} , v_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$, T_c , P_c and v_c for the 1252 NSA and 548 SA compounds are shown in **Table 3.4**. It can be observed that for both SAFT-type EoS (PC-SAFT and *I*-PC-SAFT), the difference in performance between NSA and SA compounds is more pronounced than with the *tc*-PR EoS. When SAFT-type EoS are used, the global average deviation increases of about 1% when we move from the NSA to the SA compounds. Although significant, this increase is not very large and the deviations observed for SA compounds remain quite acceptable for most of practical applications. As it was previously observed with CEoS¹²⁷, the most impacted property is $c_{P,liq}^{sat}$ for which the deviation more than doubles when switching from NSA to SA compounds. It is however believed that the large MAPEs on $c_{P,liq}^{sat}$ observed for SA compounds are not very significant for 2 reasons: (i) less than 200 SA compounds have experimental $c_{P,liq}^{sat}$ data and (ii) the calculated standard deviation on heat capacities is high (> 5%) as a consequence of huge deviations observed for a small number of components. In other words, a small number of huge deviations tend to increase a lot the value of the average MAPE, making it biased.

Table 3.4. MAPE on P^{sat} , v_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$, T_c , P_c and v_c depending on the associating character (NSA or SA) of the fluids as predicted by the PC-SAFT, I-PC-SAFT and tc-PR EoS.

EoS		MAPE on P^{sat} (1800 fluids)	MAPE on v_{liq}^{sat} (1800 fluids) ($T_r < 0.9$)	MAPE on $\Delta_{vap}H$ (1536 fluids)	MAPE on $c_{P,liq}^{sat}$ (890 fluids)	MAPE on T_c (1800 fluids)	MAPE on P_c (1800 fluids)	MAPE on v_c (1800 fluids)	Global average deviation
PC-SAFT	NSA	0.97% (1252 fluids)	0.85% (1252 fluids)	3.04% (1114 fluids)	3.35% (695 fluids)	2.34% (1252 fluids)	20.5% (1252 fluids)	3.95% (1252 fluids)	2.0% (219 406 data points)
	SA	1.66% (548 fluids)	1.19% (548 fluids)	3.78% (422 fluids)	7.07% (195 fluids)	2.15% (548 fluids)	21.5% (548 fluids)	5.34% (548 fluids)	2.8% (87 294 data points)
I-PC-SAFT	NSA	1.83%	4.35%	3.68%	3.27%	0% ^(*)	0% ^(*)	12.1%	3.3%
	SA	2.65%	5.18%	4.84%	7.05%	0% ^(*)	0% ^(*)	13.0%	4.5%
tc-PR	NSA	0.91%	2.00%	1.96%	2.07%	0% ^(*)	0% ^(*)	19.1%	1.8%
	SA	1.15%	2.28%	1.83%	4.17%	0% ^(*)	0% ^(*)	20.7%	2.1%

(*) such MAPEs are exactly zero since the I-PC-SAFT and tc-PR EoS are parameterized in order to exactly reproduce $T_{c,exp}$ and $P_{c,exp}$.

From **Table 3.5** and **Table 3.6**, which give the MAPE on P^{sat} , v_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$, T_c , P_c and v_c for each chemical family of compounds as defined in Table 2, the same conclusion is reached: alcohols, amines/amides, nitriles, nitrogen compounds, organic acids and peroxides that tend to self-associate show higher deviations than hydrocarbons (alkanes, alkenes, alkynes) but the difference in accuracy due to association is not always obvious. As an example, regardless of the SAFT-type EoS, the global average deviation on amines/amides, nitrogen compounds and epoxides is similar to the average deviation observed on alkenes.

Table 3.5 and **Table 3.6** also highlight that the highest deviations are obtained with nitriles. Such an unexpected result can be explained by noticing that most of the 31 nitriles available in the DIPPR are polyfunctional (in addition to the nitrile group, some contains double bonds, other contain a hydroxyl group, a NH_2 group, a methoxy group ...). It is believed that such a complexity explains better the observed loss of accuracy than the associating character of such components.

Table 3.5. MAPE on P^{sat} , v_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$, T_c , P_c and v_c as predicted by the PC-SAFT EoS for the 20 chemical families defined in **Table 3.2**

Chemical family	P^{sat}	ρ_{liq}^{sat}	$\Delta_{vap}H$	$c_{P,liq}^{sat}$	T_c	P_c	v_c	Global average deviation
Alcohols	2.23	1.33	4.47	10.6	1.23	14.8	5.21	3.6
Alkanes	0.55	0.62	2.30	1.85	2.15	18.4	3.49	1.4
Alkenes	0.78	0.71	3.13	3.03	2.18	18.5	2.79	2.0
Alkynes	1.05	0.84	3.08	3.08	1.84	14.2	2.81	2.0
Amines/Amides	1.28	0.85	3.27	5.08	2.01	18.6	5.68	2.2
Aromatics	0.84	0.95	3.05	2.53	2.80	25.6	3.03	1.9
Epoxides	0.60	0.73	2.85	3.88	2.61	19.9	4.73	2.0
Esters/Ethers	1.10	0.71	2.94	3.65	2.15	21.5	4.45	1.9
Halogen compounds	1.04	0.91	3.32	4.41	2.51	20.1	3.18	2.2
Inorganic compounds	2.04	1.52	4.42	7.32	2.34	19.1	9.89	3.5
Ketones/Aldehydes	0.99	0.84	3.34	3.59	2.70	23.5	2.10	2.0
Nitriles	2.42	2.81	5.80	7.50	5.67	56.2	5.25	4.4
Nitrogen compounds	1.38	1.32	3.60	3.41	2.82	25.3	5.61	2.3
Organic acids	1.53	0.97	3.83	9.01	1.96	23.6	5.15	2.7
Organic salts	1.72	1.49	3.61	3.48	3.01	27.0	8.01	2.4
Other compounds	2.27	1.32	4.57	3.25	2.55	21.8	6.17	2.8
Peroxides	1.30	1.18	3.16	3.57	0.82	8.38	6.79	2.0
Polyfunctional compounds	1.32	1.02	3.08	8.44	1.86	17.4	5.08	2.3
Silicon compounds	1.26	0.88	3.12	5.91	1.62	15.4	4.28	2.2
Sulfur compounds	0.80	0.77	2.54	2.78	2.34	18.9	4.78	1.7

Table 3.6. MAPE on P^{sat} , v_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$, T_c , P_c and v_c as predicted by the *I*-PC-SAFT EoS for the 20 chemical families defined in **Table 3.2**

Chemical family	P^{sat}	ρ_{liq}^{sat}	$\Delta_{vap}H$	$c_{P,liq}^{sat}$	T_c	P_c	v_c	Global average deviation
Alcohols	3.5	4.1	5.8	10.8	0.0	0.0	9.89	5.1
Alkanes	1.2	4.5	3.0	1.8	0.0	0.0	11.1	2.7
Alkenes	1.7	4.1	3.4	3.0	0.0	0.0	10.7	3.1
Alkynes	2.2	2.7	3.6	2.4	0.0	0.0	9.25	2.7
Amines/Amides	2.3	4.2	4.2	4.4	0.0	0.0	9.51	3.6
Aromatics	1.7	4.9	3.7	2.9	0.0	0.0	13.7	3.3
Epoxides	1.2	4.0	3.1	3.3	0.0	0.0	12.8	2.9
Esters/Ethers	2.2	4.9	4.1	3.2	0.0	0.0	14.2	3.7
Halogen compounds	1.8	4.0	3.5	4.2	0.0	0.0	10.8	3.3
Inorganic compounds	2.7	4.5	3.6	8.1	0.0	0.0	16.2	4.4
Ketones/Aldehydes	1.6	4.3	4.2	3.9	0.0	0.0	12.0	3.4
Nitriles	2.3	16.0	5.7	8.7	0.0	0.0	26.9	8.2
Nitrogen compounds	2.2	4.9	4.6	3.8	0.0	0.0	11.7	3.8
Organic acids	2.9	5.2	5.7	9.1	0.0	0.0	16.1	4.9
Organic salts	2.8	6.2	5.4	3.8	0.0	0.0	17.8	4.8
Other compounds	2.9	4.4	7.4	2.7	0.0	0.0	16.2	4.6
Peroxides	2.1	2.6	3.9	3.5	0.0	0.0	8.57	2.9
Polyfunctional compounds	2.3	4.2	4.5	8.0	0.0	0.0	10.8	3.9
Silicon compounds	2.4	4.0	4.2	5.3	0.0	0.0	9.56	3.7
Sulfur compounds	1.5	4.0	3.2	1.8	0.0	0.0	12.9	2.7

To have a deeper insight into the role played by association and to better understand the relationship between the ability of an EoS to accurately reproduce the properties of pure species

and the strength of association, it is now decided to use the criterion for *quality modelling* defined in our previous paper¹²⁷. Using this latter, molecules will be labelled as *well* or *badly* represented and it will be possible to analyze how the SA and NSA fluids distribute between the 2 categories. The proposed criterion of modelling quality compares the deviations obtained on P^{sat} and v_{liq}^{sat} for a given fluid to the mean deviations obtained for all the NSA fluids. For a given molecule, if deviations on P^{sat} and v_{liq}^{sat} are slightly lower than the corresponding mean values for NSA fluids, the molecule is considered as *well-modeled*. Otherwise, it falls in the *badly-modeled* category.

Quantitatively speaking, a pure component j will be considered as *well-modeled* by a given EoS provided:

$$\left\{ \begin{array}{l} \left(MAPE_{P^{sat}}^{EoS} \right)_j \leq \overline{MAPE}_{P^{sat}}^{EoS,NSA} + SD_{P^{sat}}^{EoS,NSA} \\ \text{and} \\ \left(MAPE_{v_{liq}^{sat}}^{EoS} \right)_j \leq \overline{MAPE}_{v_{liq}^{sat}}^{EoS,NSA} + SD_{v_{liq}^{sat}}^{EoS,NSA} \end{array} \right. \quad (3.14)$$

Where $SD_X^{EoS,NSA}$ and $\overline{MAPE}_X^{EoS,NSA}$ denote the mean standard deviation (SD) and MAPE for property X calculated with a given EoS over the 1 252 NSA components of the database (see **Table 3.7** for the numerical values).

Table 3.7. Average MAPE on P^{sat} and v_{liq}^{sat} as predicted by the PC-SAFT and I-PC-SAFT for the 1252 NSA compounds and corresponding standard deviations (SD).

PC-SAFT			
MAPE on P^{sat} (%)	0.97	MAPE on v_{liq}^{sat} (%)	0.85
SD on P^{sat} (%)	0.95	SD on v_{liq}^{sat} (%)	0.74
MAPE + SD	1.92	MAPE + SD	1.59
I-PC-SAFT			
MAPE on P^{sat} (%)	1.83	MAPE on v_{liq}^{sat} (%)	4.35
SD on P^{sat} (%)	1.54	SD on v_{liq}^{sat} (%)	2.95
MAPE + SD	3.38	MAPE + SD	7.30

If one or both conditions of Eq. (3.14) are not satisfied, the pure component is considered as *badly-modeled*. Results are presented in **Figure 3.9** and **Figure 3.10** for the PC-SAFT and *I*-PC-SAFT EoS and deserve discussion. For possible comparison, results obtained with the *tc*-PR EoS, as published in our previous paper¹²⁷, are recalled in **Figure 3.11**.

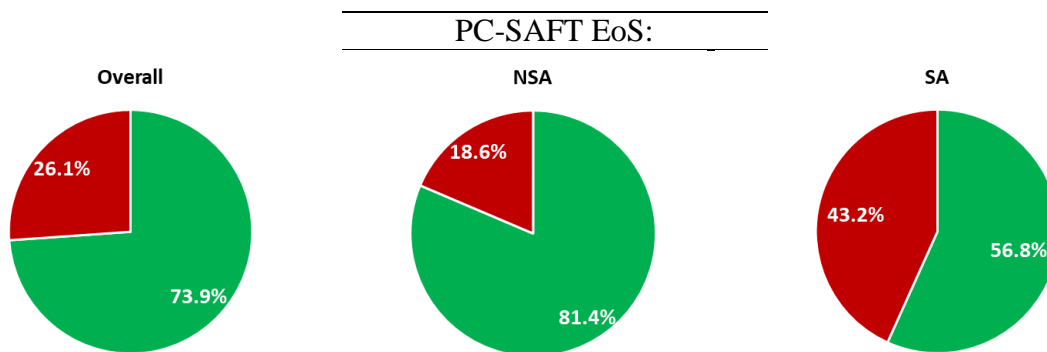


Figure 3.9. Ratio of well and badly modeled molecules by the PC-SAFT EoS classified into non-self-associating (NSA) and self-associating (SA) fluids. Green: Well-modeled molecules. Red: Badly-modeled molecules.

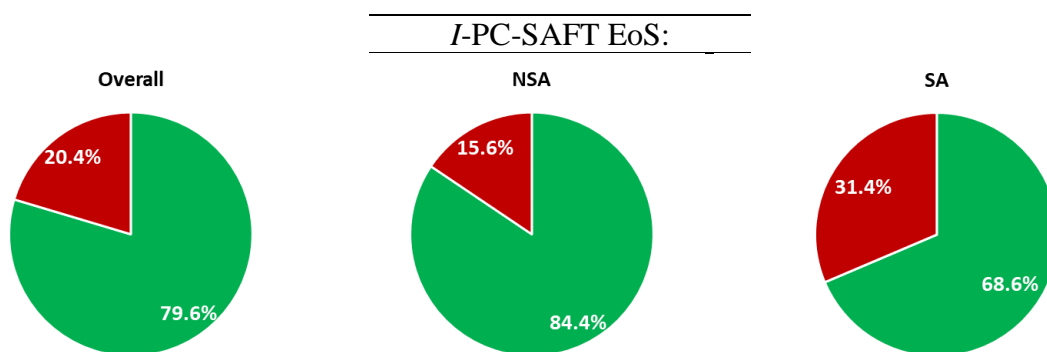


Figure 3.10. Ratio of well and badly modeled molecules by the I-PC-SAFT EoS classified into non-self-associating (NSA) and self-associating (SA) fluids. Green: Well-modeled molecules. Red: Badly-modeled molecules.

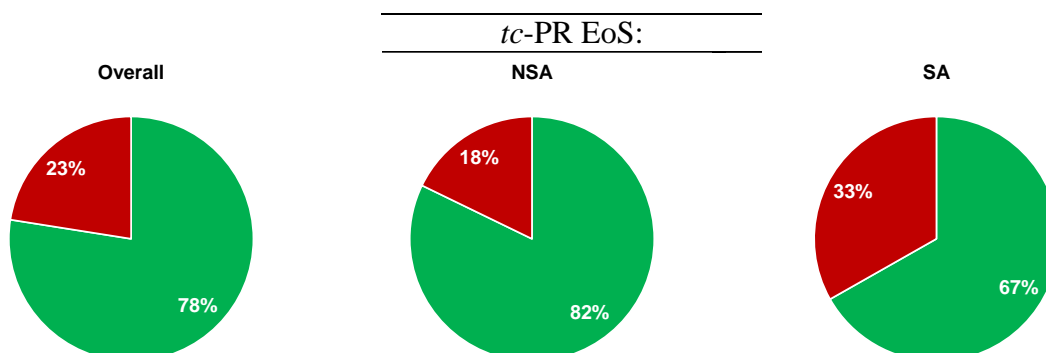


Figure 3.11. Ratio of well and badly modeled molecules by the tc-PR EoS classified into non-self-associating (NSA) and self-associating (SA) fluids. Green: Well-modeled molecules. Red: Badly-modeled molecules.

A major feature is the huge similitude between SAFT-type EoS and the *tc*-PR EoS. Indeed, regardless of the considered EoS (PC-SAFT, *I*-PC-SAFT or *tc*-PR), about 75% of the pure components are well represented, according to the criterion defined in Eq. (3.14) (see the left panel in each figure). As reported in **Table 3.2**, the database contains 70% of NSA fluids and 30% of SA components. In the absence of an association term, it could be believed that the *well-modeled* molecules are essentially NSA fluids. This is however not the case at all. Indeed, as previously reported in our paper devoted to CEoS, almost 65% of the SA molecules are *well-modeled* (see the right panel in Figures 8 to 10), while almost 17% of the NSA compounds are *badly-modeled* (refer to the middle panel in Figures 8 to 10). Once again, we might have been tempted to believe that all the NSA fluids would be *well-modeled* by SAFT-type EoS that do not embed an association term, but this is not the case. Similarly, one would not have predicted that more than half of the SA molecules would be accurately modeled in the absence of an association term.

In order to go further, it was decided to investigate a potential correlation between the strength of the hydrogen bond and the accuracy with which the experimental data were correlated. In other words, working with SA compounds, we wanted to investigate if it was possible to claim that properties of weakly-associating molecules are better correlated by non-associating versions of EoS than those of strongly-associating molecules.

To answer this question, the COSMOtherm tool for predictive property calculation of liquids that combines quantum chemistry and the COSMO-RS thermodynamic model^{118,119,124} was used to calculate the hydrogen-bond enthalpy ($-\Delta_{HB}H$) of the 548 SA fluids. The hydrogen-bond enthalpy, assumed to be proportional to the strength of the association was plotted as a function of $(\text{MAPE on } P^{sat} + \text{MAPE on } v_{liq}^{sat})$ which is believed to be a good indicator of the accuracy with which the data are correlated. The results can be seen in Figures 11 to 13 for the PC-SAFT, *I*-PC-SAFT and *tc*-PR EoS. Such figures speak by themselves: regardless of the EoS, there is absolutely no correlation between the strength of association and the EoS accuracy. It is possible to find strongly-associating molecules (for which $-\Delta_{HB}H > 25 \text{ kJ} \cdot \text{mol}^{-1}$) that are very accurately correlated. Examples are: L-phenylalanine, 1,4-cyclohexanedicarboxylic acid and Pyridine-3-carboxylic acid. Conversely, slightly-associating molecules ($-\Delta_{HB}H < 3 \text{ kJ} \cdot \text{mol}^{-1}$) that exhibit very large deviations can be found. Among others, examples are: Ethylene carbonate, Nitroethane or Succinic Anhydride that are highlighted from **Figure 3.12** to **Figure 3.14**.

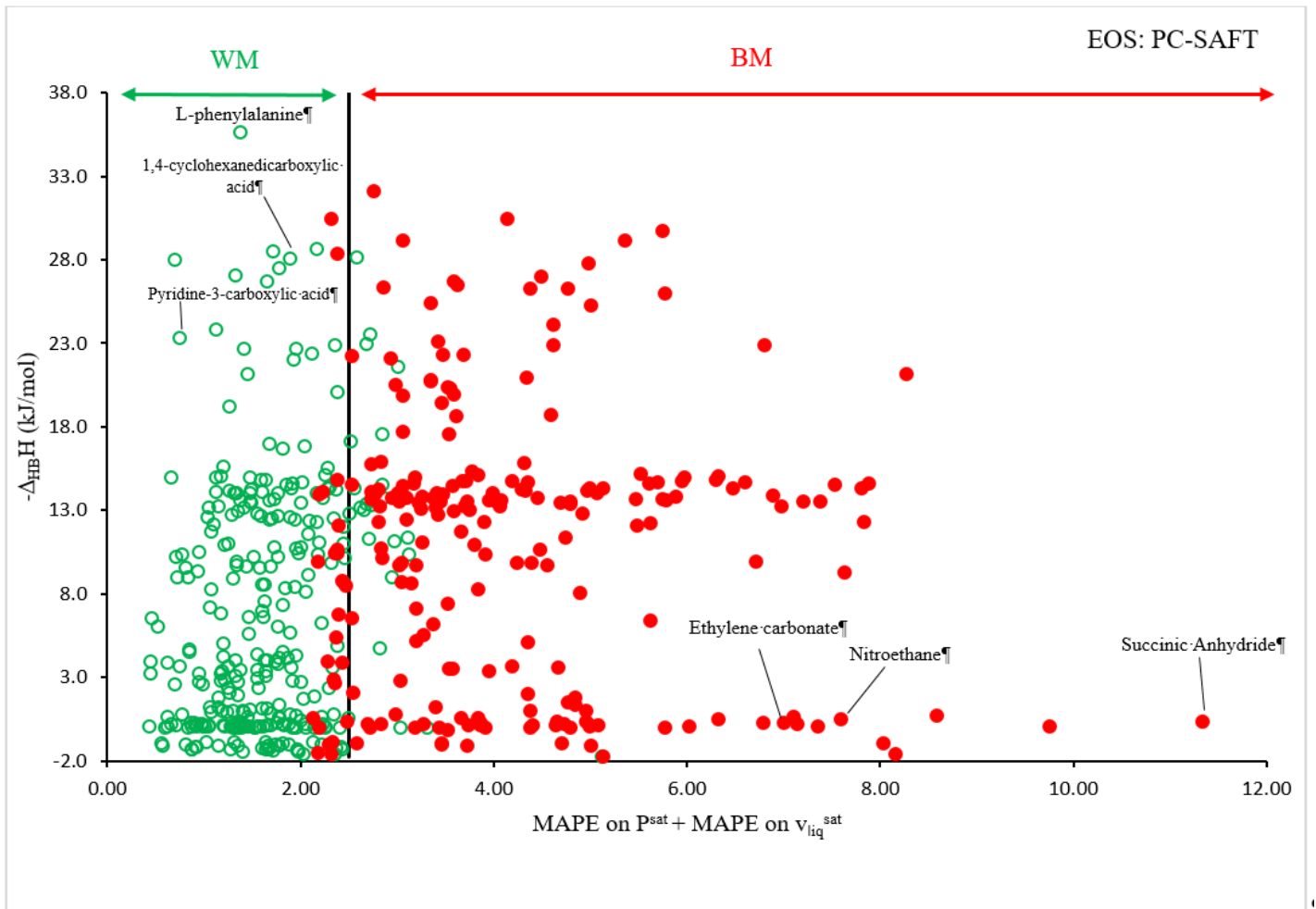


Figure 3.12. Hydrogen bond enthalpy vs. $(\text{MAPE on } P^{sat} + \text{MAPE on } v_{liq}^{sat})$ for the 548 SA compounds modeled with the PC-SAFT EoS. \circ : 311 well-modeled components. \bullet : 237 badly-modeled components. The vertical line is an approximate border between the region where the fluids are well-modeled (WM) and badly-modeled (BM).

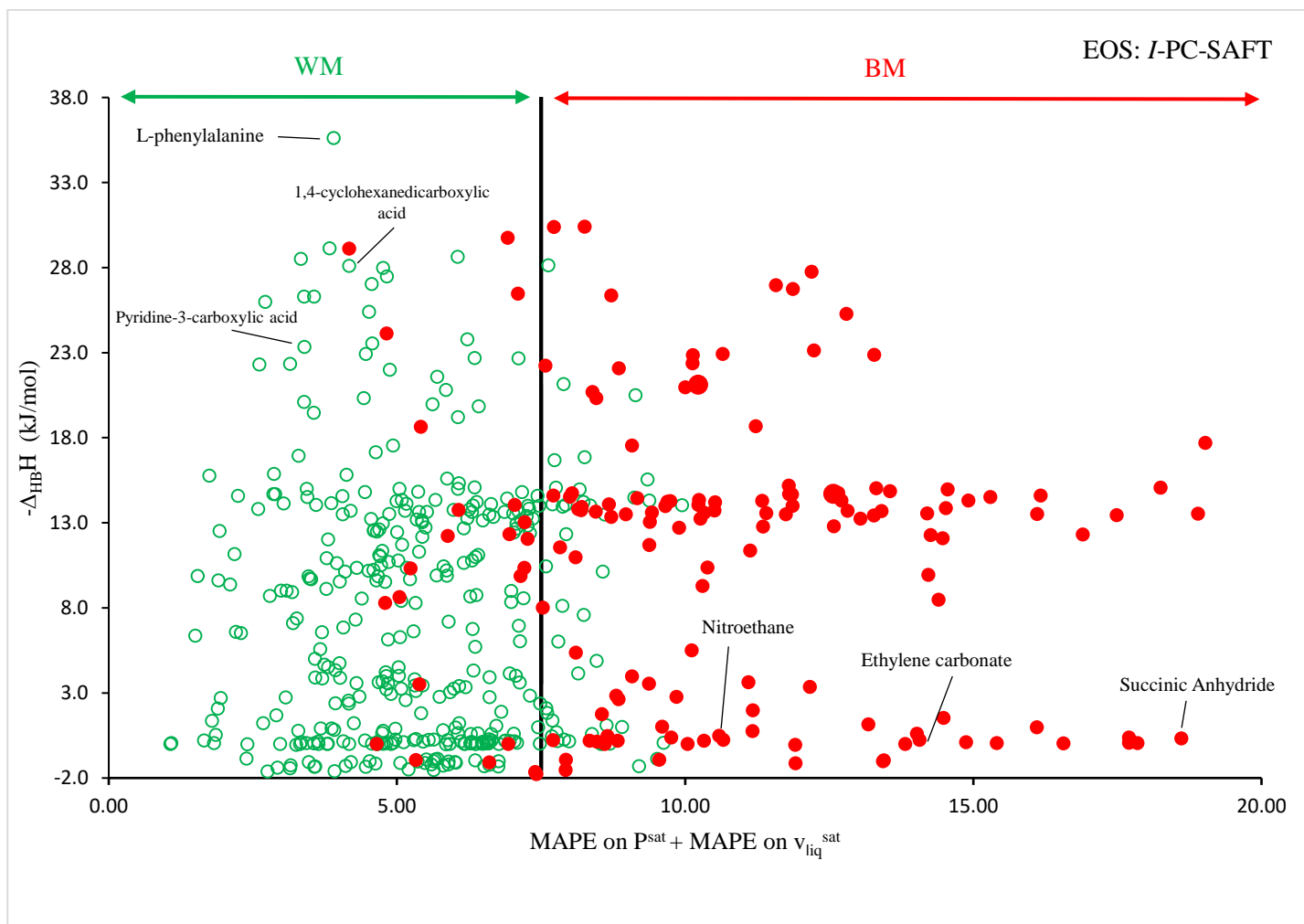


Figure 3.13. Hydrogen bond enthalpy vs. (MAPE on P^{sat} + MAPE on $v_{\text{liq}}^{\text{sat}}$) for the 548 SA compounds modeled with the I-PC-SAFT EoS. ○: 377 well-modeled components. ●: 171 badly-modeled components. The vertical line is an approximate border between the region where the fluids are well-modeled (WM) and badly-modeled (BM).

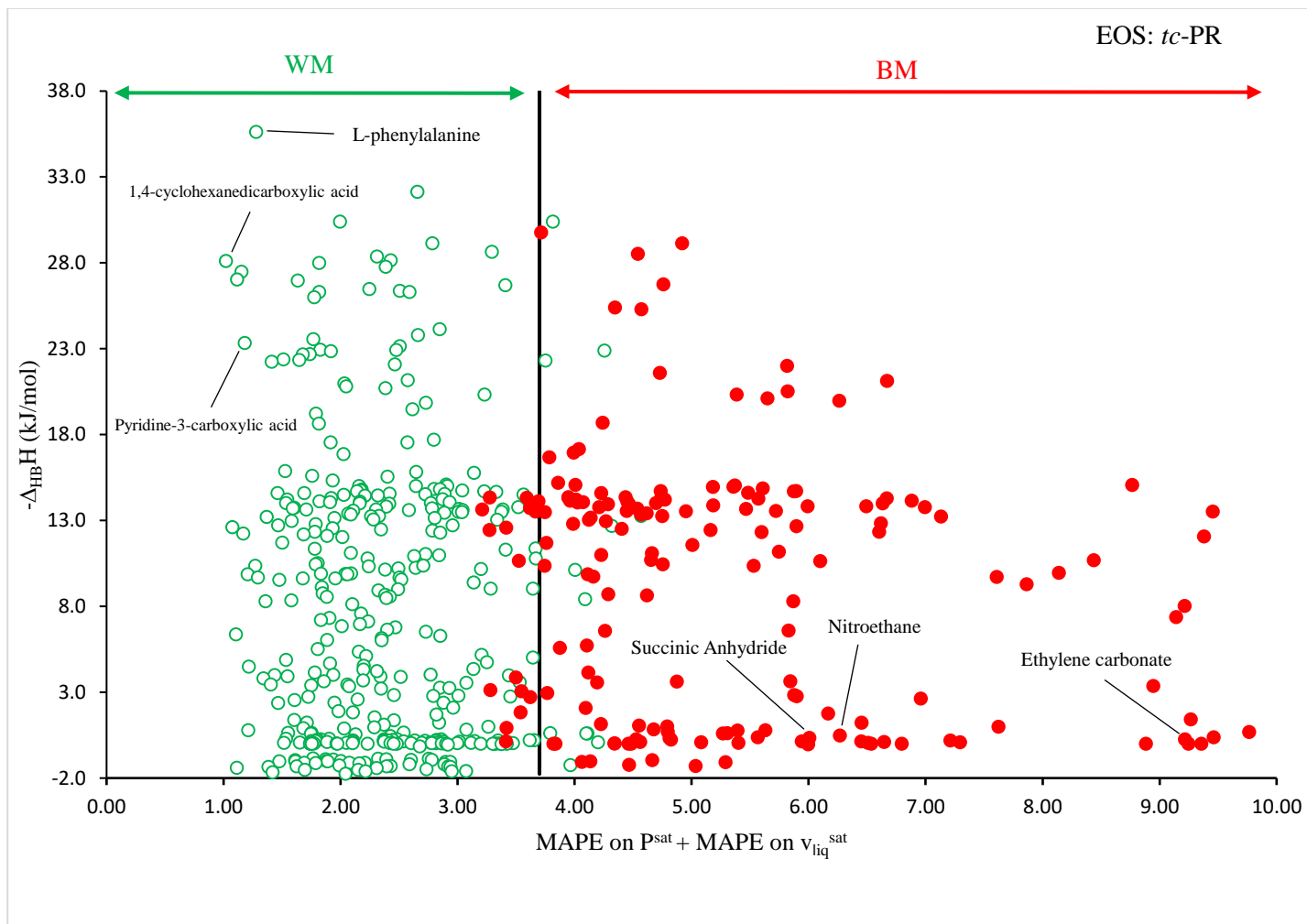


Figure 3.14. Hydrogen bond enthalpy vs. (MAPE on P^{sat} + MAPE on $v_{\text{liq}}^{\text{sat}}$) for the 548 SA compounds modeled with the tc-PR EoS. \circ : 366 well-modeled components. \bullet : 182 badly-modeled components. The vertical line is an approximate border between the region where the fluids are well-modeled (WM) and badly-modeled (BM).

From **Figure 3.12** to **Figure 3.14**, we can even assert that regardless of the EoS, the component that has the highest hydrogen-bond enthalpy is *well-represented*, while the SA compound having the smallest hydrogen-bond enthalpy is *badly-represented*. Such results do not help to decide in which direction efforts have to be devoted to improve SAFT-type and CEoS without association term. It seems thus legitimate to wonder if the addition of an association term is really the most suited solution.

Finally, a closer inspection across various chemical families (as defined by the DIPPR) is proposed. **Table 3.8** shows the distribution of *well-modeled* compounds for different chemical families and for the three EoS (PC-SAFT, *I*-PC-SAFT and *tc*-PR). Once again, the similitude of the results obtained with SAFT-type and cubic EoS can be highlighted. It is possible to observe that the three EoS have a ratio of *well-modeled* molecules greater than 65% and often close to 80% for alkanes, alkenes, alkynes, aromatics, esters, ethers, ketones, aldehydes, epoxides, peroxides, halogen compounds, amines, amides, sulfur and silicon compounds. Alcohols have >50% of well-modeled molecules except with the PC-SAFT model which yields a ratio of 32%.

Table 3.8. Distribution of well-modeled compounds across different chemical families for the PC-SAFT, *I*-PC-SAFT and *tc*-PR EoS.

Chemical family	PC-SAFT	<i>I</i> -PC-SAFT	<i>tc</i> -PR ^(*)
Alcohols	32%	54%	53%
Alkanes	96%	96%	94%
Alkenes	93%	88%	87%
Alkynes	67%	83%	83%
Amines/Amides	69%	79%	68%
Aromatics	85%	88%	83%
Epoxides	94%	94%	83%
Esters/Ethers	83%	78%	79%
Halogen Compounds	74%	84%	80%
Inorganic Compounds	60%	69%	60%
Ketones/Aldehydes	83%	86%	93%
Nitriles	29%	36%	35%
Nitrogen Compounds	69%	72%	75%
Organic Acids	59%	65%	79%
Organic Salts	54%	62%	46%
Other Compounds	56%	78%	44%
Peroxides	73%	91%	73%
Polyfunctional Compounds	72%	82%	74%

Silicon Compounds	64%	71%	72%
Sulfur compounds	88%	97%	90%

(*) Reproduced from our previous article¹²⁷.

3.5.4. Conclusion

In this chapter, two non-associating versions of the popular PC-SAFT EoS were evaluated and contrasted in their performance on the basis of pure-compound property prediction. The first version was the original PC-SAFT EoS with a recently proposed parametrization strategy in which the three molecular parameters m , σ , ε/k_B are fitted to experimental P^{sat} and ρ_{liq}^{sat} data with specific weights assigned to them in the objective function to be minimized. The second version was the *industrialized* PC-SAFT or *I-PC-SAFT* EoS which estimates the three molecular parameters by exactly reproducing the experimental critical coordinates and acentric factor ($T_{c,exp}$, $P_{c,exp}$, ω_{exp}). Such an EoS is volume-translated and the volume shift (c) is determined in order to exactly reproduce the saturated liquid molar volume at the reduced temperature of 0.8.

The assessment was performed over 1800 molecules that have accurate P^{sat} and ρ_{liq}^{sat} correlations in the DIPPR databank making possible to generate accurate pseudo-experimental data. Among the 1 800 fluids, 1 536 also possess an accurate correlation for $\Delta_{vap}H$ and 890 for $c_{P,liq}^{sat}$ making possible to generate 50 data points for such properties. The critical properties (T_c , P_c and v_c) are available for the 1 800 components so that in the end, the resulting database contains 306 700 high-quality pseudo-experimental points. These 1800 molecules were divided into 1252 non-self-associating (NSA) compounds and 548 self-associating (SA) compounds.

Results obtained over the entire database highlight:

- The very high accuracy of both SAFT-type EoS that got an average overall deviation of 2.2% and 3.6% over the 306 700 experimental data points respectively. Deviations on the derived properties ($\Delta_{vap}H$ and $c_{P,liq}^{sat}$) are around 4% which is higher than those observed for vapor pressures and liquid densities. For possible comparison, the *tc-PR*

EoS, which was found to be the most accurate cubic EoS got an average deviation of 1.9% over the entire database.

- The strong influence of the parameterization: the PC-SAFT EoS is parameterized in order to minimize the deviations between experimental and calculated P^{sat} and v_{liq}^{sat} data so that such properties are perfectly correlated. In return, the price to pay is a large deviation on the critical pressure. On the other hand, the *I*-PC-SAFT is parameterized in order to exactly reproduce the critical coordinates in a (P,T) plane but the prize to pay is a loss of accuracy in the correlation of liquid densities, especially the critical volume although a volume translation is applied.
- The absence of correlation between the strength of association and the EoS accuracy. Among the 548 self-associating components, the one that has the highest hydrogen-bond enthalpy is *well-represented*, whereas the one that has the smallest hydrogen-bond enthalpy is *badly-represented*. In addition, poor results are obtained for more than 15% of the non-self-associating compounds. Such a disappointing result was not expected from molecular-based equations of state. Simultaneously, the PC-SAFT equation is able to correlate with high accuracy (deviations lower than 2%) the vapor pressures and the liquid densities of about 60% of the self-associating compounds. This second result is even less expected since no association term was included in the considered equations of state. Such results do not help to decide in which direction efforts have to be devoted to improve SAFT-type and cubic EoS that do not embed an association term. Is the addition of an association term really the most suited solution?

Let us also recall that this paper is the first one in which molecular parameters suitable for the PC-SAFT and *I*-PC-SAFT EoS are published for 1 800 pure compounds. Such parameters can be used immediately in any commercial process simulator.

Finally, the authors hope that the database used in this paper and also in a previous one dedicated to cubic EoS will be widely adopted by the scientific community to identify the strengths and weaknesses of a given thermodynamic model to correlate (or predict) the properties of pure compounds.

Chapter 4 : Parametrization of SAFT EoS for associating compounds – overview of the association schemes and parametrization trends

Within the SAFT framework and associating models in general, associating effects are taken into account independently of the other interactions as a function of the associating energy and associating volume, which refer to the strength and size of the interaction of the HB. These two magnitudes are incorporated in the model as component-dependent parameters and are usually fitted to experimental data in order to estimate their values. However, this is not as straightforward as the parameters accounting for the dispersive forces in the molecule: the associating parameters depend on the number of sites available in the molecule to form HB in what is known as an association scheme. The most employed approach to work around this issue is utilizing the approximations and nomenclature proposed by Huang and Radosz⁴⁵ (usually referred to as association schemes directly in the literature). These approximative schemes define the number of available sites and therefore the expressions that will be used in order to obtain the associating parameters.

Although many authors have used the above-mentioned method, the use of association schemes is not systematic: some authors use different approaches to select them, with discrepancies in the selected scheme between similar compounds. Furthermore the parameter estimation is not methodical between authors and thus raises the question of how can the associating contribution of SAFT EoS be treated in order to have a transparent and systematic way to select the proper associating schemes and to obtain the corresponding parameters.

This chapter will be dedicated to reviewing the current state of association scheme selection as well as the parametrization for associating models such as the SAFT family of EoS and the Cubic Plus Association model (CPA).

4.1. The Association schemes

We begin by recalling Eq. (1.71) presented in **Chapter 1**. The final version of this equation presented here comes from several extensions of Wertheim's first order thermodynamic perturbation theory^{47-49,134} (TPT1). At this order, only dimer formation is allowed for molecules with attractive sites, meaning that one site A can only form a single HB with a second site B and none of them can participate in further HB, meaning that double or triple hydrogen-bonding is not allowed (e.g. no ABA HB are allowed only AB or BA). Wertheim's theory was developed for single spherical equal-sized particles with multiple attractive sites. Chapman^{4,5,135} extended this to mixtures of non-spherical molecules with different number of attraction sites. With this, TPT1 allows to determine the fraction of unbonded attractive sites from Eq. (1.71). The reader is directed to Zmpitas & Gross¹³⁶ for a more detailed explanation on the derivation of Eq. (1.71).

It is clear that the fraction of unbonded molecules is not explicit and therefore an analytical solution is not possible at this stage. Huang and Radosz⁴⁵ addressed this issue by introducing a series of approximations to X^A in which specific bonding constraints were assumed e.g. attractive site A of molecule i can only bond to attractive site B of molecule j . Limiting the bonding-scheme to specific site-site interactions simplifies Eq. (1.71) and allows it to be analytically solved in some cases. This allows for interactions such as the HB, in which only a donor and an acceptor site can interact, to be properly modeled.

These approximations to X^A can be made according to previous physical knowledge about the associating sites of the studied molecules, more specifically, if one has prior knowledge of the compound's structure, ideally from spectroscopic data. However, since this information is scarce and is mostly qualitative, a more empirical approach, based on the knowledge of the compound's chemical structure is often the tool employed to perform such approximations.

Consider a molecule with a given number of association sites. Since the location of these sites is not taken into account, we differentiate each site by assigning it a capital letter (A, B, C, etc.). A site with a lone pair of electrons is viewed as a negative site, which takes the role of attracting a hydrogen proton (HA site), while a site in which a hydrogen proton is labile is deemed as a positive site, taking the role of providing the hydrogen to form the HB (HD site). A third type of site can be found in which site A would be attracted to either an HA or HD site. Usually referred to as a binary¹³⁷ or bipolar¹³⁸ site.

Depending on the number of sites (and roughly the kind of site), Huang and Radosz⁴⁵ proposed an array of types of association schemes which are still used to this day. The notations include a number which represents the number of association sites and the letters, to a less strict sense, the kind of association site (HA, HD or binary). In order to best describe this notation, we will consider a generic association scheme $\alpha\beta$, where α represents the number of sites (HD, HA or bipolar) and β represents the assumptions made for the particular scheme. These assumptions can be of the following types:

- **A type:** where all sites are bipolar and the association strength is equal for all site-site bonds, i.e. $\Delta^{site A, site B} = \Delta^{site A, site A} = \Delta^{site A, site B} \neq 0$.
- **B type:** where one site is HA and the rest of the sites are HD. No bonding between like sites is allowed and the association strength is equal for all bonds, i.e.: $\Delta^{site HA, site HA} = \Delta^{site HD, site HD} = 0$; $\Delta^{site HA, site HD} \neq 0$.
- **C type:** where at least two sites are HA and the rest are HD. No bonding between like sites is allowed and the association strength is equal for all bonds, i.e. $\Delta^{site HA, site HA} = \Delta^{site HD, site HD} = 0$; $\Delta^{site HA, site HD} \neq 0$

With these association schemes, Eq. (1.71) can be analytically solved in most cases for pure species. We recall that, for pure species, Eq. (1.71) for any site A can be written as:

$$X^A \left[1 + \rho \sum_{sites B_j} \Delta^{AB_j} X^{AB_j} \right] = 1 \quad (4.1)$$

And for mixtures:

$$X^A \left[1 + \rho \sum_{components k} x_k \sum_{sites B_j} \Delta^{AB_j} X^{AB_j} \right] = 1 \quad (4.2)$$

The 1A schemes (or A schemes in general) are the ones given to molecules for which only a binary association site is present. Carboxylic acids fall under this category. This scheme assumes that the dimerization of organic acids is due to a single HB of greater strength rather

than a double HB (which is physically correct), since Wertheim's theory⁴⁷⁻⁴⁹ does not allow for this type of interaction. Another example of one-site schemes corresponds to tertiary amines, in which only a single HA site exists. However, due to the steric hindrance of the three alkyl groups, these molecules are considered as non-associating or cross-associating only. Taking into consideration the assumptions for **A type** sites for a 1A scheme, Eq. (4.1) becomes:

$$\begin{aligned}
 \Delta^{AA} &\neq 0 \\
 X^A [1 + \rho \Delta^{AA} X^A] &= 1 \\
 \therefore \rho \Delta^{AA} (X^A)^2 + X^A - 1 &= 0 \\
 \therefore X^A &= \frac{-1 + \sqrt{1 + 4\rho \Delta^{AA}}}{2\rho \Delta^{AA}}
 \end{aligned} \tag{4.3}$$

A molecule may have two bipolar sites, leading to a 2A scheme. For a 2A association scheme with the **A type** assumptions:

Bonding	A	B
A	Y	Y
B	Y	Y

Thus for site A:

$$\begin{aligned}
 \Delta^{AA} = \Delta^{BB} = \Delta^{AB} &\neq 0 \\
 X^A [1 + \rho \Delta^{AA} X^A + \rho \Delta^{AB} X^B] &= 1 \\
 \therefore X^A [1 + \rho \Delta X^A + \rho \Delta X^B] &= 1
 \end{aligned} \tag{4.4}$$

In addition, for site B:

$$\begin{aligned}
 \Delta^{AA} = \Delta^{BB} = \Delta^{AB} &\neq 0 \\
 X^B [1 + \rho \Delta^{AB} X^A + \rho \Delta^{BB} X^B] &= 1 \\
 \therefore X^B [1 + \rho \Delta X^A + \rho \Delta X^B] &= 1
 \end{aligned} \tag{4.5}$$

The ratio between Eqs. (4.4) and (4.5) leads to

$$\begin{aligned}
 \frac{X^A [1 + \rho \Delta X^A + \rho \Delta X^B]}{X^B [1 + \rho \Delta X^A + \rho \Delta X^B]} &= 1 \\
 \therefore \frac{X^A}{X^B} &= 1 \\
 \therefore X^A &= X^B
 \end{aligned} \tag{4.6}$$

Replacing Eq. (4.6) in Eq. (4.4) we obtain:

$$\begin{aligned}
X^A [1 + \rho\Delta X^A + \rho\Delta X^A] &= 1 \\
\therefore X^A [1 + 2\rho\Delta X^A] &= 1 \\
\therefore 2\rho\Delta (X^A)^2 + X^A - 1 &= 0 \\
\therefore X^A &= \frac{-1 + \sqrt{1 + 8\rho\Delta}}{4\rho\Delta}
\end{aligned} \tag{4.7}$$

A molecule may also have three bipolar sites. For a 3A association scheme with the **A type** assumptions:

Bonding	A	B	C
A	Y	Y	Y
B	Y	Y	Y
C	Y	Y	Y

For a site A:

$$\begin{aligned}
\Delta^{AA} = \Delta^{BB} = \Delta^{CC} = \Delta^{AB} = \Delta^{AC} = \Delta^{BC} &\neq 0 \\
X^A [1 + \rho\Delta^{AA} X^A + \rho\Delta^{AB} X^B + \rho\Delta^{AC} X^C] &= 1 \\
\therefore X^A [1 + \rho\Delta X^A + \rho\Delta X^B + \rho\Delta X^C] &= 1
\end{aligned} \tag{4.8}$$

For a site B:

$$\begin{aligned}
\Delta^{AA} = \Delta^{BB} = \Delta^{CC} = \Delta^{AB} = \Delta^{AC} = \Delta^{BC} &\neq 0 \\
X^B [1 + \rho\Delta^{AB} X^A + \rho\Delta^{BB} X^B + \rho\Delta^{BC} X^C] &= 1 \\
\therefore X^B [1 + \rho\Delta X^A + \rho\Delta X^B + \rho\Delta X^C] &= 1
\end{aligned} \tag{4.9}$$

In addition, for site C:

$$\begin{aligned}
\Delta^{AA} = \Delta^{BB} = \Delta^{CC} = \Delta^{AB} = \Delta^{AC} = \Delta^{BC} &\neq 0 \\
X^C [1 + \rho\Delta^{AC} X^A + \rho\Delta^{BC} X^B + \rho\Delta^{CC} X^C] &= 1 \\
\therefore X^C [1 + \rho\Delta X^A + \rho\Delta X^B + \rho\Delta X^C] &= 1
\end{aligned} \tag{4.10}$$

Taking the ratio between Eqs. (4.9) and (4.10) we obtain:

$$\begin{aligned}
\frac{X^B [1 + \rho\Delta X^A + \rho\Delta X^B + \rho\Delta X^C]}{X^C [1 + \rho\Delta X^A + \rho\Delta X^B + \rho\Delta X^C]} &= 1 \\
\therefore \frac{X^B}{X^C} &= 1 \\
\therefore X^B &= X^C
\end{aligned} \tag{4.11}$$

Similarly, taking the ratio between Eqs. (4.8) and (4.10) we get:

$$\frac{X^A [1 + \rho\Delta X^A + \rho\Delta X^B + \rho\Delta X^C]}{X^C [1 + \rho\Delta X^A + \rho\Delta X^B + \rho\Delta X^C]} = 1$$

$$\therefore \frac{X^A}{X^C} = 1 \quad (4.12)$$

$$\therefore X^A = X^C$$

Replacing Eqs. (4.11) and (4.12) into Eq. (4.8) we finally obtain:

$$X^A [1 + \rho\Delta X^A + \rho\Delta X^A + \rho\Delta X^A] = 1$$

$$\therefore X^A [1 + 3\rho\Delta X^A] = 1$$

$$\therefore 3\rho\Delta (X^A)^2 + X^A - 1 = 0 \quad (4.13)$$

$$\therefore X^A = \frac{-1 + \sqrt{1 + 12\rho\Delta}}{6\rho\Delta}$$

The 2B scheme describes a molecule with two sites in which only unlike site-site interaction is allowed (i.e. only HA-HD interactions are permitted). A simple example of this are secondary amines in which a site A is of the HA kind and a site B of the HD kind. A-A and B-B interactions are not considered and are assumed to be equal to zero. A more nuanced case for the 2B scheme are alcohols, in particular 1-alkanols: both electron pairs of the oxygen atom are combined into a single HA site, while the hydrogen is taken as the second site. Using the **B type** assumptions, for a 2B scheme, assuming site A as HD and site B as HA we obtain:

Bonding	A	B
A	N	Y
B	Y	N

For site A:

$$\Delta^{AA} = \Delta^{BB} = 0$$

$$\Delta^{AB} \neq 0$$

$$X^A [1 + \rho\Delta^{AA} X^A + \rho\Delta^{AB} X^B] = 1 \quad (4.14)$$

$$\therefore X^A [1 + \rho\Delta X^B] = 1$$

Then, for site B:

$$\Delta^{AA} = \Delta^{BB} = 0$$

$$\Delta^{AB} \neq 0$$

$$X^B [1 + \rho\Delta^{AB} X^A + \rho\Delta^{BB} X^B] = 1 \quad (4.15)$$

$$\therefore X^B [1 + \rho\Delta X^A] = 1$$

The ratio between Eqs. (4.14) and (4.15) leads to:

$$\begin{aligned}
\frac{X^A [1 + \rho \Delta X^B]}{X^B [1 + \rho \Delta X^A]} &= 1 \\
\therefore X^A [1 + \rho \Delta X^B] &= X^B [1 + \rho \Delta X^A] \\
\therefore X^A + \rho \Delta X^A X^B &= X^B + \rho \Delta X^A X^B \\
\therefore X^A &= X^B
\end{aligned} \tag{4.16}$$

Replacing the result obtained in Eq. (4.16) into Eq. (4.14) we finally obtain:

$$\begin{aligned}
X^A [1 + \rho \Delta X^A] &= 1 \\
\therefore \rho \Delta (X^A)^2 + X^A - 1 &= 0 \\
\therefore X^A &= \frac{-1 + \sqrt{1 + 4\rho \Delta}}{2\rho \Delta}
\end{aligned} \tag{4.17}$$

The 3B scheme is used for molecules which have three sites in which only unlike site interactions are allowed. This is the case for primary amines in which sites A and B (hydrogen atoms) are HD sites while site C (electron pair) is HA. Strictly speaking, alcohols are also of this kind, having both pair of electrons as sites A and B and the hydrogen atom as site C. Applying the **B type** assumptions to a 3B scheme, assuming sites A and B as HD and site C as HA, we obtain

Bonding	A	B	C
A	N	N	Y
B	N	N	Y
C	Y	Y	N

For site A:

$$\begin{aligned}
\Delta^{AA} = \Delta^{BB} = \Delta^{CC} = \Delta^{AB} &= 0 \\
\Delta^{AC} = \Delta^{BC} &\neq 0 \\
X^A [1 + \rho \Delta^{AA} X^A + \rho \Delta^{AB} X^B + \rho \Delta^{AC} X^C] &= 1 \\
\therefore X^A [1 + \rho \Delta X^C] &= 1
\end{aligned} \tag{4.18}$$

Equivalently for site B:

$$\begin{aligned}
\Delta^{AA} = \Delta^{BB} = \Delta^{CC} = \Delta^{AB} &= 0 \\
\Delta^{AC} = \Delta^{BC} &\neq 0 \\
X^B [1 + \rho \Delta^{AB} X^A + \rho \Delta^{BB} X^B + \rho \Delta^{BC} X^C] &= 1 \\
\therefore X^B [1 + \rho \Delta X^C] &= 1
\end{aligned} \tag{4.19}$$

And for site C:

$$\begin{aligned}
\Delta^{AA} &= \Delta^{BB} = \Delta^{CC} = \Delta^{AB} = 0 \\
\Delta^{AC} &= \Delta^{BC} \neq 0 \\
X^C \left[1 + \rho\Delta^{AC} X^A + \rho\Delta^{BC} X^B + \rho\Delta^{CC} X^C \right] &= 1 \\
\therefore X^C \left[1 + \rho\Delta (X^A + X^B) \right] &= 1
\end{aligned} \tag{4.20}$$

The ratio of Eqs. (4.18) and (4.19) naturally leads to:

$$\begin{aligned}
\frac{X^A \left[1 + \rho\Delta X^C \right]}{X^B \left[1 + \rho\Delta X^C \right]} &= 1 \\
\therefore \frac{X^A}{X^B} &= 1 \\
\therefore X^A &= X^B
\end{aligned} \tag{4.21}$$

Therefore, we can write Eq. (4.20) as:

$$X^C \left[1 + 2\rho\Delta X^A \right] = 1 \tag{4.22}$$

We take note that we can rewrite Eq. (4.22) as:

$$X^C + 2\rho\Delta X^A X^C = 1 \tag{4.23}$$

We can rewrite Eq. (4.18) as well:

$$\begin{aligned}
X^A + \rho\Delta X^A X^C &= 1 \\
\therefore \rho\Delta X^A X^C &= 1 - X^A
\end{aligned} \tag{4.24}$$

Replacing this result into Eq. (4.23) we finally obtain:

$$\begin{aligned}
X^C + 2(1 - X^A) &= 1 \\
\therefore X^C + 2 - 2X^A &= 1 \\
\therefore X^C &= 2X^A - 1
\end{aligned} \tag{4.25}$$

We insert this result into Eq. (4.18) to finally obtain:

$$\begin{aligned}
X^A \left[1 + \rho\Delta (2X^A - 1) \right] &= 1 \\
\therefore X^A \left[1 + 2X^A \rho\Delta - \rho\Delta \right] &= 1 \\
\therefore 2\rho\Delta (X^A)^2 + X^A - \rho\Delta X^A - 1 &= 0 \\
\therefore 2\rho\Delta (X^A)^2 + (1 - \rho\Delta) X^A - 1 &= 0 \\
\therefore X^A &= \frac{-(1 - \rho\Delta) + \sqrt{(1 - \rho\Delta)^2 + 4\rho\Delta}}{4\rho\Delta}
\end{aligned} \tag{4.26}$$

Associating schemes with four sites (4B and 4C) are used to describe molecules which are highly hydrogen bonded. The most common example of these schemes is water (4C) with two HA and two HD sites. Similar examples of these schemes would be glycols (4C) and ammonia (4B), although the latter presents three HD sites and only one HA site. Water and ammonia, however, can also be modeled by a 3B or even 2B scheme, given that one combines two likewise sites into a single one. These approximations have been discussed in the literature and will be addressed later on. Using the **C type** assumptions for a 4C scheme, where sites A and B are HD and sites C and D are HA, we obtain:

Bonding	A	B	C	D
A	N	N	Y	Y
B	N	N	Y	Y
C	Y	Y	N	N
D	Y	Y	N	N

For site A we have:

$$\begin{aligned}
 \Delta^{AA} &= \Delta^{BB} = \Delta^{CC} = \Delta^{DD} = \Delta^{AB} = \Delta^{CD} = 0 \\
 \Delta^{AC} &= \Delta^{BC} = \Delta^{AD} = \Delta^{BD} \neq 0 \\
 X^A [1 + \rho\Delta^{AA} X^A + \rho\Delta^{AB} X^B + \rho\Delta^{AC} X^C + \rho\Delta^{AD} X^D] &= 1 \\
 \therefore X^A [1 + \rho\Delta(X^C + X^D)] &= 1
 \end{aligned} \tag{4.27}$$

For site B:

$$\begin{aligned}
 \Delta^{AA} &= \Delta^{BB} = \Delta^{CC} = \Delta^{DD} = \Delta^{AB} = \Delta^{CD} = 0 \\
 \Delta^{AC} &= \Delta^{BC} = \Delta^{AD} = \Delta^{BD} \neq 0 \\
 X^B [1 + \rho\Delta^{AB} X^A + \rho\Delta^{BB} X^B + \rho\Delta^{BC} X^C + \rho\Delta^{BD} X^D] &= 1 \\
 \therefore X^B [1 + \rho\Delta(X^C + X^D)] &= 1
 \end{aligned} \tag{4.28}$$

Next, for site C:

$$\begin{aligned}
 \Delta^{AA} &= \Delta^{BB} = \Delta^{CC} = \Delta^{DD} = \Delta^{AB} = \Delta^{CD} = 0 \\
 \Delta^{AC} &= \Delta^{BC} = \Delta^{AD} = \Delta^{BD} \neq 0 \\
 X^C [1 + \rho\Delta^{AC} X^A + \rho\Delta^{BC} X^B + \rho\Delta^{CC} X^C + \rho\Delta^{CD} X^D] &= 1 \\
 \therefore X^C [1 + \rho\Delta(X^A + X^B)] &= 1
 \end{aligned} \tag{4.29}$$

Lastly for site D we have:

$$\begin{aligned}
\Delta^{AA} &= \Delta^{BB} = \Delta^{CC} = \Delta^{DD} = \Delta^{AB} = \Delta^{CD} = 0 \\
\Delta^{AC} &= \Delta^{BC} = \Delta^{AD} = \Delta^{BD} \neq 0 \\
X^D \left[1 + \rho\Delta^{AD} X^A + \rho\Delta^{BD} X^B + \rho\Delta^{CD} X^C + \rho\Delta^{DD} X^D \right] &= 1 \\
\therefore X^D \left[1 + \rho\Delta (X^A + X^B) \right] &= 1
\end{aligned} \tag{4.30}$$

The ratio between Eqs. (4.27) and (4.28) yields:

$$\begin{aligned}
\frac{X^A \left[1 + \rho\Delta (X^C + X^D) \right]}{X^B \left[1 + \rho\Delta (X^C + X^D) \right]} &= 1 \\
\therefore \frac{X^A}{X^B} &= 1 \\
\therefore X^A &= X^B
\end{aligned} \tag{4.31}$$

In similar fashion, we have, from the ratio of Eqs. (4.29) and (4.30):

$$\begin{aligned}
\frac{X^C \left[1 + \rho\Delta (X^A + X^B) \right]}{X^D \left[1 + \rho\Delta (X^A + X^B) \right]} &= 1 \\
\therefore \frac{X^C}{X^D} &= 1 \\
\therefore X^C &= X^D
\end{aligned} \tag{4.32}$$

Thus, we can reduce Eqs. (4.27) and (4.29) to the following form:

$$X^A \left[1 + 2\rho\Delta X^C \right] = 1 \tag{4.33}$$

$$X^C \left[1 + 2\rho\Delta X^A \right] = 1 \tag{4.34}$$

Rewriting both equations, we observe that:

$$2\rho\Delta X^A X^C = 1 - X^A \tag{4.35}$$

$$2\rho\Delta X^A X^C = 1 - X^C \tag{4.36}$$

Thus making evident that

$$\begin{aligned}
1 - X^A &= 1 - X^C \\
\therefore X^A &= X^C
\end{aligned} \tag{4.37}$$

Taking this result into Eq. (4.33) we get:

$$\begin{aligned}
X^A [1 + 2\rho\Delta X^A] &= 1 \\
\therefore 2\rho\Delta (X^A)^2 + X^A - 1 &= 0 \\
\therefore X^A &= \frac{-1 + \sqrt{1 + 8\rho\Delta}}{4\rho\Delta}
\end{aligned} \tag{4.38}$$

In more recent studies, some authors have proposed new association schemes with several different approximations: the 2C and 3A scheme, developed by De Villiers et al.¹³⁷ were developed for alcohols and monoethylamine (MEA) respectively. The 3A scheme follows the same set of approximations as presented above and the unbonded site fraction is obtained by Eq. (4.13). The 2C scheme takes one HA site and the HD site and combines them into a single binary site and it is mostly employed in alcohol mixtures with water. Abolala et al.¹³⁹ extended this scheme to glycols and glycerol, as well as proposing a 1-site scheme for esters when solvating. The 2C scheme is then a combination of the **A type** and **C type** assumptions, in which one site is bipolar and the remaining site is either HD or HA. Bonding between like sites is allowed only for bipolar sites and the association strength is equal for all bonds, i.e. $\Delta^{\text{site HA, site HA}} = \Delta^{\text{site HD, site HD}} = 0$; $\Delta^{\text{bipolar site, bipolar site}} = \Delta^{\text{bipolar site, site HA}} = \Delta^{\text{bipolar site, site HD}} = \Delta^{\text{site HA, site HD}} \neq 0$.

With these assumptions, for a 2C scheme with site A being either HA or HD and site B being, bipolar, we obtain:

Bonding	A	B
A	N	Y
B	Y	Y

For site A we have:

$$\begin{aligned}
\Delta^{AA} &= 0 \\
\Delta^{AB} &= \Delta^{BB} \neq 0 \\
X^A [1 + \rho\Delta^{AA} X^A + \rho\Delta^{AB} X^B] &= 1 \\
\therefore X^A [1 + \rho\Delta X^B] &= 1
\end{aligned} \tag{4.39}$$

For the bipolar site B:

$$\begin{aligned}
\Delta^{AA} &= 0 \\
\Delta^{AB} &= \Delta^{BB} \neq 0 \\
X^B [1 + \rho\Delta^{AB} X^A + \rho\Delta^{BB} X^B] &= 1 \\
\therefore X^B [1 + \rho\Delta (X^A + X^B)] &= 1
\end{aligned} \tag{4.40}$$

Equating Eqs. (4.39) and (4.40) we obtain:

$$\begin{aligned}
X^A [1 + \rho\Delta X^B] &= X^B [1 + \rho\Delta X^A + \rho\Delta X^B] \\
\therefore X^A + \rho\Delta X^A X^B &= X^B + \rho\Delta X^A X^B + \rho\Delta (X^B)^2 \\
\therefore X^A &= X^B + \rho\Delta (X^B)^2 \\
\therefore \frac{X^A}{X^B} &= 1 + \rho\Delta X^B
\end{aligned} \tag{4.41}$$

Replacing Eq. (4.41) into Eq. (4.39) we get:

$$\begin{aligned}
X^A \frac{X^A}{X^B} &= 1 \\
\therefore (X^A)^2 &= X^B
\end{aligned} \tag{4.42}$$

Using this result we now find the unbonded site fraction through Eq. (4.39):

$$\begin{aligned}
X^A [1 + \rho\Delta (X^A)^2] &= 1 \\
\therefore \rho\Delta (X^A)^3 + X^A - 1 &= 0 \\
\therefore X^A &= \frac{12^{1/3} \left[\left(9 + (\rho\Delta)^2 \sqrt{\frac{3(4 + 27\rho\Delta)}{\rho\Delta}} \right)^{2/3} - 12^{1/3} \rho\Delta \right]}{6\rho\Delta \left(9 + (\rho\Delta)^2 \sqrt{\frac{3(4 + 27\rho\Delta)}{\rho\Delta}} \right)^{1/3}}
\end{aligned} \tag{4.43}$$

Kruger et al.¹³⁸ proposed three new association schemes for glycols: the 3C scheme where both HA and HD sites of one side of the glycol are combined into a binary site; the 4E scheme where the HA sites and the HD sites on one side of the glycol are combined into two binary sites and the 4F scheme where both sides of the glycol have a binary site and an HA site.

The 3C scheme is a natural extension of the 2C scheme, meaning that it follows the same assumptions, with the difference that the molecule has a bipolar site as well as a HD and an HA site. For these assumptions taken for a 3C scheme, with Site A being HD, site B being HA and site C being a bipolar site, we obtain:

Bonding	A	B	C
A	N	Y	Y
B	Y	N	Y
C	Y	Y	Y

For site A we obtain:

$$\begin{aligned}
\Delta^{AA} &= \Delta^{BB} = 0 \\
\Delta^{AB} &= \Delta^{AC} = \Delta^{BC} = \Delta^{CC} \neq 0 \\
X^A [1 + \rho\Delta^{AA} X^A + \rho\Delta^{AB} X^B + \rho\Delta^{AC} X^C] &= 1 \\
\therefore X^A [1 + \rho\Delta(X^B + X^C)] &= 1
\end{aligned} \tag{4.44}$$

Similarly, for site B:

$$\begin{aligned}
\Delta^{AA} &= \Delta^{BB} = 0 \\
\Delta^{AB} &= \Delta^{AC} = \Delta^{BC} = \Delta^{CC} \neq 0 \\
X^B [1 + \rho\Delta^{AB} X^A + \rho\Delta^{BB} X^B + \rho\Delta^{BC} X^C] &= 1 \\
\therefore X^B [1 + \rho\Delta(X^A + X^C)] &= 1
\end{aligned} \tag{4.45}$$

Finally, for bipolar site C:

$$\begin{aligned}
\Delta^{AA} &= \Delta^{BB} = 0 \\
\Delta^{AB} &= \Delta^{AC} = \Delta^{BC} = \Delta^{CC} \neq 0 \\
X^C [1 + \rho\Delta^{AC} X^A + \rho\Delta^{BC} X^B + \rho\Delta^{CC} X^C] &= 1 \\
\therefore X^C [1 + \rho\Delta(X^A + X^B + X^C)] &= 1
\end{aligned} \tag{4.46}$$

Equating Eqs. (4.44) and (4.45) we obtain:

$$\begin{aligned}
X^A [1 + \rho\Delta(X^B + X^C)] &= X^B [1 + \rho\Delta(X^A + X^B)] \\
\therefore X^A + \rho\Delta X^A X^B + \rho\Delta X^A X^C &= X^B + \rho\Delta X^A X^B + \rho\Delta X^B X^C \\
\therefore X^A [1 + \rho\Delta X^C] &= X^B [1 + \rho\Delta X^C] \\
\therefore X^A &= X^B
\end{aligned} \tag{4.47}$$

At the same time, we find that we can rewrite Eq. (4.45) so that:

$$\begin{aligned}
X^B [1 + \rho\Delta(X^B + X^C)] &= 1 \\
\therefore 1 + \rho\Delta X^B + \rho\Delta X^C &= \frac{1}{X^B}
\end{aligned} \tag{4.48}$$

Rewriting Eq. (4.46) yields:

$$\begin{aligned}
X^C [1 + \rho\Delta X^A + \rho\Delta X^B + \rho\Delta X^C] &= 1 \\
\therefore X^C [\rho\Delta X^A + 1 + \rho\Delta X^B + \rho\Delta X^C] &= 1 \\
\therefore X^C \left[\rho\Delta X^A + \frac{1}{X^B} \right] &= 1 \\
\therefore \rho\Delta X^A + \frac{1}{X^A} &= \frac{1}{X^C} \\
\therefore \frac{1 + \rho\Delta (X^A)^2}{X^A} &= \frac{1}{X^C} \\
\therefore X^C &= \frac{X^A}{1 + \rho\Delta (X^A)^2}
\end{aligned} \tag{4.49}$$

Replacing Eq. (4.49) into Eq. (4.44) we obtain:

$$\begin{aligned}
X^A \left[1 + \rho\Delta X^A + \frac{\rho\Delta X^A}{1 + \rho\Delta (X^A)^2} \right] &= 1 \\
\therefore X^A + \rho\Delta (X^A)^2 + \frac{\rho\Delta (X^A)^2}{1 + \rho\Delta (X^A)^2} &= 1 \\
\therefore \frac{X^A + \rho\Delta (X^A)^3 + \rho\Delta (X^A)^2 + (\rho\Delta)^2 (X^A)^3 + \rho\Delta (X^A)^2}{1 + \rho\Delta (X^A)^2} &= 1 \\
\therefore \rho\Delta(1 + \rho\Delta)(X^A)^3 + 2\rho\Delta(X^A)^2 + X^A &= 1 + \rho\Delta(X^A)^2 \\
\therefore \rho\Delta(1 + \rho\Delta)(X^A)^3 + \rho\Delta(X^A)^2 + X^A - 1 &= 0
\end{aligned} \tag{4.50}$$

Solving the non-linear Eq. (4.50) yields the value of X^A for a 4E scheme.

For the 4F scheme, the assumptions needed to solve for X^A can be conceived as an extension of those made for the 2C scheme to a four-site molecule, with the special condition of having two HA sites. Therefore, for a 4F scheme in which site A is HA, site B is bipolar, site C is HA and site D is bipolar we have:

Bonding	A	B	C	D
A	N	Y	N	Y
B	Y	Y	Y	Y
C	N	Y	N	Y
D	Y	Y	Y	Y

For site A we have:

$$\begin{aligned}
\Delta^{AA} &= \Delta^{AC} = \Delta^{CC} = 0 \\
\Delta^{AB} &= \Delta^{AD} = \Delta^{BB} = \Delta^{BC} = \Delta^{BD} = \Delta^{CD} = \Delta^{DD} \neq 0 \\
X^A \left[1 + \rho\Delta^{AA} X^A + \rho\Delta^{AB} X^B + \rho\Delta^{AC} X^C + \rho\Delta^{AD} X^D \right] &= 1 \\
\therefore X^A \left[1 + \rho\Delta (X^B + X^D) \right] &= 1
\end{aligned} \tag{4.51}$$

For site B:

$$\begin{aligned}
\Delta^{AA} &= \Delta^{AC} = \Delta^{CC} = 0 \\
\Delta^{AB} &= \Delta^{AD} = \Delta^{BB} = \Delta^{BC} = \Delta^{BD} = \Delta^{CD} = \Delta^{DD} \neq 0 \\
X^B \left[1 + \rho\Delta^{AB} X^A + \rho\Delta^{BB} X^B + \rho\Delta^{BC} X^C + \rho\Delta^{BD} X^D \right] &= 1 \\
\therefore X^B \left[1 + \rho\Delta (X^A + X^C + X^D) \right] &= 1
\end{aligned} \tag{4.52}$$

For site C:

$$\begin{aligned}
\Delta^{AA} &= \Delta^{AC} = \Delta^{CC} = 0 \\
\Delta^{AB} &= \Delta^{AD} = \Delta^{BB} = \Delta^{BC} = \Delta^{BD} = \Delta^{CD} = \Delta^{DD} \neq 0 \\
X^C \left[1 + \rho\Delta^{AC} X^A + \rho\Delta^{BC} X^B + \rho\Delta^{CC} X^C + \rho\Delta^{DC} X^D \right] &= 1 \\
\therefore X^C \left[1 + \rho\Delta (X^B + X^D) \right] &= 1
\end{aligned} \tag{4.53}$$

For site D:

$$\begin{aligned}
\Delta^{AA} &= \Delta^{AC} = \Delta^{CC} = 0 \\
\Delta^{AB} &= \Delta^{AD} = \Delta^{BB} = \Delta^{BC} = \Delta^{BD} = \Delta^{CD} = \Delta^{DD} \neq 0 \\
X^D \left[1 + \rho\Delta^{AD} X^A + \rho\Delta^{BD} X^B + \rho\Delta^{CD} X^C + \rho\Delta^{DD} X^D \right] &= 1 \\
\therefore X^D \left[1 + \rho\Delta (X^A + X^B + X^C + X^D) \right] &= 1
\end{aligned} \tag{4.54}$$

From Eqs. (4.51) and (4.53) we observe immediately that:

$$\begin{aligned}
X^A \left[1 + \rho\Delta (X^B + X^D) \right] &= X^C \left[1 + \rho\Delta (X^B + X^D) \right] = 1 \\
\therefore X^A &= X^C
\end{aligned} \tag{4.55}$$

Equivalently, from Eqs. (4.52) and (4.54) we gather:

$$\begin{aligned}
X^B \left[1 + \rho\Delta (X^B + X^D + X^B + X^D) \right] &= X^D \left[1 + \rho\Delta (X^B + X^D + X^B + X^D) \right] \\
\therefore X^B &= X^D
\end{aligned} \tag{4.56}$$

Replacing Eq. (4.55) into Eq. (4.52) and Eq. (4.56) into Eq. (4.51) we get:

$$X^A \left[1 + 2\rho\Delta X^B \right] = 1 \tag{4.57}$$

$$X^B \left[1 + 2\rho\Delta X^A + 2\rho\Delta X^B \right] = 1 \tag{4.58}$$

We can rewrite Eq. (4.57) into:

$$\rho\Delta X^A = \frac{\rho\Delta}{1+2\rho\Delta X^B} \quad (4.59)$$

Introducing Eq. (4.59) into (4.58) we obtain:

$$\begin{aligned} X^B \left[1 + \frac{2\rho\Delta}{1+2\rho\Delta X^B} + 2\rho\Delta X^B \right] &= 1 \\ \therefore X^B \left[\frac{1+2\rho\Delta X^B + 2\rho\Delta + 2\rho\Delta X^B + 4(\rho\Delta)^2 (X^B)^2}{1+2\rho\Delta X^B} \right] &= 1 \\ \therefore X^B \left[1+2\rho\Delta X^B + 2\rho\Delta + 2\rho\Delta X^B + 4(\rho\Delta)^2 (X^B)^2 \right] &= 1+2\rho\Delta X^B \\ \therefore 4(\rho\Delta)^2 (X^B)^3 + 4\rho\Delta (X^B)^2 + X^B - 1 &= 0 \end{aligned} \quad (4.60)$$

Solving the non-linear equation (4.60) yields the value of X^B , which in turn, coupled with Eq. (4.59) leads to the value of X^A .

The 4E scheme can be seen as a more general case of the 4F scheme, in which the molecule possesses two bipolar sites, one HA site and one HD site. For a scheme in which A is an HA site, B is a HD site and both C and D are bipolar sites we obtain:

Bonding	A	B	C	D
A	N	Y	Y	Y
B	Y	N	Y	Y
C	Y	Y	Y	Y
D	Y	Y	Y	Y

For site A we have:

$$\begin{aligned} \Delta^{AA} = \Delta^{BB} &= 0 \\ \Delta^{AB} = \Delta^{AC} = \Delta^{AD} = \Delta^{BC} = \Delta^{BD} = \Delta^{CC} = \Delta^{CD} = \Delta^{DD} &\neq 0 \\ X^A \left[1 + \rho\Delta^{AA} X^A + \rho\Delta^{AB} X^B + \rho\Delta^{AC} X^C + \rho\Delta^{AD} X^D \right] &= 1 \\ \therefore X^A \left[1 + \rho\Delta (X^B + X^C + X^D) \right] &= 1 \end{aligned} \quad (4.61)$$

Next, for site B, we obtain:

$$\begin{aligned} \Delta^{AA} = \Delta^{BB} &= 0 \\ \Delta^{AB} = \Delta^{AC} = \Delta^{AD} = \Delta^{BC} = \Delta^{BD} = \Delta^{CC} = \Delta^{CD} = \Delta^{DD} &\neq 0 \\ X^B \left[1 + \rho\Delta^{AB} X^A + \rho\Delta^{BB} X^B + \rho\Delta^{BC} X^C + \rho\Delta^{BD} X^D \right] &= 1 \\ \therefore X^B \left[1 + \rho\Delta (X^A + X^C + X^D) \right] &= 1 \end{aligned} \quad (4.62)$$

For sites C we find that:

$$\begin{aligned}
\Delta^{AA} &= \Delta^{BB} = 0 \\
\Delta^{AB} &= \Delta^{AC} = \Delta^{AD} = \Delta^{BC} = \Delta^{BD} = \Delta^{CC} = \Delta^{CD} = \Delta^{DD} \neq 0 \\
X^C \left[1 + \rho \Delta^{AC} X^A + \rho \Delta^{BC} X^B + \rho \Delta^{CC} X^C + \rho \Delta^{CD} X^D \right] &= 1 \\
\therefore X^C \left[1 + \rho \Delta (X^A + X^B + X^C + X^D) \right] &= 1
\end{aligned} \tag{4.63}$$

Which is equivalent to site D, thus:

$$X^D \left[1 + \rho \Delta (X^A + X^B + X^C + X^D) \right] = 1 \tag{4.64}$$

From Eqs. (4.63) and (4.64) it becomes evident that $X^C = X^D$, therefore we can rewrite Eqs. (4.61)-(4.63) as:

$$X^A \left[1 + \rho \Delta X^B + 2\rho \Delta X^C \right] = 1 \tag{4.65}$$

$$X^B \left[1 + \rho \Delta X^A + 2\rho \Delta X^C \right] = 1 \tag{4.66}$$

$$X^C \left[1 + \rho \Delta X^A + \rho \Delta X^B + 2\rho \Delta X^C \right] = 1 \tag{4.67}$$

Equating Eqs. (4.65) and (4.66) we obtain:

$$\begin{aligned}
X^A \left[1 + \rho \Delta X^B + 2\rho \Delta X^C \right] &= X^B \left[1 + \rho \Delta X^A + 2\rho \Delta X^C \right] \\
\therefore X^A + \rho \Delta X^A X^B + 2\rho \Delta X^A X^C &= X^B + \rho \Delta X^A X^B + 2\rho \Delta X^B X^C \\
\therefore X^A \left[1 + 2\rho \Delta X^C \right] &= X^B \left[1 + 2\rho \Delta X^C \right] \\
\therefore X^A &= X^B
\end{aligned} \tag{4.68}$$

We take this result into Eq. (4.67) to obtain:

$$\begin{aligned}
X^C \left[1 + 2\rho \Delta X^A + 2\rho \Delta X^C \right] &= 1 \\
\therefore 1 + 2\rho \Delta X^C &= \frac{1}{X^C} - 2\rho \Delta X^A
\end{aligned} \tag{4.69}$$

Additionally, Eq. (4.65) can be rewritten to obtain:

$$1 + 2\rho \Delta X^C = \frac{1}{X^A} - \rho \Delta X^A \tag{4.70}$$

Equating both equations, we get:

$$\begin{aligned}
\frac{1}{X^C} - 2\rho\Delta X^A &= \frac{1}{X^A} - \rho\Delta X^A \\
\therefore \frac{1}{X^C} &= \frac{1}{X^A} + \rho\Delta X^A \\
\therefore X^C &= \frac{X^A}{1 + \rho\Delta(X^A)^2}
\end{aligned} \tag{4.71}$$

Using Eq. (4.71) and replacing it in Eq. (4.66) we obtain:

$$\begin{aligned}
X^B \left[1 + \rho\Delta X^A + \frac{2\rho\Delta X^A}{1 + \rho\Delta(X^A)^2} \right] &= 1 \\
\therefore X^A + \rho\Delta(X^A)^2 + \frac{2\rho\Delta(X^A)^2}{1 + \rho\Delta(X^A)^2} &= 1 \\
\therefore X^A + \rho\Delta(X^A)^3 + \rho\Delta(X^A)^2 + (\rho\Delta)^2(X^A)^4 + 2\rho\Delta(X^A)^2 &= 1 + \rho\Delta(X^A)^2 \\
\therefore (\rho\Delta)^2(X^A)^4 + \rho\Delta(X^A)^3 + 2\rho\Delta(X^A)^2 + X^A - 1 &= 0
\end{aligned} \tag{4.72}$$

Solving Eq. (4.72) yields the value of X^A for a 4E scheme.

Other schemes have been presented in the literature and although they are worth of mentioning, due to their complexity, specificity or exclusive application to mixtures they will be only referenced and the reader is directed to the original publications for further information. Janecek & Paricaud.¹⁴⁰ presented an association scheme that accounts for dimer formation in carboxylic acids, named DBD (doubly bonded dimers) scheme, for pure compounds and mixtures with hydrocarbons. This scheme has an additional adjustable parameter f_v that accounts for cyclic dimer formation. In other studies, Tan and Piri.¹⁴¹ used the 1A scheme to model nitrogen dioxide and nitrogen monoxide, while proposing an association scheme with 1 HD site and 2.5 HA sites, based on the results obtained in binary HNO₃/H₂O calculations. Dietz et al.¹⁴² proposed a 2-site scheme for deep eutectic solvents (DES) with one HD and one HA site. Cripwell et al.¹⁴³ proposed an N-scheme and a P-scheme specifically for molecules with only one site (HA and HD respectively) to account for the HB effects in cross association.

Table 4.1 presents a summary of the association schemes described above, as well as a graphical representation of them for illustration purposes.

Table 4.1. Association schemes and their structural representation. Red circles correspond to HA sites, blue circles to HD sites and black circles to binary sites.

Scheme type	Chemical species	Structural representation
1A	Acids	
	Nitriles	
	Tertiary amines	
2B	NO ₂ , NO	
	Alcohols	
	Secondary Amines	
2C	DES	
	Alcohols	
3B	Alcohols	
	Primary amines	
3A	MEA	
3C	Glycols	
4C	Water	
	Glycols	

Scheme type	Chemical species	Structural representation
4E	Glycols	
4F	Glycols	

Table 4.2 presents the approximations to the association strength (Δ) and the non-bonded site fraction (X^A) and the respective analytical expressions that can be derived from them for all the association schemes presented.

Table 4.2. Associating scheme types, associating strength approximations, unbonded monomer fraction approximations and expressions.

Scheme type	Δ approximation	X^A approximation	X^A
1A	$\Delta^{AA} \neq 0$	-	$\frac{-1 + \sqrt{1 + 4\rho\Delta^{AA}}}{2\rho\Delta^{AA}}$
2B	$\Delta^{AA} = \Delta^{BB} = 0$ $\Delta^{AB} \neq 0$	$X^A = X^B$	$\frac{-1 + \sqrt{1 + 4\rho\Delta^{AB}}}{2\rho\Delta^{AB}}$
2C	$\Delta^{BB} = 0$ $\Delta^{AA} = \Delta^{AB} \neq 0$	$X^B = \sqrt{X^A}$	$X^A = \frac{12^{1/3} \left[\left(9 + (\rho\Delta)^2 \sqrt{\frac{3(4+27\rho\Delta)}{\rho\Delta}} \right)^{2/3} - 12^{1/3} \rho\Delta \right]}{6\rho\Delta \left(9 + (\rho\Delta)^2 \sqrt{\frac{3(4+27\rho\Delta)}{\rho\Delta}} \right)^{1/3}}$
3A	$\Delta^{AA} = \Delta^{AB} = \Delta^{AC} = \Delta^{BB} = \Delta^{BC} = \Delta^{CC} \neq 0$	$X^A = X^B = X^C$	$\frac{-1 + \sqrt{1 + 12\rho\Delta^{AA}}}{6\rho\Delta^{AA}}$
3B	$\Delta^{AA} = \Delta^{BB} = \Delta^{CC} = \Delta^{AB} = 0$ $\Delta^{AC} = \Delta^{BC} \neq 0$	$X^A = X^B$ $X^C = 2X^A - 1$	$\frac{-(1 - \rho\Delta^{AC}) + \sqrt{(1 + \rho\Delta^{AC})^2 + 4\rho\Delta^{AC}}}{4\rho\Delta^{AC}}$
4B	$\Delta^{AA} = \Delta^{AB} = \Delta^{BB} = \Delta^{AC} = \Delta^{BC} = \Delta^{CC} = \Delta^{DD} = 0$ $\Delta^{AD} = \Delta^{BD} = \Delta^{CD} \neq 0$	$X^A = X^B = X^C$ $X^D = 3X^A - 2$	$\frac{-(1 - 2\rho\Delta^{AD}) + \sqrt{(1 + 2\rho\Delta^{AD})^2 + 4\rho\Delta^{AD}}}{6\rho\Delta^{AD}}$
4C	$\Delta^{AA} = \Delta^{BB} = \Delta^{CC} = \Delta^{DD} = \Delta^{AB} = \Delta^{CD} = 0$ $\Delta^{AC} = \Delta^{BC} = \Delta^{AD} = \Delta^{BD} \neq 0$	$X^A = X^B = X^C = X^D$	$\frac{-1 + \sqrt{1 + 8\rho\Delta^{AC}}}{4\rho\Delta^{AC}}$

Scheme type	Δ approximation	X^A approximation	X^A
4F	$\Delta^{AA} = \Delta^{BB} = 0$ $\Delta^{AB} = \Delta^{AC} = \Delta^{AD} = \Delta^{BC} = \Delta^{BD} = \Delta^{CC} = \Delta^{CD} = \Delta^{DD} \neq 0$	$X^A = X^B$ $X^C = X^D$ $\rho\Delta X^A = \frac{\rho\Delta}{1 + 2\rho\Delta X^B}$	$4(\rho\Delta)^2 (X^B)^3 + 4\rho\Delta (X^B)^2 + X^B - 1 = 0$
4E	$\Delta^{BB} = \Delta^{CC} = \Delta^{BC} = 0$ $\Delta^{AB} = \Delta^{AD} = \Delta^{AA} = \Delta^{AC} = \Delta^{BD} = \Delta^{CD} = \Delta^{DD} \neq 0$	$X^A = X^D$ $X^B = X^C$ $X^C = \frac{X^A}{1 + \rho\Delta (X^A)^2}$	$(\rho\Delta)^2 (X^A)^4 + \rho\Delta (X^A)^3 + 2\rho\Delta (X^A)^2 + X^A - 1 = 0$

4.2. Association Scheme Selection: literature review and trends

Association schemes have been studied in the past by many authors in order to understand which one is the most adequate for a given family of associating compounds both in terms of rigorous physical representation of the molecules and performance once selected and coupled with the EoS.

This process, however, is not standardized and it still relies heavily on both the expertise of the user/developer and the studied compounds and data available to them. This section is aimed at investigating how association schemes are selected and treated in the literature.

Although highly accepted, the association schemes from Huang and Radosz are at times not a straightforward option, meaning that one cannot always assort a molecule into one of the categories easily at first glance. This fact is even highlighted in their paper when they use the 2B scheme instead of the 3B scheme (the more rigorous one) for alcohols. They state that:

“(...) we felt that the limited experimental data used for fitting did not justify the use of the rigorous type 3B. Therefore we report results for alkanols of type 2B(...)”.

A similar approximation is done to water and ammonia; both modeled using the 3B scheme although a more rigorous 4-site scheme should be used in theory. They parametrized two of the non-associating parameters (m and ε) coupled with the associating parameters $\varepsilon^{A_i B_j}$ and $\kappa^{A_i B_j}$ by fitting them to experimental vapor pressure and liquid density data. The segment volume (and therefore the segment diameter) was held constant in all cases for associating compounds (12 in all cases, except for water, ammonia and hydrogen sulfide where it was set at 10 and carboxylic acids where it was approximated to the corresponding n-alkane). They obtained (on average) an average absolute deviation error (AAD %) of 0.65 % for vapor pressure (P^{sat} , number of data points (NP) = 170) and 0.91 % for liquid volume (v_{liq}^{sat} , equivalent to ρ_{liq}^{sat} , NP = 108) for alcohols with the 2B scheme (15 alcohols including the first 10 1-alkanols, 2 branched 1-alkanols and phenol). For primary amines (3B scheme) they obtained an AAD % of 1.4 % and 1.61 % for P^{sat} (NP = 89) and v_{liq}^{sat} (NP=77), which includes the first 7 n-alkylamines and aniline. On the other hand secondary amines (2B scheme) had an AAD % for P^{sat} equal to 1.96 % (NP = 23). No volumetric experimental data was collected for either of the compounds (dimethylamine and diethylamine). They also reported for the first 10 carboxylic acids (1A scheme) and benzoic acid an AAD % of 0.52 % for P^{sat} (NP = 88) and 0.54 % for v_{liq}^{sat} (NP = 48). Volume data from hexanoic acid to decanoic acid was not reported. Finally for ammonia (3B scheme) they reported an AAD % of 1.6 % for P^{sat} and 3.2 % for v_{liq}^{sat} (NP =10 in both cases). For water (3Bscheme) they reported 1.3 % for P^{sat} and 3.2 % for v_{liq}^{sat} (NP =13 in both cases) and for hydrogen sulfide (3B scheme) 0.69 % for P^{sat} and 1.4 % for v_{liq}^{sat} (NP =14 in both cases). The highest deviations in vapor pressure for each family were 2.1 % for alcohols (1-decanol), 2.3 % for primary amines (1-pentamine), 3.2 % for secondary amines (diethylamine), 1.6 % (ethanoic acid) and 1.6 % for the remainder three molecules (ammonia). In the case of the molar volume, they obtained (in the same order, except for secondary amines, which do not have data) 1.4 % (2-methyl-1-propanol), 2.6 % (1-

butanamine), 1.0 % (pentanoic acid) and 3.2 % (water and ammonia). The authors do not comment about the results with other schemes (i.e. for alcohols where they state that they performed the same calculations with a 3B scheme).

This selection via approximation has also been used by other authors. Gross and Sadowski on their follow-up PC-SAFT paper¹³ chose a 2B scheme for all treated molecules, which included 11 alcohols (C1-C9 1-alkanols, 2-propanol, 2-methyl-2-butanol), water, five amines (C1-C3 alkylamines, 2-propylamine and aniline) and acetic acid. They selected this scheme following the suggestions of Suresh and Elliott¹⁴⁴ who found similar performances between two-sites and higher order sites such as the 4C scheme for water. Nonetheless, Gross and Sadowski mention that water is best represented by a 4C scheme. Using the 2B scheme they obtained an AAD % for alcohols of 1.06 % for P^{sat} and 3.2 % for ρ_{liq}^{sat} (NP not specified); for amines they obtained 0.41 % and 0.74 %; for acetic acid 2.12 % and 1.36 % and for water 1.88 % and 6.83 %. The highest deviations for alcohols were obtained for methanol (2.36 % P^{sat} , 2.01 % ρ_{liq}^{sat}), while aniline had the highest vapor pressure deviation (0.79 %) and ethylamine for liquid density (1.15 %) for amines. Water had the highest deviation for the latter property with 6.83 % and methanol had the highest deviation for vapor pressure overall. It is clear that the 2B approximation is not enough to represent the complex HB occurring in compounds like water and acetic acid, where formation of cyclic dimers is present. To some extent, this approach is also not as well suited for methanol as it was the worst performing of the alcohols. The authors reach similar conclusion and they add that the PC-SAFT did not account for dipole-dipole interactions. They agree that the directional interactions have a significant impact on the behavior of these molecules, especially for water. They compared their results to those obtained by Huang and Radosz (referred to as SAFT in their paper) for pure compounds and binary mixtures. **Figure 4.1** (taken from Gross and Sadowski¹³) shows VLE for three alcohols in a T- ρ diagram and an isobaric phase diagram for a mixture of methanol and cyclohexane.

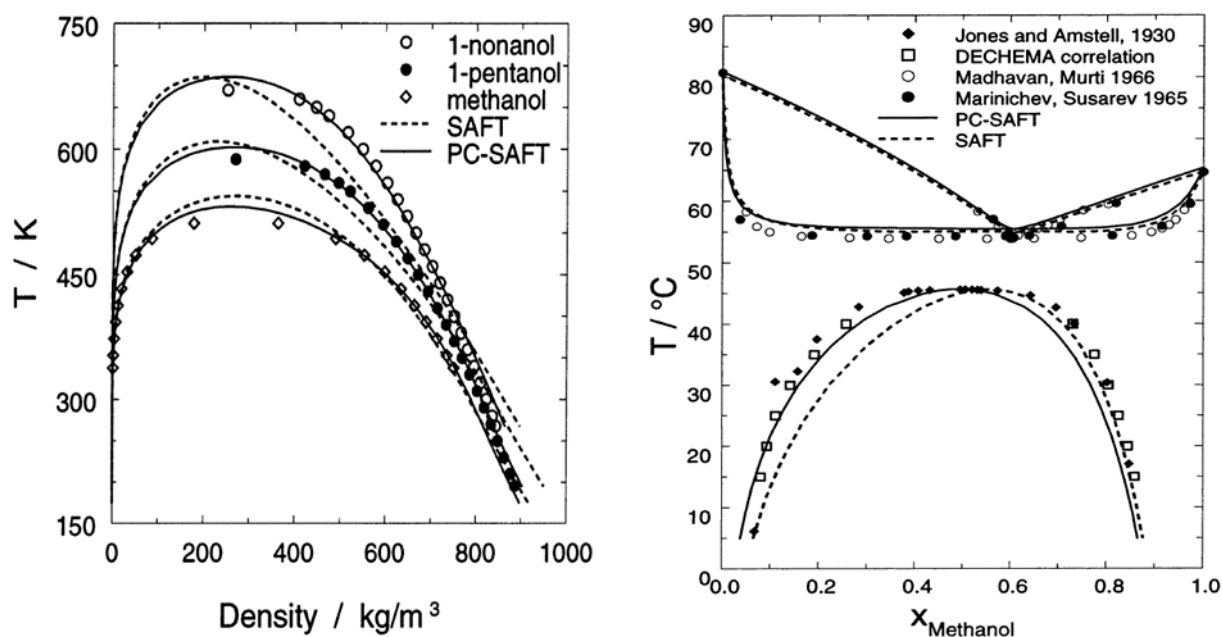


Figure 4.1. (left) Saturated liquid and vapor densities for methanol, 1-pentanol and 1-nonanol. Comparison of PC-SAFT (solid) and SAFT (dashed) to experimental data; (right) Isobaric vapor-liquid equilibrium and liquid-liquid equilibria for methanol at $P = 1.013$ bar. Comparison of experimental data to PC-SAFT ($k_{ij} = 0.051$) and SAFT ($k_{ij} = 0.044$). Taken from Gross & Sadowski¹³ DOI: 10.1021/ie010954d.

It is clear that the proposed schemes with PC-SAFT work better with the representation of pure compounds when compared to the results of Huang and Radosz' SAFT. However, it is apparent that neither is the most appropriate for methanol when contrasted to experimental data. Given that the main difference between this two versions comes from the dispersive terms one can conclude that improvements describing dispersive interactions seem to lead to better results for pure associating compounds, which agrees to the authors' findings. Looking into a binary mixture containing methanol and cyclohexane one can see that both models (both with 2B schemes) perform similarly, with higher deviations for the PC-SAFT in the LLE curve near the methanol-rich phase. It becomes apparent that although the 2B scheme selected seems to perform well, it still does not represent accurately the associating nature of methanol (which is known to be highly associating) neither in pure compounds nor in binary mixtures.

Von Solms et al.¹⁴⁵ tested different association schemes for the PC-SAFT and the cubic plus association (CPA) EoS. In particular, they tested the 2B scheme proposed for water from Gross and Sadowski¹³ to the more physically rigorous 3B and 4C schemes. A similar comparison was done for the first three 1-alkanols and 1-octanol between the 2B scheme and the 3B scheme. They parametrized the PC-SAFT by fixing the segment number and fitting the remaining four parameters to P^{sat} and ρ_{liq}^{sat} . In the particular case of water, they tested seven parameters sets, with m going from 2.0 to 3.5 in 0.25 increments. They tested the ability of these parameters to predict unbonded fraction (X^{A_i}) data obtained from spectroscopy, as a way to assess the parametrization of a scheme. They justified this by observing that all seven parameters sets provided better results than the ones obtained with the 2B parameter set obtained from Gross and Sadowski. Furthermore, they stated,

“Using density and vapor pressure data alone cannot help in choosing association schemes”.

They used the accuracy in reproducing X^A data as a way to validate the parameter set. This does not guarantee that the best VLE set corresponds to the best X^A set, nor that including this type of data in the fitting process may result in a parameter although they stated that this might be the case. Using this information, they reached the conclusion that the 4C scheme for water is better than the 2B scheme, with an AAD % on vapor pressure of 0.58 % on average for the seven water sets and 1.23 % for liquid density, versus the 1.88 % and 6.83 % reported by Gross and Sadowski's 2B scheme. **Figure 4.2** (taken from von Solms et al.¹⁴⁵) presents a comparison of the monomer fraction (product of all unbonded fractions) between the 4C scheme calculated at $m = 2$ and $m = 3.5$ (first and last value for segment numbers) the 2B scheme and experimental data from Luck¹⁴⁶. The authors included CPA with 3B and 4C schemes to assess the EoS as well.

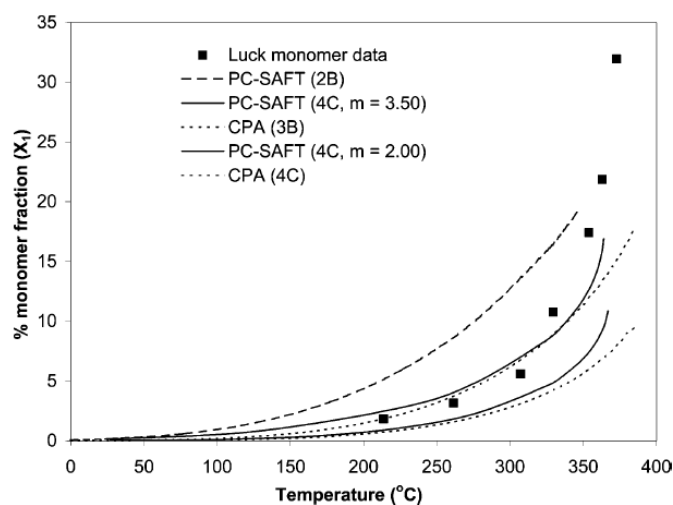


Figure 4.2. Comparison of the predictions of various models and schemes for the monomer fraction of pure water. Taken from von Solms et al.¹⁴⁵ DOI: 10.1021/ie051341u.

Figure 4.2 shows that the PC-SAFT with a 2B scheme (dashed line) over predicts the monomer fraction. The 4C scheme with 3.5 segments (upper solid line) perform the best, alongside with CPA with a 3B scheme (upper dotted line). The other two models under predict the monomer fraction across the temperature range. The above illustration highlighted the difficulty of using just VLE data to both select the appropriate association scheme and parametrize the pure compound parameters, however they conclude that the 4C scheme is best suited for the PC-SAFT EoS.

They ran a similar test for the studied alcohols and found that a 3B scheme is best suited for methanol, as it is more highly associating than heavier alcohols for which a 2B scheme seems to be enough. They state,

“There is a volume dilution effect of the increasingly larger non-associating groups, meaning that the concentration of associating sites on larger alcohols is lower.”

The authors also claim that an additional guide to test association scheme for a compound is to study the results obtained when dealing with mixtures, using VLE or LLE data as an assessment tool (without including it into the parameter fitting) as suggested by Kontogeorgis et al.¹⁴⁷. Clark et al.¹⁴⁸ reached a similar conclusion saying,

“(…) one cannot discriminate between these (association schemes) with the usual technique of regressing the parameters to vapor pressure and saturated liquid density data”.

They do, however, agree that water is best represented by a 4C scheme and methanol a 3B scheme. They go further with the associating scheme for water showing that it is best suited for mixtures with hydrocarbons and in general conclude that using VLE data of mixtures can be of great aid when working with associating compounds.

Ferrando et al.⁸⁷ proposed a method to select association schemes both qualitatively and quantitatively from Monte Carlo simulations. The first one is to obtain information about the distribution of HB in a molecule and to determine which configuration of HB per molecule are significant. They tested this on methanol and their results are shown in Figure 3 (taken from Ferrando et al.⁸⁷).

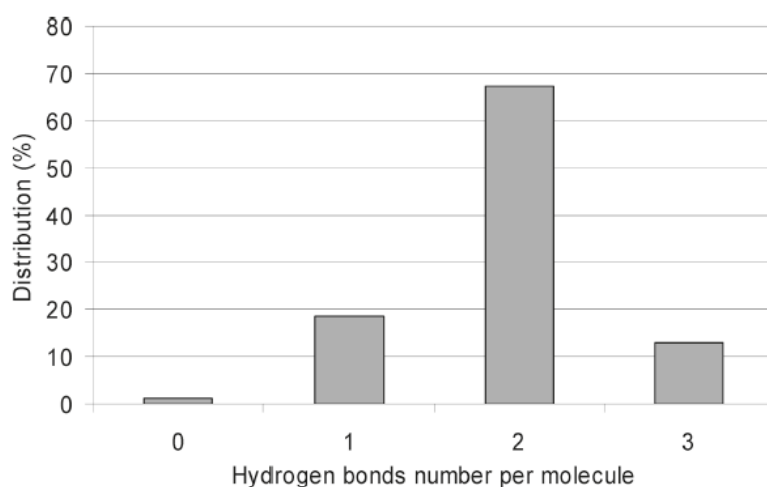


Figure 4.3. Distribution of HB number per molecule of methanol at 300K. Taken from Ferrando et al.⁸⁷ DOI: 10.1021/jp209313a.

They highlighted that most of the molecules are involved at maximum in two HB. However, this figure shows that there is an unneglectable portion of molecules that participate in three HB. For this reason, they consider that the number of sites to be considered for methanol should preferentially be three (3B scheme).

Their quantitative approach relates the monomer fraction and the free hydrogen fraction, X^H . They consider the monomer fraction (similar to the mentioned before) as

$$X^m = \prod_{i=1}^N X^{A_i} \quad (4.73)$$

Taking the 3B and 2B schemes discussed by the authors, equation (4.73) becomes, respectively:

$$X^m = X^{O_1} X^{O_2} X^H \quad (4.74)$$

$$X^m = X^O X^H \quad (4.75)$$

If one assumes that both oxygen sites have an equal probability of forming an HB they can be related in the form of:

$$X^m = (X^H)^2 \quad (4.76)$$

Additionally, for every H site involved in a HB an O site in the system is also bonded. Performing a material balance over the number of sites for both schemes one obtains:

$$1 - X^H = 2(1 - X^{O_1}) \quad (4.77)$$

$$1 - X^H = 1 - X^O \quad (4.78)$$

Equation (4.77) corresponds to the 3B scheme and equation (4.78) to the 2B scheme. Using both of them, equations (4.79) and (4.80) can be written in terms of free hydrogen fractions:

$$X^m = \frac{(X^H + 1)^2 X^H}{4} \quad (4.79)$$

$$X^m = (X^H)^2 \quad (4.80)$$

Equation (4.79) corresponds to the 3B scheme and equation (4.80) to the 2B scheme. The authors used these equations to compare against Monte Carlo simulation monomer fraction data of the first eight 1-alkanol and understand which scheme provides the best reproduction of said data. Figure 4 (taken from Ferrando et al⁸⁷) shows the results obtained by the authors

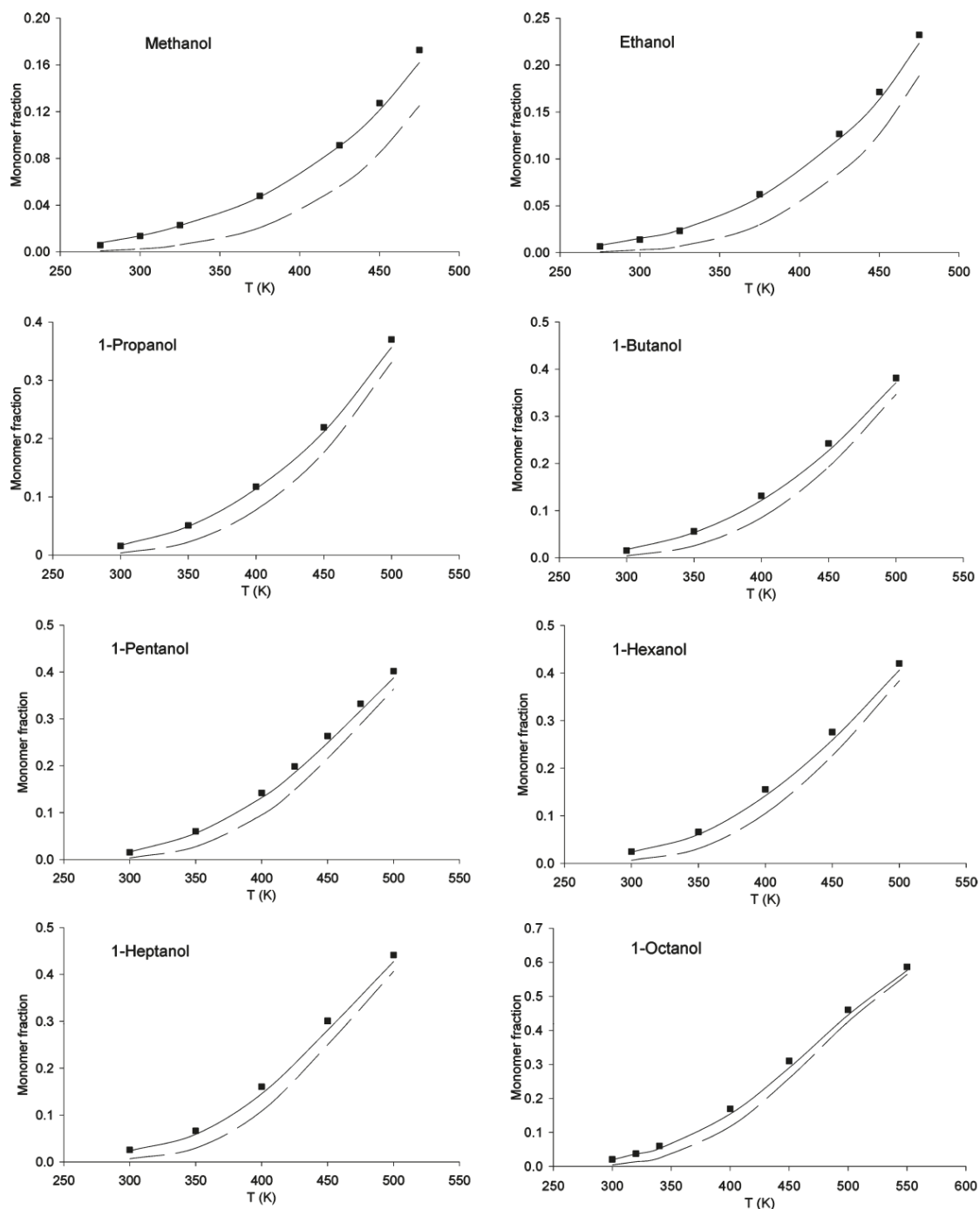


Figure 4.4. Monomer fraction for the first eight 1-alkanols from Monte Carlo simulations (square symbols), the 3B scheme (solid lines) and 2B scheme (dashed lines). Taken from Ferrando et al⁸⁷ DOI: 10.1021/jp209313a.

From these results, the authors conclude that the 3B scheme is best suited for alcohols. The authors limit this study to alcohols and further application of this methodology to other association schemes is not presented.

Authors also choose association schemes for non-self-associating compounds that might form HB when in mixtures. Mac Dowell et al.¹⁴⁹ treat CO₂ as a non-associating pure compound, but when in mixture with MEA they add 2 HA sites to account for cross-association. In a similar

fashion, Cripwell et al.¹⁴³ use the N and P scheme for HA and HD molecules to account only for solvation in mixtures. Some authors use different schemes even for self-associating compounds as it may enhance binary calculations as shown for water by Haarman et al.¹⁵⁰ where the 2B scheme seemed to work better for mixtures. It should be noted that mixtures with only one associating substance do not require mixing rules for the associating term⁶⁰, a point also highlighted by Kontogeorgis et al.¹⁴⁷, when explaining that adding binary interaction parameters to associating compounds in mixtures did not improve significantly results obtained by SAFT EoS.

In spite of evidence in efforts of having a selection methodology for associating schemes, the comparison of an association scheme's performance against VLE parametrization results is still the guide used in many studies, in spite of several authors^{145,147,149} advising against this, as VLE data alone does not provide enough information on the correct selection on association schemes.

To highlight this, figure 5 shows the AAD % for vapor pressure of methanol for several of the mentioned authors as well as the association scheme employed

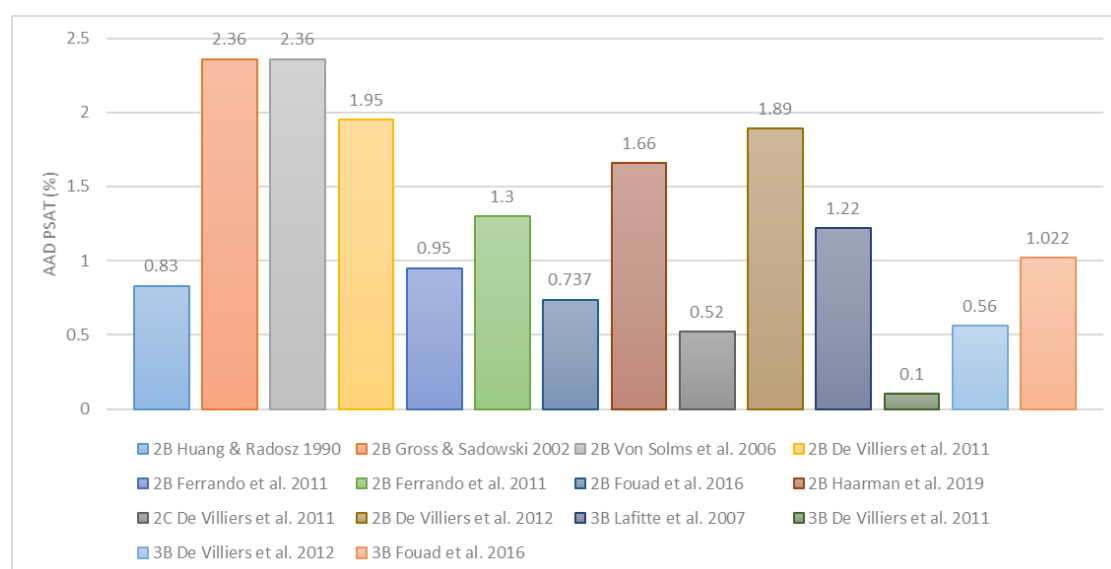


Figure 4.5. AAD (%) for P^{sat} of Methanol for various association schemes as reported by several authors.

It is evident that choosing based solely on this information is difficult. One may choose a 3B scheme knowing beforehand the physical nature of methanol (empirically or through experimental data) but even then the results seem to be scattered. Furthermore one can argue that not every time a better result is obtained with a 3B scheme, as seen with the result from Fouad et al.¹⁵¹, when compared to the less rigorous 2B or 2C schemes used by Huang and Radosz⁴⁵ and De Villiers¹³⁷ et al. respectively. The only two results that seem truly consistent amongst themselves are the ones obtained by Gross and Sadowski¹³ and von Solms et al.¹⁴⁵, both using a 2B scheme. Although experimental information such as monomer data from spectroscopy, Monte Carlo simulation and quantum chemical data^{152,153} strongly suggest that Methanol should be modeled as a 3B molecule (the same could be said about water with a 4C scheme). This example highlights that it is not a straightforward answer, and much ground needs to be covered on the appropriate selection of associating schemes.

4.3. Parametrization of SAFT EoS for associating compounds: literature review and trends

In the previous section, we presented a review on the common decisions used in research for using association schemes. We observed that it is in fact very reliant on the user's expertise to select an association scheme and that results may not always tell the complete story when it comes to selecting them.

Another issue that arises from this is the impact on the parametrization of the SAFT or CPA model: the selection of the association scheme changes the shape of the expression for non-bonded site fraction and thus changes the model to be optimized for fitting parameters. This has led to different parametrization strategies to obtain ε^{AB} and κ^{AB} , which will be the object of this section. The amount of strategies alongside standardization issues such as the number of data points or the domains of said points (temperature or pressure ranges) tie in with the discrepancies presented in **Figure 4.5** of the previous section.

Different authors have approached this issue with different strategies. The most straightforward one is to fit all five parameters to vapor pressure and liquid density data as done by Gross and Sadowski¹³, Llovel and Vega¹⁵⁴, and Tan et al.¹⁴¹ for their studied molecules. As mentioned before the oversimplification of scheme 2B for water in Gross and Sadowski's work led to higher deviations in both target properties when contrasted to the other compounds. Llovel and Vega showed accurate results, although no explicit mention of the scheme used, they mention that the hydroxyl group is modeled by two square-well sites following Pamiès¹⁵⁵, which makes it equivalent to the 2B association site although for a LJ fluid. Tan & Piri¹⁴¹ obtained good results for pure nitrogen oxides and nitric acid, with the latter having the highest AAD % for vapor pressure of 1.23 %. The latter team suggested that the number of association sites could be treated as a fitting parameter granted the knowledge of molecular structures.

A second common approach is to fit all five SAFT parameters to VLE data and an experimental new property. Lafitte et al.⁶⁹, Kontogeorgis et al.¹⁵⁶ and De Villiers et al.¹⁰³ included enthalpy of vaporization ($\Delta_{vap}H$) as a third target property. Lafitte et al. justified this inclusion saying

“($\Delta_{vap}H$) has been found in this case to be of interest to ensure that the association parameters have sound physical meaning and good predictive capability”.

They fitted the associating parameters to the enthalpy of vaporization and used the isobaric heat capacity (C_p) as a reference to assess the parametrization stating,

“This property is mainly governed by the association capability and molecular size”

Adding that this property is mostly governed by the ideal and associative term of the SAFT EoS (SATF-VR in their case). They found high accuracy for the treated 1-alkanols regardless of the scheme and model. It is worth noting that methanol had AAD % for $\Delta_{vap}H$ above 4.5 % in all their studied cases. Kontogeorgis et al.¹⁵⁶ used the enthalpy of vaporization data to study the capabilities of the model (CPA and simplified PC-SAFT) to predict accurately monomer fraction data. They found out that VLE data alone underestimates the latter, and the inclusion of the third property does not show notable improvements. They performed another test where

they included the monomer fraction data as a target property for water but saw little improvement on the VLE calculations. They also found that the 2B and 3B schemes had little differences with their parametrization routine. De Villiers et al.¹⁰³ on the other hand reached the conclusion that PC-SAFT works best for alcohols using the 3B scheme with their parametrization routine including enthalpy of vaporization and weighting their objective function to give higher priority to vapor pressure and liquid density. Other authors have included different properties to their O.F to better estimate ε^{A,B_j} and κ^{A,B_j} : Fouad et al.¹⁵¹ used activity coefficient data to fit non-associating parameters (σ and ε) to minimize the contributions of associating and polar interactions while Oliveira et al.⁸⁶ added C_p data as it offered better results for associating compounds (in particular alcohols heavier than ethanol and water) both in VLE properties as well as in second derivative properties. Ribeiro et al.¹⁵⁷ tested coupling VLE data with several properties such as enthalpy of vaporization, isobaric heat capacity, compressibility factor, speed of sound and second virial coefficient to observe the performance of CPA and sPC-SAFT in calculating them for acetic acid. They found out that VLE data was well calculated with both the 1A and 2B scheme, with the latter being slightly better. Nonetheless, the 1A scheme provided better results overall for the remainder of the properties. Kruger et al.¹³⁸ studied the sensitivity of the CPA parameters including the associating ones for the 3C, 4C, 4E and 4F schemes for MEG and its mixtures with hydrocarbons and water for gas-hydration applications. They used a weighted relative squared error function in which higher importance is given to large data sets such as vapor pressure data, but also increasing the weight of individual points for small data sets, including LLE data used for mixtures. They found out that the 3C scheme provided the best results for pure MEG and liquid phase MEG-water systems, when including vapor pressure, liquid density and LLE data.

Their sensitivity analysis for pure MEG with the 4C scheme with literature parameters showed that the association energy has a major impact on the prediction of vapor pressure and the covolume parameter has the biggest influence on the liquid density. Meanwhile, the association volume show little impact in both the vapor pressure and liquid density, as shown in **Figure 4.6**

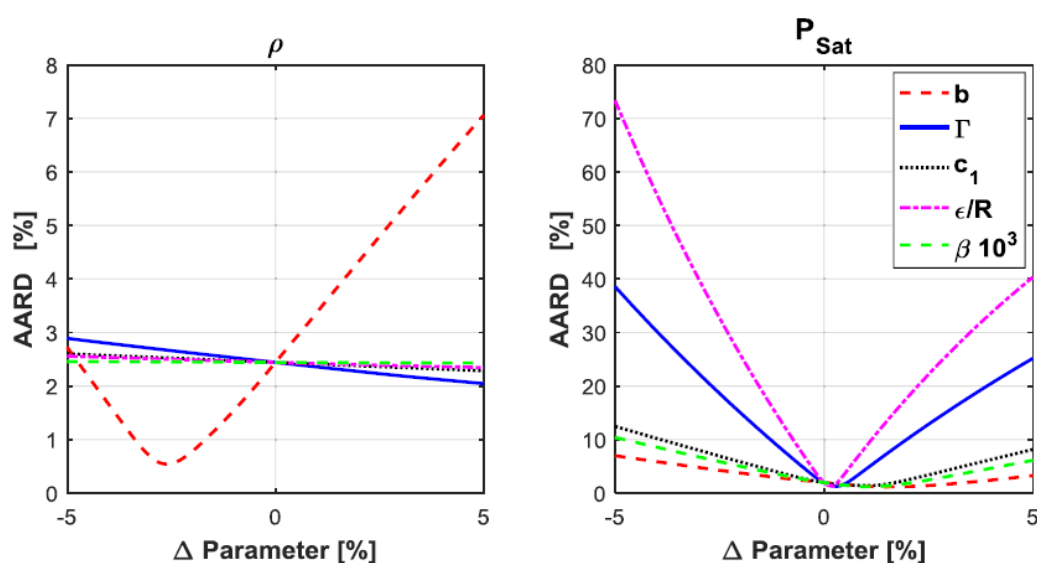


Figure 4.6. Single parameter sensitivity analysis for pure MEG density and vapor pressure using the 4C scheme. Taken from Kruger et al.¹³⁸ DOI: 10.1016/j.fluid.2017.11.026.

The authors also conclude that their 4E and 4F schemes perform similar but state that the 4F scheme with binary interaction parameters fitted to vapor-phase data provided the best results for ternary MEG-H₂O-CH₄ systems and liquid phase MEG-Hexane systems.

Liang et al.^{72,73} included speed of sound data (u) in addition to vapor pressure and liquid density in their parametrization routine. They proposed two approaches to include this data:

- Using speed of sound data in the parameter regression.
- Using speed of sound data in the universal constant regression of the PC-SAFT EoS (see Eqs. (1.63) and (1.64) from **Chapter 1**) and then in the parameter regression.

They used these approaches to estimate the five parameters for 1-alkanols⁷³ and observed that the second approach yielded the best results for speed of sound predictions, but sacrificed accuracy on vapor pressure. The first approach showed the same performance than not including speed of sound in the regression for P^{sat} , but had slightly higher deviations on ρ_{liq}^{sat} . For u the performance is improved, but it still worse than the one shown by the second approach.

Finally, one of the most common practices for parametrization of associating species is to fix one of the parameters to lower the computational burden. Fixing the segment number is one of the most common practices among literature^{45,140,145,149,151,158,159}, mostly approximating small molecules to low segment numbers (water, CO₂, methanol, etc.). Although in most of these cases the gain of computational performance is the objective, it is also apparent that letting m to vary leads to better estimations of VLE. The second common practice of this nature is to fix the association parameters and to fit the remaining parameters. Grenner et al.¹⁶⁰ fitted the five pure-component parameters for vapor pressure and liquid density for eight 1-alkanols. They took the geometric mean of $\varepsilon^{A_i B_j}$ and $\kappa^{A_i B_j}$ and assumed it as constant for all the alcohols employed after comparing these values to literature. Llovell and Vega¹⁵⁴ fitted the five parameters for methanol and ethanol and assumed $\varepsilon^{A_i B_j}$ constant from 1-propanol onwards and $\kappa^{A_i B_j}$ from ethanol onwards. Belkadi et al.¹⁶¹ used a similar treatment for nitriles from C1 to C3 and then fixed both associating parameters for all subsequent nitriles. Yushu et al.¹⁶² set the associating parameters of acetic acid as constants while fitting the rest of the parameters for heavier acids to vapor pressure. Fuenzalida et al.⁸⁸ fixed the value of $\kappa^{A_i B_j}$ for alcohols and n-alkylamines after performing a sensitivity test for all parameters of the PC-SAFT EoS. Dietz et al.¹⁴² used density data to fit the non-associating parameters for several DES, while using suggested values from literature for the associating parameters. Cripwell et al.¹⁴³ proposed to fit all five parameters for methanol, ethanol, isopropanol and 1-butanol and then extend their associating parameters to esters.

In conclusion, associating scheme selection is far from being trivial and it has a deep impact in the accuracy of the model, the physical soundness of it and the performance required to execute the calculations. Selection based only on VLE deviations is risky as not much information is provided. Introducing additional data such as monomer fraction data or adding properties may help into selecting the appropriate scheme, but cannot avoid raising questions, such as which properties are more closely linked to the associating parameters and therefore to the associating scheme? Should they be included into the parametrization routine or are they best left as a reference such as LLE data? Is there a physical giveaway of the associating scheme aside from

complex and scarce data such as monomer fraction data, spectroscopic, NMR or Monte Carlo data? Must all five parameters be estimated at the same time or should one first obtain the non-associating set and then the associating one? Why do some associating schemes perform badly when in pure components but better when in mixtures (such as the 2B for water)?

**Chapter 5 : On the effect of the associating term on
the performance of the PC-SAFT EOS**

5.1.Introduction

The Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT) equation of state (EoS) proposed by Gross & Sadowski^{12,13} is acknowledged as one of the most popular thermodynamic models due to its capacity to reproduce phase equilibria for pure compounds and binary mixtures, especially those including associating compounds. These chemical species are often deemed as more complex than non-associating compounds (e.g. n-alkanes) due to their strong and directional intermolecular forces, in particular the hydrogen bond (HB). It is in fact the existence of a term within the SAFT framework, which specifically accounts for these interactions, that makes this family of EoS an appealing choice to both developers, researchers and process engineers.

However, the addition of this associating term is followed by a compromise in computational speed and time, as the associating term introduces additional adjustable parameters to the model and, depending on the approximations to the association scheme⁴⁵, additional mathematical complexity to both pure compound and mixture calculations, an issue that is not often discussed by researchers and developers. Furthermore, the question of how much does the associating term improve predictions done by the PC-SAFT for associating compounds is not addressed in the open literature. Nonetheless, some authors have raised observations that can open the discussion towards answering these questions for non-associating EoS in general, such as Postnikov et al.⁷⁰, which used the CP-PC-SAFT¹⁷ to estimate pure compound properties for 1-alkanols, whom noticed that vapor pressure predictions improved in function of the molecular weight (inversely to the associating strength), suggesting that the effects of HB seem to dilute with the carbon chain, making the model perform better. It should be noted that they did not take into account an associating term, therefore hinting that the PC-SAFT model may be robust enough without an associating term. It should be noted that the CP-PC-SAFT estimates the non-associating pure-component parameters (m , σ and ε/k_B) by reproducing the critical point and the triple point density.

Pina-Martinez et al.¹²⁷ tested the accuracy of cubic equations of state (CEoS) to reproduce vapor pressure (P^{sat}), liquid density at saturation (ρ_{liq}^{sat}), vaporization enthalpy ($\Delta_{vap}H$) and liquid heat capacities at saturation ($c_{P,liq}^{sat}$), as well as the critical pressure (P_c), temperature (T_c) and molar volume (v_c), for 1800 compounds, including 548 self-associating (SA) pure compounds. They used the original Peng-Robinson (PR)³⁴ and Soave-Redlich-Kwong (SRK)³³ EoS, as well as a translated and consistent version of each of these EoS (tc -PR and tc -RK respectively), as proposed by Le Guennec et al.³². They showed that well over 50% of the SA compounds treated were modeled satisfactorily, with the tc -RK having up to 70% of pure SA compounds well-modeled. This highlights the capabilities of non-associating EoS in reproducing complex species such as SA compounds. It should be noted that they obtained the pure component parameters for the translated and consistent EoS (L , M , N) by fitting them to at least vapor pressure data, as suggested on a preceding work⁹⁶.

In a similar spirit, Ramirez-Velez et al.¹⁶³ compared the performance of the PC-SAFT and the industrialized-PC-SAFT (I-PC-SAFT) proposed by Moine et al.¹⁸ and contrasted their

performance against the same database used by Pina Martinez et al.¹²⁷ For the PC-SAFT, they used a non-associating version with a special focus in the parameter estimation routine. They utilized a weighted objective function (OF) which was selected after extensive property combination testing over 1252 non-associating compounds. Their final OF used vapor pressure and liquid-density data to fit the PC-SAFT parameters. They used this to calculate the same target properties (vapor pressure, liquid density, enthalpy of vaporization, liquid heat capacity, critical temperature, critical pressure and critical molar volume) and derived a strict criteria to categorize well-modeled (WM) badly-modeled compounds (BM). They contrasted the performance of the non-associating PC-SAFT when reproducing these properties for SA compounds and gave each compound a WM or BM classification according to their proposed criteria. More details about the parameter estimation method, as well as the WM/BM criteria can be found in their original publications^{95,163} and in **Chapter 3**.

Their study showed that the PC-SAFT EoS with their parametrization routine is able to predict 56.8% of the SA compounds accurately, with a global average deviation for SA compounds of 2.8%. Regarding the two main properties (included in the OF), vapor pressure had an average deviation of 1.66% and the liquid density had a deviation of 1.19% for the PC-SAFT EoS. Likewise, for the I-PC-SAFT EoS, they found that 68% of the SA compounds were correctly predicted by the model, with a global average deviation of 4.5%. For the vapor pressure an average deviation of 2.65% was obtained and 5.2% average deviation was found for the liquid density. This comes to show that the PC-SAFT framework may be robust enough to be able to accurately predict pure self-associating compounds.

However, although these results are indeed promising, they are not sufficient to yield the conclusion that the associating term can be neglected for SA compounds. In fact, the authors showed in the same study that there was no clear relation between the association energy (represented by the hydrogen bonding enthalpy $-\Delta_{HB}H$) and the quality of the predictions done by the model. This means, that there was no evident trend between how much a molecule tends to form self-associated complexes and how well predicted the target properties are with respect to their used data, especially for the two key properties: vapor pressure and liquid density. Thus, further explorations must be done with the PC-SAFT EoS and its associating term in order to truly assess the need of including it in the model.

The aim of this work is to study well-known self-associating families of compounds included in the database proposed by Ramirez-Velez et al.¹⁶³ to assess the impact of including an associating term. Furthermore, the optimal parameter space will be explored to investigate whether the associating parameters need to be fitted for each pure component or if a general set of associating parameters is enough for a given SA family.

5.2. Methodology

5.2.1. Chemical family and compound selection

Due to the heterogenic behavior between the performance of the PC-SAFT EoS and the association energy of the 548 SA compounds found in the database proposed by Ramirez-Velez et al.¹⁶³, investigating the entire SA compound set may lead to erroneous conclusions.

In other words, in spite of all 548 compounds showing self-association due to HB, the associating energy for hydrogen bond formation $\Delta_{HB}H$ can change dramatically between one chemical family and other. For example, for ethanol we have $-\Delta_{HB}H = 14.7 \text{ kJ/mol}$ while ethylamine has a value of $-\Delta_{HB}H = 4.5 \text{ kJ/mol}$. We see that their HB energies are rather different, with ethanol being higher, in spite of having structures differentiated by the functional group. Both compounds exhibit, however, self-association. It was also observed that compounds of an homologous series from a same chemical family (e.g. n-alcohols, n-aliphatic acids, etc.) share a similar HB enthalpy e.g. n-alcohols and n-aliphatic acids have a $-\Delta_{HB}H \approx 14 \text{ kJ/mol}$, while n-aliphatic primary amines have a value of $\Delta_{HB}H \approx 4 \text{ kJ/mol}$ or formats (esters of formic acid) which have a $-\Delta_{HB}H \approx 0.18 \text{ kJ/mol}$. This observation gives us a first selection criterion, in which each compound set to be studied will include members of the same homologous series of the same chemical family. With this in mind, it was decided to study the Alcohol family which are well-known self-associating compounds with high energies of association.

As a second selection criterion, we aim to understand the effect of the associating term on SA compounds. This means, in this context, that we wish to observe if activating the associating term for the PC-SAFT EoS changes the quality of its predictions and ultimately changes the WM/BM classification for the studied compounds (whether it goes from BM to WM, from BM to WM or it remains unchanged). With this in mind it is decided to make the set as homogenous as possible regarding the HB enthalpy. Thus 11 members of the linear series for the n-alcohols are included (from ethanol to 1-dodecanol). Methanol is not included as it usually behaves as an outlier, meaning that its properties tend to stray away from the trend shared by heavier linear alcohols. A second reason is to follow their WM/BM classification after calculating their properties with an associating PC-SAFT EoS and compare them to the previous results¹⁶³ without it. The selected alcohols are all classified as BM, which will allow for initial perspectives for this classification. **Table 5.1** show the list of selected compounds, their non-associating parameters and the mean average percent error (MAPE) for each of the four target properties (P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$) and their modeling classification.

Table 5.1. List of selected **n-alcohols** with their PC-SAFT non-associating parameters and MAPE on vapor pressure, liquid density, enthalpy of vaporization and liquid heat capacity and their modeling classification. WM means well-modeled and BM means badly-modeled.

Compound name	PC-SAFT non-associating parameters					MAPE* (%) on			Modeling Classification
	CAS	m	σ	ε/k_B	P^{sat}	ρ_{liq}^{sat}	$\Delta_{vap}H$	$c_{P,liq}^{sat}$	
ETHANOL	64-17-5	5.8651	2.3092	187.7	1.18	2.54	5.14	46.68	BM
1-PROPANOL	71-23-8	6.0994	2.4830	191.4	3.06	2.91	2.58	33.72	BM
1-BUTANOL	71-36-3	5.9827	2.6867	201.4	4.23	2.07	3.56	18.44	BM
1-PENTANOL	71-41-0	5.7447	2.8915	213.6	3.62	1.90	4.45	11.58	BM
1-HEXANOL	111-27-3	5.6799	3.0511	223.0	4.63	1.85		10.89	BM
1-HEPTANOL	111-70-6	5.7031	3.2161	230.1	5.26	0.63		10.40	BM
1-OCTANOL	111-87-5	5.7253	3.3260	237.7	4.57	0.42	7.49	10.93	BM
1-NONANOL	143-08-8	5.6314	3.4621	247.5	4.02	0.95		14.82	BM
1-DECANOL	112-30-1	5.7798	3.5603	251.7	3.61	0.48		12.27	BM
1-UNDECANOL	112-42-5	5.5399	3.7354	263.8	2.58	0.68		13.73	BM
1-DODECANOL	112-53-8	5.7898	3.7840	265.6	2.48	0.29		12.59	BM

$$* MAPE_X = \frac{100}{N_T} \sum_{i=1}^{N_T} \left| \frac{X_{j,\text{exp}}(T_i) - X_{j,\text{calc}}(T_i)}{X_{j,\text{exp}}(T_i)} \right| \text{ where } X \in \{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, c_{P,liq}^{sat}\}$$

5.2.2. Parametrization of the PC-SAFT EoS

The PC-SAFT EoS without association was presented previously by Gross & Sadowski¹² and the reader is referred to the original publication for further details of the model. In here we include the associating term, originally proposed by Chapman et al.^{6,7} which is the one used across all SAFT variants. We recall that the associating contribution to the Helmholtz energy for the SAFT framework for a pure compound is given by:

$$\frac{a^{assoc}}{Nk_B T} = \sum_A \left(\ln(X^A) - \frac{X^A}{2} \right) + \frac{1}{2} M \quad (5.1)$$

Where M is the **number of association sites** of molecule and X^A is the **fraction of molecules not bonded to site A** which is given by:

$$X^A = \left[1 + \sum_B \rho X^B \Delta^{AB} \right] \quad (5.2)$$

Where x_j is the mole fraction of j and Δ^{AB_j} is the **association strength** between two sites A and B belonging to two different molecules i and j which is expressed as:

$$\Delta^{AB} = d_i^3 g_{ii}^{hs}(\sigma_{ii}) \kappa^{AB} \left[\exp\left(\frac{\varepsilon^{AB}}{k_B T}\right) - 1 \right] \quad (5.3)$$

Where $g_{ii}^{hs}(\sigma_{ii})$ is the **radial distribution function** of the hard spheres and d_i is the **temperature-dependent diameter**. The expressions for the latter two variables can be found in the appendices of the original PC-SAFT publication¹².

The inclusion of Eq. (5.1) into the PC-SAFT EoS adds two component-dependent parameters per HB between two sites A and B, which appear in Eq. (1.72), namely the **association energy** (ε^{AB}/k_B) and the **association volume** (κ^{AB}). With the already mentioned non-associating parameters m , σ and ε/k_B the PC-SAFT for a SA fluid must fit experimental data to $3 + 2N_{HB}$ component-dependent parameters (where N_{HB} is the number of possible H bonds between molecule sites). Furthermore, Eq. (5.2) is not explicit on X^A , thus adding further complexity. However, to alleviate this issue, we use the approximations for the association schemes proposed by Huang & Radosz⁴⁵, in particular we will use the 2B scheme for the alcohols (for which $N_H = 1$), as suggested by these authors.

To estimate the three non-associating parameters, we will use the methodology proposed by Ramirez-Velez et al.⁹⁵ in which the following weighted OF will be minimized:

$$\left\{ \begin{aligned} OF_{\text{component } j} &= \frac{1}{N_T} \left[3 \sum_{i=1}^{N_T} \left[\frac{P_{j,calc}^{sat}(T_i) - P_{j,exp}^{sat}(T_i)}{P_{j,exp}^{sat}(T_i)} \right]^2 + 2 \sum_{i=1}^{N_T} \left[\frac{\rho_{liq,j,calc}^{sat}(T_i) - \rho_{j,exp}^{sat}(T_i)}{\rho_{liq,j,exp}^{sat}(T_i)} \right]^2 \right] \\ N_T &= 50 \text{ is the number of temperature points} \end{aligned} \right. \quad (5.4)$$

This OF proved to yield the safest results for both properties present in them as well as for $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ (when the pseudo-experimental data was available). Thus for each alcohol, m , σ and ε/k_B will be fitted to P^{sat} and ρ_{liq}^{sat} for the temperature ranges described in Table S1 of **Appendix A5**.

It is worth noting that, although Eq. (5.4) was validated for non-associating compounds, the conclusions are still valid for self-associating compounds. In order to demonstrate this assessment, four of the objective functions presented in **Chapter 2** were tested using 152 SA compounds for which all four target properties are available (all belonging to the set of 1800 compounds treated throughout this dissertation). **Table 5.2** presents the average MAPE values for all target properties using four objective functions with different combinations of the four target properties (always including vapor pressure and liquid density).

Table 5.2. Average values of the MAPEs on $\{P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, C_{P,liq}^{sat}\}$, calculated over 152 self-associating pure species, corresponding each to a different combination of property data on which the PC-SAFT parameters were adjusted

MAPE (%)						
OF	Properties included	P^{sat}	ρ_{liq}^{sat}	$\Delta_{vap}H$	$C_{P,liq}^{sat}$	Sum of the 4 MAPEs on $P^{sat}, \rho_{liq}^{sat}, \Delta_{vap}H, C_{P,liq}^{sat}$
1	$(P^{sat} + \rho_{liq}^{sat} + \Delta_{vap}H + C_{P,liq}^{sat})$	1.65	1.29	3.45	5.45	11.85
13	$(P^{sat} + \rho_{liq}^{sat} + C_{P,liq}^{sat})$	1.66	1.10	3.69	5.31	11.77
6	$(P^{sat} + \rho_{liq}^{sat})$	1.42	1.03	3.75	5.91	12.11
12	$(P^{sat} + \rho_{liq}^{sat} + \Delta_{vap}H)$	1.57	1.33	3.40	5.68	11.98

As seen in the table, including any of the auxiliary properties does not bring a drastic improvement on any of the properties. Evidently, including one or both of them improves the value of the MAPE obtained, at the expense of slightly sacrificing accuracy on the vapor pressure and the liquid density. Thus, we can conclude that for SA compounds, only vapor pressure and liquid density data are needed in the OF to reach the minimization objectives set in **Chapter 2**.

In order to assess the impact of the associating term on the selected compounds, the parameter space of the associating parameters ε^{AB}/k_B and κ^{AB} must be investigated. Instead of including them in the regression, they will be given fixed values over a specified range for each parameter. The procedure to do this is carried out as follows:

- I. Initialize each non-associating parameter according to the proposed method found in **Appendix A5**.
- II. Input ε^{AB}/k_B and κ^{AB} as fixed parameters.
- III. Run 11 optimization algorithms in which Eq. (5.4) is minimized for each alcohol. If any parameter after the parametrization takes place, converges in either of the boundary values they are expanded by multiplying k_{\min} or k_{\max} by 0.9 and 1.5 respectively and restart optimization.
- IV. Save the new parameter set and restore initial values.
- V. Move back to step I until there are no more pairs of ε^{AB}/k_B and κ^{AB} .

Figure 5.1 shows a short schematic of the parametrization strategy used here.

In the case where the same values of ε^{AB}/k_B and κ^{AB} are used for all the alcohols, it becomes possible to construct a parameter mesh in which the behavior of the average MAPE over all the alcohols of the key properties with respect to both associating parameters can be investigated through a contour plot.

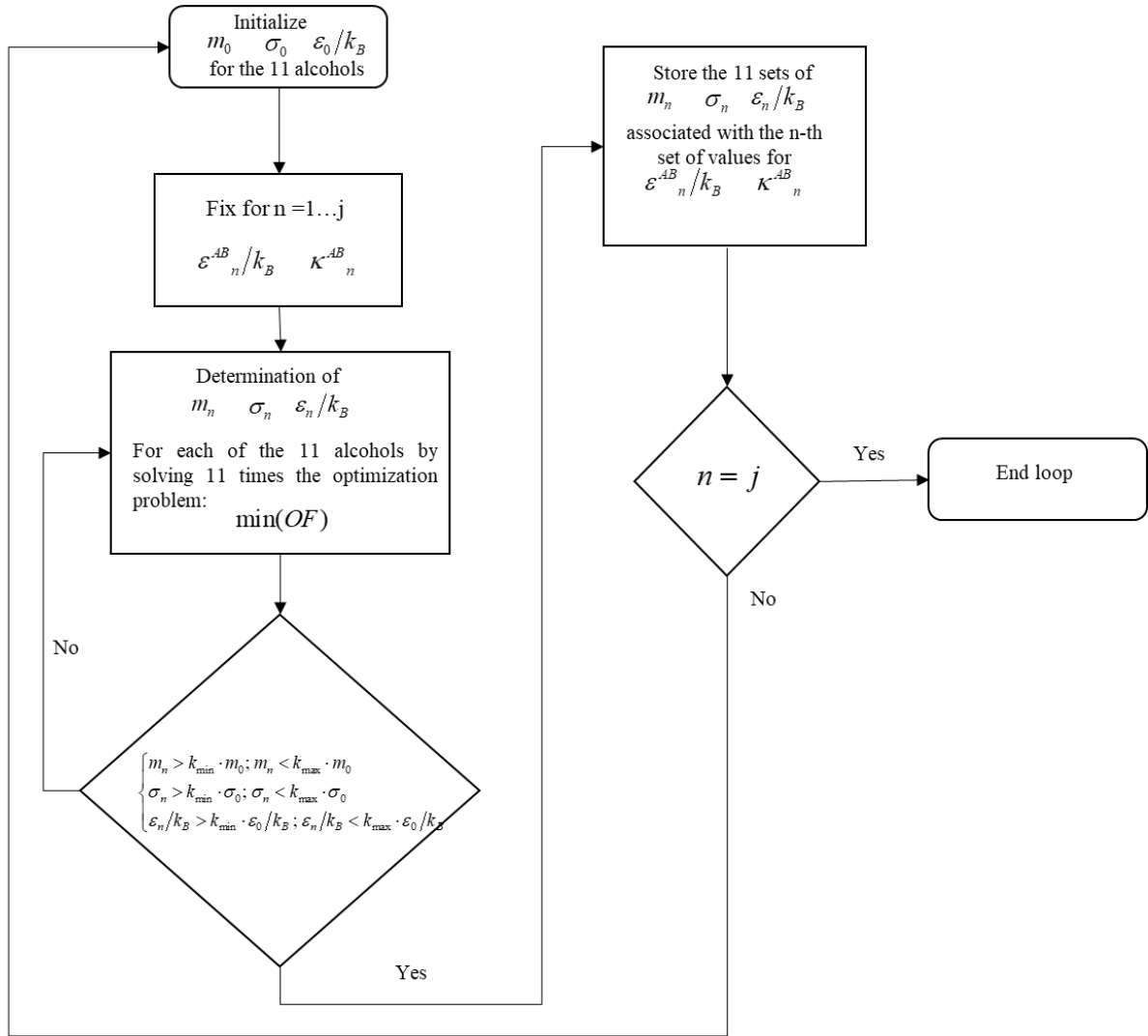


Figure 5.1. Strategy for the calculation of the associating parameter mesh, where n is the current pair of associating parameters and j is the total number of associating parameter pairs.

Each of the chemical species studied will have different ranges for the associating parameters. The selected ranges for ϵ^{AB}/k_B and κ^{AB} for the n -alcohols are:

$$\begin{cases} \epsilon^{AB}/k_B \in [1000K - 3000K] \\ \kappa^{AB} \in [0 - 0.1] \end{cases} \quad (5.5)$$

The associating energy range was divided in 41 equidistant points while the associating volumes were divided into 101 equidistant points for a total of 4141 pairs of parameters to construct the mesh.

For each set of five parameters obtained this way, the MAPE on P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ is calculated on a component-by-component basis. The calculations were done through the AspenPlus V10 software¹⁶⁴, selecting the Britt-Luecke optimization algorithm¹⁶⁵ (default mode for AspenPlus) in the regression mode functionality. The process was automated through Python¹⁶⁶ taking advantage of AspenPlus' variable explorer, which allows to input data and

collect results systematically. Once the results are obtained, the contour plot was created through Python's matplotlib¹⁶⁷ library.

A comparison between (i) results obtained by using a general set of associating parameters for the alcohol family (i.e., the same associating parameters for the 11 alcohols), (ii) results obtained by considering associating parameters specific to each compound; and (iii) the results obtained with the non-associating PC SAFT parameters will take place in the following section.

5.3. Results and discussion

Assuming that the same values of ε^{AB}/k_B and κ^{AB} can be used for the 11 alcohols and defining global MAPE for each property by averaging the MAPE over the 11 alcohols, we begin by analyzing the behavior of the global MAPE for vapor pressure and liquid density, as well as the sum of both properties (as a measure of the behavior of the OF) with respect to both the association energy and the association volume. **Figure 5.2** shows the contour plot for the three mentioned quantities. We define global here as the average MAPE over the 11 alcohols for a given property

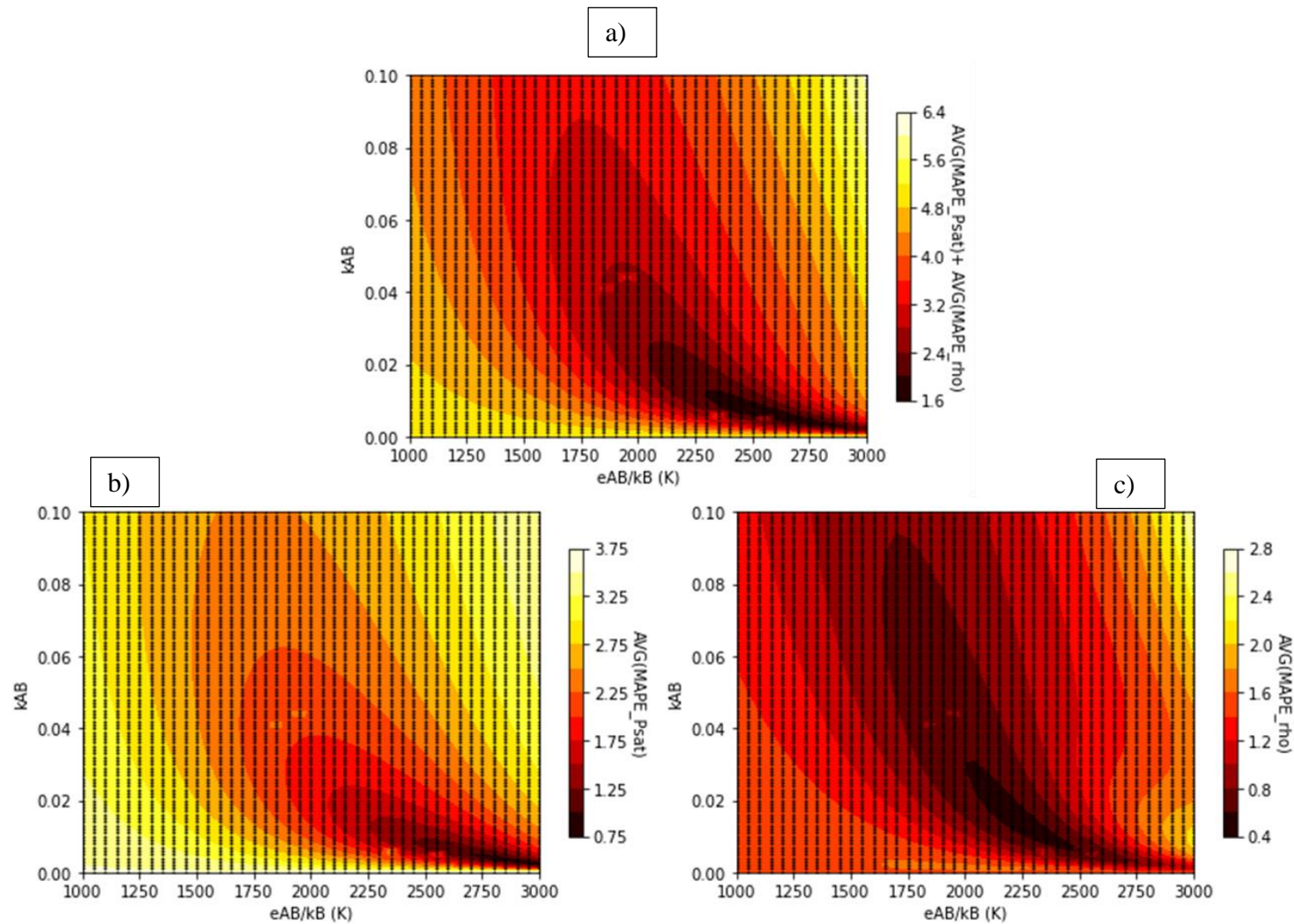


Figure 5.2. Contour plot of the associating parameter mesh (black dots) constructed for a) The sum of the global MAPE (global means that the MAPE is calculated by averaging the MAPEs of the 11 alcohols) on vapor pressure and liquid density, b) the global MAPE on vapor pressure and c) the global MAPE on liquid density. All MAPE values are in percentage (%).

We observe that the vapor pressure is best estimated when having higher values for the association energy (above 2500 K) while maintaining lower values for the association volume (below 0.01 approximately). However, for the liquid density the optimal region is shifted towards lower values of the association energy (between 2000 – 2500 K) and associating volumes (from 0.01 to 0.03). It is worth noting that the minima for the liquid density is lower than the minima for the vapor pressure, meaning that the associating parameters could have a stronger influence in predicting the volumetric properties when contrasted with the vapor pressure. The difference is not large enough however to indicate that one property is superior than the other in their respective optimal regions.

When taking into account both properties, we effectively observe that the optimal regions are intersected ($\varepsilon^{AB}/k_B \in [2300K - 2800K]$ and $\kappa^{AB} < 0.01$). This is a measure of the optimal region which meets the goals set back in **Chapter 2**. We observe that the minima region yields an OF of 1.6%, which gives us a first qualitative indication that the associating parameters can improve the PC-SAFT predictions for the two main properties. Looking into the associating parameter pair that minimizes the OF we find that the best pair corresponds to $\varepsilon^{AB}/k_B = 2650 K$ and $\kappa^{AB} = 0.005$ which yields an average MAPE for vapor pressure of 0.91% and 0.84% for liquid density.

In order to assess better the impact of the associating term for the n-alcohols, a case-by-case of the studied compounds is proposed. **Table 5.3** present the results using the optimal associating parameters for the 11 alcohols. For the the results found without including an associating term the reader is referred to **Table 5.1**.

Table 5.3. PC-SAFT parameters including association and MAPE for P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$ for the 11 studied n-alcohols. The associating parameters are chosen so that the vapor pressure and the liquid density are minimized.

MAPE ON (%)										
Compound name	CAS	ϵ^{AB} / k (K)	κ^{AB}	m	σ (Å)	ϵ / k (K)	P^{sat}	ρ_{liq}^{sat}	$\Delta_{vap}H$	$c_{P,liq}^{sat}$
ETHANOL	64-17-5	2650.00	0.005	1.6434	3.6866	285.3	1.50	1.75	4.75	7.22
1-PROPANOL	71-23-8	2650.00	0.005	2.2022	3.6233	268.9	0.62	0.85	3.34	7.76
1-BUTANOL	71-36-3	2650.00	0.005	2.5664	3.6928	268.5	0.12	0.76	3.66	4.34
1-PENTANOL	71-41-0	2650.00	0.005	2.7207	3.8345	277.4	0.63	0.44	2.53	2.74
1-HEXANOL	111-27-3	2650.00	0.005	3.1054	3.8431	275.2	0.65	0.40	-	3.82
1-HEPTANOL	111-70-6	2650.00	0.005	3.5486	3.8627	270.6	1.39	1.62	-	3.46
1-OCTANOL	111-87-5	2650.00	0.005	3.8811	3.8688	271.2	1.03	0.36	2.40	3.66
1-NONANOL	143-08-8	2650.00	0.005	4.0077	3.9540	278.1	1.14	0.55	-	4.50
1-DECANOL	112-30-1	2650.00	0.005	4.4259	3.9557	275.1	1.03	0.32	-	2.87
1-UNDECANOL	112-42-5	2650.00	0.005	4.2738	4.1378	288.5	1.56	0.80	-	4.98
1-DODECANOL	112-53-8	2650.00	0.005	4.7595	4.0920	283.3	1.58	0.20	-	3.70
Average							1.02	0.73	3.34	4.46

We observe that the associating term for the PC-SAFT, using a family-wide set of associating parameters, improves the MAPE across all properties for all alcohols. The vapor pressure is reduced on average from 3.52 % to 1.02%, while the liquid density is reduced nearly in half from 1.44% to 0.73% when including association. The enthalpy of vaporization, although improved seems to be the less sensitive to the inclusion of an associating term. The liquid heat capacity is the property which is improved the most, going from 19.1% to 4.46%.

These results show that the optimization objective was indeed attained (minimize vapor pressure and liquid density), with the improvement of the two auxiliary properties as an additional feature. However, it would be reasonable to assume that, in order to guarantee accurate results the four properties using an associating PC-SAFT, that they should be minimized by the OF. **Table 5.4** shows the results found by including both $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ in the minimization objective for the 11 alcohols.

Table 5.4. PC-SAFT parameters including association and MAPE for P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$ for the 11 studied n-alcohols. The associating parameters are chosen so that the all four target properties are minimized.

Compound name	CAS	ϵ^{AB} / k (K)	κ^{AB}	m	σ (Å)	ϵ / k (K)	MAPE ON (%)			
							P^{sat}	ρ_{liq}^{sat}	$\Delta_{vap}H$	$c_{P,liq}^{sat}$
ETHANOL	64-17-5	2750.00	0.004	1.4274	3.8784	299.5392	1.13	2.14	4.84	7.33
1-PROPANOL	71-23-8	2750.00	0.004	1.9570	3.7800	281.7478	0.46	1.23	3.78	6.57
1-BUTANOL	71-36-3	2750.00	0.004	2.3307	3.8240	279.4416	0.19	1.05	4.21	3.22
1-PENTANOL	71-41-0	2750.00	0.004	2.5066	3.9504	287.4590	0.80	0.66	2.87	2.28
1-HEXANOL	111-27-3	2750.00	0.004	2.9372	3.9224	281.9742	0.55	0.29	-	3.01
1-HEPTANOL	111-70-6	2750.00	0.004	3.4284	3.9123	274.7265	1.13	1.69	-	2.81
1-OCTANOL	111-87-5	2750.00	0.004	3.7931	3.9020	274.0440	0.78	0.39	2.02	3.07
1-NONANOL	143-08-8	2750.00	0.004	3.9402	3.9791	280.2861	1.00	0.54	-	3.88
1-DECANOL	112-30-1	2750.00	0.004	4.3828	3.9703	276.3933	0.91	0.33	-	2.29
1-UNDECANOL	112-42-5	2750.00	0.004	4.2396	4.1503	289.6897	1.54	0.78	-	4.39
1-DODECANOL	112-53-8	2750.00	0.004	4.7402	4.0983	283.9273	1.54	0.18	-	3.09
Average							0.91	0.84	3.54	3.81

We observe that including all four properties as the minimization objective yields an improvement on P^{sat} and $c_{P,liq}^{sat}$ while decreasing ρ_{liq}^{sat} and $\Delta_{vap}H$. It should be noted that, in order to minimize all four properties, the associating energy PC-SAFT parameter is higher than before. The improvement on the liquid heat capacity suggests a relationship between this parameter and itself. Nevertheless, we can see that on average having only vapor pressure and liquid density as the minimization objectives performs just as well as having all four properties in the OF. This means that for a family-wide parameter set, fitting to P^{sat} and ρ_{liq}^{sat} is enough to guarantee an improved performance over the non-associating PC-SAFT.

Noting that the common practice is to minimize the five PC-SAFT parameters (when the association term is used), meaning that all parameters are treated as component-dependent, we analyze the case where each pair of associating parameters is chosen so that the sum of MAPE for each compound is minimized, thus effectively searching for five parameters per compound. **Table 5.5** shows the parameters and MAPE for the 11 alcohols when the five parameters are assumed component dependent.

Table 5.5. PC-SAFT parameters including association and MAPE for P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$ for the 11 studied n-alcohols. The associating parameters are assumed component-dependent and chosen so that the four properties are minimized.

MAPE ON (%)										
Compound name	CAS	ε^{AB} / k (K)	κ^{AB}	m	σ (Å)	ε / k (K)	P^{sat}	ρ_{liq}^{sat}	$\Delta_{vap}H$	$c_{P,liq}^{sat}$
ETHANOL	64-17-5	2600.00	0.025	2.2676	3.2445	212.6312	0.12	0.49	3.83	1.84
1-PROPANOL	71-23-8	2650.00	0.007	2.1608	3.6432	262.9744	0.18	1.02	4.17	5.63
1-BUTANOL	71-36-3	2750.00	0.004	2.3307	3.8240	279.4416	0.19	1.05	4.21	3.22
1-PENTANOL	71-41-0	2650.00	0.005	2.7207	3.8345	277.4443	0.63	0.44	2.53	2.74
1-HEXANOL ^a	111-27-3	3000.00	0.002	2.6546	4.0702	297.0260	0.76	0.31	-	1.39
1-HEPTANOL ^a	111-70-6	3000.00	0.002	3.3019	3.9667	280.9284	0.47	1.63	-	1.25
1-OCTANOL ^a	111-87-5	3050.00	0.002	3.5555	3.9968	282.5011	0.28	0.45	1.12	1.51
1-NONANOL ^a	143-08-8	3350.00	0.001	3.6225	4.1053	292.2088	0.80	0.56	-	1.14
1-DECANOL ^a	112-30-1	3100.00	0.002	4.1416	4.0557	283.2257	0.52	0.28	-	1.04
1-UNDECANOL	112-42-5	2950.00	0.002	4.4153	4.0862	286.1919	1.43	0.56	-	2.23
1-DODECANOL ^a	112-53-8	3350.00	0.001	4.7106	4.1077	285.7755	1.44	0.14	-	1.14
Average							0.62	0.63	3.17	2.10

^a These compounds converged to boundary values for one or both associating parameters, thus their parameter ranges were extended.

At first glance, we observe that using five component-dependent parameters for an associating PC-SAFT gives the best results across all properties. It should be noted that the OF here is set to minimize all four target properties, in particular the $c_{P,liq}^{sat}$. To better explain the reasoning, **Figure 5.3** shows the MAPE on liquid density against the MAPE on vapor pressure for 1-pentanol for every evaluated pair of associating parameters.

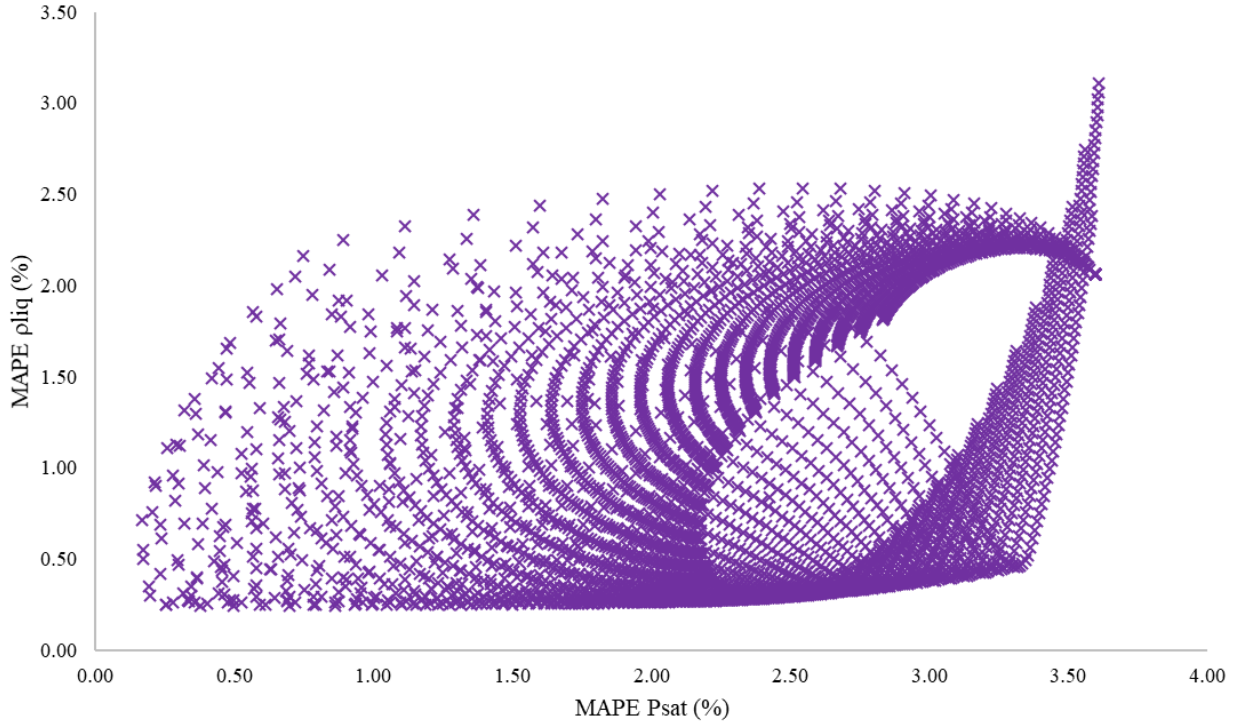


Figure 5.3. MAPE on liquid density vs. MAPE on vapor pressure obtained for every combination of associating parameters for 1-pentanol.

Inspecting the figure, we observe that when we move to the left on the P^{sat} we obtain lower deviations for this property. The same is true when moving from up to down on the ρ_{liq}^{sat} axis. Therefore, when both properties tend to zero, we should find the minimum value for the OF. However, near the value of 0% we observe that there is a collection of points very closely placed. These points are essentially equivalent solutions for the OF. Thus, P^{sat} and ρ_{liq}^{sat} data alone are not enough to determine the optimal value for the OF using an associating PC-SAFT EoS that uses all five parameters as component-dependent. Some of these values, although optimal for P^{sat} and ρ_{liq}^{sat} are not as accurate for the other properties. Taking a specific case from the example with 1-pentanol, we have:

$$\left\{ \begin{array}{l} \varepsilon^{AB}/k_B = 2350 \text{ K} \\ \kappa^{AB} = 0.008 \\ MAPE_{P^{sat}} = 0.17\% \\ MAPE_{\rho_{liq}^{sat}} = 0.50\% \\ MAPE_{\Delta_{vap}H} = 1.20\% \\ MAPE_{c_{p,liq}^{sat}} = 10.6\% \end{array} \right.$$

We see that for the two main properties, the MAPE are excellent. The MAPE for the enthalpy of vaporization is also quite outstanding. However, the liquid heat capacity is not satisfactory. Thus, if the PC-SAFT EoS is to be parametrized with an associating term with five pure-compound parameters, vapor pressure and liquid density data are not enough. At least one of the two auxiliary properties (enthalpy of vaporization or liquid heat capacity) must be included in order to discriminate from equivalent solutions to the OF and collect the true optimal parameter set. ***Thus, the main conclusion for this chapter is that vapor pressure and liquid density data are enough to fit parameters for the PC-SAFT EoS without an associating term or with an associating term which uses family-wide associating parameters (equal associating parameters for all compounds). However, if all five parameters are included in the fitting, auxiliary properties are needed to find the optimal parameter set.***

In order to validate this conclusion, we tested the behavior of the sum of the average MAPE for the four key properties when parametrized with an OF that only includes P^{sat} and ρ_{liq}^{sat} (OF1) and with an OF that includes all four target properties (OF2), as a function of the number of alcohols included in the average MAPE. **Figure 5.4** shows the plot of the SUM of the average MAPE for the four properties as a function of the number of alcohols included in the OF.

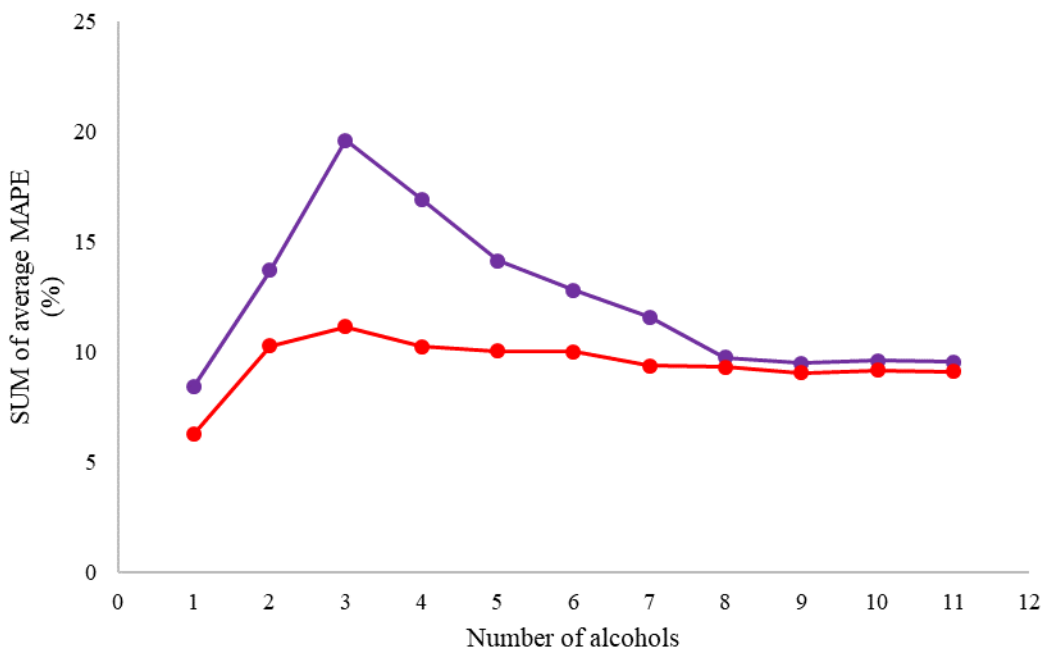


Figure 5.4. Sum of the average MAPE of P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$, $c_{P,liq}^{sat}$ and as a function of the number of alcohols included in the OF. The purple line represents OF1 which only includes P^{sat} and ρ_{liq}^{sat} in the minimization objective. The red line represents OF2 in which all four target properties are included in the minimization objective. Dots represent the value of the OF at a given number of alcohols.

Both OFs begin with ethanol at point 1. At this point, it is clear that there is a need for all four properties due to the fact having only one compound makes all five parameters component-dependent. However, when adding more alcohols we observe a rising discrepancy between the two OF, in which OF1 diverges after including two and three alcohols. At this point, when only ethanol, 1-propanol and 1-butanol are present, the maximum difference in sum of average MAPE is found between OF1 and OF2. This implies that if only light members of the family are included, the all five parameters should be treated as component-dependent.

Next, we see that both curves begin to converge after adding four or more alcohols. In fact, once eight alcohols are present in the OF, both OF1 and OF2 become equivalent, meaning that the sum of the average MAPE for all four properties is nearly equal. From this, we can gather that, in order to use family-wide parameters, at least eight members of the chemical family must be present in the OF. Otherwise, using component-dependent parameters is recommended.

Regarding the modeling classification given to these alcohols, we recall that the threshold value for P^{sat} is 1.92% and 1.59% for ρ_{liq}^{sat} . Comparing the values obtained by each alcohol in each of the three presented cases (family parameters with OF minimizing P^{sat} and ρ_{liq}^{sat} ; family parameters with OF minimizing all four properties and component-dependent parameters) we observe that 1-heptanol is still classified as BM regardless of the case. This means that the PC-

SAFT with or without association is not able to describe this compound entirely (in particular the liquid density is above the threshold). On the other hand, ethanol appears as BM in both

family-parameter cases, meaning that this compound requires component-dependent parameters in order to be correctly modeled.

5.4. Conclusions

The influence of the associating term of the PC-SAFT was tested for a number of highly associating alcohols. The methodology included creating an associating parameter mesh in which the associating parameters were fixed in the OF and the non-associating parameters were fitted to experimental vapor pressure and liquid density data.

The results showed that this type of experimental data is sufficient to obtain safe results and optimal parameters without using association and when using association with equal parameters across the chemical family (family-wide parameters). Although there is improvement if more properties are included in the minimization objective, the results do not show enough incentive to add more properties to an objective function. It should be noted, that this is only true if enough members of the chemical family are included in the OF. Indeed, for the alcohol family, at least eight members must be present in the OF to obtain equivalent results using a OF with family-wide parameters.

When working with component-dependent parameters with the PC-SAFT, vapor pressure and liquid density data alone are not enough, as this leads to a large number of equivalent solutions that may be inadequate for other properties such as the heat capacity of mixing. Thus, if five parameters are being fitted with the PC-SAFT EoS using the associating term, at least enthalpy of vaporization or liquid-heat capacity data must be included in order to correctly discriminate the optimal parameter set from equivalent one.

Finally, although this study was limited to a small number of alcohols, its conclusions lead to a new perspective regarding association in the PC-SAFT framework. Further studies which include other associating families such as amines and organic acids, (the latter which is notable doubly associated) which are often modeled with different association schemes, are needed in order to reach general conclusions for associating compounds and their need for an associating term within the SAFT framework.

**Chapter 6 Development of a database of reference
binary system data to evaluate the performance of
equations of state**

This chapter will present in form of a published article the development of a database made up of 200 binary mixtures of different associating characters and over 300.000 data points including VLE, LLE and VLLE data, mixing enthalpy and heat capacity data, critical point and azeotropic data. It will also present a robust methodology to use this database to assess the performance of any EoS. The paper was published in July 2020 in the Journal of Industrial & Engineering Chemistry Research under the name “Benchmark Database Containing Binary-System-High-Quality-Certified Data for Cross-Comparing Thermodynamic Models and Assessing Their Accuracy”.

This project was not included in the mainline of this dissertation given that I took a support role in its development. My contributions to this project include:

- Review of the experimental data used for the database, including addition of new data, extraction of data (when we could not confirm its validity, or we decided to remove the system) and data arrangement.
- Execute calculations with the PR EoS with classical mixing rules and temperature-dependent binary interaction parameters for a number of systems
- Summarizing and performing basic statistics for the experimental data (number points, percentage of each type of data with respect to the total amount of points, etc.).
- Draft reviewing.

6.1. Introduction

Commercially available computer-aided-process-design software require thermodynamic models to design, develop, analyze and optimize chemical processes. As a result of their great potential, equations of state represent the cornerstone of thermodynamic models¹⁶⁸. Indeed, combining an EoS and ideal-gas heat capacities enables to calculate not only phase equilibria, but also all 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, industry sometimes seems skeptical when weighing the value gained by using a more complex model, and rarely updates¹⁶⁹ or replaces its thermodynamic models with newer ones unless a clear advantage is evident. As a rule of thumb, it takes 10 years² 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 question of their accuracy inevitably arises because these models are, by definition, a simplification of reality.

In this paper, in order 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 published² 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 non-electrolytic binary systems was selected to cover all categories of mixtures and divided into 9 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 is indeed considered as 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 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.

6.2. Criterion to build a benchmark database

6.2.1. 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>), that 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 in 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. Firstly, they are so comprehensive that a model evaluation procedure accounting for all the data would require an excessive amount of time. Secondly, 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 sub-database 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 non-electrolytic and non-polymeric systems available in the literature is the one proposed by Danner and Gess in 1990¹⁷⁰. 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 non-ideal 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 inch 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 Gess¹⁷⁰ 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?

6.2.2. *Which thermophysical properties should be included?*

To answer this question, we must be aware of the industrial needs. The paper by Hendriks et al.² 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 EoS 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 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 lines¹⁷¹ leads to an accurate restitution of phase diagrams on the entire temperature and pressure ranges. Such lines indeed fix the global topology¹⁷² of the isothermal and isobaric phase diagrams for any fixed temperature or pressure, respectively. Convinced by the importance of critical points, a 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 a 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 to determine the temperature dependence of the phase equilibrium what 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.¹³¹ 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, Qian¹⁷³ 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 are 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 used mixing rules. This implies that before grading a thermodynamic model with the proposed database, it is necessary to give 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 adsorption¹⁷⁴ equilibrium data.

6.2.3. *Which binary systems should be included?*

Danner and Gess database retained our attention as it does not only compile experimental data but also provides a classification for binary systems revealing their thermodynamic complexity (here *thermodynamic complexity* means a measure of the non-ideal 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 for a molecule to donate or accept a hydrogen atom and the presence of hydrogen bonding. Starting from these 4 categories of pure compounds, Danner and Gess defined 9 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 non-ideal. 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^{26,108,147} or SAFT^{8,12,154,175-183} EoS clearly indicate that an actual scientific challenge for EoS is their ability to properly describe the very complex association phenomena.

6.2.3.1. Definition of the “associating character” of a pure component.

In this paper, “association” means association only by hydrogen bonding. In classical physical chemistry¹⁸⁴, 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 cut-off for an ability to participate in hydrogen bonding but nitrogen (N), oxygen (O) or fluor (F) atoms participate most effectively. From the definition above, the formation of a hydrogen bond can be regarded as the electrostatic and partially covalent 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 Fig. 6.1). 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 6.1. (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 in 4 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 “Non-Associating”): the molecule has neither a labile hydrogen atom nor a lone pair of electrons. It is nonpolar. Molecules like alkanes and mono-halogenated compounds are included in this family. In short, this category includes nonpolar/non-associating 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 non-associating 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-, tri-halogenated 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 non-associating 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 **Appendix A9** lists the 107 pure compounds included in the proposed database and indicates for each of them the corresponding *associating character* among “Non-Associating” (NA), “Hydrogen-Acceptor” (HA), “Hydrogen-Donor” (HD) or “Self-Associating” (SA).

6.2.3.2. *Definition of binary association codes 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 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 for 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 that are both non-associating mixtures, into a single family, thus reducing the number of BACs to nine.

Table 6.1. Definition of the ten families of binary systems and their corresponding BAC (binary association code).

Component 1	Component 2	Binary association code (BAC)	Type of exhibited association
NA (Non-Associating) <i>nonpolar</i>	NA (Non-Associating) <i>nonpolar</i>	1	Mixtures without association
HA (Hydrogen-Acceptor) <i>polar but non-associating</i>	NA (Non-Associating) <i>nonpolar</i>	2	
HD (Hydrogen-Donor) <i>polar but non-associating</i>	NA (Non-Associating) <i>nonpolar</i>	3	
HA (Hydrogen-Acceptor) <i>polar but non-associating</i>	HA (Hydrogen-Acceptor) <i>polar but non-associating</i>	4	
HD (Hydrogen-Donor) <i>polar but non-associating</i>	HD (Hydrogen-Donor) <i>polar but non-associating</i>		
SA (Self-Associating) <i>polar and associating</i>	NA (Non-Associating) <i>nonpolar</i>	5	Mixtures in which self-association takes place (but tends to be broken)
HD (Hydrogen-Donor) <i>polar but non-associating</i>	HA (Hydrogen-Acceptor) <i>polar but non-associating</i>	6	Mixtures in which cross-association takes place alone
SA (Self-Associating) <i>polar and associating</i>	HD (Hydrogen-Donor) <i>polar but non-associating</i>	7	Mixtures in which both cross-association and self-association take place
SA (Self-Associating) <i>polar and associating</i>	HA (Hydrogen-Acceptor) <i>polar but non-associating</i>	8	
SA (Self-Associating) <i>polar and associating</i>	SA (Self-Associating) <i>polar and associating</i>	9	

From Table 6.1, 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, the labile hydrogen atom and the lone pair of electrons originate from the 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 no-association, 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 thermodynamic-complexity degree (for small BAC value, the thermodynamic complexity is low and this complexity increases with the BAC).
- In binary systems belonging to the BAC 5, a NA (Non-Associating) component faces a SA (Self-Associating) component so that self-association (at least partially) persists in the mixture. The non-associating 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: “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 mixture than when they are pure; therefore, such mixtures usually exhibit negative deviations from ideality.
- For binary association codes 7 to 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.

6.2.3.3. *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 both from quantitative and qualitative viewpoints. Qualitatively, a system will be named ideal if it is formed by molecules having (i) similar sizes, (ii) similar shapes, and (iii) showing similar energetic interactions (nature & strength), regardless of the temperature, pressure and composition¹⁸⁵. On the contrary, a system is considered as non-ideal 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 non-ideal 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) terms. In order 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 non-ideal, including enthalpic, entropic and combined effects). Doing so, our database will allow the identification of model failures in their enthalpic and/or entropic modelling 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 by using the VLE relationship stemming from the γ - ϕ approach:

$$\gamma_i(T, \mathbf{x}) = P_{\text{exp}} \cdot y_{i,\text{exp}} / [P_i^{\text{sat}}(T_{\text{exp}}) \cdot x_{i,\text{exp}}] \quad (6.1)$$

Eq. (6.1) 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 6.2.

For each binary system for which subcritical VLE data were available, a set of 4 parameters (p_1, p_2, p_3, p_4) of the Margules excess Gibbs energy model were fit over both VLE data and enthalpy of mixing data (when available).

$$\begin{cases} \frac{g^E(T, \mathbf{x})}{RT} = x_1 \cdot x_2 \cdot A(T) \\ A(T) = p_1 - p_2 T - p_3 \ln T + p_4 \exp\left(\frac{1}{T}\right) \end{cases} \quad (6.2)$$

The p_i parameters were determined in order 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. (6.2):

$$h^E = g^E - T \left(\frac{\partial g^E}{\partial T} \right)_{\mathbf{x}} \quad (6.3)$$

For VLE calculations, the γ - ϕ approach was used assuming that the gas phase is perfect and by neglecting the Poynting factor. In other words, the following classical VLE relation, especially suitable to correlate subcritical data, was used:

$$p y_i = p_i^{sat} x_i \gamma_i \quad (6.4)$$

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

Once the 4 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 as *ideal* (see Table 6.2) if $\left| g^E / RT \right|_{x=0.5} < 0.1$ for each of the considered temperatures. If not, the system is declared non-ideal.

For non-ideal 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 non-ideal systems, when h^M data were lacking, the systems were thus declared (see Table 6.2): *non-ideal with non-assessed causes*. In turn, when h^M data were available:

1. If $\left| (h^E / RT) / (s^E / R) \right|_{x=0.5} > 2$ for all temperatures, it was considered that non-ideality stemmed from enthalpic effects. In Table 2, the system is labelled: *non-ideal with enthalpic causes*.
2. If $\left| (h^E / RT) / (s^E / R) \right|_{x=0.5} < \frac{1}{2}$ for all temperatures, it was considered that non-ideality stemmed from entropic effects. In Table 2, the system is labelled: *non-ideal 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 6.2, the system is labelled: *non-ideal with enthalpic and entropic causes*.

An overview of how the deviations from ideality are distributed among the nine BACs can be found in Table 6.2 whereas the different steps that were followed to build the proposed database are summarized in Fig. 6.2.

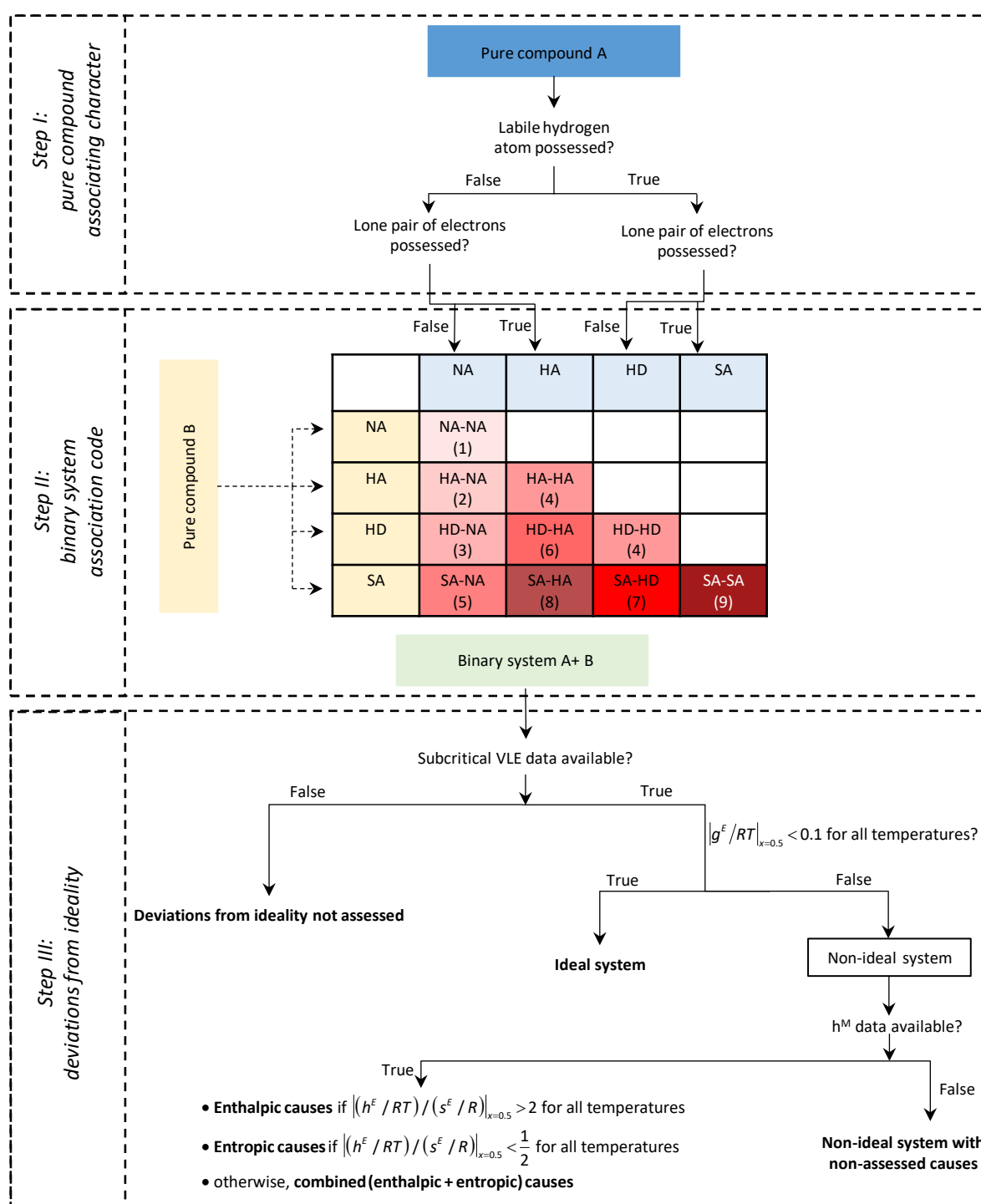


Figure 6.2. Procedure followed to build the proposed database.

Table 6.2. 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 (the abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”).

Binary association code (BAC)	Deviations from ideality not assessed ^(*)	Ideal	Non-ideal with enthalpic causes	Non-ideal with entropic causes	Non-ideal with enthalpic and entropic causes	Non-ideal with non-assessed causes ^(**)
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%

(*) non-availability of subcritical VLE data (refer to Fig. 2)

(**) non-availability of h^M data (refer to Fig. 2)

6.2.4. 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 in order 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 well representative of their family. Among these systems, our ambition is to reach a distribution of $1/4$ of systems containing high-pressure VLE data (for which deviations from ideality cannot be assessed), $1/4$ of ideal systems and $1/2$ of non-ideal systems. The non-ideal systems should include similar number 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. In order 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 were checked with the help of four consistency tests: the point test¹⁸⁶, the integral test¹⁸⁷, the differential test and the infinite-dilution test¹⁸⁸, 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 non-ideal systems, the point test and two of the three remaining tests had to be passed in order to keep the experimental data in our database. Indeed, as explained by Wisniak et al.¹⁸⁹ 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, 8,500 h^M data, 1,500 c_p^M data, and 2,000 data points relative to critical points, azeotropic points or three-phase lines).

6.2.5. The built database

An extensive screening of thousands of binary systems was first realized and a complex strategy was developed in order to only keep the 200 systems that met our criteria in terms of (i) types of association, (ii) deviations from ideality, (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.

As previously stated, an overview of how the deviations from ideality are distributed among the nine BACs can be found in Table 6.2. Similarly, an overview of how the different types of data are distributed among the 9 BACs can be found in Table 6.3. For each BAC, Tables 6.4 to 6.12 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.

Remark: Table 6.3 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 for some azeotropic systems to interpolate the experimental VLE data in order to determine the temperature, pressure and composition of the azeotropic point.

Several Excel files are available in **Appendix A8**:

- The first one, named Database.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 200 other sheets contain each the data related to a given binary system.
- The nine others, one for each BAC, and named BAC_i with visualization of the data.xlsx (i=1 to 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 contain each, the data related to a given binary system.

Table 6.3. 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 (the abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”).

Binary association code (BAC)	Subcritical liquid phase ^(*) composition	Subcritical vapor phase (or 2 nd liquid phase ^(**)) composition	Supercritical liquid phase ^(*) composition	Supercritical vapor phase (or 2 nd liquid phase ^(**)) 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	12249	12181	6172	6036	225	1116	8570	1234	66	47849	
%	25,6%	25,5%	12,9%	12,6%	0,47%	2,33%	17,91%	2,58%	0,14%		

(*) *Liquid phase* refers indifferently to a VLE or a LLE data point. For a LLE, it designates the composition of the α -liquid phase.

(**) 2nd liquid phase designates the composition of the β -liquid phase in the case of a LLE.

Table 6.4. List of the 26 binary systems for which the binary association code is: BAC=1 (NA-NA). Such a BAC corresponds to a binary system involving a “Non-Associating” (NA) molecule + another “Non-Associating” (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.

<i>Origin of the deviations from ideality</i>	<i>Molecule 1</i>	<i>Molecule 2</i>	<i>References</i>
Deviations from ideality not assessed	methane	propane	190–202
	methane	n-hexane	200,203–210
	methane	n-heptane	200,211–214
	nitrogen	ethane	215–222
	methane	n-decane	223–228
	ethane	n-heptane	229–234
	nitrogen	n-pentane	235–237
	nitrogen	n-decane	238,239
	methane	n-tetracosane	240–243
	ethane	n-hexatriacontane	244–246
Ideal	n-hexane	cyclohexane	247–259
	benzene	toluene	260–269
	propane	isopentane	270
	cyclohexane	methylcyclohexane	248,269,271–274
Non-ideal with non-assessed causes	ethane	propane	275–287
	methane	n-butane	200,210,288–292
Non-ideal with enthalpic causes	argon	methane	293–302
	n-heptane	monochlorobenzene	303–309
	cyclohexane	monochlorobenzene	272,309–314
	1,2-dichloroethane	carbon tetrachloride	315–320
Non-ideal with entropic causes	1,2-dichloroethane	toluene	264,321–325
Non-ideal with enthalpic and entropic causes	Nitrogen	methane	293,326–331,220,332,333,301,334,302
	methane	ethane	198,200,219,220,335–339
	benzene	n-heptane	248,269,304,340–356
	benzene	cyclohexane	250,259,350,357–374
	ethylene	xenon	375–377

Table 6.5. List of the 24 binary systems for which the binary association code is: BAC=2 (HA-NA). Such a BAC corresponds to a binary system involving a “Hydrogen-Acceptor” (HA) molecule + a “Non-Associating” (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.

<i>Origin of the deviations from ideality</i>	<i>Molecule 1</i>	<i>Molecule 2</i>	<i>References</i>
Deviations from ideality not assessed	carbon dioxide	toluene	378–392
	carbon dioxide	n-decane	393–404
	methane	carbon dioxide	194,338,405–414
	carbon dioxide	cyclopentane	415,416
	nitrogen	carbon dioxide	217,406–408,412,417–428
	methane	hydrogen sulfide	429–431
	carbon dioxide	n-dotriacontane	432–434
Ideal	methyl tert-butyl ether	n-heptane	435–439
	ethyl acetate	toluene	440–443
	carbon tetrachloride	1,4-dioxane	444–449
	methyl ethyl ketone	benzene	450–453
	methyl tert-pentyl ether	n-heptane	454–457
	methyl tert-butyl ether	toluene	458–461
	1,2,3,4-tetrahydronaphthalene	quinoline	462,463
Non-ideal with non-assessed causes	ethylene	carbon dioxide	464–470
	carbon dioxide	propane	194,201,286,418,471–479
Non-ideal with enthalpic causes	acetone	n-hexane	480–486
	n-pentane	acetone	480,484,486–488
	acetone	cyclohexane	257,357,489–496
Non-ideal with entropic causes	benzene	n-methyl-2-pyrrolidone	497–502
Non-ideal with enthalpic and entropic causes	carbon dioxide	ethane	338,476,503–512
	carbon dioxide	n-butane	286,420,465,475–478,513–520
	n-hexane	methyl ethyl ketone	346,453,521–524
	acetone	benzene	357,445,525–533

Table 6.6. List of the 20 binary systems for which the binary association code is: BAC=3 (HD-NA). Such a BAC corresponds to a binary system involving a “Hydrogen-Donor” (HD) molecule + a “Non-Associating” (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.

<i>Origin of the deviations from ideality</i>	<i>Molecule 1</i>	<i>Molecule 2</i>	<i>References</i>
Deviations from ideality not assessed	ethylene	dichloromethane	534
	nitrogen	chlorodifluoromethane	535–538
	chloroform	Benzene	264,530,539–545
Ideal	chloroform	1,2-dichloroethane	546–548
	chloroform	carbon tetrachloride	549–552
	1,1,1-trifluoroethane	2,3,3,3-tetrafluoropropene	553
	ethyl fluoride	1,1,1,2-tetrafluoroethane	554
	propylene	chlorodifluoromethane	555
	difluoromethane	Propane	556–560
	trifluoromethane	Ethane	561,562
Non-ideal with non-assessed causes	carbon tetrafluoride	chlorodifluoromethane	563,564
	pentafluoroethane	Propane	557,559,565–567
	carbon tetrafluoride	trifluoromethane	568
	hexafluoroethane	1,1,1,2-tetrafluoroethane	555,569
	decafluorobutane	1,1,1,3,3-pentafluorobutane	570
	chlorodifluoromethane	dichlorodifluoromethane	571–576
	dichloromethane	carbon tetrachloride	316,319,550,577
Non-ideal with enthalpic causes	chloroform	n-hexane	578–584
	chloroform	n-heptane	578,581,582,584–586
Non-ideal with enthalpic and entropic causes	dichloromethane	n-pentane	587–589

Table 6.7. List of the 22 binary systems for which the binary association code is: BAC=4 (HA-HA or HD-HD). 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.

<i>Origin of the deviations from ideality</i>	<i>Molecule 1</i>	<i>Molecule 2</i>	<i>References</i>
Deviations from ideality not assessed	carbon dioxide	dimethyl ether	590–592
	carbon dioxide	hydrogen sulfide	593–596
	carbon dioxide	ethyl acetate	597–601
	carbon dioxide	carbon disulfide	602,603
	carbon dioxide	dimethyl carbonate	604–609
	carbon monoxide	carbon dioxide	610–612
	oxygen	carbon dioxide	423,424,613–616
Ideal	pentafluoroethane	1,1,1,2-tetrafluoroethane	617–621
	chlorodifluoromethane	1,1,1,2-tetrafluoroethane	622,623
	difluoromethane	1,1,1,2-tetrafluoroethane	617,618,620,621,624–628
	1,1,1,2-tetrafluoroethane	1,1-difluoroethane	555,629,630
	ethyl acetate	1,4-dioxane	444,631–633
	dimethyl carbonate	diethyl carbonate	634–636
	1,2-epoxybutane	dimethyl carbonate	637
Non-ideal with non-assessed causes	dimethyl ether	sulfur dioxide	638–640
	trifluoromethane	chlorodifluoromethane	641,642
Non-ideal with enthalpic causes	diethyl ether	acetone	542,643,644
	carbon disulfide	acetone	645–647
	triethylamine	1,4-dioxane	648,649
Non-ideal with entropic causes	thiophene	sulfolane	650
Non-ideal with enthalpic and entropic causes	tetrahydrofuran	N,N-dimethylformamide	651,652
	n-butyl acetate	N,N-dimethylformamide	653,654

Table 6.8. List of the 18 binary systems for which the binary association code is: BAC=5 (SA-NA). Such a BAC corresponds to a binary system involving a “Self-Associating” (SA) molecule + a “Non-Associating” (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.

<i>Origin of the deviations from ideality</i>	<i>Molecule 1</i>	<i>Molecule 2</i>	<i>References</i>
Deviations from ideality not assessed	n-butane	water	655–659
	water	benzene	660–664
	ethane	1-propanol	665–670
	nitrogen	ammonia	671–673
	ethane	water	656
	nitrogen	water	674–684
Ideal	diethylamine	benzene	304,685,686
	diethylamine	monochlorobenzene	304,687
Non-ideal with non-assessed causes	ethane	methanol	667,688–693
	propane	methanol	694–698
Non-ideal with enthalpic causes	1-propanol	benzene	359,699–707
	ethanol	benzene	349,352,367,539,704,707–717
	isopropanol	2,2,4-trimethylpentane	718–725
	2-butanol	cyclohexane	726–731
Non-ideal with enthalpic and entropic causes	1-propanol	n-hexane	732–738
	ethanol	n-heptane	739–755
	methanol	n-hexane	738,747,756–764
	methanol	benzene	704,707,714,765–775

Table 6.9. List of the 25 binary systems for which the binary association code is: BAC=6 (HD-HA). 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.

<i>Origin of the deviations from ideality</i>	<i>Molecule 1</i>	<i>Molecule 2</i>	<i>References</i>
Deviations from ideality not assessed	carbon dioxide	chlorodifluoromethane	535,536,642,776
	carbon dioxide	1,1,1,2-tetrafluoroethane	777–780
	carbon dioxide	1,1,1,2,3,3,3-heptafluoropropane	781,782
	trifluoromethane	carbon disulfide	642
	chloroform	diisopropyl ether	584,649,783,784
	1,1,1-trifluoroethane	dimethyl ether	785
	chloroform	n-butyl ethyl ether	783,786
Ideal	carbon dioxide	difluoromethane	628,787–789
	difluoromethane	dimethyl ether	790–792
	difluoromethane	sulfur dioxide	793
	ethyl acetate	trichloroethylene	794
Non-ideal with non-assessed causes	sulfur dioxide	1,1,1,2,3,3,3-heptafluoropropane	795
	chlorodifluoromethane	dimethyl ether	796
	chlorodifluoromethane	carbon disulfide	642
	pentafluoroethane	dimethyl ether	566,797
	3-pentanone	1,1,2,2-tetrachloroethane	798
	dimethyl ether	1,1,1,3,3,3-hexafluoropropane	799,800
Non-ideal with enthalpic causes	dichloromethane	carbon disulfide	801,802
Non-ideal with enthalpic and entropic causes	acetone	chloroform	531,533,543,579,584,649,803–810
	chloroform	ethyl acetate	811–814
	chloroform	tetrahydrofuran	546,584,815–818
	chloroform	di-n-propyl ether	584,783,784,786,819,820
	methyl acetate	chloroform	584,811,821,822
	cyclopentanone	1,1,2,2-tetrachloroethane	823–825
	ethyl acetate	1,1,2,2-tetrachloroethane	826,827

Table 6.10. List of the 16 binary systems for which the binary association code is: BAC=7 (SA-HD). Such a BAC corresponds to a binary system involving a “Self-Associating” (SA) molecule + a “Hydrogen-Donor” (HD) 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.

<i>Origin of the deviations from ideality</i>	<i>Molecule 1</i>	<i>Molecule 2</i>	<i>References</i>
Deviations from ideality not assessed	chloroform	1-butanol	541,828,829
	1-propanol	trichloroethylene	830,831
	trichloroethylene	1-butanol	831,832
	isopropanol	trichloroethylene	830,833
	2-butanol	trichloroethylene	832,833
	1-hexyne	acetonitrile	834,835
	isopropanol	chloroform	829,836,837
Non-ideal with enthalpic causes	ethanol	1-heptyne	838,839
Non-ideal with entropic causes	ethanol	chloroform	541,586,829,840–845
	chloroform	acetic acid	846–850
	methanol	halothane	851–853
	trichloroethylene	2-methoxyethanol	854,855
Non-ideal with enthalpic and entropic causes	chloroform	acetonitrile	856–861
	ethyl formate	chloroform	811,813
	chloroform	1-propanol	542,829,862,863
	n-propyl formate	1,1,2,2-tetrachloroethane	826,864

Table 6.11. List of the 26 binary systems for which the binary association code is: BAC=8 (SA-HA). 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.

<i>Origin of the deviations from ideality</i>	<i>Molecule 1</i>	<i>Molecule 2</i>	<i>References</i>
Deviations from ideality not assessed	carbon dioxide	water	865–883
	carbon dioxide	ethanol	378,401,666,738,884–898
	ethanol	methyl tert-butyl ether	439,899–903
	carbon dioxide	2-methyl-1-propanol	904–909
	carbon monoxide	methanol	910–912
	carbon dioxide	1-pentanol	401,906,913–916
Ideal	diethylamine	ethyl acetate	632,633
	diethylamine	triethylamine	917–920
	2-methyl-2-propanol	methyl tert-butyl ether	921–924
	acetonitrile	1,4-dioxane	925–927
Non-ideal with non-assessed causes	dimethyl ether	water	592,928–931
	carbon dioxide	methanol	379,380,401,592,738,890,895,898,910,932–942
Non-ideal with enthalpic causes	methanol	ethyl acetate	943–950
	isopropanol	diisopropyl ether	720,901,951,952
	methanol	n-butyl acetate	948,953–955
	diethyl ether	ethanol	956–958
	methanol	1,4-dioxane	959–964
	methanol	thiophene	765
	ethanol	di-n-butyl ether	958,965–967
Non-ideal with entropic causes	methanol	diisopropyl ether	901,968–970
	methanol	methyl tert-butyl ether	436,438,439,900,969,971–975
	ethanol	ethyl acetate	945,948,949,967,976–983
Non-ideal with enthalpic and entropic causes	acetone	water	494,769,984–995
	ethanol	methyl ethyl ketone	450,996–1003
	ethanol	acetone	745,1004–1009
	methanol	acetone	490,494,989,1010–1015

Table 6.12. List of the 23 binary systems for which the binary association code is: BAC=9 (SA-SA). 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.

<i>Origin of the deviations from ideality</i>	<i>Molecule 1</i>	<i>Molecule 2</i>	<i>References</i>
Deviations from ideality not assessed	water	ethylenediamine	1016–1018
	water	1-pentanol	1019–1022
	methanol	1-butanol	769,1023–1027
	ethanol	acetic acid	983,1028–1031
Ideal	methanol	ethanol	814,1027,1032–1038
	2-methyl-2-propanol	1-butanol	1039–1041
	ethanol	3-methyl-1-butanol	1042–1044
	methanol	3-methyl-1-butanol	1044–1046
	methanol	1-propanol	755,992,1027,1037,1038,1047–1050
	ammonia	water	1051–1060
Non-ideal with non-assessed causes	ammonia	acetonitrile	1061
	water	allyl alcohol	1062,1063
	water	phenol	1064–1070
Non-ideal with enthalpic causes	methyl formate	methanol	1071–1075
	ethyl formate	water	1076,1077
	ethanol	ethyl formate	1075,1078–1080
	1-butanol	nitromethane	1038,1081–1085
	water	2-butoxyethanol	1086–1091
Non-ideal with entropic causes	water	propylene glycol monomethyl ether	1087
	ethanol	water	976,992,1033,1092–1112
Non-ideal with enthalpic and entropic causes	water	acetonitrile	1113–1122
	methanol	water	989,1095,1109,1110,1123–1140
	isopropanol	water	745,1097,1141–1147

The following part of this article (section 6.3) aims at explaining how the proposed database should be used to grade a thermodynamic model in order to assess its accuracy. For illustrative purpose, section 6.4 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.

6.3. Grading of a thermodynamic model by means of the proposed database in order to assess its accuracy

This section focuses initially on the methodology that has to be followed in order 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.

6.3.1. Evaluation of the deviations between model predictions and experimental data

In order 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 the Gibbs's phase rule there is not a 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, 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 two others. The arbitrary 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 is somehow similar to a T,P-flash calculation¹¹⁴⁸. For each property available in the proposed database, Table 13 reports the variance, the specified and the calculated variables. In other words, Table 6.13 dictates the methodology that has to be strictly followed in order to evaluate the deviations between model predictions and experimental data by means of the proposed database.

Table 6.13 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.

Table 6.13. 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	1	T, P, x_1	T	P, x_1
Azeotropic point				
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	$\begin{cases} x_1, y_1 & \text{for VLE} \\ x_1^\alpha, x_1^\beta & \text{for LLE} \end{cases}$
Three-phase equilibrium data (VLLE)	1	$T, P, x_1^\alpha, x_1^\beta, y_1$	T	$P, x_1^\alpha, x_1^\beta, y_1$
Enthalpy of mixing	N.A. ^(*)	T, P, z_1, h^M	T, P, z_1	h^M
Heat capacity of mixing		T, P, z_1, c_p^M		c_p^M

^(*) 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.

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, the pressure, the 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 first to be performed at specified temperature, pressure and global composition in order to determine the number of phases in equilibrium, their composition and their proportions. Once done, h^M or c_p^M can be straightforwardly calculated for the specified (T, P, z_1) values¹²⁸. 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 Excel files *database.xlsx* and *BACi with visualization of the data.xlsx* (i=1 to 9) – available in **Appendix A9** – that contain all 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 Fig. 6.3. In this example, the unknown (not stated) experimental pressure has to be replaced by the atmospheric pressure (1.0132 bar).

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)
$h^M / \text{J.mol}^{-1}$	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 6.3. Notation used in the files database.xlsx and BACi with visualization of the data.xlsx (i=1 to 9) when the experimental pressure is not mentioned.

Lastly, for any calculated property X , the MAPE (Mean Absolute Percentage Error) was selected to quantify the deviation between experimental and calculated data:

$$MAPE_X(\%) = \frac{1}{N_{data}} \sum_{i=1}^{N_{data}} 100 \cdot \left| \frac{X_i^{EXP} - X_i^{MODEL}}{X_i^{EXP}} \right| \quad (6.5)$$

6.3.2. 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. (6.5) to evaluate the $MAPE_X(\%)$. In other words, we simply apply: $N_{data} = N_{data} - 1$ in Eq. (6.5).** Here below, are detailed all 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 2-phase system is experimentally observed whereas the model predicts a 1-phase system. All the experimental data points for which the model predicts a 1-phase system are declared "out of model". This case is illustrated in Fig. 6.4 (panel a).

Case 2: at specified T and P ($T = T_{exp}$ and $P = P_{exp}$), a 2-phase system is experimentally observed and a 2-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 these experimental data points are declared *out of model*. This case – that typically appears when the azeotropic composition is not properly predicted by the model – is illustrated in Fig. 6.4 (panel b).

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 Fig. 6.4 (panel b and c).

Case 4: a 3-phase line (VLLE) is experimentally observed at $T = T_{exp}$ whereas the model does not predict such a behavior. The experimental 3-phase line is thus declared "out of model". This case is illustrated in Fig. 6.4 (panel d).

Case 5: the number of calculated critical points at $T = T_{\text{exp}}$ is different to the number of critical points experimentally observed. As an example, the binary system may exhibit 2 experimental critical points whereas 1 or zero are returned by the model (see e.g. Fig. 6.4 – panel e). The opposite may also happen: the binary system exhibits a unique critical point but 2 are returned by the model (see, e.g., Fig. 6.4 – panel f).

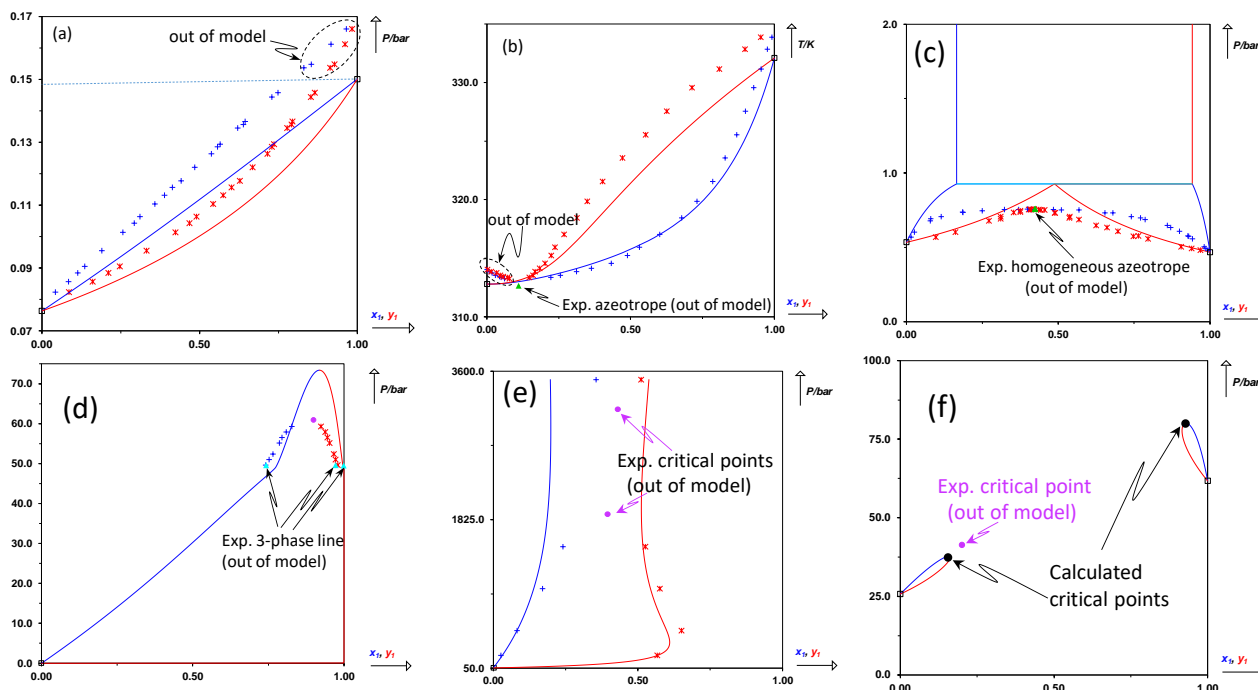


Figure 6.4. Illustration of all the cases in which out of model data points can appear. For such exp. data points, the MAPE cannot be evaluated. (a): experimentally 2-phase data points that are found to be 1-phase by the model. (b) An azeotropic system is predicted as a zeotropic system so that the homogeneous azeotrope is declared out of model. In addition, for small mole fractions, $y_{1,\text{exp}} > x_{1,\text{exp}}$ whereas the model predicts the opposite. (c) A homogeneous azeotrope is predicted as heterogeneous. (d) A 3-phase line is not predicted by the model. (e) 2 critical points that are not predicted by the model are experimentally observed. (f) The model predicts 2 critical points whereas only one is experimentally observed.

6.3.3. 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 only obtained if the model is able to exactly reproduce (with 0% deviation) all 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. (6.5)), 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 ten marks (one for each of the ten calculated properties defined in the last column of Table 13), that are:

- | | |
|---|--|
| (1) critical pressure, | (6) gas phase (or 2 nd liquid phase) composition (y_1, x_1^β |
| (2) critical composition, |), |
| (3) azeotropic pressure, | (7) three-phase pressure, |
| (4) azeotropic composition, | (8) three-phase compositions, |
| (5) liquid phase composition (x_1, x_1^α), | (9) mixing enthalpy, |

(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 nine to four by averaging the marks got by some BACs in order 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 these systems do not exhibit association (see Table 6.1). In Eq. (6.6), 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 systems - and only in this one - self-association tends to be broken (see Table 6.1). In Eq. (6.6), $mark_{BAC_5}$ 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 systems - 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 6.1). In Eq. (6.6), $mark_{BAC_6}$ is noted $mark_{CA}$ (where CA stands for "cross-association")
- The marks obtained by $BAC_7 + BAC_8 + BAC_9$ are averaged because all these systems both exhibit cross-association and self-association (see Table 6.1). In Eq. (6.6), 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. (6.6)) relative to (i) 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.

$$\left. \begin{array}{l}
 \text{Final mark} \\
 \text{of a thermodynamic model} \\
 \text{(over 20)} \\
 \\
 \text{with:} \\
 \\
 \\
 \\
 \end{array} \right\} = \frac{1}{4} \times \underbrace{\left[\underbrace{mark_{NA}}_{\text{no association}} + \underbrace{mark_{SA}}_{\text{self-association}} + \underbrace{mark_{CA}}_{\text{cross-association}} + \underbrace{mark_{CA+SA}}_{\text{cross-association + self-association}} \right]}_{\text{average of 4 marks}} \quad (6.6)$$

$$\left. \begin{array}{l}
 mark_{NA} = \frac{mark_{BAC_1} + mark_{BAC_2} + mark_{BAC_3} + mark_{BAC_4}}{4} \\
 mark_{SA} = mark_{BAC_5} \\
 mark_{CA} = mark_{BAC_6} \\
 mark_{CA+SA} = \frac{mark_{BAC_7} + mark_{BAC_8} + mark_{BAC_9}}{3}
 \end{array} \right\}$$

The procedure aimed at giving a mark over 20 to a given BAC ($mark_{BAC_i}$) 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 2nd liquid phase) composition y (or x^β), three-phase pressure P_{LLV} , three-phase compositions 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 liquid phase composition (x for VLE and x^α for LLE):

$$Mark_{x \text{ or } x^\alpha} = 20 - 0.5 \times \left[\frac{MAPE \text{ on } x_1 \text{ or } x_1^\alpha (\%) + MAPE \text{ on } x_2 \text{ or } x_2^\alpha (\%)}{2} \right] \quad (6.7)$$

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

- (2) Mark in gas phase (y) or 2nd liquid phase (x^β) composition:

$$Mark_{y \text{ or } x^\beta} = 20 - 0.5 \times \left[\frac{MAPE \text{ on } y_1 \text{ or } x_1^\beta (\%) + MAPE \text{ on } y_2 \text{ or } x_2^\beta (\%)}{2} \right] \quad (6.8)$$

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 $x_{1,exp} = 0.000002$. In the case a model calculates $x_1 = 0.000082$, the corresponding $\frac{1}{2} \times (MAPE \text{ on } x_1 + MAPE \text{ on } x_2)$ relative to this unique data point is about 2000 % even though the absolute deviation is extremely small ($|x_{1,exp} - x_{1,cal}| = 0.00008$). Such a datapoint can thus have a huge influence on the calculated

$Mark_{x \text{ or } x^\alpha}$ (or $Mark_{y \text{ or } x^\beta}$). To avoid such a bias, if:

$$\begin{cases} z_{1,exp} < 0.01 \\ \text{or} \\ z_{1,exp} > 0.99 \end{cases} \text{ and simultaneously } \frac{1}{2} \times (MAPE \text{ on } z_1 + MAPE \text{ on } z_2) > 45\% \quad (6.9)$$

where z_1 stands for the mole fraction of component 1 in the liquid or gas phase of a 2-phase system (VLE or LLE), the corresponding datapoint is **rejected** (we here mean, it is not taken into account in Eq. (6.5) in order to annihilate its influence on the calculated $Mark_{x \text{ or } x^\alpha}$ (or $Mark_{y \text{ or } x^\beta}$)). **In other**

words, we simply apply: $x_i^{MODEL} = x_i^{EXP}$ and $N_{data} = N_{data} - 1$ in Eq. (6.5).

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

$$Mark_{P_{LLV}} = 20 - 0.50 \times MAPE \text{ on } P_{LLV} (\%) \quad (6.10)$$

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

$$Mark_{z_{LLV}} = 20 - 0.5 \times \sum_{i=1}^2 \left[\frac{MAPE \text{ on } x_i^\alpha (\%) + MAPE \text{ on } x_i^\beta (\%) + MAPE \text{ on } y_i (\%)}{6} \right] \quad (6.11)$$

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

- (5) Mark in critical pressure, P_c :

$$Mark_{P_c} = 20 - 0.75 \times MAPE \text{ on } P_c (\%) \quad (6.12)$$

- (6) Mark in critical composition, x_c :

$$Mark_{x_c} = 20 - 0.5 \times \left[\frac{MAPE \text{ on } x_{1,c} (\%) + MAPE \text{ on } x_{2,c} (\%)}{2} \right] \quad (6.13)$$

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

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

$$Mark_{P_{az}} = 20 - 0.50 \times MAPE \text{ on } P_{az} (\%) \quad (6.14)$$

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

$$Mark_{x_{az}} = 20 - 0.5 \times \left[\frac{MAPE \text{ on } x_{1,az} (\%) + MAPE \text{ on } x_{2,az} (\%)}{2} \right] \quad (6.15)$$

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

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

$$Mark_{h^M} = 20 - 0.25 \times \frac{1}{N_{data}} \sum_{i=1}^{N_{data}} \frac{1}{2} \left(100 \cdot \left| \frac{h_i^{M,EXP} - h_i^{M,MODEL}}{h_i^{M,EXP}} \right| + 100 \cdot \left| \frac{h_i^{M,EXP} - h_i^{M,MODEL}}{h_i^{M,MODEL}} \right| \right) \quad (6.16)$$

Remarks:

1. h^M goes to zero when the mole fraction of the studied phase (z_1) goes to zero or one. 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. (6.16):

$$\frac{1}{2} \left(100 \cdot \left| \frac{h_i^{M,EXP} - h_i^{M,MODEL}}{h_i^{M,EXP}} \right| + 100 \cdot \left| \frac{h_i^{M,EXP} - h_i^{M,MODEL}}{h_i^{M,MODEL}} \right| \right) > 80\%, \text{ this quantity is set to } 80\%.$$

2. Eq. (6.16) highlights that we here decided to make the average between 2 MAPEs: one calculated with the classical definition (see Eq. (6.5)) and one obtained by introducing $h_i^{M,MODEL}$ (i.e., the calculated value) at the denominator. This procedure is selected in order 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 $h^{M,EXP} = 100 \text{ J} \cdot \text{mol}^{-1}$. If the calculated value is 50 times too small, let us say: $h^{M,MODEL} = 2 \text{ J} \cdot \text{mol}^{-1}$ then Eq. (6.5) returns a $MAPE_{h^M}(\%) = 98\%$. In contrast, if the calculated value is 50 times too large, that is: $h^{M,MODEL} = 5000 \text{ J} \cdot \text{mol}^{-1}$ then Eq. (6.5) returns a $MAPE_{h^M}(\%) = 4900\%$. 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 ($h^{M,MODEL} = 2 \text{ J} \cdot \text{mol}^{-1}$ or $h^{M,MODEL} = 5000 \text{ J} \cdot \text{mol}^{-1}$), the average of the 2 MAPEs embedded in Eq. (6.16) is exactly the same. For the selected example:

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

3. In practice, h^M is used to evaluate molar enthalpies of the streams ($h_{stream} = z_1 h_1 + z_2 h_2 + h^M$) that are involved in the energy balance of a given process. The mark determined by Eq. (6.16) thus needs to capture the influence of h^M on such a balance. One possibility to reach

this target is to convert the difference $\left| h_i^{M,EXP} - h_i^{M,MODEL} \right|$ into terms of temperature effect¹²⁸

ΔT_h through:

$$\Delta T_h = \frac{\left| h_i^{M,EXP} - h_i^{M,MODEL} \right|}{c_p} \quad (6.17)$$

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. (6.16) is conceived so that with this deviation the mark is equal to 15/20.

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

$$Mark_{c_p^M} = 20 - 0.10 \times \frac{1}{N_{data}} \sum_{i=1}^{N_{data}} \frac{1}{2} \left(100 \cdot \left| \frac{c_{p,i}^{M,EXP} - c_{p,i}^{M,MODEL}}{c_{p,i}^{M,EXP}} \right| + 100 \cdot \left| \frac{c_{p,i}^{M,EXP} - c_{p,i}^{M,MODEL}}{c_{p,i}^{M,MODEL}} \right| \right) \quad (6.18)$$

This mark was built 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 zero when the mole fraction of the studied phase (z_1) goes to zero or one. 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. (6.18):

$$\frac{1}{2} \left(100 \cdot \left| \frac{c_{p,i}^{M,EXP} - c_{p,i}^{M,MODEL}}{c_{p,i}^{M,EXP}} \right| + 100 \cdot \left| \frac{c_{p,i}^{M,EXP} - c_{p,i}^{M,MODEL}}{c_{p,i}^{M,MODEL}} \right| \right) > 200\% \text{ this quantity is set to } 200\%.$$

2. The choice of Eq. (6.18) 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 lead to an average deviation of only 2% on the molar isobaric heat capacity of the corresponding stream calculated as: $c_{p,stream} = z_1 c_{p,1} + z_2 c_{p,2} + c_p^M$. In consequence, Eq. (6.18) is built so that a deviation of 50% on c_p^M leads to a good mark of 15/20.

Important remark: any mark below zero is raised to zero.

And, in the end:

$$Mark_{BAC_i} = average \left(\begin{matrix} Mark_{x \text{ or } x^\alpha}; Mark_{y \text{ or } x^\beta}; Mark_{P_{LLV}}; Mark_{z_{LLV}}; Mark_{P_c}; \\ Mark_{x_c}; Mark_{P_{az}}; Mark_{x_{az}}; Mark_{h^M}; Mark_{c_p^M} \end{matrix} \right) \quad (6.19)$$

To conclude, ten 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. (6.19). As an example, none of the binary systems embedded in BAC₂ contain 3-phase equilibrium data so that $Mark_{P_{LLV}}$ and $Mark_{z_{LLV}}$ cannot be evaluated. For BAC₂, the given mark (Eq. (6.19)) is the average of only 8 marks (instead of 10).

It is worth noting that the previous equations (from Eq. (6.7) to Eq. (6.18)) 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. (6.12), 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. (6.18), a similar MAPE of 13 % on the mixing heat capacities leads to a $Mark_{c_p^M}$ of 18.7/20 and a MAPE of 26 % leads to a $Mark_{c_p^M}$ of 17.4/20.

6.4. Illustration: grading and discussion around the accuracy of the Peng-Robinson EoS with classical mixing rules and a temperature-dependent BIP

6.4.1. The 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^{34,1149} (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 the experimental properties contained in the database are unaffected by a temperature-independent volume translation^{41,133}.

For a pure component, the PR EoS is:

$$P = \frac{RT}{v - b_i} - \frac{a_i(T)}{v(v + b_i) + b_i(v - b_i)} \quad (6.20)$$

Although non-consistent^{32,35,97} at very high temperatures, it was decided to classically use the Soave-type³³ α -function proposed by Peng and Robinson¹¹⁴⁹ in 1978. An updated version has however recently been developed by Piña-Martinez¹¹⁵⁰ and coworkers (including Peng). We thus used:

$$\text{and} \left\{ \begin{array}{l} R = 8.314472 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1} \\ X = \left[1 + \sqrt[3]{4 - 2\sqrt{2}} + \sqrt[3]{4 + 2\sqrt{2}} \right]^{-1} \approx 0.253076587 \\ b_i = \Omega_b \frac{RT_{c,i}}{P_{c,i}} \text{ with: } \Omega_b = \frac{X}{X + 3} \approx 0.0777960739 \\ a_i(T) = a_{c,i} \alpha_i(T) \text{ with } \left\{ \begin{array}{l} a_{c,i} = \Omega_a \frac{R^2 T_{c,i}^2}{P_{c,i}} \text{ and } \Omega_a = \frac{8(5X + 1)}{49 - 37X} \approx 0.457235529 \\ \alpha_i(T) = \left[1 + m_i \left(1 - \sqrt{\frac{T}{T_{c,i}}} \right) \right]^2 \end{array} \right. \\ \text{if } \omega_i \leq 0.491 \text{ then } m_i = 0.37464 + 1.54226\omega_i - 0.26992\omega_i^2 \\ \text{if } \omega_i > 0.491 \text{ then } m_i = 0.379642 + 1.48503\omega_i - 0.164423\omega_i^2 + 0.016666\omega_i^3 \end{array} \right. \quad (6.21)$$

where P is the pressure, R is the gas constant, T is the temperature, a_i and b_i are the cohesive parameter and molar co-volume of 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 methods¹¹⁵¹.

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 rules¹¹⁵² are used in this study:

$$\begin{cases} a(T, \mathbf{z}) = \sum_{i=1}^N \sum_{j=1}^N z_i z_j \sqrt{a_i(T) \cdot a_j(T)} [1 - k_{ij}(T)] \\ b(\mathbf{z}) = \sum_{i=1}^N z_i b_i \end{cases} \quad (6.22)$$

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. (6.23)) is the one used in the well-established PPR78^{1153–1158} and PR₂SRK¹¹⁵⁹ models and contains 2 parameters (A_{ij} and B_{ij}) for the binary system $i + j$.

$$k_{ij}(T) = \frac{A_{ij} \left(\frac{298.15}{T} \right)^{B_{ij}-1} - \left(\frac{\sqrt{a_i}}{b_i} - \frac{\sqrt{a_j}}{b_j} \right)^2}{2 \times \frac{\sqrt{a_i}}{b_i} \times \frac{\sqrt{a_j}}{b_j}} \quad (6.23)$$

6.4.2. The fitting procedure

The selected model is a correlative (i.e., non-predictive) model and for a given binary system, the two parameters involved in Eq. (6.23) have to be fitted against experimental data. In this work, it was decided that the two parameters would be determined, system by system, in order 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 data, heat capacity of mixing data and enthalpy of mixing data) and model predictions. The selected objective function expression is:

$$F_{\text{obj}} = \frac{\left(F_{\text{obj}, x \text{ or } x^\alpha} + F_{\text{obj}, y \text{ or } x^\beta} + F_{\text{obj}, P_{LLV}} + F_{\text{obj}, z_{LLV}} + F_{\text{obj}, P_c} \right) + F_{\text{obj}, x_c} + F_{\text{obj}, P_{az}} + F_{\text{obj}, x_{az}} + F_{\text{obj}, h^M} + F_{\text{obj}, c_p^M}}{n_{x \text{ or } x^\alpha} + n_{y \text{ or } x^\beta} + 2n_{\text{triph}} + 2n_{\text{crit}} + 2n_{\text{az}} + n_{h^M} + n_{c_p^M}} \quad (6.24)$$

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

$$\begin{cases} F_{\text{obj}, x \text{ or } x^\alpha} = 100 \sum_{i=1}^{n_{x \text{ or } x^\alpha}} 0.5 \left(\frac{|\Delta x|}{x_{1, \text{exp}} \text{ (or } x_{1, \text{exp}}^\alpha)} + \frac{|\Delta x|}{x_{2, \text{exp}} \text{ (or } x_{2, \text{exp}}^\alpha)} \right) \\ \text{with: } |\Delta x| = |x_{1, \text{exp}} \text{ (or } x_{1, \text{exp}}^\alpha) - x_{1, \text{cal}} \text{ (or } x_{1, \text{cal}}^\alpha)| \end{cases} \quad (6.25)$$

$$F_{\text{obj}, x \text{ or } x^\alpha} / n_{x \text{ or } x^\alpha}$$

$n_{x \text{ or } x^\alpha}$ 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 in order to reduce this huge deviation to the detriment of other compositions. To avoid such a bias, if $x_{1, \text{exp}} < 0.01$ (or $x_{1, \text{exp}} > 0.99$) and simultaneously $50 \left(\frac{|\Delta x|}{x_{1, \text{exp}} \text{ (or } x_{1, \text{exp}}^\alpha)} + \frac{|\Delta x|}{x_{2, \text{exp}} \text{ (or } x_{2, \text{exp}}^\alpha)} \right) > 45\%$, the corresponding deviation was not included in the calculation of $F_{\text{obj}, x \text{ or } x^\alpha}$.

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

$$\left\{ \begin{array}{l} F_{\text{obj}, y \text{ or } x^\beta} = 100 \sum_{i=1}^{n_{y \text{ or } x^\beta}} 0.5 \left(\frac{|\Delta y|}{y_{1, \text{exp}} \text{ (or } x_{1, \text{exp}}^\beta)} + \frac{|\Delta y|}{x_{2, \text{exp}} \text{ (or } x_{2, \text{exp}}^\beta)} \right)_i \\ \text{with: } |\Delta y| = |y_{1, \text{exp}} \text{ (or } x_{1, \text{exp}}^\beta) - y_{1, \text{cal}} \text{ (or } x_{1, \text{cal}}^\beta)| \end{array} \right. \quad (6.26)$$

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

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

$$F_{\text{obj}, P_{\text{LLV}}} = 100 \sum_{i=1}^{n_{\text{triph}}} \left(\frac{|P_{\text{LLV}, \text{exp}} - P_{\text{LLV}, \text{cal}}|}{P_{\text{LLV}, \text{exp}}} \right)_i \quad (6.27)$$

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

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

$$F_{\text{obj}, z_{\text{LLV}}} = 100 \sum_{i=1}^{n_{\text{triph}}} \frac{1}{6} \left(\frac{|\Delta x^\alpha|}{x_{1, \text{exp}}^\alpha} + \frac{|\Delta x^\alpha|}{x_{2, \text{exp}}^\alpha} + \frac{|\Delta x^\beta|}{x_{1, \text{exp}}^\beta} + \frac{|\Delta x^\beta|}{x_{2, \text{exp}}^\beta} + \frac{|\Delta y|}{y_{1, \text{exp}}} + \frac{|\Delta y|}{y_{2, \text{exp}}} \right)_i \quad (6.28)$$

with:
$$\left\{ \begin{array}{l} |\Delta x^\alpha| = |x_{1, \text{exp}}^\alpha - x_{1, \text{cal}}^\alpha| = |x_{2, \text{exp}}^\alpha - x_{2, \text{cal}}^\alpha| \\ |\Delta x^\beta| = |x_{1, \text{exp}}^\beta - x_{1, \text{cal}}^\beta| = |x_{2, \text{exp}}^\beta - x_{2, \text{cal}}^\beta| \\ |\Delta y| = |y_{1, \text{exp}} - y_{1, \text{cal}}| = |y_{2, \text{exp}} - y_{2, \text{cal}}| \end{array} \right.$$

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

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

$$F_{\text{obj}, P_c} = 100 \sum_{i=1}^{n_{\text{crit}}} \left(\frac{|P_{c, \text{exp}} - P_{c, \text{cal}}|}{P_{c, \text{exp}}} \right)_i \quad (6.29)$$

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

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

$$F_{\text{obj}, x_c} = 100 \sum_{i=1}^{n_{\text{crit}}} 0.5 \left(\frac{|\Delta x_c|}{x_{c1, \text{exp}}} + \frac{|\Delta x_c|}{x_{c2, \text{exp}}} \right) |\Delta x_c| = |x_{c1, \text{exp}} - x_{c1, \text{cal}}| = |x_{c2, \text{exp}} - x_{c2, \text{cal}}| \quad (6.30)$$

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

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

$$F_{\text{obj}, P_{\text{az}}} = 100 \sum_{i=1}^{n_{\text{az}}} \left(\frac{|P_{\text{az}, \text{exp}} - P_{\text{az}, \text{cal}}|}{P_{\text{az}, \text{exp}}} \right)_i \quad (6.31)$$

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

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

$$F_{\text{obj}, x_{\text{az}}} = 100 \sum_{i=1}^{n_{\text{az}}} 0.5 \left(\frac{|\Delta x_{\text{az}}|}{x_{\text{az1}, \text{exp}}} + \frac{|\Delta x_{\text{az}}|}{x_{\text{az2}, \text{exp}}} \right) |\Delta x_{\text{az}}| = |x_{\text{az1}, \text{exp}} - x_{\text{az1}, \text{cal}}| = |x_{\text{az2}, \text{exp}} - x_{\text{az2}, \text{cal}}| \quad (6.32)$$

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

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

$$F_{\text{obj}, h^M} = 100 \sum_{i=1}^{n_{h^M}} 0.5 \left(\left| \frac{h_{\text{exp}}^M - h_{\text{cal}}^M}{h_{\text{exp}}^M} \right| + \left| \frac{h_{\text{exp}}^M - h_{\text{cal}}^M}{h_{\text{cal}}^M} \right| \right)_i \quad (6.33)$$

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

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

$$F_{\text{obj}, c_p^M} = 100 \sum_{i=1}^{n_{c_p^M}} 0.5 \left(\left| \frac{c_{p, \text{exp}}^M - c_{p, \text{cal}}^M}{c_{p, \text{exp}}^M} \right| + \left| \frac{c_{p, \text{exp}}^M - c_{p, \text{cal}}^M}{c_{p, \text{cal}}^M} \right| \right)_i \quad (6.34)$$

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

Important remark: Section 6.3 of this paper, devoted to the grading of a thermodynamic model, dictates the methodology that has to be strictly followed in order to evaluate the deviations between model predictions and experimental data by means of 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. (6.23). In the case our goal would have been to assess the accuracy of a predictive thermodynamic model in which the binary interaction parameters are determined by group-contribution (e.g., PSRK^{1160,1161}, VTPR^{1162,1163}, UMR-PRU^{19,20}, PPR78¹¹⁵³, MHV1-UNIFAC¹¹⁶⁴, etc.), the experimental data of the proposed database would not have been used for parameterization purpose.

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 zero. 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 experience¹⁸ that such an influence may be huge.

6.4.3. 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 Supporting Information. This very detailed analysis (over 1000 pages) includes:

1. information on how the system deviates from ideality,
2. the values of the *A* and *B* optimal parameters (see Eq.(6.23)),
3. the values of the ten objective functions (from Eq. (6.25) to Eq.(6.34)). In the Supporting Information,
 - *MAPE on x* refers to Eq. (6.25)
 - *MAPE on y* refers to Eq. (6.26)
 - *MAPE on p_{LLV}* refers to Eq. (6.27)
 - *MAPE on z_{LLV}* refers to Eq. (6.28)
 - *MAPE on p_c* refers to Eq. (6.29)
 - *MAPE on x_c* refers to Eq. (6.30)
 - *MAPE on p_{oz}* refers to Eq. (6.31)
 - *MAPE on x_{oz}* refers to Eq. (6.32)
 - *MAPE on h^M* refers to Eq. (6.33)
 - *MAPE on c_p^M* refers to Eq. (6.34)
4. the so-called GPED (global phase equilibrium diagram) – calculated by the PR EoS – enabling to immediately identify the binary system class according to the scheme proposed by Van Konynenburg and Scott¹⁷²,
5. all the experimental data with the corresponding references,
6. all 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 Supporting Information.

6.4.4. *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 6.14.

Table 6.14. 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 9 binary association codes (BACs). The abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”.

Binary association code	Type of association	MAPE on:									
		x Eq. (6.25)	y Eq. (6.26)	P_{LLV} Eq. (6.27)	z_{LLV} Eq. (6.28)	P_c Eq. (6.29)	x_c Eq. (6.30)	P_{az} Eq. (6.31)	x_{az} Eq. (6.32)	h^M Eq. (6.33)	c_p^M Eq. (6.34)
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%

Such MAPEs make it possible to give a score over 20 to each of the 9 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. (6.19)). Such marks can be found in Table 6.15. At the end, as previously explained, the marks obtained by BACs 1 to 4 and BACs 7 to 9 are averaged in order to only retain 4 categories (BAC₁-BAC₄; BAC₅; BAC₆; BAC₇-BAC₉) of binary systems based on the type of association they exhibit. By averaging the marks of these 4 categories of binary systems (see Eq.(6.6)), the model: {PR EoS + classical mixing rules with a T-dependent k_{ij} } receives the final mark of **12.3/20**.

Table 6.15. Rating of the 9 binary association codes in order to finally grade the model: {PR EoS + classical mixing rules with a T-dependent k_{ij} }. The abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”.

Binary association code (BAC)	Type of association	Mark on:										Binary association code mark Eq. (6.19)	Mark (over 20) by type of association Eq. (6.6)	Final mark of the PR EoS with classical MR and T-dependent BIPS Eq. (6.6)
		x Eq. (6.7)	y Eq. (6.8)	P_{LLV} Eq. (6.10)	z_{LLV} Eq. (6.11)	P_c Eq. (6.12)	x_c Eq. (6.13)	p_{az} Eq. (6.14)	x_{az} Eq. (6.15)	h^M Eq. (6.16)	c_p^M Eq. (6.18)			
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	$mark_{NA}$ = 15.5 no association	12.3/20
2 (HA-NA)		15.6	16.6	-	-	18.2	15.5	19.5	16.9	15.9	4.0	15.3		
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	$mark_{SA}$ = 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	$mark_{CA}$ = 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	$mark_{CA+SA}$ = 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		

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 Fig. 6.5 for each category of binary systems based on the type of association they exhibit.

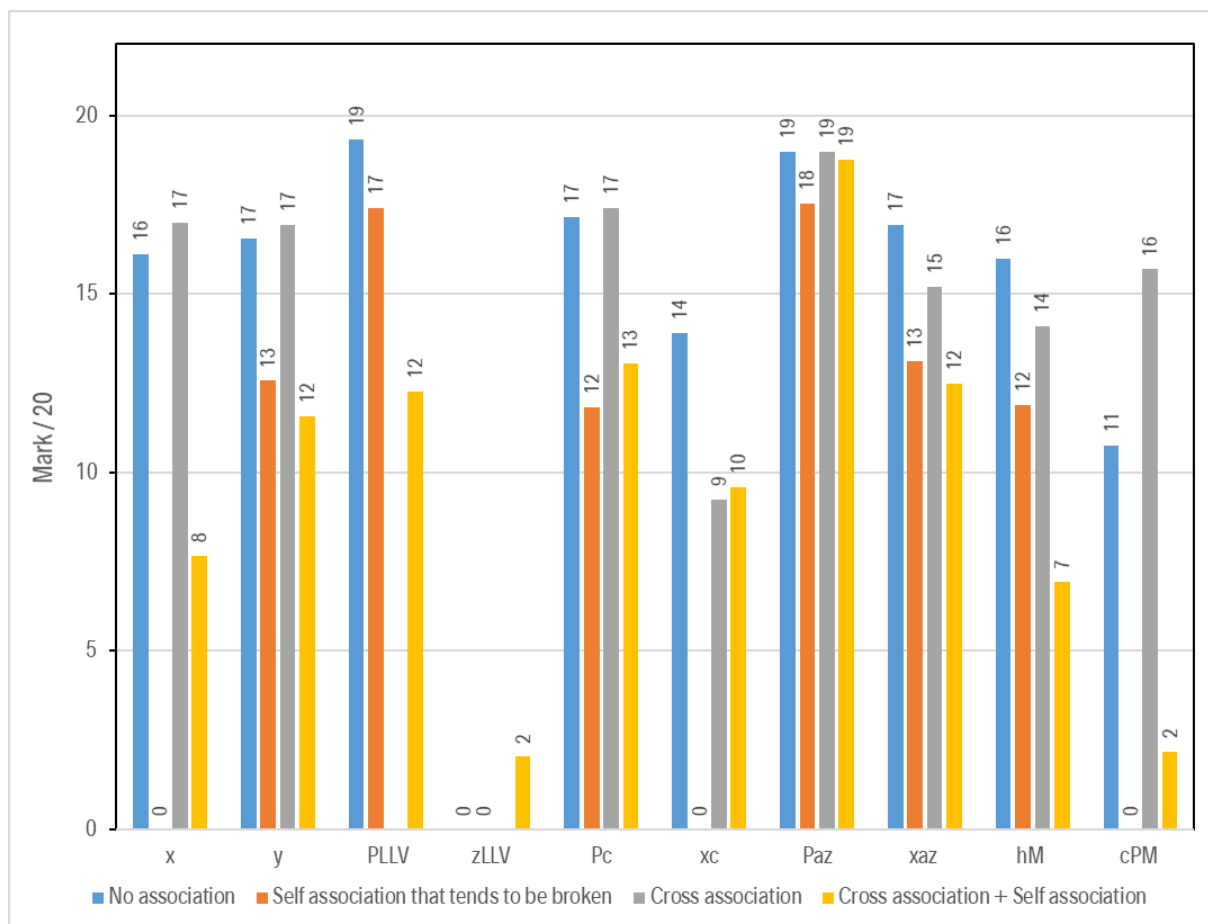


Figure 6.5 . Overview of the accuracy of the model: {PR EoS + classical mixing rules with a T-dependent k_{ij} } by plotting the marks in ten properties for the four categories of binary systems based on the type of association they exhibit.

Fig. 6.5 and Table 6.15 highlight that with an excellent mark of 15.6/20, the binary systems that exhibit cross-association alone are those which 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 from 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 zero. In such systems, a non-associating component is mixed with a self-associating compound so that self-association (partially) persists in the mixture. The non-associating 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 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 to 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 the very good mark of 15.5/20. The identified weakness is the inaccurate correlation of the composition of the phases in equilibrium when the system exhibits a three-phase line. This weakness highlights the difficulty to simultaneously correlate VLE and LLE data with a unique set of adjustable parameters. Non-associating systems often belong to type-I systems but some fall into type-III, especially when the 2 compounds show a high size-asymmetry.

This analysis allows 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 to form new ones are not involved.

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

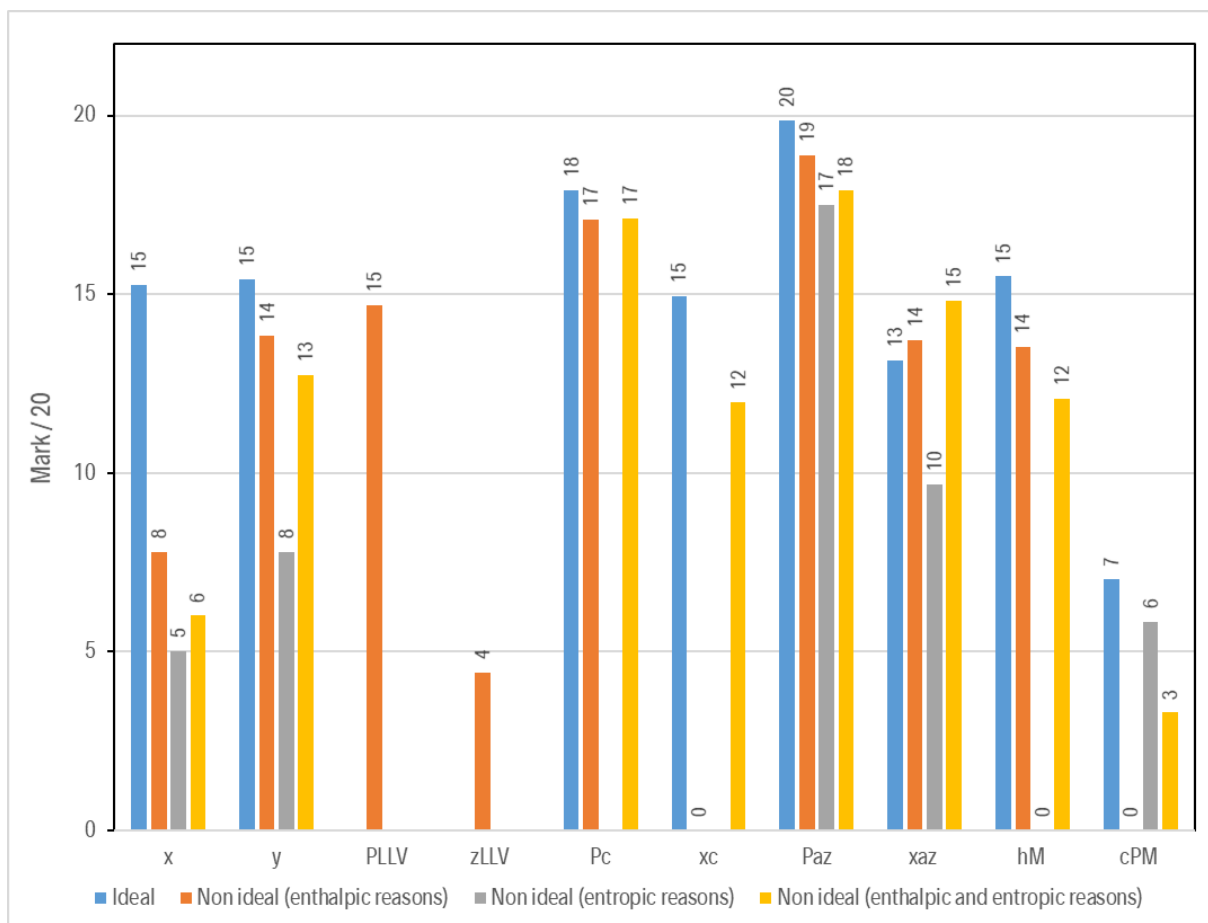


Figure 6.6. Marks in 10 properties calculated for five categories of binary systems based on how they deviate from ideality (marks on VLLE data are not shown due to a lack of information for some categories of binary systems).

Fig. 6.6 shows that except for the liquid phase composition (including the critical composition), all the other properties are correlated with a similar accuracy both for ideal and non-ideal 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.

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.

6.5. Conclusion

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 database's systems on the base 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 non-ideal. 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 the 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 weak point is the poor correlation of systems in which hydrogen bonds are broken without the possibility to form 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 to improve the model efficiency.

Last but not 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.

**Chapter 7 : Evaluation of the Universal Mixing Rule
Peng-Robinson EoS with UNIFAC-type model using
a benchmark database for thermodynamic models**

7.1 Introduction

In the past, the Universal Mixing Rule Peng-Robinson with a UNIFAC-type model (UMR-PRU) model, proposed by Voutsas et al.^{19,20}, has shown accurate predictions of a wide array of mixtures: Louli et al.¹¹⁶⁵ used it to predict dew point experimental data for six mixtures of synthetic natural gas and two of real natural gas. They compared the performance of the UMR-PRU with the PR EoS (with zero binary interaction parameters) and the PPR78 EoS¹¹⁶⁶ (with temperature-dependent binary interaction parameters) in describing dew point data for their natural gas mixtures. They found that the UMR-PRU performs just as well as the PR (AAD = 0.8% overall for both models over all mixtures studied) and slightly better than the PPR78 (which has an AAD=1.1%). A similar study for natural gas mixtures was performed by Novak et al.¹¹⁶⁷ where they found that the UMR-PRU performs best for dew point data predictions over the PC-SAFT, the Soave-Redlich-Kwong (SRK) EoS³³ and the PR EoS and that both the UMR-PRU and PR are best suited for liquid dropout calculations. In a following study, Novak et al. used the UMR-PRU with the Mathias-Copeman¹¹⁶⁸ (MC) $\alpha(T)$ function to predict VLE and dew point data for natural gas mixtures finding overall improvement over UMR-PRU with the Soave $\alpha(T)$ function.

Petropoulou et al.¹¹⁶⁹ compared the performance of the UMR-PRU with the PR with the Van der Waals one-fluid mixing rules and the Cubic-Plus Association (CPA)¹⁰⁸ PR in describing different natural gas mixtures with associating molecules, such as water, methanol and mono ethylene glycol (MEG). They showed that the CPA-PR predicted better the solubility of methane in the methane-water-methanol system (AAD in $x_{\text{methane}}=32\%$) than the UMR-PRU (AAD in $x_{\text{methane}}=90\%$). The opposite was found to be true, where the UMR-PRU performed better describing the solubility of methane for methane-water-MEG mixtures (AAD in $x_{\text{methane}}=25\%$) than the CPA-PR (AAD in $x_{\text{methane}}=32\%$). They also showed that both models performed better than the PR EoS at predicting dew point data. On a followup study, Petropoulou & Voutsas¹¹⁷⁰ extended the model to mixtures with triethylene glycol (TEG) mixtures to simulate natural gas dehydration with satisfactory results.

Koulocheris et al.¹¹⁷¹ used the UMR-PRU model to describe hydrocarbon mixtures containing hydrogen. They compared their VLE predictions to the PPR78 and found that both models are capable of accurate VLE predictions, with the UMR-PRU yielding the lowest deviations from experimental data, with global average deviation of 4.7% over the 7.5% of the PPR78.

On a different study, Koulocheris et al. used the UMR-PRU to describe various mixtures containing mercury. They found an overall deviation of 4.38% for all mixtures studied. They compared their results with the MC-PR EoS (overall deviations equal to 5.6%) and the SRK EoS with a Twu $\alpha(T)$ ¹¹⁷² (overall deviations of 6.31% with optimized k_{ij}) and concluded that, in spite of all models being able to describe mixtures containing mercury, the UMR-PRU was the most accurate.

Plakia et al.¹¹⁷³ used the UMR-PRU model to perform phase equilibrium calculations for CO₂-water-alkanolamine mixtures. They found an average deviation in pressure of 36.4% for mixtures including monoethanolamine, and 31.5% for methyldiethanolamine. They compared

their results with the electrolyte Non-Random Two Liquid (e-NRTL)¹¹⁷⁴ model finding similar accuracy between the two models.

The purpose of this study is to evaluate the accuracy of the Universal Mixing Rule Peng-Robinson with a UNIFAC-type model (UMR-PRU) according to the previously proposed database²¹ for benchmarking thermodynamic models. In this report, the UMR-PRU model is described in the first section, followed by a description of the main characteristics of the benchmark database. Next, grading procedure is detailed in the third section along with two modifications with respect to the original grading procedure introduced by Pina-Martinez et al.¹³⁰. The Simulis Thermodynamics Software used for the thermodynamic calculations and additional considerations for the UMR-PRU model are discussed in the fourth section. The results obtained with the UMR-PRU and the grading are discussed in the fifth section. Finally, a discussion of the results compared to other benchmarked models will be presented in the sixth section.

7.2. UMR-PRU model

The UMR-PRU model^{19,20} is an EoS/g^E type thermodynamic model, where the universal mixing rule (UMR) is applied by coupling the Peng-Robinson (PR) equation of state (EoS) with an UNIFAC-type model¹¹⁷⁵. The Peng-Robinson (PR) equation of state (EoS)^{34,1149} writes,

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} \quad (7.1)$$

In the equation, P is pressure, T is temperature, and v is molar volume. The gas constant $R = 8.314472 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$. The PR-EoS includes two parameters: the attractive term parameter a and the co-volume parameter b . For a pure component i , a and b are given by

$$\begin{cases} a_i = 0.45724 \frac{R^2 T_{c,i}^2}{P_{c,i}} \alpha(T) \\ b_i = 0.0778 \frac{RT_{c,i}}{P_{c,i}} \end{cases} \quad (7.2)$$

$T_{c,i}$ is the critical temperature, and $P_{c,i}$ is the critical pressure of component i . The function $\alpha(T)$ can be estimated by the Mathias-Copeman (MC) equation¹¹⁶⁸,

$$\begin{cases} \text{if } T \leq T_{c,i}, \alpha(T) = \left[1 + c_{1,i} \left(1 - \sqrt{\frac{T}{T_{c,i}}} \right) + c_{2,i} \left(1 - \sqrt{\frac{T}{T_{c,i}}} \right)^2 + c_{3,i} \left(1 - \sqrt{\frac{T}{T_{c,i}}} \right)^3 \right]^2 \\ \text{if } T > T_{c,i}, \alpha(T) = \left[1 + c_{1,i} \left(1 - \sqrt{\frac{T}{T_{c,i}}} \right) \right]^2 \end{cases} \quad (7.3)$$

The pure-compound-specific parameters $c_{1,i}$, $c_{2,i}$, and $c_{3,i}$ are determined by fitting vapor pressure data of pure component i . Alternatively, if the parameters are not available due to a lack of experimental data, the Soave³³ $\alpha(T)$ function, as defined by Peng and Robinson³⁴, is used instead:

$$\begin{cases} \text{if } \omega_i \leq 0.491, c_{1,i} = 0.37464 + 1.54226\omega_i - 0.26992\omega_i^2, \\ \text{if } \omega_i > 0.491, c_{1,i} = 0.379642 + 1.48503\omega_i - 0.164423\omega_i^2 + 0.016666\omega_i^3 \\ c_{2,i} = 0 \\ c_{3,i} = 0 \end{cases} \quad (7.4)$$

For a mixture, the following Universal Mixing Rule (UMR)²⁰ is applied for calculating parameters a and b ,

$$\begin{cases} \frac{a}{bRT} = \sum_i x_i \frac{a_i}{b_i RT} + \frac{1}{A_c} \frac{g_{AC}^{E,SG} + g_{AC}^{E,res}}{RT} \\ b = \sum \sum x_i x_j b_{ij}, \text{ with } b_{ij} = (b_i^{1/2} + b_j^{1/2})^2 \end{cases} \quad (7.5)$$

A_c in the above equation is a constant that depends on the cubic EoS used. For the PR EoS $A_c = -0.53$. The terms $g_{AC}^{E,SG}$ and $g_{AC}^{E,res}$ in equation (5) are the Staverman-Guggenheim term of the combinatorial part and the residual part of the excess Gibbs free energy (g^E), respectively, obtained from the UNIFAC (UNIQUAC Functional-group Activity Coefficient) model¹¹⁷⁵. In the latter, molecules are considered as consisting of functional groups, and the activity coefficients of the components in a mixture are calculated by using a group contribution method. To be specific, in the UNIFAC model $g_{AC}^{E,SG}$ and $g_{AC}^{E,res}$ are computed with the equations,

$$\frac{g_{AC}^{E,SG}}{RT} = 5 \sum_i x_i q_i \ln \frac{\theta_i}{\phi_i} \quad (7.6)$$

$$\frac{g_{AC}^{E,res}}{RT} = \sum_i x_i v_k^i (\ln \Gamma_k - \ln \Gamma_k^{(i)}) \quad (7.7)$$

In equation (6), x_i is the mole fraction of component i in the mixture. θ_i and ϕ_i are the surface area fraction and the volume fraction of component i in the mixture, respectively. θ_i and ϕ_i are calculated from the Van der Waals surface area parameter q_i and volume parameter r_i ,

$$\theta_i = \frac{q_i}{\sum_j x_j q_j} \quad (7.8)$$

$$\phi_i = \frac{r_i}{\sum_j x_j r_j} \quad (7.9)$$

The Van der Waals surface area parameter q_i and volume parameter r_i of component i are calculated by a group contribution method,

$$q_i = \sum_k v_k^i Q_k \quad (7.10)$$

$$r_i = \sum_k v_k^i R_k \quad (7.11)$$

Q_k and R_k indicate the Van der Waals surface area and volume contributions of group k , and v_k^i indicates the number of occurrences of group k in the molecule i .

In the equation (7.7), Γ_k is the residual activity coefficient of group k in the mixture. $\Gamma_k^{(i)}$ is the residual activity coefficient of group k in the system consisting only of molecule i (i.e. pure component i system). Γ_k and $\Gamma_k^{(i)}$ are calculated with the equation,

$$\ln \Gamma_k = Q_k \left[1 - \ln \sum_m \Theta_m \Psi_{mk} - \sum_m \frac{\Theta_m \Psi_{km}}{\sum_n \Theta_n \Psi_{nm}} \right] \quad (7.12)$$

Θ_m , which is the surface area fraction of group m in the system (mixture or pure-component), is calculated with the equation,

$$\Theta_m = \frac{Q_m X_m}{\sum_n Q_n X_n} \quad (7.13)$$

X_m is the mole fraction of group m in the system.

In the equation (7.12), Ψ_{nm} indicates the interaction between group n and group m . It can be calculated with

$$\Psi_{nm} = \exp \left[-\frac{A_{nm} + B_{nm} (T - 298.15) + C_{nm} (T - 298.15)^2}{T} \right] \quad (7.14)$$

A_{nm} , B_{nm} and C_{nm} are binary interaction parameters between group n and group m .

It is worth noting that the group area parameter Q_k and volume parameter R_k , as well as the group interaction parameters A_{nm} , B_{nm} and C_{nm} used with the UMR-PRU are not the same as those of the original UNIFAC model¹¹⁷⁵, and they were determined by correlating experimental data in the works of several authors^{19,20,1165,1170,1176,1177}. In order to establish a distinction between the original UNIFAC model and the UNIFAC model applied in the UMR-PRU, we denote the latter as UNIFAC-UMR-PRU in this work.

7.3.PSRK model

The predictive-Soave-Rdlich-Kwong (PSRK) EoS¹¹⁷⁸⁻¹¹⁸¹ is a predictive model which combines the SRK EoS with an excess molar Gibbs energy (g^E) mixing rule estimated through a UNIFAC group contribution method. It uses the original SRK EoS³³ with the MC $\alpha(T)$ function from Eq. (3) and the following mixing rule:

$$\begin{cases} \frac{a_m(T)}{b_m} = \sum z_i \frac{a_i(T)}{b_i} + \frac{g_0^E + RT \sum \ln\left(\frac{b}{b_i}\right)}{-0.64663} \\ b_m = \sum z_i b_i \end{cases} \quad (7.15)$$

It should be noted that the UNIFAC group interaction parameters are temperature-dependent, expressed by:

$$\Psi_{nm} = \exp\left[-\frac{A_{nm}}{T}\right] \quad (7.16)$$

7.4.*tc*-PR-UNIQUAC model

This model uses the translated-consistent Peng-Robinson (*tc-PR*) EoS proposed by Le Guennec et al.³² coupled with the residual part of the UNIQUAC¹¹⁸² activity coefficient model as presented by Pina-Martinez et al.¹³⁰:

$$\begin{aligned} \frac{a_{res}^{E,UNIQUAC}(T, \mathbf{z})}{RT} = & -q_1 z_1 \left[\frac{z_1 q_1}{z_1 q_1 + z_2 q_2} + \frac{z_2 q_2}{z_1 q_1 + z_2 q_2} \exp\left(-\frac{A_{12}}{T}\right) \right] \\ & -q_2 z_2 \left[\frac{z_2 q_2}{z_1 q_1 + z_2 q_2} + \frac{z_1 q_1}{z_1 q_1 + z_2 q_2} \exp\left(-\frac{A_{21}}{T}\right) \right] \end{aligned} \quad (7.17)$$

Where q_1 and q_2 are the Van der Waals surface areas of molecules 1 and 2 divided by a reference surface of $2.5 \times 10^9 \text{ cm}^2 \text{ mol}^{-1}$. The parameters A_{12} and A_{21} are temperature-independent and are fitted to experimental data.

7.5. Benchmark database

The benchmark database was detailed in the paper²¹. The database consists of nine families of binary systems, each identified by a binary association code (BAC) depending on the associating character of the components present in the mixture: non-associating (NA), hydrogen-acceptor (HA), hydrogen-donor (HD) or self-associating (SA). These nine families

are divided into four categories of mixtures, depending on the type of association they exhibit. These categories are defined as: 1) mixtures without association, which include BACs 1 to 4; 2) mixtures in which self-association tends to be broken, corresponding to BAC₅; 3) mixtures from BAC₆ in which only cross-association takes place; and 4) mixtures from BACs 7 to 9 in which both cross- and self-association take place. A summary of the nine BAC and the four categories mentioned previously is given in *Table 7.1*.

For each system of the database, ten properties at most are experimentally available: liquid phase composition x , gas phase composition (or second liquid 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 .

Table 7.1. Definition of the ten families of binary systems and their corresponding BAC (binary association code).

Component 1	Component 2	Binary association code (BAC)	Categories of exhibited association
NA (Non-Associating) <i>nonpolar</i>	NA (Non-Associating) <i>nonpolar</i>	1	Mixtures without association
HA (Hydrogen-Acceptor) <i>polar but non-associating</i>	NA (Non-Associating) <i>nonpolar</i>	2	
HD (Hydrogen-Donor) <i>polar but non-associating</i>	NA (Non-Associating) <i>nonpolar</i>	3	
HA (Hydrogen-Acceptor) <i>polar but non-associating</i>	HA (Hydrogen-Acceptor) <i>polar but non-associating</i>	4	
HD (Hydrogen-Donor) <i>polar but non-associating</i>	HD (Hydrogen-Donor) <i>polar but non-associating</i>		
SA (Self-Associating) <i>polar and associating</i>	NA (Non-Associating) <i>nonpolar</i>	5	Mixtures in which self-association takes place (but tends to be broken)
HD (Hydrogen-Donor) <i>polar but non-associating</i>	HA (Hydrogen-Acceptor) <i>polar but non-associating</i>	6	Mixtures in which cross-association takes place alone
SA (Self-Associating) <i>polar and associating</i>	HD (Hydrogen-Donor) <i>polar but non-associating</i>	7	Mixtures in which both cross-association and self-association take place
SA (Self-Associating) <i>polar and associating</i>	HA (Hydrogen-Acceptor) <i>polar but non-associating</i>	8	
SA (Self-Associating) <i>polar and associating</i>	SA (Self-Associating) <i>polar and associating</i>	9	

7.6. Grading procedure

The grading procedure consists of the following steps:

- I. Calculation of the Mean Average Percentage Errors (MAPEs) of each property, BAC by BAC, considering all the points of the BAC without considering the binary systems from which they originate.**

a. MAPE on liquid phase composition x (VLE data) or x^α (LLE data):

$$\left\{ \begin{array}{l} \text{MAPE}_{x \text{ or } x^\alpha} = 100 \sum_{i=1}^{n_{x \text{ or } x^\alpha}} 0.5 \left(\frac{|\Delta x|}{x_{1, \text{exp}} \text{ (or } x_{1, \text{exp}}^\alpha)} + \frac{|\Delta x|}{x_{2, \text{exp}} \text{ (or } x_{2, \text{exp}}^\alpha)} \right)_i \\ \text{with: } |\Delta x| = |x_{1, \text{exp}} \text{ (or } x_{1, \text{exp}}^\alpha) - x_{1, \text{cal}} \text{ (or } x_{1, \text{cal}}^\alpha)| = |x_{2, \text{exp}} \text{ (or } x_{2, \text{exp}}^\alpha) - x_{2, \text{cal}} \text{ (or } x_{2, \text{cal}}^\alpha)| \end{array} \right. \quad (7.18)$$

$n_{x \text{ or } x^\alpha}$ is the number of data points for which the liquid phase composition x_1 (VLE data) or the 1st liquid phase composition x_1^α (LLE data) is known considering all the binary systems of a given BAC.

Note: as explained in the original procedure ²¹, very small mole fractions may lead to huge percent deviations, even though the absolute deviation is extremely small. When this happens, such datapoints can have a huge influence on the calculated $\text{MAPE}_{x \text{ or } x^\alpha}$. To avoid such a bias, if $x_{1, \text{exp}} < 0.01$ (or $x_{1, \text{exp}} > 0.99$)

and simultaneously $0.5 \left(\frac{|\Delta x|}{x_{1, \text{exp}} \text{ (or } x_{1, \text{exp}}^\alpha)} + \frac{|\Delta x|}{x_{2, \text{exp}} \text{ (or } x_{2, \text{exp}}^\alpha)} \right)_i > 0.45$, the

corresponding deviation is not included in the calculation of $\text{MAPE}_{x \text{ or } x^\alpha}$.

b. MAPE on gas phase composition y (VLE data) or 2nd liquid phase composition x^β (LLE data):

$$\left\{ \begin{array}{l} \text{MAPE}_{y \text{ or } x^\beta} = 100 \sum_{i=1}^{n_{y \text{ or } x^\beta}} 0.5 \left(\frac{|\Delta y|}{y_{1, \text{exp}} \text{ (or } x_{1, \text{exp}}^\beta)} + \frac{|\Delta y|}{y_{2, \text{exp}} \text{ (or } x_{2, \text{exp}}^\beta)} \right)_i \\ \text{with: } |\Delta y| = |y_{1, \text{exp}} \text{ (or } x_{1, \text{exp}}^\beta) - y_{1, \text{cal}} \text{ (or } x_{1, \text{cal}}^\beta)| = |y_{2, \text{exp}} \text{ (or } x_{2, \text{exp}}^\beta) - y_{2, \text{cal}} \text{ (or } x_{2, \text{cal}}^\beta)| \end{array} \right. \quad (7.19)$$

$n_{y \text{ or } x^\beta}$ is the number of data points for which the gas phase composition y_1 (VLE data) or the 2nd liquid phase composition x_1^β (LLE data) is known.

Note: in order to avoid a bias, if $y_{1, \text{exp}} > 0.99$ (or $y_{1, \text{exp}} < 0.01$) and simultaneously

$0.5 \left(\frac{|\Delta y|}{y_{1, \text{exp}} \text{ (or } x_{1, \text{exp}}^\beta)} + \frac{|\Delta y|}{y_{2, \text{exp}} \text{ (or } x_{2, \text{exp}}^\beta)} \right)_i > 0.45$, the corresponding deviation is

not included in the calculation of $\text{MAPE}_{y \text{ or } x^\beta}$.

c. MAPE on critical pressure P_c (critical point data):

$$\text{MAPE}_{P_c} = 100 \sum_{i=1}^{n_{\text{crit}}} \left(\frac{|P_{c, \text{exp}} - P_{c, \text{cal}}|}{P_{c, \text{exp}}} \right)_i \quad (7.20)$$

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

d. MAPE on critical composition x_c (critical point data):

$$\left\{ \begin{array}{l} \text{MAPE}_{x_c} = 100 \sum_{i=1}^{n_{\text{crit}}} 0.5 \left(\frac{|\Delta x_c|}{x_{c,1, \text{exp}}} + \frac{|\Delta x_c|}{x_{c,2, \text{exp}}} \right)_i \\ \text{with: } |\Delta x_c| = |x_{c,1, \text{exp}} - x_{c,1, \text{cal}}| = |x_{c,2, \text{exp}} - x_{c,2, \text{cal}}| \end{array} \right. \quad (7.21)$$

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

e. MAPE on azeotropic pressure P_{az} (azeotropic point data):

$$\text{MAPE}_{P_{\text{az}}} = 100 \sum_{i=1}^{n_{\text{az}}} \left(\frac{|P_{\text{az, exp}} - P_{\text{az, cal}}|}{P_{\text{az, exp}}} \right)_i \quad (7.22)$$

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

f. MAPE on azeotropic composition x_{az} (azeotropic point data):

$$\left\{ \begin{array}{l} \text{MAPE}_{x_{\text{az}}} = 100 \sum_{i=1}^{n_{\text{az}}} 0.5 \left(\frac{|\Delta x_{\text{az}}|}{x_{\text{az},1, \text{exp}}} + \frac{|\Delta x_{\text{az}}|}{x_{\text{az},2, \text{exp}}} \right)_i \\ \text{with: } |\Delta x_{\text{az}}| = |x_{\text{az},1, \text{exp}} - x_{\text{az},1, \text{cal}}| = |x_{\text{az},2, \text{exp}} - x_{\text{az},2, \text{cal}}| \end{array} \right. \quad (7.23)$$

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

g. MAPE on three-phase equilibrium pressure P_{LLV} (VLLE data):

$$\text{MAPE}_{P_{\text{LLV}}} = 100 \sum_{i=1}^{n_{\text{triph}}} \left(\frac{|P_{\text{LLV, exp}} - P_{\text{LLV, cal}}|}{P_{\text{LLV, exp}}} \right)_i \quad (7.24)$$

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

h. MAPE on three-phase equilibrium composition x^α , x^β , and y (VLLE data):

$$\left\{ \begin{aligned} \text{MAPE}_{z_{\text{LLV}}} &= 100 \sum_{i=1}^{n_{\text{triph}}} \frac{1}{6} \left(\frac{|\Delta x^\alpha|}{x_{1,\text{exp}}^\alpha} + \frac{|\Delta x^\alpha|}{x_{2,\text{exp}}^\alpha} + \frac{|\Delta x^\beta|}{x_{1,\text{exp}}^\beta} + \frac{|\Delta x^\beta|}{x_{2,\text{exp}}^\beta} + \frac{|\Delta y|}{y_{1,\text{exp}}} + \frac{|\Delta y|}{y_{2,\text{exp}}} \right)_i \\ \text{with:} \\ |\Delta x^\alpha| &= |x_{1,\text{exp}}^\alpha - x_{1,\text{cal}}^\alpha| = |x_{2,\text{exp}}^\alpha - x_{2,\text{cal}}^\alpha| \\ |\Delta x^\beta| &= |x_{1,\text{exp}}^\beta - x_{1,\text{cal}}^\beta| = |x_{2,\text{exp}}^\beta - x_{2,\text{cal}}^\beta| \\ |\Delta y| &= |y_{1,\text{exp}} - y_{1,\text{cal}}| = |y_{2,\text{exp}} - y_{2,\text{cal}}| \end{aligned} \right. \quad (7.25)$$

n_{triph} is the number of three-phase equilibrium composition data.

Note: A modification to the original grading procedure, introduced by Pina-Martinez et al.¹³⁰, is used. In here, very small (or close to 1) mole fractions may lead to huge percent deviations and introduce a bias in the grade of a given BAC.

To avoid such a bias, if $z_{1,\text{exp}} < 0.01$ (or $z_{1,\text{exp}} > 0.99$) and simultaneously

$0.5 \left(\frac{|\Delta z|}{z_{1,\text{exp}}} + \frac{|\Delta z|}{z_{2,\text{exp}}} \right)_i > 0.45$, the corresponding deviation is not included in the

$\text{MAPE}_{z_{\text{LLV}}}$ calculation. Here, z_1 stands for the mole fraction of component 1 in the first liquid phase α (x_1^α) or in the gas phase (y_1) or the second liquid phase β (x_1^β).

i. MAPE on mixing enthalpy h^M (enthalpy of mixing data):

$$\text{MAPE}_{h^M} = 100 \sum_{i=1}^{n_{h^M}} 0.5 \left(\left| \frac{h_{\text{exp}}^M - h_{\text{cal}}^M}{h_{\text{exp}}^M} \right| + \left| \frac{h_{\text{exp}}^M - h_{\text{cal}}^M}{h_{\text{cal}}^M} \right| \right)_i \quad (7.26)$$

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

Note: in order to obtain the same mark when calculated values of h^M are n times smaller or n times larger than the experimental values, h_{exp}^M and h_{cal}^M are respectively set as the denominator to calculate the average MAPE at each data point. Besides, h^M goes to zero when the mole fraction of the studied phase (z_1) tends to zero or one. In such cases, huge percent deviations (and consequently

very bad marks) on h^M can be obtained. To avoid such a bias, if in equation

$$(7.26): 0.5 \left(\left| \frac{h_{\text{exp}}^M - h_{\text{cal}}^M}{h_{\text{exp}}^M} \right| + \left| \frac{h_{\text{exp}}^M - h_{\text{cal}}^M}{h_{\text{cal}}^M} \right| \right)_i > 0.8, \text{ this quantity is set to } 0.8.$$

j. MAPE on mixing heat capacity c_p^M (heat capacity of mixing data):

$$\text{MAPE}_{c_p^M} = 100 \sum_{i=1}^{n_{c_p^M}} 0.5 \left(\left| \frac{c_{p,\text{exp}}^M - c_{p,\text{cal}}^M}{c_{p,\text{exp}}^M} \right| + \left| \frac{c_{p,\text{exp}}^M - c_{p,\text{cal}}^M}{c_{p,\text{cal}}^M} \right| \right) \quad (7.27)$$

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

Note: similarly as the mixing enthalpy h^M , if in equation (7.27):

$$0.5 \left(\left| \frac{c_{p,\text{exp}}^M - c_{p,\text{cal}}^M}{c_{p,\text{exp}}^M} \right| + \left| \frac{c_{p,\text{exp}}^M - c_{p,\text{cal}}^M}{c_{p,\text{cal}}^M} \right| \right)_i > 2, \text{ this quantity is set to } 2.$$

II. Calculation, BAC by BAC, of the mark obtained by a given BAC for each property.

In the previous grading procedure, the general expression for a property j , is given by:

$$\text{mark}_j^{\text{BAC}_i} = 20 - \alpha_j \times \text{MAPE}_j^{\text{BAC}_i} \quad (7.28)$$

Where $\alpha_j = 0.5$ with the exception of $\alpha_{P_c} = 0.75$, $\alpha_{h^M} = 0.25$ and $\alpha_{c_p^M} = 0.1$. In this work, the second modification introduced by Pina-Martinez et al.¹³⁰ is employed to take into account the effect of the “out-of-model” (OM) points in the grading procedure.

$$\begin{cases} \text{mark}_j^{\text{BAC}_i} = (20 - \alpha_j \times \text{MAPE}_j^{\text{BAC}_i}) \times \text{SR}_j^{\text{BAC}_i} \\ \text{SR}_j^{\text{BAC}_i} = 1 - \frac{N_{\text{OM},j}^{\text{BAC}_i}}{N_{\text{exp},j}^{\text{BAC}_i}} \end{cases} \quad (7.29)$$

Where $\text{SR}_j^{\text{BAC}_i}$, $N_{\text{OM},j}^{\text{BAC}_i}$ and $N_{\text{exp},j}^{\text{BAC}_i}$ correspond respectively to the success ratio of the model, the number of “out-of-model” points and the number of experimental data points for the property j from BAC_i . Therefore, $\text{SR}_j^{\text{BAC}_i}$ represents the actual number of points considered in the MAPE calculation, i.e., not declared “out-of-model”, with respect to the number of experimental points.

III. Calculation of the final mark obtained by each BAC by averaging the marks obtained in each of the available properties, i.e. for which at least one deviation has been calculated, among x , y , P_{LLV} , z_{LLV} , P_c , x_c , P_{az} , x_{az} , h^M and c_p^M .

$$\text{mark}_{\text{BAC}_i} = \text{average} \left(\begin{array}{l} \text{mark}_{x \text{ or } x^{\alpha}}^{\text{BAC}_i}; \text{mark}_{y \text{ or } x^{\beta}}^{\text{BAC}_i}; \text{mark}_{P_c}^{\text{BAC}_i}; \text{mark}_{x_c}^{\text{BAC}_i}; \text{mark}_{P_{az}}^{\text{BAC}_i}; \\ \text{mark}_{x_{az}}^{\text{BAC}_i}; \text{mark}_{P_{LLV}}^{\text{BAC}_i}; \text{mark}_{z_{LLV}}^{\text{BAC}_i}; \text{mark}_{h^M}^{\text{BAC}_i}; \text{mark}_{c_p^M}^{\text{BAC}_i} \end{array} \right) \quad (7.30)$$

I. Calculation of the mark attributed to each of the four categories of binary systems by averaging, if necessary, the marks obtained by the BACs belonging to each of them.

II. .

$$\left\{ \begin{array}{l} \text{mark}_{\text{NA}} = \frac{\text{mark}_{\text{BAC}_1} + \text{mark}_{\text{BAC}_2} + \text{mark}_{\text{BAC}_3} + \text{mark}_{\text{BAC}_4}}{4} \\ \text{mark}_{\text{SA}} = \text{mark}_{\text{BAC}_5} \\ \text{mark}_{\text{CA}} = \text{mark}_{\text{BAC}_6} \\ \text{mark}_{\text{CA+SA}} = \frac{\text{mark}_{\text{BAC}_7} + \text{mark}_{\text{BAC}_8} + \text{mark}_{\text{BAC}_9}}{3} \end{array} \right. \quad (7.31)$$

III. Calculation of the final mark of the thermodynamic model by averaging the mark of the four considered categories of binary systems.

$$\text{Final mark of a thermodynamic model (over 20)} = \frac{1}{4} \times \underbrace{\left[\underbrace{\text{mark}_{\text{NA}}}_{\text{no association}} + \underbrace{\text{mark}_{\text{SA}}}_{\text{self-association}} + \underbrace{\text{mark}_{\text{CA}}}_{\text{cross-association}} + \underbrace{\text{mark}_{\text{CA+SA}}}_{\text{cross-association + self-association}} \right]}_{\text{average of 4 marks}} \quad (7.32)$$

7.7. Simulis thermodynamics

Simulis Thermodynamics, which can be available as a Microsoft Excel Add-In, is a calculation server for thermophysical properties and phase equilibria properties of pure substances or multi-component mixtures. Using this software, the user can easily define the substances, the thermodynamic models (e.g., EoS or activity coefficient models), and the functions (e.g., the calculations of phase equilibrium, critical property, enthalpy, or heat capacity) inside a Microsoft Excel worksheet. In this work, Simulis Thermodynamics is used for the calculations of thermodynamic properties with the UMR-PRU model.

The Mathias-Copeman parameters $c_{1,i}$, $c_{2,i}$, and $c_{3,i}$ of most relevant pure substances are already provided by Simulis Thermodynamics, except 4 substances (1,1,1,3,3,3-hexafluoropropane, 1,1,1,2,3,3,3-heptafluoropropane, 1,1,1,3,3-pentafluorobutane and 2,3,3,3-tetrafluoropropene), for which the Soave $\alpha(T)$ function is used instead, as presented in equation (7.3), due to the lack of experimental data to determine these parameters. On the other hand, it is not possible to decompose 18 molecules into elementary units using the 54 available groups in the UNIFAC-

UMR-PRU model. For this reason, any binary system containing any of these 18 molecules (presented in *Table 7.2*) will be excluded from the benchmarking of the UMR-PRU, since the pure compounds cannot be decomposed into elementary groups and thus their properties cannot be calculated.

Table 7.2. Summary of the 18 compounds that cannot be decomposed with the available groups defined in the UNIFAC- UMR-PRU model, the associated binary systems to be excluded from the benchmarking and their respective BACs.

Compounds that cannot be decomposed into elementary groups	Associated excluded binary system	System codes	BAC
AMMONIA	nitrogen + ammonia	905_1911	BAC5
	ammonia + acetonitrile	1911_1772	BAC9
	ammonia + water	1911_1921	BAC9
ARGON	argon + methane	914_1	BAC1
CARBON MONOXIDE	carbon monoxide + carbon dioxide	908_909	BAC4
	methanol + carbon monoxide	908_1101	BAC8
CARBON TETRAFLUORIDE	trifluoromethane + carbon tetrafluoride	1616_1615	BAC3
	chlorodifluoromethane + carbon tetrafluoride	1616_1604	BAC3
DIFLUOROMETHANE	difluoromethane + propane	1614_3	BAC3
	difluoromethane + 1,1,1,2-tetrafluoroethane	1614_2650	BAC4
	difluoromethane + sulfur dioxide	1614_910	BAC6
	carbon dioxide + difluoromethane	909_1614	BAC6
	difluoromethane + dimethyl ether	1614_1401	BAC6
ETHYL FLUORIDE	1,1,1,2-tetrafluoroethane + ethyl fluoride	1617_2650	BAC3
ETHYLENE	ethylene + xenon	201_959	BAC1
	ethylene + carbon dioxide	201_909	BAC2
	dichloromethane + ethylene	201_1511	BAC3
HYDROGEN SULFIDE	methane + hydrogen sulfide	1_1922	BAC2
	carbon dioxide + hydrogen sulfide	909_1922	BAC4
OXYGEN	oxygen + carbon dioxide	901_909	BAC4
PENTAFLUOROETHANE	pentafluoroethane + propane	1646_3	BAC3
	pentafluoroethane + 1,1,1,2-tetrafluoroethane	1646_2650	BAC4
	pentafluoroethane + dimethyl ether	1646_1401	BAC6
SULFOLANE	thiophene + sulfolane	1821_1845	BAC4
SULFUR DIOXIDE	dimethyl ether + sulfur dioxide	1401_910	BAC4

Compounds that cannot be decomposed into elementary groups	Associated excluded binary system	System codes	BAC
	trifluoromethane + ethane	1615_2	BAC3
TRIFLUOROMETHANE	trifluoromethane + chlorodifluoromethane	1615_1604	BAC4
	trifluoromethane + carbon disulfide	1615_1938	BAC6
1,1-DIFLUOROETHANE	1,1,1,2-tetrafluoroethane + 1,1-difluoroethane	2650_1640	BAC4
	1,1,1,2,3,3,3-heptafluoropropane + sulfur dioxide	2630_910	BAC6
1,1,1,2,3,3,3-HEPTAFLUOROPROPANE	carbon dioxide + 1,1,1,2,3,3,3-heptafluoropropane	909_2630	BAC6
	1,1,1,2-tetrafluoroethane + hexafluoroethane	2693_2650	BAC3
1,1,1,2-TETRAFLUOROETHANE	chlorodifluoromethane + 1,1,1,2-tetrafluoroethane	1604_2650	BAC4
	carbon dioxide + 1,1,1,2-tetrafluoroethane	909_2650	BAC6
2,3,3,3-TETRAFLUOROPROPENE	1,1,1-trifluoroethane + 2,3,3,3-tetrafluoropropene	1619_3608	BAC3

A total of 35 binary systems are removed from the benchmarking of the UMR-PRU model due to being comprised of either one or two of these molecules that cannot be decomposed into elementary groups. It should be noted that nine of the removed systems belong to BAC3; ten belong to BAC4 and eight belong to BAC6. This indicates that the UMR-PRU model is particularly lacking in parameters for polar compounds, especially fluorinated hydrocarbons like difluoromethane (DIPPR id: 1614) and 1,1,1,2-tetrafluoroethane (DIPPR id: 2650) which have the highest number of associated systems removed of any of the molecules presented in **Table 7.2**, with five and 7 respectively.

Finally, an additional collection of 13 binary systems are also excluded from the calculations and final grading of the UMR-PRU model. Despite having available groups decompositions for each of the molecules that make up each of the systems listed in **Table 7.3**, they cannot be modeled due to the lack of group-interaction parameters in the UNIFAC-UMR-PRU parameter matrix.

Table 7.3 List of 13 binary mixtures for which no UMR-PRU group-interaction parameters are available and their respective BACs.

Binary Mixtures	System Codes	BAC
nitrogen + chlorodifluoromethane	905_1604	BAC3
propylene + chlorodifluoromethane	202_1604	BAC3
carbon dioxide + carbon disulfide	909_1938	BAC4
carbon dioxide + dimethyl carbonate	909_2391	BAC4

Binary Mixtures	System Codes	BAC
1,1,1-trifluoroethane + dimethyl ether	1619_1401	BAC6
dichloromethane + carbon disulfide	1511_1938	BAC6
carbon dioxide + chlorodifluoromethane	909_1604	BAC6
chlorodifluoromethane + carbon disulfide	1604_1938	BAC6
dimethyl ether + 1,1,1,3,3,3-hexafluoropropane	1401_1620	BAC6
methanol + halothane	1101_2640	BAC7
trichloroethylene + 2-methoxyethanol	1541_2860	BAC7
n-propyl formate + 1,1,2,2-tetrachloroethane	1303_1529	BAC7
ethyl formate + water	1302_1921	BAC9

Once again, we take notice that most of the removed systems belong to either BAC3, BAC4 or BAC6, although in this case, the latter has the most removed systems with five in total. At this stage we can conclude that the UMR-PRU cannot describe many systems related to fluorinated or chlorofluorinated molecules due to the lack of model parameters. *Table 7.4* presents a summary of the number of removed systems per BAC.

Table 7.4. Summary of number of systems removed in each BAC.

BAC	Number of systems removed
BAC1	2
BAC2	2
BAC3	11
BAC4	12
BAC5	1
BAC6	13
BAC7	3
BAC8	1
BAC9	3
Total	48

In the end, 48 mixtures (24% of the total number of binary systems present in the database) will be removed from the benchmarking of the UMR-PRU EoS, leaving 152 available for the evaluation. After creating a Simulis Thermodynamics calculator in the worksheet of Excel, the components of the binary mixture and the thermodynamic model (i.e., UMR-PRU model) can be easily set, following the instruction of the software.

7.8. Results and Discussion

For each BAC family evaluated with the UMR-PRU model, the MAPEs on each property are listed in *Table 7.5* while the success ratio (SR) is listed on *Table 7.6*. Based on these two calculated quantities, the thermodynamic model can be scored first by giving a mark over 20 for each property in each BAC family, as presented in section 3. The marks of each property are listed in *Table 7.7*, as well as the average mark for each of the four categories of mixtures presented in *Table 7.1* followed by the final mark obtained by the UMR-PRU model.

Table 7.5. Overview of the MAPE between experimental data and values calculated with the UMR-PRU model for the 152 binary systems included in the proposed database that are classified in nine binary association codes (BACs). The abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”.

Binary association code (BAC)	Type of association	MAPE on:									
		x or x^α Eq. (1)	y or x^β Eq. (2)	P_c Eq. (3)	x_c Eq. (4)	P_{az} Eq. (5)	x_{az} Eq. (6)	P_{LLV} Eq. (7)	z_{LLV} Eq. (8)	h^M Eq. (9)	c_p^M Eq. (10)
1 (NA - NA)	Mixtures without association	14.55%	10.76%	8.01%	10.19%	5.96%	15.73%	2.72%	41.88%	48.79%	198.69%
2 (HA-NA)		22.96%	12.30%	8.72%	17.04%	8.06%	9.31%	-	-	46.90%	175.51%
3 (HD-NA)		32.78%	24.67%	1.78%	47.76%	0.41%	3.07%	-	-	57.27%	193.85%
4 (HA-HA or HD-HD)		21.71%	15.89%	9.16%	12.03%	10.73%	24.94%	-	-	55.34%	200.00%
5 (SA-NA)	Mixtures in which self-association tends to be broken	24.17%	9.30%	8.85%	50.28%	3.25%	6.22%	3.37%	37.20%	42.57%	122.08%
6 (HD-HA)	Mixtures in which cross-association takes place alone	15.15%	22.54%	1.09%	49.87%	2.56%	13.74%	-	-	36.41%	121.90%
7 (SA-HD)	Mixtures in which both cross-association and self-association take place	19.80%	12.14%	-	-	7.95%	10.48%	-	-	64.35%	78.56%
8 (SA-HA)		24.32%	12.10%	6.37%	25.92%	4.21%	15.90%	7.88%	18.26%	45.81%	113.60%
9 (SA-SA)		54.76%	20.28%	9.80%	24.86%	5.02%	29.76%	5.33%	65.41%	70.60%	93.80%

Table 7.6. Overview of the Success Ratio (SR) between experimental data and values calculated with the UMR-PRU model for the 152 binary systems included in the proposed database that are classified in nine binary association codes (BACs). The abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”.

Binary association code (BAC)	Type of association	Success ratio (SR) on:										BAC Average
		x or x^α	y or x^β	P_c	x_c	P_{az}	x_{az}	P_{LLV}	z_{LLV}	h^M	c_p^M	
1 (NA - NA)	Mixtures without association	0.98	0.95	0.87	0.87	1.00	1.00	0.56	0.31	1.00	1.00	0.85
2 (HA-NA)		0.96	0.96	0.94	0.94	0.94	0.94	-	-	1.00	1.00	0.96
3 (HD-NA)		0.90	0.90	1.00	1.00	0.29	0.29	-	-	1.00	1.00	0.80
4 (HA-HA or HD-HD)		0.98	0.98	1.00	1.00	1.00	1.00	-	-	1.00	1.00	0.99
5 (SA-NA)	Mixtures in which self-association tends to be broken	0.85	0.92	0.88	0.87	0.90	0.90	0.58	0.27	1.00	1.00	0.82
6 (HD-HA)	Mixtures in which cross-association takes place alone	0.82	0.80	1.00	1.00	0.70	0.70	-	-	1.00	1.00	0.88
7 (SA-HD)	Mixtures in which both cross-association and self-association take place	0.97	0.97	-	-	1.00	1.00	-	-	1.00	1.00	0.99
8 (SA-HA)		0.93	0.94	0.73	0.73	0.98	0.98	0.50	0.50	1.00	1.00	0.83
9 (SA-SA)		0.92	0.93	0.87	0.87	0.50	0.50	1.00	0.90	1.00	1.00	0.85
Overall		0.92	0.93	0.91	0.91	0.81	0.81	0.66	0.50	1.00	1.00	0.84

Table 7.7. Rating of the nine binary association codes in order to finally grade the UMR-PRU model. The abbreviations used for the associating character of a pure compound are: NA for “Non-Associating”, HA for “Hydrogen-Acceptor”, HD for “Hydrogen-Donor” and SA for “Self-Associating”.

Binary association code (BAC)	Type of association	Mark on:										Binary association code mark	Mark (over 20) by type of association	Final mark of the UMRPRU model
		x or x^α	y or x^β	P_c	x_c	P_{az}	x_{az}	P_{LLV}	z_{LLV}	h^M	c_p^M			
1 (NA - NA)	Mixtures without association	12.42	13.89	12.14	12.93	17.02	12.13	10.48	0.00	7.80	0.13	9.89	$\underbrace{\text{mark}_{NA}}_{\text{no association}} = 9.09$	9.3/20
2 (HA-NA)		8.20	13.27	12.70	10.83	14.97	14.39	-	-	8.27	2.45	10.63		
3 (HD-NA)		3.24	6.89	18.67	0.00	5.66	5.28	-	-	5.68	0.61	5.75		
4 (HA-HA or HD-HD)		8.96	11.80	13.13	13.98	14.64	7.53	-	-	6.16	0.00	9.53		
5 (SA-NA)	Mixtures in which self-association tends to be broken	6.70	14.05	11.72	0.00	16.60	15.25	10.57	0.38	9.36	7.79	9.24	$\underbrace{\text{mark}_{SA}}_{\text{self-association}} = 9.29$	
6 (HD-HA)	Mixtures in which cross-association takes place alone	10.18	7.02	19.19	0.00	13.11	9.19	-	-	10.90	7.81	9.67	$\underbrace{\text{mark}_{CA}}_{\text{cross-association}} = 9.7$	
7 (SA-HD)	Mixtures in which both cross-association and self-association take place	9.76	13.50	-	-	16.02	14.76	-	-	3.91	12.14	11.68	$\underbrace{\text{mark}_{CA+SA}}_{\text{cross-association + self-association}} = 9.4$	
8 (SA-HA)		7.29	13.09	11.09	5.13	17.48	11.77	8.03	5.43	8.55	8.64	9.65		
9 (SA-SA)		0.00	9.15	11.02	6.59	8.75	2.56	17.33	0.00	2.35	10.62	6.84		

We observe that the UMR-PRU model obtains an overall mark of 9.3/20 with an overall success ratio of 0.84, meaning that the model was able to predict 84% of the experimental data points.. The liquid phase composition (x for VLE or x^α for LLE) as well as the vapor/second liquid phase composition (y or x^β) have an overall SR of 0.92 and 0.93 respectively. For the liquid phase composition, we see that the highest SR is found in BACs 1 and 4, while Bacs 4 and 7 have the top SR for vapor/second liquid phase compositions. The lowest SR for each of these properties is found in BAC₆ which indicates that the UMR-PRU has a lower capacity of predicting VLE data for systems that tend to show negative deviations from ideality such as BAC₆, although the SR is over 0.8, which is not undesirable by any means.

The lowest SR comes from the three-phase properties, with 0.66 for the three-phase pressure (P_{LLV}) and 0.50 for the three-phase composition (z_{LLV}) with BAC₈ having the lowest SR for the three-phase pressure and BAC₅ having the lowest SR for three-phase composition with 0.27. We can deduct from these observations that the UMR-PRU has a low capability of predicting the phase behavior topology of these binary mixtures, when contrasted to the other properties and this highly affects the overall SR of the UMR-PRU (which would be 0.91 if the three-phase properties were to be excluded).

We now turn our attention towards the marks obtained by the UMR-PRU for each of the four categories. In general, we observe that all four categories have very similar marks, with the highest mark being mixtures with cross-association only, which corresponds to BAC₆, with 9.7/20, followed by mixtures with both cross and self-association (BACs 7-9) with a mark of 9.4/20. The UMR-PRU is capable of capturing complex directional phenomena such as hydrogen bonding that is present in associating mixtures. However, the BAC comprised of mixtures with presence of only self-associating compounds (BAC₉,) has the lowest mark amongst the associating BAC categories with 6.84/20. This BAC has a mark of 0/20 for both VLE/LLE composition and three-phase composition, which helps explain the low mark obtained for the BAC. The mark obtained for the azeotropic composition is also low, with a 2.56/20. It seems that the UMR-PRU has difficulties in predicting the phase behavior of mixtures of self-associating compounds. On the other hand, mixtures with self-associating compounds and hydrogen-donors (BAC₇) received the highest mark among all BACs with 11.68/20. The UMR-PRU has higher capabilities to reproduce the azeotropic behavior of these mixtures and to a lesser extent their phase equilibria. The only downside is that the enthalpy of mixture is poorly predicted with a mark of 3.91/20.

Looking into BAC₆, (mark = 9.7/20) where only cross-association is present in the binary mixtures, we immediately observe the near-to perfect score on the critical pressure. This, coupled with the 1.0 SR makes it the highest mark obtained by the UMR-PRU. In contrast, the critical composition gets a mark of 0.0 due to the high deviations observed (49.87%). The model has also acceptable marks for the liquid phase and compositions with 10.18/20 and 9.19/20 respectively. The azeotropic pressure also received a high score with 13.11/20. On a similar fashion, BAC₅ shows a high grade on the critical pressure (11.72/20), but also receives a 0 on the critical composition due to high deviations (50.28%). The azeotropic pressure has a high mark of 16.6 and the azeotropic composition 15.25/20 (making it the highest grade for this property). The vapor/second liquid composition has a high mark (14.059/20), contrasted by the poor description of the liquid phase composition (6.70/20). Furthermore, the three-phase composition received a mark of 0.38/20 with a SR of 0.27, making it clear that the UMR-PRU struggles describing these types of phase behavior.

We now turn to the lowest-scoring category, mixtures without association (BACs 1-4), which received a score of 9.0/20. A closer inspection on each individual BAC for this category reveals that BACs 1, 2 and 4 have similar marks of 9.89/20, 10.63/20 and 9.53/20 respectively. However, BAC₃ received a mark of 5.75/20, making it not only the lowest score for this category but also for all the BACs, which strikes as a surprise, due to the fact that mixtures in this category usually have less complexity in their interactions when compared to the other three categories. Looking into BAC₃, we see that the only remarkable grade was obtained for the critical pressure (18.67/20) with a SR of 1.0. The remaining properties all received marks below 7.0/20 with the critical composition and the heat capacity of mixing being the lowest scores (0.0/20 and 0.61/20 respectively). It should also be noted that the SR for the azeotropic pressure and composition was rather low for this BAC, with 0.29 in both cases, meaning that the UMR-PRU cannot successfully predict all azeotropic behaviors in association code. A common feature among the four BACs in these categories is that both the enthalpies of mixing and heat capacities of mixing reduced their final score. In the cases of BACs 1 and 4 the three-phase composition also contributes to the lowering of their overall score

BAC₁ (which is often referred to as the simplest BAC) has marks above 10/20 for all properties, with the azeotropic pressure scoring 17/20. However, the 0.0/20 mark for the three-phase composition and 0.31/20 for the mixing heat capacity (as well as the mixing enthalpy, although to a lesser extent, with a mark of 7.80/20) evidently bring down the overall score for this BAC. If we remove the poor scores on these three properties, the BAC would have earned a 13.0/20. For this BAC we see that the SR on both three-phase properties is below 0.6, with the three-phase composition being the lowest of the two with 0.31.

BAC₂ has a similar situation, although this time the liquid phase composition is below 10/20 with the enthalpy and heat capacity of mixing. The azeotropic properties are above 14/20, making them the highest marks for this BAC. Nonetheless, it seems the model struggles with the liquid phase part of the phase equilibrium for these systems. Nevertheless, this is the second highest rated BAC for this model.

On a similar note, BAC₄ shows similar trends in its marks as the previously mentioned BAC. However, in this case the azeotropic composition has a mark of 7.53/20 and the mixing heat capacity a mark of 0.0/20.

Overall, BACs 3 and 9 are below par with respect to the remaining ones. The UMR-PRU model showed low marks on the phase equilibrium, critical, azeotropic and three-phase line only for BAC₉) compositions, with the latter being obtaining consistently low marks for all BACs. The mixing heat capacities were also below par (except for BACs 7 and 9) followed by the mixing enthalpies (except for BAC₇). The BACs 1, 2 and 4 were the only ones with marks above 10/20 for the critical composition. BACs 1 and 6 were the only ones to obtained grades above 10/20 for the liquid phase composition. Ranking the BACs based on their individual marks we obtain: 7-2-1-6-8-4-5-9-3.

Figure 7.1 shows an overview of the overall marks obtained by the UMR-PRU for each property for the four categories of binary mixtures.

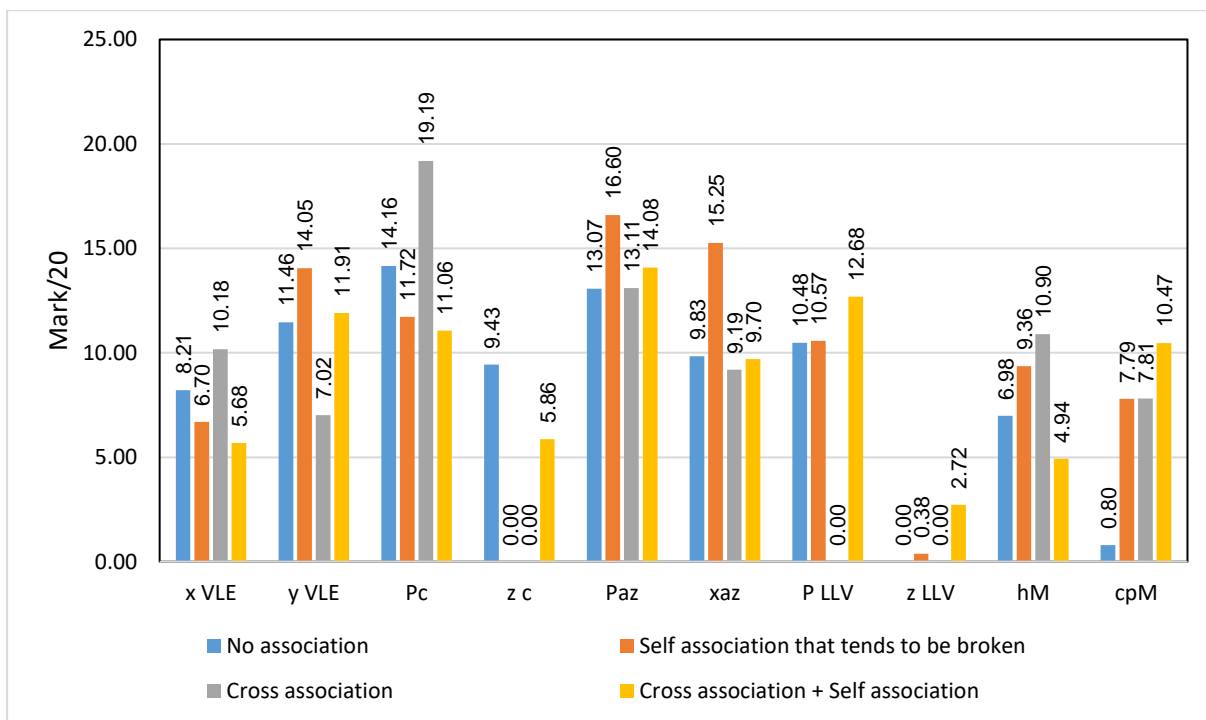


Figure 7.1. Overview of the marks obtained by the UMR-PRU model for each property over the four categories of binary systems of the benchmark database.

The VLE/LLE liquid composition are below 10/20 for all categories, except for the cross-associating binary mixtures, which has a score of 10.18/20. The vapor/second-liquid phase compositions on the other hand are over 11.0/20, except for the cross-associating mixtures. We then observe that the model has scored over 11.0/20 for all categories for the critical pressure (with the cross-associating mixtures obtaining the highest mark of 19.19/20). However, only the non-associating mixtures and the cross-associating + self-associating mixtures have scores different from zero, with the former having the highest (9.43/20). The four categories have marks of 13.0/20 for the azeotropic pressure (with the mixtures where self-association tends to be broken being the highest with 16.6/20). The azeotropic composition had marks over 9.0/20 for all categories, with the mixtures where self-association tends to break standing out with 15.25/20. The model obtained marks over 10.0/20 for all categories, except for the cross-associating mixtures which had a mark of 0.0/20. The three-phase composition showed marks below 3.0/20, with only two categories obtaining grades above zero (mixtures where self-association tends to be broken and mixtures where cross and self-association occurs). The marks for enthalpies of mixing were above 6.0/20 except for the mixtures with cross and self-association with a mark of 4.94/20. Finally, the enthalpies of mixing obtained marks above 7.0/20, except for the non-associating mixtures with a mark of 0.80/20.

At this point, we can immediately deduce that the UMR-PRU model struggles describing the critical and three-phase compositions. The latter in particular had very low marks across all four categories of binary mixtures, which indicates in itself, that the model cannot predict accurately this kind of phase behavior. The same is concluded for the critical composition for the mixtures where self-associating tends to be broken and the cross-associating mixtures, where the model is not able to predict this property accurately.

In order to better understand the overall performance of the UMR-PRU model, as well as its performance on the remaining properties, a comparison to other benchmarked models will be carried out throughout this section. Pina-Martinez et al.¹³⁰ benchmarked the translated-consistent PR (*tc*-PR) EoS coupled several advanced EoS/ $a_{res}^{E,\gamma}$ mixing rules including Wilson (*tc*-PR-Wilson), UNIQUAC (*tc*-PR-UNIQUAC), NRTL (*tc*-PR-NRTL). They also included the PR with Van Laar mixing rules (PR-Van Laar). On a separate work, Nikolaidis et al.¹²⁹ benchmarked the PC-SAFT EoS with Van der Waals one-fluid mixing rules and no binary interaction parameters (PC-SAFT-kij=0). Xu et al.¹¹⁸³ benchmarked the predictive SRK (PSRK) which uses a mixing rule with UNIFAC parameters. We will compare these models to understand the performance of the UMR-PRU. **Figure 7.2** presents an overview of the final score obtained by each of these models.

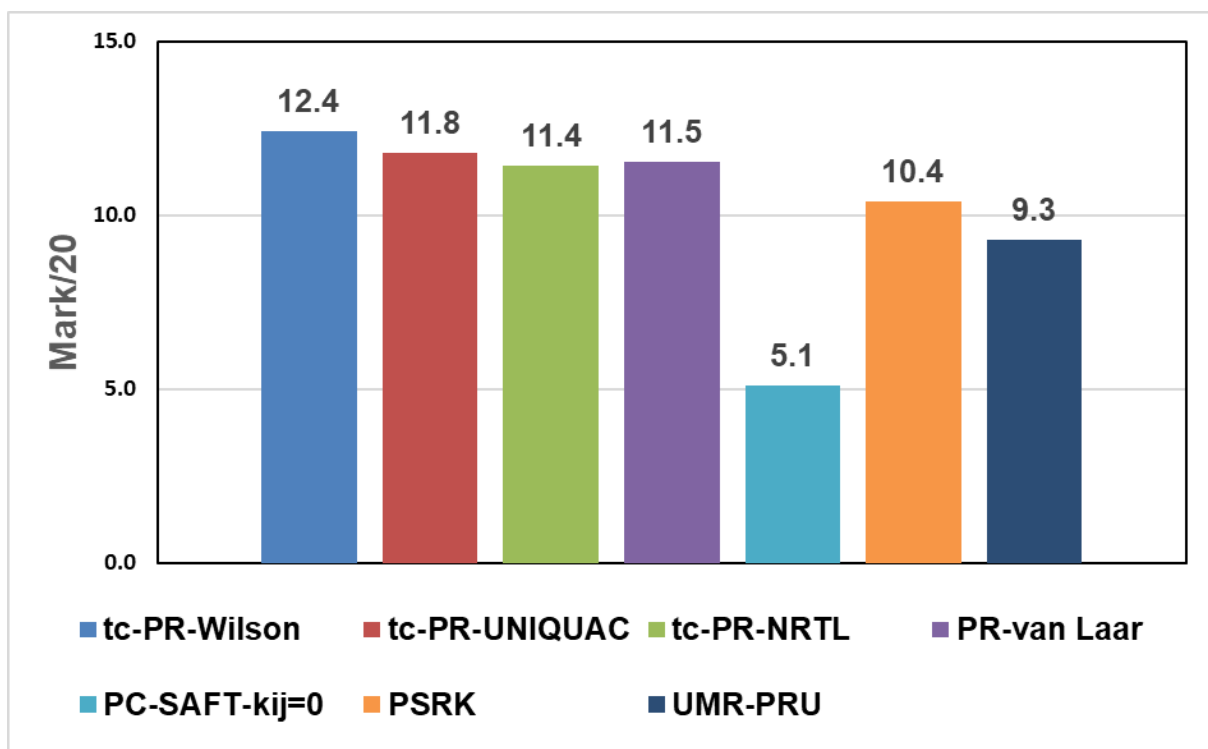


Figure 7.2. Overview of the final marks obtained for the *tc*-PR-Wilson, *tc*-PR-UNIQUAC, *tc*-PR-NRTL, PR-van Laar, PC-SAFT-vdW1f, PSRK and UMR-PRU.

We see that the *tc*-PR-Wilson is the best performing of the seven models with a mark of 12.4/20, followed by the *tc*-PR-UNIQUAC, *tc*-PR-NRTL and PR-van Laar, all with similar marks around 11.0/20. The PSRK comes in third place with 10.4/20, followed by the UMR-PRU with 9.3/20 and the PC-SAFT-kij=0 with 5.1/20. It is clear that the simpler mixing rules used with the PC-SAFT have played a role in the overall mark, as nearly all the other models double its score. The UMR-PRU in spite of performing better than the PC-SAFT-kij=0 is still below average when compared to the rest of the models.

It is interesting to notice that models that have similarities in their formulation, such as *tc*-PR-UNIQUAC, PSRK and UMR-PRU have different marks (even if they are close marks as the case of PSRK and *tc*-UNIQUAC). However, despite these common grounds, the UMR-PRU seems to fall short when compared to the other two models. **Figure 7.3** presents an overview

of the marks obtained for each one of the four categories of binary mixtures for the t_c -PR-UNQUAC, PSRK and UMR-PRU.

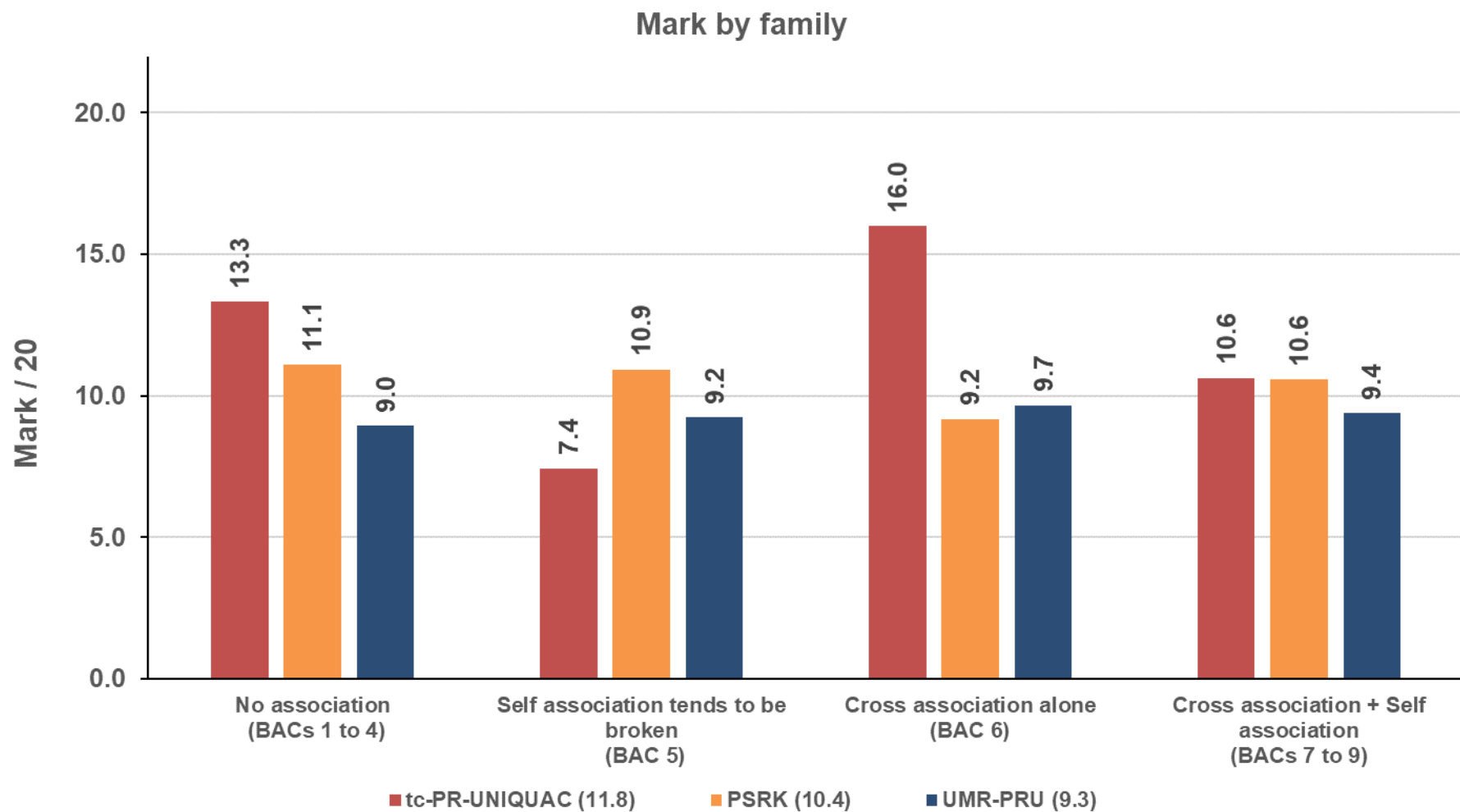


Figure 7.3. Mark obtained by the tc-PR-UNIQUAC, PSRK and UMR-PRU for the four categories of binary mixtures. In parenthesis, besides each of the model's name, we find the final mark obtained by each one.

For the non-associating binary mixtures, we observe that the *tc*-PR-UNIQUAC is well above the other two models with a mark of 13.3/20. The PSRK has a mark of 11.1/20 and the UMR-PRU a mark of 9.0/20. We see that the first two models do not have a broad difference in their respective scores (1.8 difference) but a larger difference when contrasted to the UMR-PRU (2.5 for PSRK and 4.3 for *tc*-PR-UNIQUAC). It would seem that the model has less success in describing non-associating binary mixtures, which are often deemed as simple systems. In order to understand this behavior, we must analyze the scores for each property to determine where is the UMR-PRU underperforming with respect to the remaining two models. **Figure 7.4** presents the scores obtained by the three EoS for the first category (mixtures with no association).

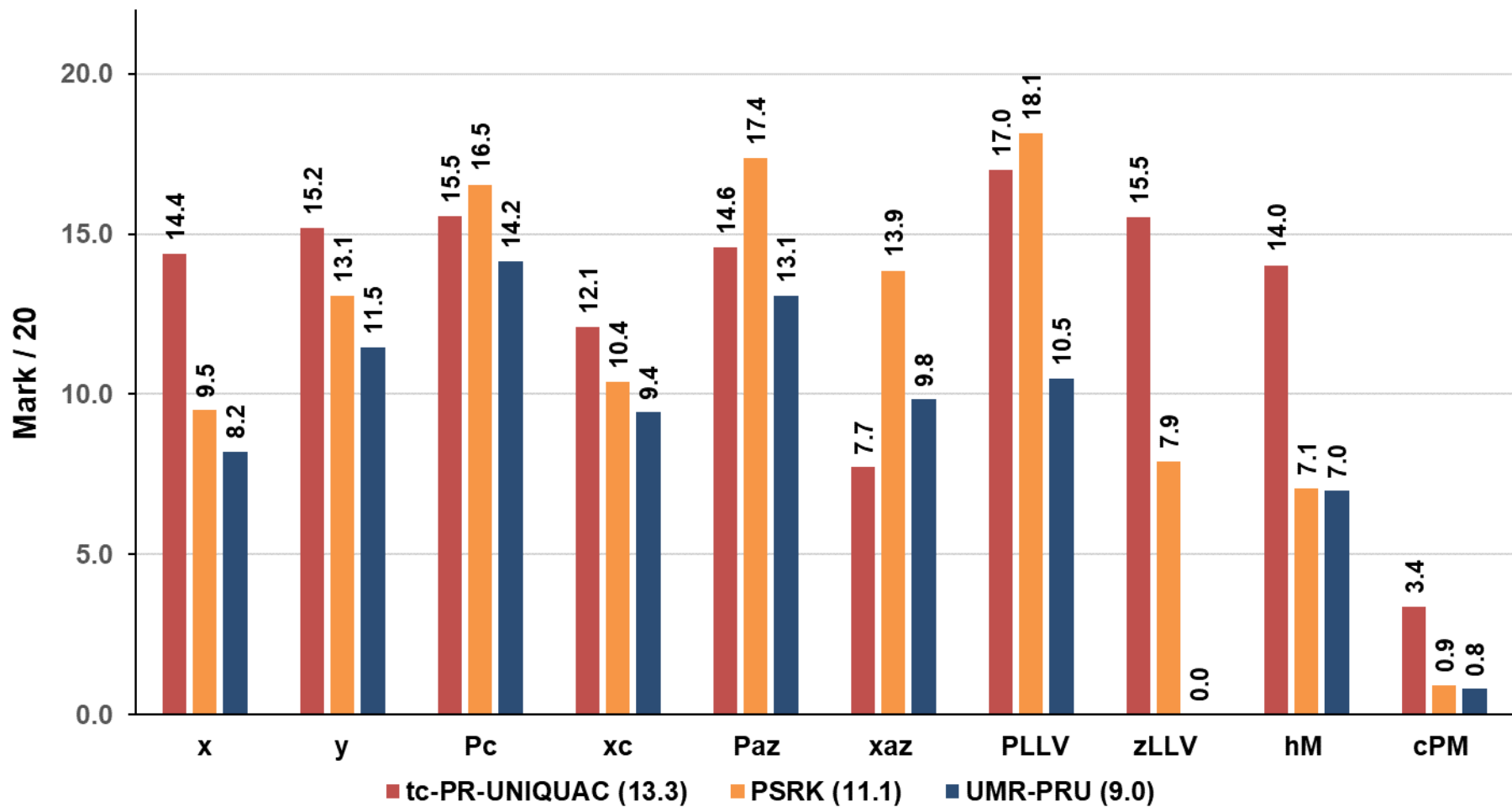


Figure 7.4. Marks obtained by the *tc*-PR-UNIQUAC, PSRK and UMR-PRU for each property for the first category of binary mixtures (mixtures with no association). In parenthesis, besides the name of each model we find the mark obtained by each one for this category.

We observe that both VLE properties x (8.2/20) and y (11.5/20) for the UMR-PRU and are below those of the tc -PR-UNIQUAC (14.4/20 for x and 15.2/20 for y) and the PSRK (9.5/20 for x and 13.1/20 for y). For all three models, the respective y marks are higher than those of the x marks. It should be noted that the PSRK and the UMR-PRU models obtained closer marks for VLE/LLE data between them than each one individually when compared to the tc -UNIQUAC., which indicates that the use of the consistent Twu91 $\alpha(T)$, as proposed by Le Guennec et al.³², improves the prediction on VLE properties. We recall that both the PSRK and the UMR-PRU use the MC $\alpha(T)$. Regarding the marks of PSRK and UMR-PRU, it would seem that the differences in estimation of the group interaction parameters between PSRK^{1160,1161,1178–1181,1184} and the UMR-PRU^{19,20,1165,1167,1169–1171,1173} work in favor of the PSRK model for both VLE properties. **Figure 7.5** and **Figure 7.6** present a side-by-side comparison of the predictions in phase behavior for both models for some a binary system of each BAC comprising the non-associating category.

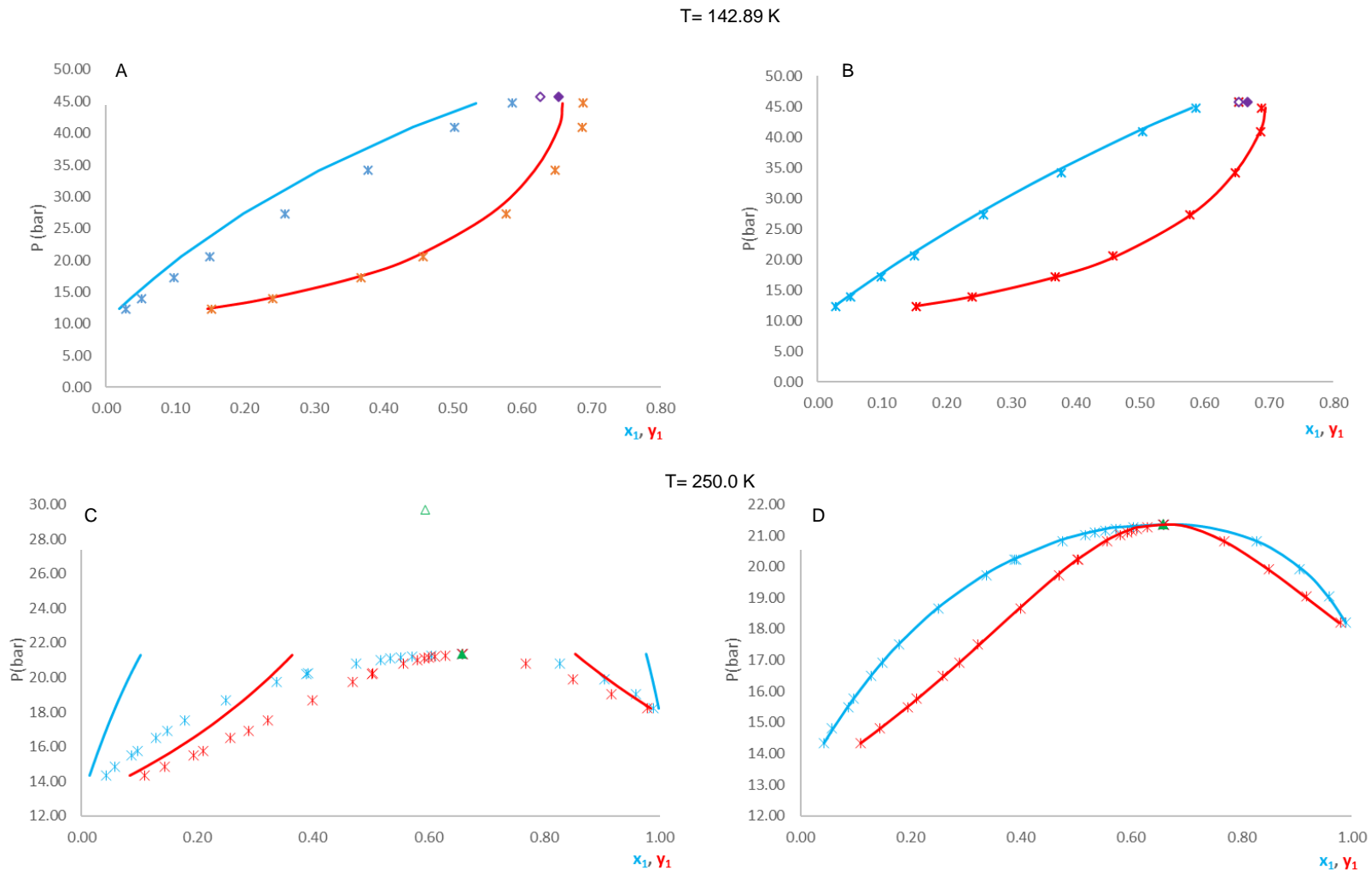


Figure 7.5. VLE diagram for A) nitrogen-methane @T=142.89 K with the UMR-PRU ; B) nitrogen-methane @ T=142.89 K with the PSRK; C) CO₂-ethane @ T= 250 K with the UMR-PRU; D) CO₂-ethane @ T = 250 K with the PSRK. Blue colors symbolize liquid phases, while red colors symbolize vapor phases. Solid lines represent calculated VLE data. Asterisks represent experimental VLE data. Solid diamonds and triangles represent experimental critical and azeotropic data respectively. Hollow diamonds and triangles represent calculated critical and azeotropic data. Diagrams A and B belong to BAC 1 while diagrams C and D belong to BAC 2.

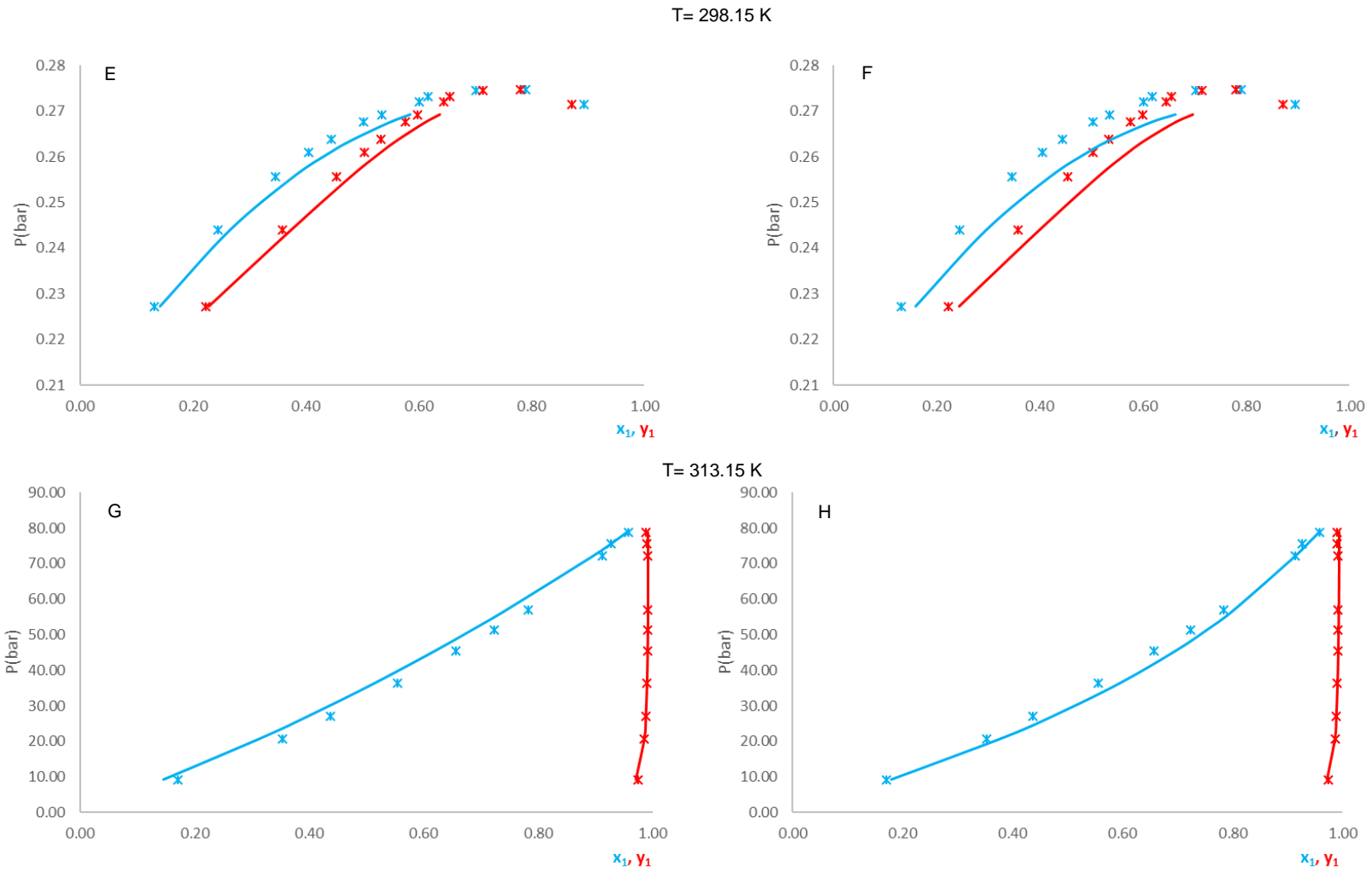


Figure 7.6. VLE diagram for E) chloroform-n-hexane @T =298.15 K with the UMR-PRU; F) chloroform-n-hexane @T =298.15 K with the PSRK; G) CO₂-ethyl acetate @ T= 313.15 K with the UMR-PRU; G) CO₂-ethyl acetate @ T= 313.15 K with the PSRK. Blue colors symbolize liquid phases, while red colors symbolize vapor phases. Solid lines represent calculated VLE data. Asterisks represent experimental VLE data. Diagrams E and D belong to BAC 3 while diagrams G and H belong to BAC 4.

We observe that for BAC1 and BAC2 systems both liquid phases tend to be overpredicted by the UMR-PRU as well as the azeotropic points. The critical point is shifted to a smaller composition for the nitrogen-methane system. The UMR-PRU struggles to reproduce the behavior of the CO₂-ethane mixtures at this temperature. On the other hand, the PSRK correctly models both systems, including their azeotropic and critical points. It seems that the difference of UNIFAC group parameters, such as the ones found for methane (CH₄) and CO₂ have a negative impact in the phase equilibria predictions. However, for parameters of other groups that are common in both models, like chloroform, n-hexane and ethyl acetate, show that the difference in using the original UNIFAC parameters from Hansen et al.¹¹⁸⁵ and the linear temperature-dependent UNIFAC parameters proposed by Hansen et al.¹¹⁷⁷ is somewhat beneficial. For instance, the system chloroform-n-hexane (BAC3) is underpredicted for both phases by both models. However, the UMR-PRU is closer to the experimental values in both phases. For the case of the CO₂-ethyl acetate systems, the predictions for both models regarding the vapor phase are equivalent, but their prediction of the liquid phase is inverted: UMR-PRU under predicts the experimental data, while the PSRK overpredicts it. From these four pairs of examples we can observe that the UMR-PRU model takes the biggest loss in accuracy for VLE data from BACs 1 and 2, as it seemingly struggles to reproduce the phase behavior of these mixtures. We can further corroborate this theory by looking at the individual average marks of BACs 1-4 between the UMR-PRU (see *Table 7.5*) and the PSRK (12.70/20 ; 14/20; 6.41/20 and 11.33/20 for BACs 1 to 4 respectively). We see that BAC3 is close between both EoS. However, BACs 1, 2 and 4 for the UMR-PRU have approximately 3.0 points less for each one when compared to the PSRK. This means that the difference in the UNIFAC model selected impact mixtures with non-associating compounds, especially those exhibiting critical or azeotropic points. Furthermore, it is clear from the mark obtained on the three-phase composition that the UMR-PRU is unable to reproduce this type of behavior on non-associating mixtures.

Concerning the mixing heat-capacities, it is interesting to note that all three models discussed to this point perform poorly (marks below 3.5/20). However, it should be noted that both the PSRK and the UMR-PRU models have temperature-dependent parameters, which was recognized in the past as a possible strength of some models, such as the PR-Van Laar¹³⁰. It seems this strength is not a shared feature with group-contribution models with temperature-dependent group interaction parameters, as evidenced here.

Moving onto the next category, mixtures where self-association tends to be broken (BAC5), **Figure 7.7** presents the marks obtained for each property for the *tc*-PR-UNIQUAC, the PSRK and the UMR-PRU.

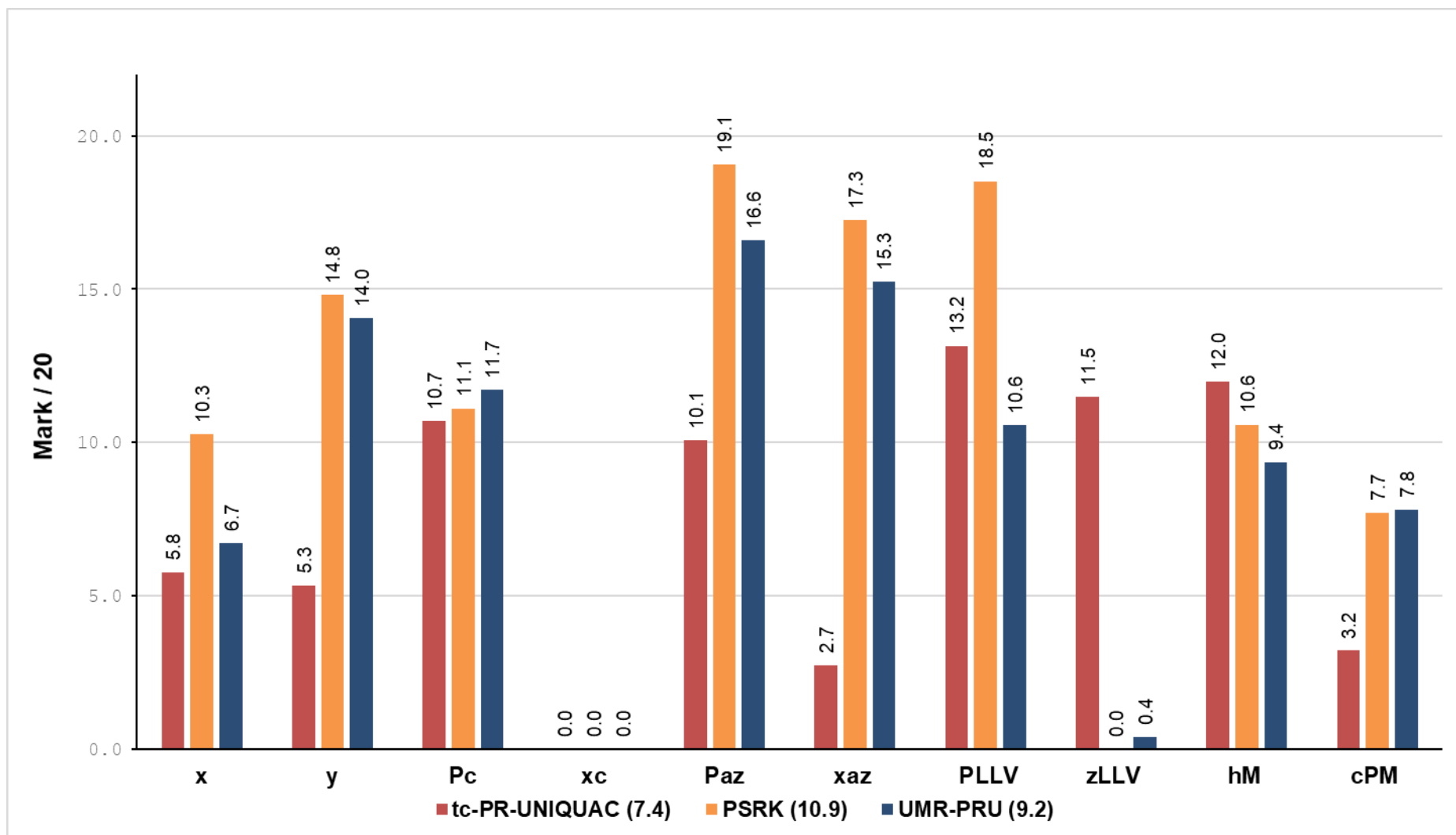


Figure 7.7. Marks obtained by the tc-PR-UNIQUAC, PSRK and UMR-PRU for each property for the second category of binary mixtures (mixtures where self-association tends to be broken). In parenthesis, besides the name of each model we find the mark obtained by each one for this category

For mixtures in BAC5 (the only member of this category), we see that the UMR-PRU performs similarly to the other two models for most properties. Most notably, the azeotropic pressure and composition have marks over 15 for the UMR-PRU, only being outperformed by the PSRK. Furthermore, the vapor/second liquid phase composition and the critical pressure has received an above average mark of 14.0/20 and the model is the best of the three regarding both the critical pressure and the heat capacities of mixing. It should be noted that all three models received a mark equal to zero for the critical composition and in the case of the PSRK and the UMR-PRU a mark of zero for the three-phase composition.

Regarding the liquid phase composition, both the *tc*-PR-UNIQUAC and the UMR-PRU receive similar marks (around 6.0/20), while the PSRK shows a clear advantage with a mark of 10.3/20. **Figure 7.8** shows the VLE diagram for a binary mixture of BAC5, modeled by the UMR-PRU and the PSRK.

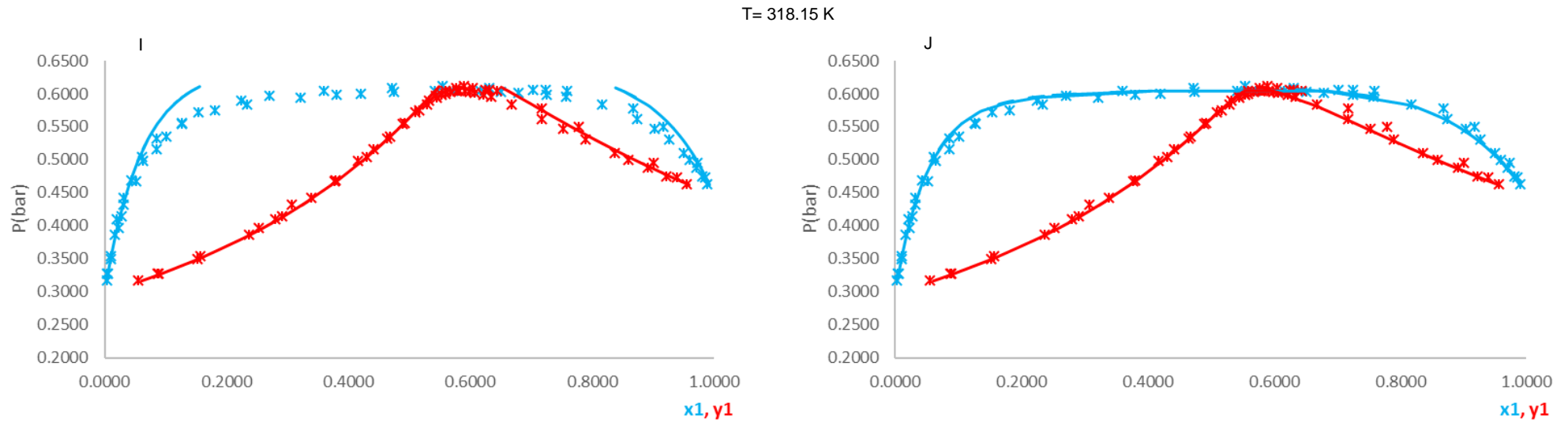


Figure 7.8. VLE diagram for I) methanol-benzene @T =318.15 K with the UMR-PRU; J) methanol-benzene @T =318.15 K with the PSRK. Blue colors symbolize liquid phases, while red colors symbolize vapor phases. Solid lines represent calculated VLE data. Asterisks represent experimental VLE data. Both diagrams belong to BAC5.

As indicated by the marks, the UMR-PRU over predicts the liquid phase and fails to reproduce the shape of the phase diagram completely. On the other hand, the PSRK shows great accuracy in the liquid phase composition. This further demonstrates the impact of the different UNIFAC approaches taken by each model, as the PSRK has a clear advantage over the UMR-PRU for this property. It should be noted that the *tc*-PR-UNIQUAC was the only model capable of describing three-phase line data, with a mark above average as well (11.5/20).

Regarding the mixing heat capacities, both the PSRK and the UMR-PRU models have an advantage over the *tc*-PR-UNIQUAC. Consequently, we are led to think that the temperature-dependent group interaction parameters have a positive influence for these types of systems. It should be noted that these mixtures are regarded as more complex than others, due to the opposing nature of the chemical species comprising them. This can be extended to the general mark for the category, in which both UNIFAC models obtained scores above 9.0/20 while the UNIQUAC model obtained a mark of 7.4/20.

Moving on to the mixtures where only cross-association happens (BAC6), we observe that the *tc*-PR-UNIQUAC has a clear advantage over the two UNIFAC models, with a score of 16.0/20. The UMR-PRU obtained a score of 9.7/20, which in turn is the highest mark for any of the four categories of binary mixtures for this model. **Figure 7.9** presents the marks obtained by the *tc*-PR-UNIQUAC, the PSRK and the UMR-PRU for this category of binary mixtures.

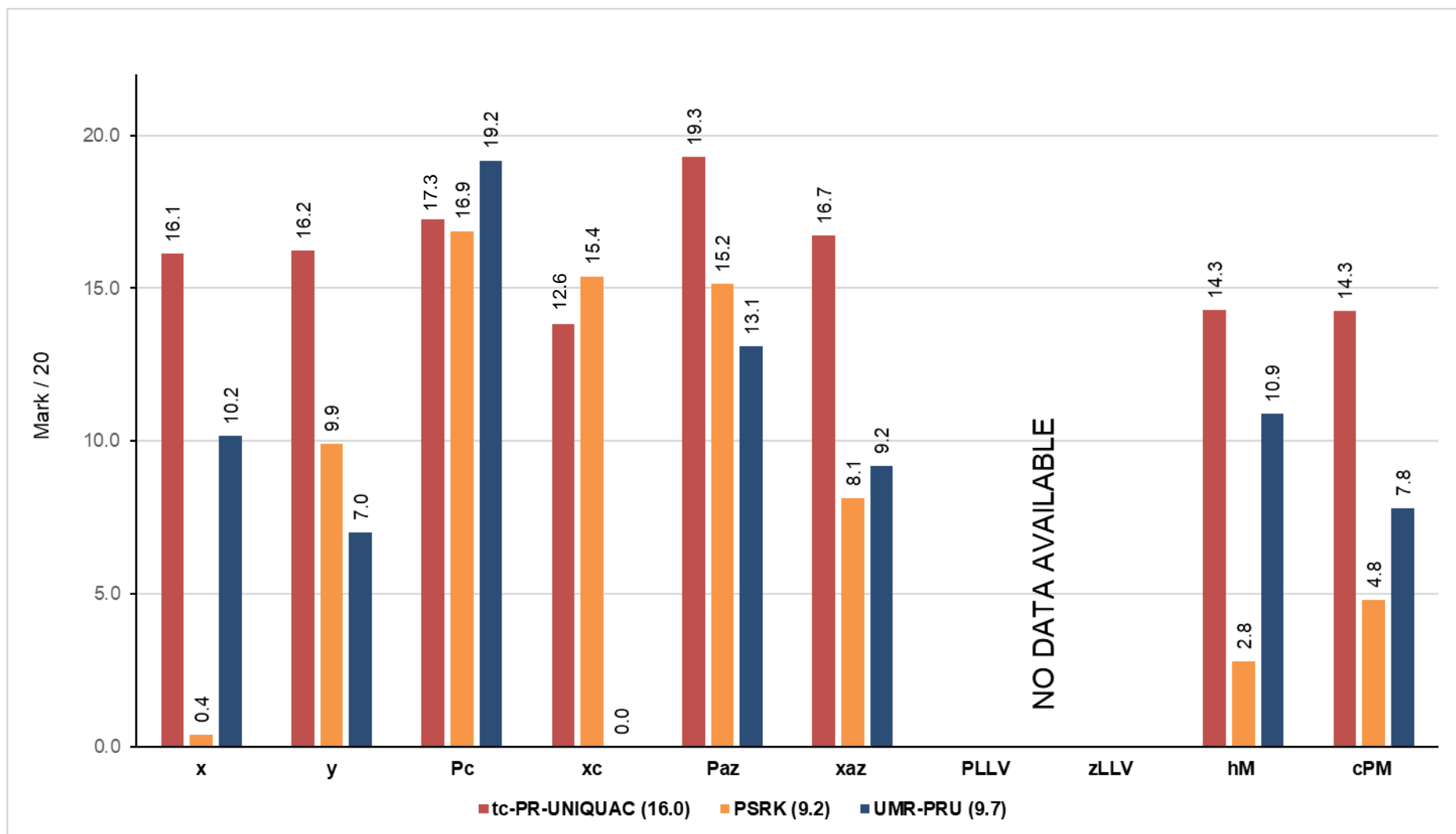


Figure 7.9. Marks obtained by the tc-PR-UNIQUAC, PSRK and UMR-PRU for each property for the third category of binary mixtures (mixtures where only cross-association takes place). In parenthesis, besides the name of each model we find the mark obtained by each one for this category.

At first glance, we note that the *tc*-PR-UNIQUAC has an advantage over the other two models in all properties, except the critical pressure and critical composition, in which the UMR-PRU and the PSRK, respectively, have the advantage. It should be noted that the mark obtained by the UMR-PRU on the critical pressure is the highest mark obtained by a single property for this model. For cross-associating only systems, it seems that the PSRK and the UMR-PRU have opposite behaviors on the VLE properties: the PSRK has a low mark on the liquid phase composition, while the vapor/second liquid composition is lower for the UMR-PRU. **Figure 7.10** presents the phase diagram for the cross-associating system chloroform-acetone.

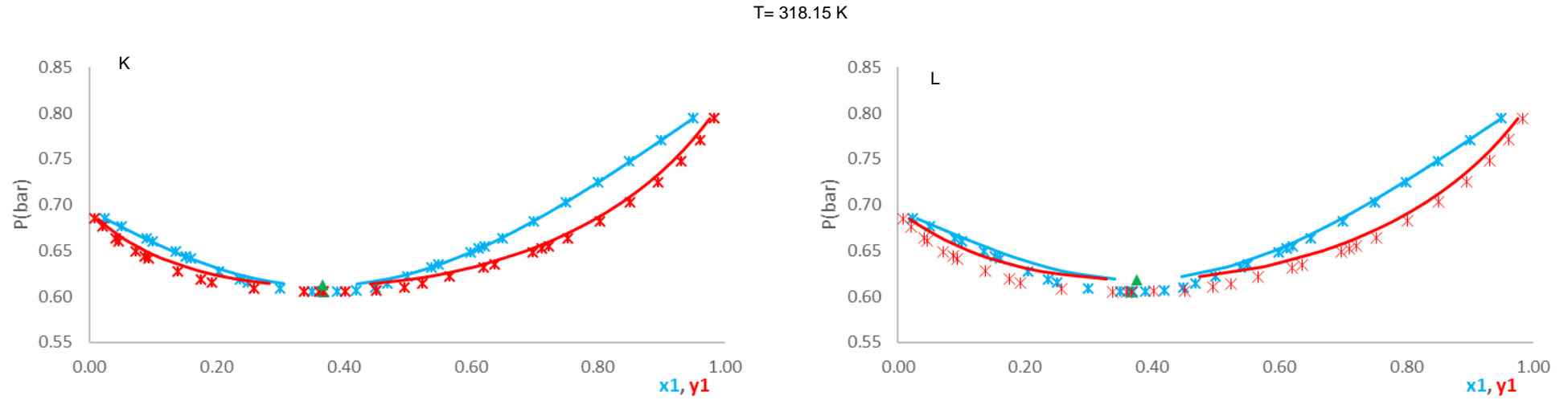


Figure 7.10. VLE diagram for K) chloroform-acetone @T =323.15 K with the UMR-PRU; L) chloroform-acetone @T =323.15 K with the PSRK;. Blue colors symbolize liquid phases, while red colors symbolize vapor phases. Solid lines represent calculated VLE data. Asterisks represent experimental VLE data. Solid triangles represent experimental azeotropic data. Hollow triangles represent calculated azeotropic data. Diagrams K and L belong to BAC 6.

We see that the UMR-PRU effectively reproduces the liquid phase composition, while over predicting both the vapor phase and the azeotropic composition, in concordance with the marks obtained by the model. However, the PSRK seems to overpredict both liquid and vapor phases, as well as the azeotropic point. The liquid phase composition although overpredicted below the azeotropic composition, it does not seem to be as far away from the experimental data, as the composition mark would suggest. The vapor phase, which is the mark that has an advantage over the UMR-PRU is overpredicted all across de composition range. We recall that BAC6 for the UMR-PRU had 13 systems removed. Taking a closer inspection to these systems, we observe that some of the removed systems had a negative impact on the marks for the liquid phase composition for the PSRK. For example, the system trifluoromethane-carbon disulfide had a MAPE on the liquid composition over 400%, which lowers the overall mark to be obtained by this model, explaining the advantage that the UMR-PRU presently has over the PSRK for this property.

Concerning the mixing enthalpies and heat capacities, we observe that the UMR-PRU has an advantage over the PSRK in both cases, which would be an indication of the model's linearly temperature-dependent parameters working for the benefit of the predictions for this model. The issue mentioned for the liquid composition is not relevant here, as all the systems that have experimental data for both these properties are among the systems retained for this BAC, thus given more strength to our previous argument. Nonetheless, the UMR-PRU still falls short for these two properties when compared to the UNIQUAC model, meaning that the group contribution approach of the UMR-PRU may not be enough to reproduce these properties accurately at this stage.

Finally, we turn our attention towards the category of mixtures with both cross and self-association (BACs 7-9). In this case, we see that both the *tc*-PR-UNIQUAC and the PSRK have almost equal marks with 10.6/20 and 10.5/20 respectively, while the UMR-PRU falls shortly behind with a mark of 9.4/20, giving a first indication that the specific UNIFAC model it uses is not as successful at predicting systems in which hydrogen bonding can occur between equal and unlike species. To better asses this, we proceed to inspect each of the properties individually. Figure YY present the marks obtained by the three mentioned models for all properties for the last category of mixtures.

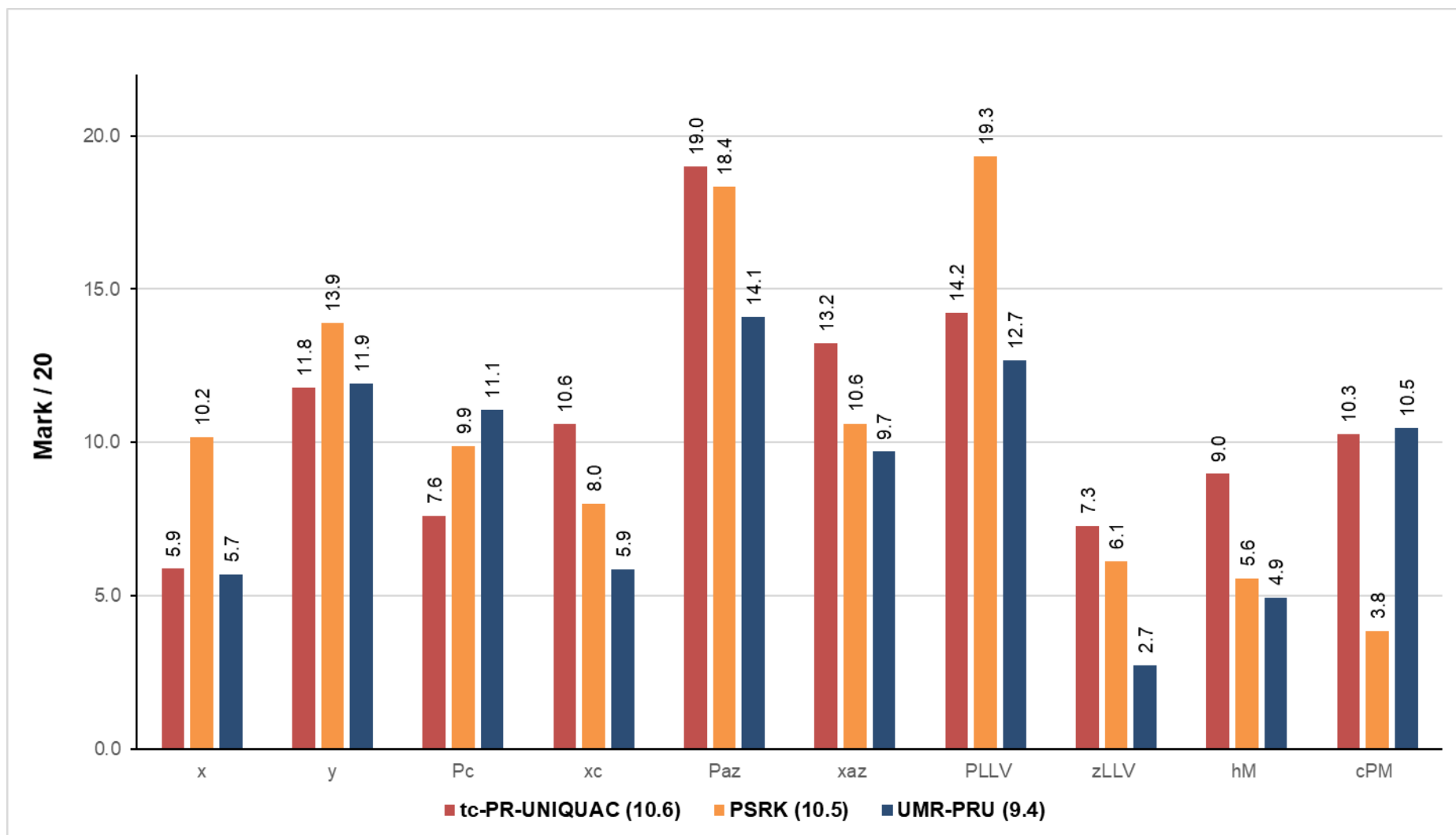


Figure 7.11. Marks obtained by the *tc*-PR-UNIQUAC, PSRK and UMR-PRU for each property for the fourth category of binary mixtures (mixtures with cross and self-association). In parenthesis, besides the name of each model we find the mark obtained by each one for this category.

We see that the PSRK has the main advantage for the VLE properties and the three-phase pressures. The *tc*-PR-UNIQUAC has the advantage in the critical, azeotropic and three-phase compositions as well as in the azeotropic pressure. For the VLE properties, the UMR-PRU obtained the same marks as the *tc*-PR-UNIQUAC. On the azeotropic and three-phase pressures the UMR-PRU also obtained lower marks than the other two models, however all of them above 12.0/20. The model obtained a low score of 2.7/20 on the three-phase composition, 9.7/20 on the azeotropic composition and 5.9/20 on the critical composition. For these three properties, the other models have the advantage over the UMR-PRU for this category of binary mixtures. However, for the critical pressure, the UMR-PRU has the advantage with a score of 11.1/20.

Apparently, the UMR-PRU has a harder time describing associating mixtures, especially in the liquid phase. It is apparent that the PSRK has a better performance on this property, which leads to believe that the differences between their UNIFAC models serve in benefit of the PSRK. This is also true for the critical and azeotropic points, as well as for the three-phase lines. **Figure 7.12** presents different phase diagrams of binary mixtures from this category.

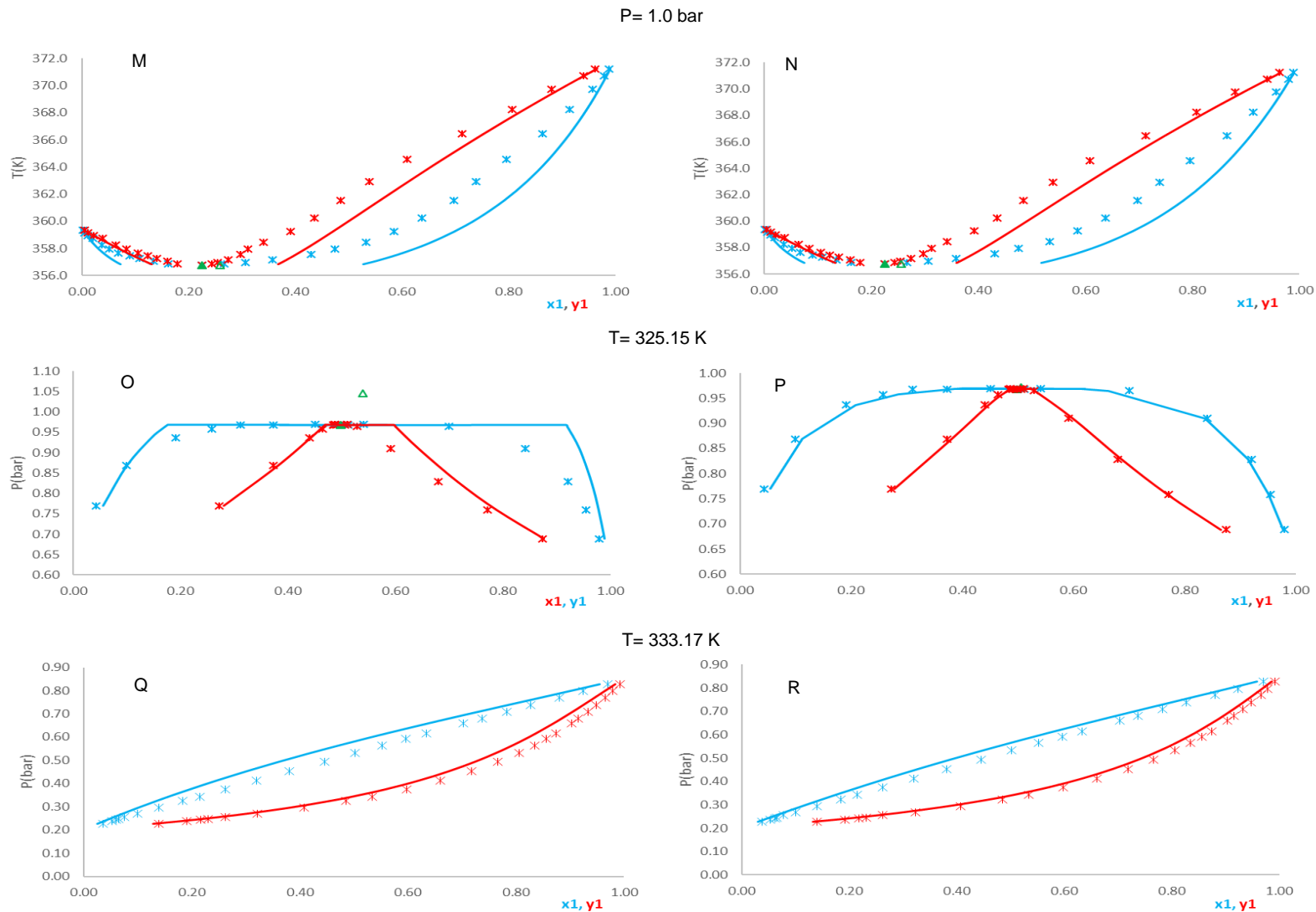


Figure 7.12. VLE diagram for M) 2-butanol-trichloroethylene @P = 1.0 bar with the UMR-PRU; N) 2-butanol-trichloroethylene @P = 1.0 bar with the PSRK; O) methanol-diisopropyl ether @ T = 325.15 K with the UMR-PRU; P) methanol-diisopropyl ether @ T = 325.15 K with the PSRK; Q) methanol-1-propanol @ T = 333.17 K with the UMR-PRU and R) methanol-1-propanol @ T = 333.17 K with the PSRK. Blue colors symbolize liquid phases, while red colors symbolize vapor phases. Solid lines represent calculated VLE data. Asterisks represent experimental VLE data. Solid triangles represent experimental azeotropic data. Hollow triangles represent calculated azeotropic data. Diagrams K and L belong to BAC 6.

For the 2-butanol-trichloroethylene mixture (BAC7) we observe that the UMR-PRU underestimates both the liquid and the vapor phases, especially after the azeotropic point. However, a similar behavior is shown by the PSRK, which indicates that mixtures of self-associating compounds with hydrogen donors are described with equivalent levels of accuracy for both models. Inspecting the methanol-diisopropyl ether (BAC8) system, we observe that the PSRK predicts both phases accurately, as well as the azeotrope. The UMR-PRU overestimates the liquid phase, as well as the azeotrope. Furthermore, it fails at reproducing the topology of the phase diagram. It seems that mixtures of self-associating compounds and hydrogen acceptors present difficulties for the UMR-PRU model. Looking into the methanol-1-propanol system, we evidence once again the overestimations of both phases with the UMR-PRU, especially in the liquid phase. We deduce that mixtures including two self-associating compounds are also a challenge for the UMR-PRU model. From this we can conclude that the differences in the marks obtained by both models for the phase equilibrium properties comes from their ability to reproduce systems in which at least a the self-associating compound present in the mixture is behaving as the hydrogen donor (SA-HA or SA-SA mixtures, BACs 8 and 9).

Concerning mixing heat capacities, we see that the UMR-PRU has the highest mark, alongside the *tc*-PR-UNIQUAC. This indicates that the model performs better than the other UNIFAC version, probably due to the difference between temperature dependent group interaction parameters.

7.9. Conclusions

In this work, the performance of the UMR-PRU was compared against the experimental data of the benchmark database proposed by Jaubert et al.²¹. The results were then compared to previously benchmarked models such as the *tc*-PR with Wilson, UNIQUAC and NRTL advanced mixing rules, the PR EoS with Van Laar mixing rules, the PC-SAFT with van der Waals one-fluid mixing rules and the PSRK EoS. A special attention was given to the *tc*-PR-UNIQUAC and the PSRK in the comparison due to their common background, especially between UMR-PRU and PSRK with their UNIFAC group contribution approach.

It was observed that the UMR-PRU has a lower performance in reproducing the experimental data than the other cubic models, being the closest to the PSRK model, indicative of their similarities in their UNIFAC approach. The UMR-PRU performs with similar capacities all types of binary mixtures, with the best performance being those where only cross-association happens, where it performs better than the PSRK. Notably, both UNIFAC models perform better than the UNIQUAC model for mixtures where self-association tends to break. The UMR-PRU performs below par regarding the other types of mixtures.

Notably, the UMR-PRU seems to struggle in reproducing phase behavior of liquid phases and three-phase topologies in general, when compared to other models. The UMR-PRU shows its main advantages for mixing heat capacities, especially for mixtures where some type of association is present, which indicates that its temperature-dependent group interaction parameters benefit positively for this property.

In the end, with a score of 9.3/20 the UMR-PRU is below average, but performs better than the PC-SAFT-vdW1f, indicating that the more advanced mixing rule improves the predictions of the EoS. It should be noted that the total amount of systems studied for the UMR-PRU was

reduced to 152 from 200 present in the benchmark database, due to shortcomings of the model regarding availability of groups or interaction parameters for the removed systems. If these shortcomings are reviewed and solved in the future, it is proposed to revisit this study in order to guarantee that the benchmark database is being used at its fullest and the benchmark is done with the complete set of systems for the UMR-PRU.

Removing the 48 systems from the results obtained by the -tc-PR-UNIQUAC and PSRK showed that the UNIFAC model improved overall in their marks and even surpassed the UNIQUAC model in all affected categories of binary mixtures. (all categories except mixtures where self-association tends to break). Furthermore, this gives an idea that the UMR-PRU is performing up to par with the other two models, in spite of the inability to model these binary systems, thus reinforcing the idea that a future review of this benchmarking is valuable to contrast the model with the benchmark database at its fullest.

CONCLUSIONS AND PERSPECTIVES
(ENGLISH)

In this thesis, a standardized and universal parametrization protocol was proposed for the SAFT family of equations of state. A deep analysis of the capabilities of the EoS in describing non-associating and associating pure compounds was performed and discussed. The intent was to answer some of the industries main concerns regarding SAFT EoS, without modifying or changing the physically solid background that accompanies the model, which is often viewed as its main feature. A valuable insight into the robustness of the SAFT framework with and without association was obtained as a result of the work presented here.

Finally, the performance of a predictive cubic equation of state with advanced mixing rules was contrasted against a benchmark database of high-quality experimental data for binary mixtures. The scores obtained by the model were contrasted against other models that are also benchmarked to obtain the true state of the current model.

Main results and contributions

How to parametrize reliably SAFT models applied to non-associating compounds in a standardized and universal manner ? Which properties are needed to guarantee that the minimization objective is safe?

One of the main foundations of this work is that the SAFT framework has a robust theoretical background, but the parametrization development has not been keeping up to the growth of the model's theory. A key development presented here is the proposed parametrization methodology. For the case study of the PC-SAFT EoS, it was found that, for non-associating compounds, safe and reliable results are obtained when the objective of the minimization includes only P^{sat} and ρ_{liq}^{sat} experimental data. This, coupled with optimization weights of 3 and 2 for each property respectively guarantees both that the deviations on these two properties are close-to-equal.

It was shown that the inclusion of auxiliary properties such as $\Delta_{vap}H$ and $c_{P,liq}^{sat}$ does not benefit the results of the optimization, however both main properties must be present in the objective function to guarantee optimal results. Using the final objective function leads to close-to-equal deviations on average for both auxiliary properties without taking priority from any of the two main properties.

For 1252 pure non-associating compounds parametrized with this methodology, the following

deviations are obtained: $MAPE_{P^{sat}} = 0.97 \%$, $MAPE_{\rho_{liq}^{sat}} = 0.85 \%$, $MAPE_{\Delta_{vap}H} = 3.04 \%$ and

$$MAPE_{c_{P,liq}^{sat}} = 3.35 \%$$

This methodology aims to contribute to the industrialization of SAFT EoS by introducing a standardized, transparent, and universal protocol to estimate pure compound parameters.

How does a non-associating EoS perform for associating compounds using a standardized parametrization protocol?

This thesis aimed at understanding the robustness of the SAFT family of EoS by parametrizing pure self-associating compounds with and without association. For the first case, the developed parametrization strategy was used to fit non-associating parameters for 548 self-associating compounds.

It was shown that the non-associating PC-SAFT EoS performed satisfactorily for the self-associating compounds, with an average deviation of 2.8% across all studied properties. A major finding is that the PC-SAFT EoS without association included can predict accurately the properties of over 60% of the treated associating compounds. Furthermore, the relation between the strength of the associating effects and the performance of the EoS is not evident, meaning that highly associated compounds can be well-modeled and poorly associated compounds could be badly-modeled.

From this work, a database containing non-associating parameters for 1800 pure compounds (1252 non-associating and 548 self-associating) has been developed. To best of the author's knowledge, this is the first database of this kind available in the open literature.

These findings help to validate the parametrization protocol and allows process engineers to use the simpler and faster non-associating version of the PC-SAFT EoS using the proposed parametrization method or already estimated parameters. It is also an indication on the power of the non-associating contributions of the SAFT family, as shown by the positive results.

What is the impact of the associating term on self-associating pure compounds within the SAFT framework?

This work presented a thorough parameter space study for the two associating parameters for the PC-SAFT over 11 linear alcohols. It was shown that when including the same pair of associating parameters for all alcohols, vapor pressure and liquid density data are sufficient to guarantee that the found solution is optimal and the parameters are safe. Including auxiliary properties improves the predictions, but the improvement is not large enough to consider modifying the parametrization methodology.

However, it was found that treating the five parameters as component-dependent demands the inclusion of at least one of the auxiliary properties studied, preferably $c_{P,liq}^{sat}$. It was found that excluding any of these properties in the minimization objective does not allow to discriminate between equivalent solutions, meaning that the vapor pressure and liquid density could have small deviations but the enthalpy of vaporization and the liquid heat capacity large ones.

Including the associating term, either family-wide or component-dependent, improves the predictions for highly associating compounds such as n-alcohols. However, some of these compounds still remain as badly modeled (e.g. 1-heptanol). This leads to think that, although the associating term has a positive impact on the predictions done by the PC-SAFT, it appears that it is still not enough to shift 100 % of the badly-modeled self-associating compounds.

Perspectives

As the development of this thesis went on, new ideas were conceived and intriguing questions were raised that set the stage for future research projects and development. These new lines of research are presented here.

- **Study of the impact of the associating term for other families of pure compounds:** the results presented in this thesis for the n-alcohols are interesting and promising. However, more research is needed in the direction of including new chemical families, such as organic acids and amines, which would allow a broader knowledge on the influence of the associating term on pure compounds. This would allow to understand the behavior of the SAFT family when dealing with compounds of different associating strengths and associating schemes.
- **Study of the performance of the new parametrization method for mixtures:** the non-associating PC-SAFT with the parametrization method showed surprising results for self-associating pure compounds. The natural extension from this is to study the performance of the parameters obtained this way when predicting mixture properties, especially with self-associating compounds.
- **Extension of the parametrization methodology to include association scheme selection:** although the results for self-associating compounds are promising when using a non-associating PC-SAFT EoS, it appears to be the case that some compounds would require an associating term. However, as shown in the literature review in **Chapter 4**, the selection of a scheme is still very much empiric and due to the lack of standardization, results found in the literature alone cannot help decide on the most appropriate scheme. Thus, a method that incorporates the association scheme selection automatically from the parametrization routine is a natural next step in its development.
- **Implementation of the parameter estimation methodology to other SAFT variants:** the results obtained in this work are based on the PC-SAFT. For this reason, the pure-compound parameters cannot be transferred to other SAFT models, such as the SAFT-VR or the soft SAFT. Furthermore, there is no guarantee that the objective function for other SAFT variants will have the same properties as the ones found for the PC-SAFT. However, the methodology itself can be transferred, as it is model-independent. This leaves room to develop pure-component databases for other SAFT variants, similar to the one proposed here for the PC-SAFT.

CONCLUSIONS ET PERSPECTIVES
(FRANÇAIS)

Dans cette thèse, une méthode de paramétrage systématique et universelle a été proposée pour les équations d'état (EoS) de type SAFT. Une analyse approfondie des capacités de l'EoS à décrire des composés purs associés et non associés a été réalisée et discutée. L'objectif visé de notre démarche était de rendre les modèles de type SAFT conforme aux principales attentes industrielles en la matière. Notons qu'en travaillant le paramétrage de ces modèles, aucune modification n'a été apportée aux bases physiques sur lesquelles il repose et qui sont souvent considérées comme sa principale force. Le travail présenté ici a permis d'obtenir un aperçu de la robustesse mais également des limitations des modèles SAFT, qu'ils contiennent ou non un terme d'association.

Enfin, les performances d'une équation d'état cubique prédictive avec des règles de mélange avancées, nommée UMR-PRU, ont été évaluées sur la base de données binaires de référence sélectionnées avec soin sur la base de leur qualité et de la nature des interactions présentes dans les systèmes binaires correspondants. Les scores obtenus par le modèle ont été comparés à ceux obtenus par les autres modèles précédemment évalués .

Principaux résultats et contributions

Comment paramétrer de manière fiable les modèles SAFT appliqués à des composés non-associés d'une manière systématique et universelle ? Quelles propriétés sont nécessaires pour garantir la qualité du paramétrage ?

Le déclenchement de ce travail résulte de l'observation que le développement des équations d'état de type SAFT au cours des 30 dernières années a été dirigé principalement vers l'amélioration des expressions des termes du modèle sur la base de considérations physiques tandis que les problématiques liées au paramétrage n'ont presque pas été abordées. Dans cette étude, une méthodologie de paramétrage est proposée. Dans le cas de l'EoS PC-SAFT, il a été constaté que, pour les composés non associés, des descriptions précises et fiables des propriétés de corps purs sont obtenues lorsque les paramètres du modèle sont régressés a minima sur des données expérimentales de type pression de vapeur saturante (P^{sat}) et masse volumique du liquide saturé (ρ_{liq}^{sat}). Dans le cadre de la procédure de régression, nous conseillons d'adopter des poids de 3 et 2 pour P^{sat} et ρ_{liq}^{sat} afin de garantir des déviations relatives entre points expérimentaux et calculés identiques pour ces deux propriétés.

Il a été démontré que l'inclusion de propriétés auxiliaires telles que $\Delta_{vap}H$ et $c_{P,liq}^{sat}$ n'améliore pas significativement les résultats de la régression. L'utilisation d'une fonction objectif telle que décrite ci-dessus conduit à des déviations sensiblement égales en moyenne pour les deux propriétés auxiliaires qui sont supérieures aux déviations observées sur les propriétés principales.

Pour 1252 composés purs non associés décrits par l'équation d'état PC-SAFT paramétrée selon

la méthodologie proposée, les écarts suivants sont obtenus : $MAPE_{P^{sat}} = 0.97 \%$, $MAPE_{\rho_{liq}^{sat}}$

$= 0.85 \%$, $MAPE_{\Delta_{vap}H} = 3.04 \%$ and $MAPE_{c_{P,liq}^{sat}} = 3.35 \%$.

En introduisant un protocole systématique, transparent et universel pour estimer les paramètres des composés purs, la méthodologie proposée constitue donc un pas en avant vers l'industrialisation des EoS de type SAFT.

Quelle qualité de description des composés associés obtient-on en paramétrant l'équation PC-SAFT sans terme d'association selon la procédure décrite précédemment ?

Dans le cadre de cette thèse, nous souhaitons mettre en évidence la nécessité d'introduire un terme d'association pour décrire les composés associés et proposer un paramétrage de ce terme.

Pour ce faire, nous avons comparé tout d'abord les prédictions de l'équation PC-SAFT obtenues en utilisant deux approches distinctes pour décrire les composés auto-associés : (i) nous les avons considérés comme des composés non-associés décrits par 3 paramètres ($m, \sigma, \frac{\varepsilon}{k}$) puis (ii) nous les avons considérés comme des composés associés décrits par 5 paramètres (voir paragraphe suivant). Dans le premier cas, la stratégie de paramétrage mentionnée dans le paragraphe précédent a été utilisée pour ajuster les 3 paramètres de chacun des 548 composés auto-associés présents dans notre banque de données.

Ainsi, une base de données contenant des paramètres ($m, \sigma, \frac{\varepsilon}{k}$) pour l'équation PC-SAFT sans terme d'association a été constituée pour 1800 corps purs (1252 constituants non-associés et 548 auto-associés). À notre connaissance, il s'agit de la première base de données de ce type disponible dans la littérature ouverte. Il a été démontré que l'EoS PC-SAFT sans terme d'association produit des résultats satisfaisants pour les composés auto-associés et a conduit à une déviation moyenne de 2,8 % sur l'ensemble des propriétés étudiées (P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ et $c_{P,liq}^{sat}$). L'une des principales conclusions est que l'EoS PC-SAFT sans terme d'association peut prédire avec précision les propriétés de plus de 60 % des composés associés traités. En outre, alors que la littérature mentionne un lien direct entre force d'association et nécessité d'inclure un terme d'association dans l'équation d'état, nous avons mis en évidence l'absence de relation entre l'enthalpie molaire de la liaison hydrogène (révélant la force d'association) et la capacité de l'EoS à décrire un constituant associé. Cela s'illustre par le fait que certains composés fortement associés sont bien décrits par l'équation d'état sans terme d'association tandis que certains composés très faiblement associés sont fort mal décrits par le modèle.

Quel est l'influence du terme d'association des équations d'état de type SAFT sur la description des propriétés thermodynamiques des composés purs auto-associés ?

Dans le cadre de ce travail, nous avons étudié l'influence des deux paramètres d'association ($\varepsilon_{AB}, \kappa_{AB}$) sur la qualité de description des propriétés thermodynamiques de 11 alcools linéaires représentés par l'équation PC-SAFT incluant un terme d'association. Différentes stratégies de paramétrage ont été envisagées : (i) ($\varepsilon_{AB}, \kappa_{AB}$) ont été considérés comme spécifiques à chaque constituant et (ii), ($\varepsilon_{AB}, \kappa_{AB}$) ont été considérés comme identiques pour tous les constituants d'une même famille chimique.

Il a été démontré que dans la configuration (ii), des valeurs optimales de $(\varepsilon_{AB}, \kappa_{AB})$ pour l'ensemble de la famille chimique et des valeurs de $(m, \sigma, \frac{\varepsilon}{k})$ spécifiques à chaque constituant peuvent être régressées sur des jeux de données n'incluant que les deux propriétés : pression de vapeur saturante et de densité liquide ; nous montrons qu'elles sont suffisantes pour garantir que la solution trouvée est optimale pour la représentation des quatre propriétés (P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ et $c_{P,liq}^{sat}$). L'inclusion de propriétés auxiliaires ($\Delta_{vap}H$ et $c_{P,liq}^{sat}$) dans la régression n'apporte pas d'amélioration significative.

Dans le cas de la configuration (i), nous avons montré que les jeux de paramètres $(\varepsilon_{AB}, \kappa_{AB}, m, \sigma, \frac{\varepsilon}{k})$ doivent être déterminés par régression sur des données incluant a minima P^{sat} , ρ_{liq}^{sat} et $c_{P,liq}^{sat}$. Si l'une de ces trois propriétés est manquante dans la régression, les deux propriétés restantes seront bien restituées mais la troisième sera très mal décrite.

Finalement, l'inclusion du terme d'association dans l'équation d'état PC-SAFT, avec des paramètres d'association spécifiques à la famille chimique ou à chaque composant, améliore sensiblement la description des propriétés thermodynamiques de la plupart des composés fortement associés tels que les n-alcools. Cependant, certains de ces composés restent encore imparfaitement modélisés (par exemple, le 1-heptanol). Ceci nous amène à nous interroger sur les raisons pour lesquelles certains composés auto-associés échappent au modèle PC-SAFT incluant un terme d'association tandis que les composés voisins en taille de la même famille chimique sont correctement décrits.

Perspectives

Au fur et à mesure de l'élaboration de cette thèse, de nouvelles idées ont été envisagées et des questionnements ont été soulevés, ouvrant la voie à de futurs projets de recherche et de développement. Ces nouvelles lignes de recherche sont présentées ici.

- **Étude de l'impact du terme associatif sur d'autres familles de composés purs** : les résultats présentés dans cette thèse pour les n-alcools sont intéressants et prometteurs. Cependant, ceux-ci nécessitent d'être confirmés en réalisant des études similaires sur d'autres familles chimiques de composés associés telles que la famille des acides organiques et celle des amines. Cette pratique nous permettra de mieux comprendre le comportement de la famille SAFT selon la famille chimique (forces d'association différentes) et la schéma d'association choisi pour la décrire.
- **Extension de la méthodologie de paramétrage incluant la sélection du schéma d'association** : bien que les résultats pour les composés auto-associés soient prometteurs lorsqu'on utilise un modèle PC-SAFT sans terme d'association, il semble que certains composés nécessitent l'usage d'un terme d'association. Cependant, comme le montre la revue de la littérature au **Chapitre 4**, la sélection d'un schéma est encore très empirique et il reste difficile de déterminer a priori quel sera le schéma d'association optimal. Ainsi, le développement d'une méthode permettant de sélectionner automatiquement le schéma d'association le mieux adapté pourrait constituer une prochaine étape naturelle de ce travail.

- **Mise en œuvre de la méthodologie d'estimation des paramètres à d'autres variantes de SAFT** : les résultats obtenus dans ce travail reposent sur le modèle PC-SAFT. Pour cette raison, les paramètres des composés purs ne peuvent pas être transférés à d'autres modèles SAFT, tels que SAFT-VR ou soft SAFT. Il serait intéressant de s'assurer que les méthodologies développées sont indépendantes du modèle considéré. Ensuite, il serait utile de développer des bases de données de paramètres de composants purs pour les modèles SAFT précédemment mentionnés.

Appendix

Appendix A1 - Parameter dependency of properties predicted from the non-associating version of the PC-SAFT model

In this study, the perturbed-chain SAFT (PC-SAFT) EoS proposed by Gross and Sadowski¹² is considered as well representative of SAFT-type EoS and is selected as base model. All our coming conclusions will be derived from calculations performed using this EoS. Note that the PC-SAFT EoS is extensively described in the literature^{12,93}. Basically, the pressure P of a non-associating compound is a function of 2 state variables (the temperature T and the molecular volume V/N , where V and N are the volume and molecule number of a pure fluid) and 3 model parameters (m , σ , ε/k); it is recalled that m denotes the segment number, σ , the segment diameter and ε/k , a temperature characterizing dispersive interactions:

$$P = f\left(T, \frac{V}{N}, m, \sigma, \frac{\varepsilon}{k}\right) \quad (\text{G.33})$$

As mentioned elsewhere⁹⁴, the PC-SAFT EoS for non-associating species obeys the 3-parameter corresponding state theorem. Introducing the reduced variables (*reduced* is a synonymous of *dimensionless* here):

$$\begin{cases} T^* = T/(\varepsilon/k) \\ P^* = P\sigma^3/\varepsilon \\ v^* = V/(N\sigma^3) \end{cases} \quad (\text{G.34})$$

the EoS can be simply expressed in a dimensionless space involving 2 dimensionless state variables and only one dimensionless model parameter:

$$P^* = f(T^*, v^*, m) \quad (\text{G.35})$$

At vapor-liquid equilibrium (VLE), the variance loses one unit and consequently, the reduced vapor pressure solely depends on one dimensionless state variable and one model parameter:

$$P^{sat,*} = f(T^*, m) \quad (\text{G.36})$$

Still as a consequence of the abovementioned theorem, it is possible to claim that the following VLE reduced properties depend on the (T^*, m) variables:

- The reduced enthalpy of vaporization $\Delta_{vap}H/(RT_c)$,
- The reduced residual isobaric heat capacity $\left(c_P^{res}\right)_{liq}^{sat}/R$ of a saturated liquid,
- The reduced saturated-liquid density $\rho_{liq}^{sat,*} = 1/v_{liq}^{sat,*}$,

While the critical reduced coordinates solely depend on the m parameter. By conjugating the reduced property definition and the 3-parameter corresponding state theorem, one obtains the results presented in **Table 2.3**.

Appendix A2 - Pure component selection

In order to study how parametrization influences the predictions of a thermodynamic model, one must use reliable experimental data. As mentioned before, previous works done over CEoS⁹⁶ showed that a safe parametrization was possible if at least accurate vapor pressure data are available. They developed a database containing two parameters for 1721 molecules, which have at least this property available.

Following the spirit of this work, we proceeded to select which pure components could be part of the present study. In this work, experimental data are generated from DIPPR correlations following a methodology carefully detailed in previous studies^{35,40,96}. To determine if any given correlation for any given property is accurate we used the three types of error proposed by Pina-Martinez et al.⁹⁶:

- Type I error: corresponding to the reported uncertainty of the correlation given by the DIPPR.
- Type II error: corresponding to the actual average uncertainty of the DIPPR correlation (updated following a methodology detailed in reference⁹⁶).
- Type III error: corresponding to the deviation between the pseudo-experimental data and the predictions from the generalized version of the translated consistent Peng-Robinson EoS (*tc*-PR) developed by Le Guennec et al.³². An excessive deviation from this model shows either that experimental data are inaccurate or, that the compound does not obey the 3-parameter corresponding state law.

It is worth noting that EoS only predicts residual properties. Consequently, for estimating the liquid heat capacity, it is necessary to add an ideal-gas heat capacity term ($C_{P,IG}$) to the residual heat capacity. Therefore, an accurate correlation for $C_{P,IG}$ is also needed.

Table A.1. presents the thresholds for the three types of error. For a detailed view on the estimation of type II and type III thresholds the reader is redirected to the original paper⁹⁶.

Table A.1. Thresholds adopted in this study for type I, type II and type III errors

Error type	P^{sat}	ρ_{liq}^{sat}	$\Delta_{vap}H$	$(c_P)_{liq}^{sat}$	$C_{P,IG}$
type I	5.0%	5.0%	5.0%	5.0%	5.0%
type II	5.0%	5.0%	5.0%	5.0%	5.0%
type III	3.4%	3.2%	4.2%	9.1%	-

It should be noted that for a property of a given component is deemed as acceptable if, at least one out of the 3 types of error is below the corresponding threshold. Furthermore, if for a compound and a given property, more than one available correlation could be selected, two scenarios may occur:

- one or more correlation validates the compound on the same type of error, in which case the one with the lowest value is selected as the valid correlation,

- two correlations validate the component on different types of error. In such a case, we define the following priority for the three types of error: $error^{typeI} > error^{typeII} > error^{typeIII}$.

Applying this methodology and doing a mapping over 2230 compounds available in the DIPPR databank, one obtained:

- 656 non-associating pure components for which the 4 properties (P^{sat} , ρ_{liq}^{sat} , $\Delta_{vap}H$ and $c_{P,liq}^{sat}$) have valid correlations.
- 1252 non-associating pure components for which the 2 properties (P^{sat} , ρ_{liq}^{sat}) have valid correlations.

Appendix A3 – Determination of the associating character of a pure component

Surface-charge distribution for a given molecule are input data for COSMO-based models^{114,118–120,1186}. The probability distribution of a molecular surface segment that has a specific charge density is known as sigma profile (σ -profile). **Erreur! Source du renvoi introuvable.** Figure A.1 presents the σ -profiles of water and propane where the two vertical dotted lines represent the sigma-value cutoff for hydrogen bonding ($\pm\sigma_{hb}$) defining the hydrogen bond donor and acceptor regions. While the σ_{hb} cutoff value suggested by Klamt et al.¹²⁰, the developer of the COSMO-RS model, is $0.0084 \text{ e}/\text{\AA}^2$, the value used in this work is $0.01 \text{ e}/\text{\AA}^2$ as suggested by Khan et al.¹²¹. The cutoff value indicates that any molecule whose σ -profile exhibits a peak at the left side of $-0.01 \text{ e}/\text{\AA}^2$ will have H-bond donor ability while those for which the peak lies at the right side of $0.01 \text{ e}/\text{\AA}^2$ will have acceptor ability.

Molecules exhibiting H-bond donor and acceptor abilities are considered as self-associating. Otherwise, they are considered as non-associating molecules. In consequence, it is possible to confirm that propane is a non-associating molecule since its σ -profile lies neither in the H-bond donor nor in H-bond acceptor region. On the other hand, for water the σ -profile covers neutral, positive and negative area, which indicates that such a molecule can act as both H-bond acceptor and donor, and is thus an associating molecule.

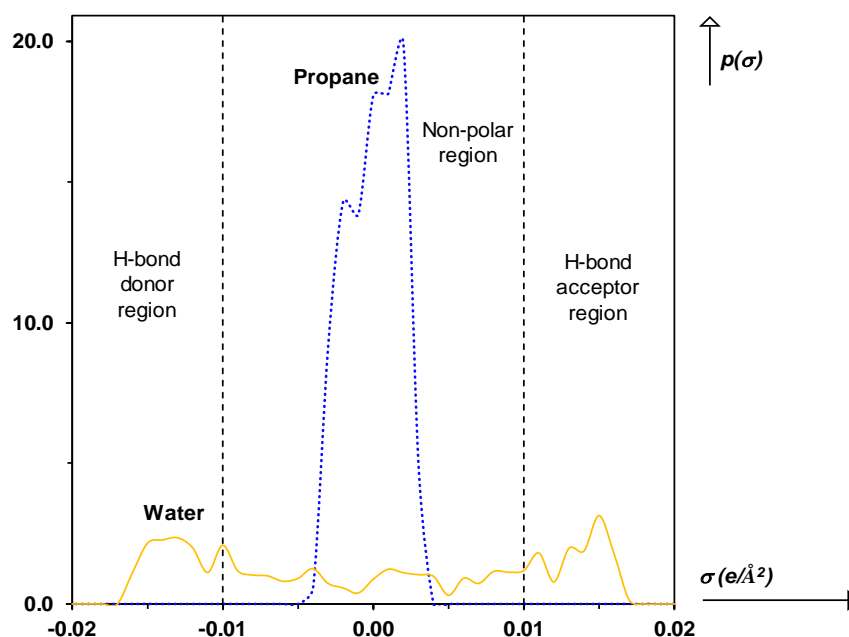


Figure A.1. σ -profile of water (solid line) and propane (dotted line). Dashed vertical lines define the H-donor and H-acceptor regions.

Appendix A4 – Initial value selection for the three PC-SAFT molecular parameters

Given the form of an OF, sometimes an initial parameter set can lead the optimization method to converge to OF value that satisfies the convergence condition but is not actually the lowest value of the OF (known as the *global minimum*). We regard this phenomenon as a convergence to a *local minimum* of the OF.

It is difficult to determine whether a final parameter set corresponds to a local or global optimum without analyzing more deeply the OF itself. To assure, as far as possible, that one has safely landed at the global minimum of the OF, one can:

- test different sets of initial parameter sets,
- evaluate if the values for the parameters and the OF are all equivalent through the different tests. If this is not the case, one needs to analyze more specifically the situation. In particular, if *most of* the initial parameter sets have led to the same minimum OF value, it can be considered that this value corresponds to the global minimum.

This is the spirit of the method used presently. To help the BFGS optimization routine converging to the global minimum of a given OF, we selected first physically-meaningful (m , σ , ε/k) initial values by using the procedure proposed for the *I*-PC-SAFT EoS^{18,94}. This simple procedure requires experimental values of the critical pressure, critical temperature and acentric factor ($P_{c,exp}$, $T_{c,exp}$, ω_{exp}) as input parameters and, in return, provides the (m , σ , ε/k) values ensuring an exact reproduction of the three aforementioned experimental data (we called this procedure “critical point parametrization”).

We used this first set of initial parameters to generate some others by creating a parameter range around these values. Defining the molecular parameter vector θ which contains m , σ and ε/k , the interval in which the initial values are generated is given by:

$$\theta_i \in [k_{\min}\theta_i^{Crit}, k_{\max}\theta_i^{Crit}] \text{ for } i \in \{1; 2; 3\} \quad (\text{G.37})$$

Where the superscript *Crit* refers to the critical point parametrization method. Factors k_{\min} and k_{\max} were specified empirically to 0.9 and 1.5, respectively, to create a parameter range around the critical point parametrization initial values. Eventually, for each OF considered, 10 initial parameter sets were randomly generated, each SAFT parameter satisfying Eq. (A.5.).

Appendix A5 – Temperature range selected for regression of pure-compound parameters and MAPE estimation

Table S1. Experimental data temperature-range selected to regress pure-component parameters and to calculate MAPE.

For each pure component and each considered temperature-dependent property (P^{sat} , $\Delta_{\text{vap}}H$, $c_{P,\text{liq}}^{\text{sat}}$, $\rho_{\text{liq}}^{\text{sat}}$), the regression of pure-component parameters and the MAPE calculations were performed on 50 experimental data points chosen on a defined temperature range. This temperature range depends on the considered property according to the conditions described in the following table. The goal of these conditions is to have the same reduced temperature range for each property for all compounds.

Property	T_{\min}	T_{\max}	Reason of modifications
P^{sat}	$\text{Max}\left\{T_{\min}^{\text{DIPPR}}; T^{\text{eb}}\left(P^{\text{sat}} = 0.1 \text{ bar}\right)\right\}$	$\text{Min}\left\{T_{\max}^{\text{DIPPR}}; T_{c,\text{exp}}\right\}$	If $P^{\text{sat}} < 0.1 \text{ bar}$, the low value of the saturation pressures handicaps the calculation of the MAPE. Moreover, very few processes work at very low pressures.
$\rho_{\text{liq}}^{\text{sat}}$	T_{\min}^{DIPPR}	$\text{Min}\left\{T_{\max}^{\text{DIPPR}}; 0.9 \times T_{c,\text{exp}}\right\}$	It is well known that EoS are inaccurate in the $(P, \rho_{\text{liq}}^{\text{sat}})$ plane for $T_r > 0.9$. This could lead to wrong evaluation of pure-component parameters.
$\Delta_{\text{vap}}H$	T_{\min}^{DIPPR}	$\text{Min}\left\{T_{\max}^{\text{DIPPR}}; 0.98 \times T_{c,\text{exp}}\right\}$	The slope in the $(T, \Delta_{\text{vap}}H)$ is too steep for $T_r > 0.98$.
$c_{P,\text{liq}}^{\text{sat}}$	$\text{Max}\left\{T_{\min,C_{P,IG}}^{\text{DIPPR}}; T_{\min,C_{P,L}}^{\text{DIPPR}}\right\}$	$\text{Min}\left\{\text{Min}\left\{T_{\max,C_{P,IG}}^{\text{DIPPR}}; T_{\max,C_{P,L}}^{\text{DIPPR}}\right\}; 0.98 \times T_{c,\text{exp}}\right\}$	The ideal gas ($C_{P,IG}$) heat capacity and the liquid heat capacity ($C_{P,L}$) must have a common range for the data to be selected. The slope in the $(T, c_{P,\text{liq}}^{\text{sat}})$ is too steep for $T_r > 0.98$.

Note also that, if the calculated property from the EoS is out this temperature range, the point is not considered in the MAPE calculation.

Appendix A6 – Parameter values of 1 800 pure components suitable for the PC-SAFT and I-PC-SAFT equations of state

Table S2. Parameter values for the PC-SAFT and I-PC-SAFT equations of state.

Name	T_c (K)	P_c (bar)	PC-SAFT parameter values			I-PC-SAFT parameter values			
			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
(3,3,3-TRIFLUOROPROPYL)METHYLDICHLOROSILANE	561.7	25.25	4.1422	3.7400	230.5	4.2681	3.8550	224.2	31.096
(3-GLYCIDOXYPROPYL)METHYLDIETHOXSILANE	698.7	15.98	6.8640	3.7093	244.4	7.1897	3.9020	236.0	85.335
(3-METHYLACRYLOXYPROPYL)TRICHLOROSILANE	708.1	21.13	5.7366	3.6975	260.7	5.9210	3.8767	253.1	62.415
[3-(2,3-EPOXYPROXY)PROPYL]TRIMETHOXSILANE	701.4	18.12	6.7007	3.5763	247.6	7.0409	3.7806	238.3	81.754
[3-(MERCAPTO)PROPYL]TRIETHOXSILANE	647.5	18.63	7.5694	3.4830	216.8	7.6927	3.5097	214.7	19.813
1-(4-ETHYLPHENYL)-2-(4-ETHYLPHENYL)ETHANE	780.9	19.17	5.1578	3.9942	302.1	5.5847	4.2382	284.3	91.355
1-(4-ETHYLPHENYL)-2-PHENYLETHANE	771	21.7	5.1465	3.8340	297.9	5.5210	4.0684	281.7	79.888
1,1,1,2,2,3,4,5,5,5-DECAFLUOROPENTANE	454.2	22.88	5.0230	3.3345	172.6	4.8829	3.5208	172.9	28.123
1,1,1,2,2-PENTAFLUOROPROPANE	380.11	31.37	3.1682	3.3695	174.2	3.3264	3.4573	167.3	18.046
1,1,1,2,3,3,3-HEPTAFLUOROPROPANE	374.83	29.12	3.6199	3.2781	162.1	3.7247	3.3832	157.6	18.514
1,1,1,2,3,3-HEXAFLUOROPROPANE	412.38	34.12	3.6949	3.1891	177.0	3.8321	3.2777	171.5	17.107
1,1,1,2-TETRACHLORODIFLUOROETHANE	552	33.4	2.8398	3.8591	266.0	2.9554	4.0017	255.4	28.747
1,1,1,2-TETRACHLOROETHANE	624	40.2	2.6005	3.8788	315.0	2.8406	3.9747	293.8	28.177
1,1,1,2-TETRAFLUROETHANE	374.18	40.56	3.2357	3.0193	171.0	3.5013	3.0980	161.2	16.817
1,1,1,3,3,3-HEXAFLUOROPROPANE	398.07	32.19	3.9434	3.1394	166.2	4.0039	3.2482	162.8	17.019
1,1,1,3,3-PENTACHLOROPROPANE	670.9	32.96	3.3916	3.8377	300.1	3.4792	4.0427	289.8	40.427
1,1,1,3,3-PENTAFLUROBUTANE	473.7	33.92	3.3460	3.5022	208.1	2.9562	3.7829	219.1	15.489
1,1,1,3,3-PENTAFLUROPROPANE	427.2	36.4	3.9063	3.0835	178.9	3.8850	3.2289	176.7	17.687

Name	T_c (K)	P_c (bar)	PC-SAFT parameter values			I-PC-SAFT parameter values			
			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
1,1,1-TRICHLOROETHANE	545	43	2.4608	3.7695	279.4	2.6555	3.8044	264.4	16.031
1,1,1-TRICHLOROFLUOROETHANE	565	39.9	2.5619	3.6993	289.9	2.9017	3.8258	263.5	34.665
1,1,1-TRICHLOROTRIFLUOROETHANE	483	33.2	2.7280	3.7984	237.4	3.0311	3.8006	221.0	21.195
1,1,1-TRIFLUOROETHANE	345.88	37.64	2.6194	3.2291	174.6	2.9897	3.2771	159.2	18.901
1,1,2,2,3-PENTAFLUOROPROPANE	447.57	39.25	3.5597	3.1772	194.9	3.7076	3.2548	188.5	15.490
1,1,2,2-TETRACHLORODIFLUOROETHANE	551	33.4	2.8998	3.8236	263.7	3.1267	3.9192	248.8	29.569
1,1,2,2-TETRACHLOROETHANE	645	40.9	3.0159	3.6470	302.2	2.8753	3.9785	302.0	34.635
1,1,2,2-TETRAFLUROETHANE	391.8	46.4	2.7228	3.1824	191.6	3.0253	3.1725	179.4	11.226
1,1,2,2-TETRAPHENYLETHANE	827	16.7	6.6217	4.0017	290.4	6.8019	4.1653	283.7	75.081
1,1,2-TRICHLOROETHANE	602	44.8	2.7468	3.5988	296.5	2.9719	3.7276	277.8	26.680
1,1,2-TRICHLOROTRIFLUOROETHANE	487.25	34.1	2.8435	3.7394	232.7	2.9127	3.8321	226.9	16.734
1,1,2-TRIFLUOROETHANE	429.8	52.41	3.4247	2.8592	190.5	3.4979	2.9799	185.3	13.537
1,1,2-TRIMETHYLCYCLOPENTANE	579.54	29.39	2.7353	4.1472	284.5	2.9188	4.2636	269.6	34.443
1,1,2-TRIPHENYLETHANE	840	20.4	5.4007	3.9415	319.4	5.7961	4.1889	302.3	91.547
1,1,3-TRIMETHYLCYCLOHEXANE	611.3	29.78	2.9548	4.2064	286.6	3.0979	4.2294	277.1	16.701
1,1,3-TRIMETHYLCYCLOPENTANE	569.54	28.27	2.6261	4.2419	283.1	2.6068	4.4688	278.7	35.497
1,1,5-TRIMETHYLINDAN	713.6	27.19	3.4340	4.1710	318.6	3.7348	4.2856	299.7	49.814
1,1-DIBROMOETHANE	628	60.3	2.6996	3.5717	295.5	1.9425	3.9686	353.6	-5.782
1,1-DICHLORO-1-FLUROETHANE	478.85	43.4	2.5390	3.5909	240.7	2.6778	3.6219	231.5	10.868
1,1-DICHLOROETHANE	523	50.7	2.7241	3.4170	253.9	2.7767	3.4966	248.7	10.653
1,1-DICHLOROETHYLENE	482	51.9	2.7657	3.3252	233.3	3.0730	3.2564	219.3	8.325
1,1-DICHLOROPROPANE	560	42.4	2.7272	3.6362	275.1	2.9237	3.7279	260.3	24.594
1,1-DICHLOROTETRAFLUROETHANE	418.55	33	2.7816	3.6409	201.8	2.9263	3.6767	194.5	12.783

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
1,1-DIETHYLCYCLOHEXANE	643	25.7	3.9464	3.9013	270.4	4.1088	4.0680	260.3	46.346
1,1-DIFLUOROETHANE	386.44	45.2	2.7007	3.0998	192.9	3.0957	3.1594	175.3	18.923
1,1-DIFLUOROETHYLENE	302.8	44.6	2.0267	3.2726	170.0	2.0276	3.3912	166.9	7.973
1,1-DIMETHOXYETHANE	507.8	37.73	3.2566	3.4591	230.3	3.5076	3.5114	218.7	19.476
1,1-DIMETHYLCYCLOHEXANE	591.15	29.38	2.6344	4.2049	295.3	2.7660	4.3745	281.6	37.610
1,1-DIMETHYLCYCLOPENTANE	547	34.45	2.8470	3.9140	261.0	3.0747	3.8930	248.8	12.686
1,1-DIPHENYLETHANE	775	26.8	4.3032	3.9449	316.1	4.5329	4.1100	302.7	53.441
1,2,3,4-TETRAHYDRONAPHTHALENE	720	36.5	3.2873	3.8827	326.5	3.5672	3.9638	307.9	34.237
1,2,3,4-TETRAMETHYLBENZENE	693	31.1	3.7369	3.8280	300.6	4.2167	3.8752	277.9	41.082
1,2,3,4-TETRAMETHYLCYCLOHEXANE	642	25.7	3.9056	3.9143	271.3	4.0925	4.0721	260.3	46.422
1,2,3,5-TETRAETHYLBENZENE	708	20.7	5.4911	3.7916	264.4	5.6512	3.9789	256.8	62.066
1,2,3,5-TETRAMETHYLBENZENE	679	29.7	3.9086	3.7805	288.5	4.2725	3.8887	271.0	44.611
1,2,3,6-TETRAHYDROBENZALDEHYDE	655	40.3	3.6137	3.5245	284.6	3.7921	3.6321	273.4	26.887
1,2,3,6-TETRAHYDROBENZYL ALCOHOL	703.7	40.5	3.9892	3.4520	296.8	4.4513	3.4928	276.7	29.832
1,2,3-TRICHLOROBENZENE	734	45.1	4.1922	3.4589	296.3	4.2895	3.4669	292.5	5.249
1,2,3-TRICHLOROPROPANE	652	38.7	2.9957	3.6686	312.5	3.3342	3.8556	286.6	41.063
1,2,3-TRIETHYLBENZENE	683	23.8	4.6794	3.7829	270.7	4.9269	3.9669	259.2	59.209
1,2,3-TRIMETHYL-4-ETHYLBENZENE	702.7	27.95	4.3175	3.7655	286.1	4.5393	3.9205	274.4	47.150
1,2,3-TRIMETHYLBENZENE	664.5	34.54	3.5372	3.7362	292.3	3.8142	3.8336	276.8	35.693
1,2,3-TRIMETHYLINDENE	726	27.7	4.0525	3.8116	305.9	4.4145	4.0187	286.3	61.565
1,2,4,5-TETRAISOPROPYLBENZENE	703	15.56	5.8753	4.0667	256.1	5.9978	4.2597	250.3	75.823
1,2,4,5-TETRAMETHYLBENZENE	676	29	3.9495	3.7621	286.1	4.2526	3.9210	270.2	51.673
1,2,4-TRICHLOROBENZENE	725	37.2	3.4481	3.7283	323.8	3.7474	3.8759	304.1	42.580

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
1,2,4-TRIETHYLBENZENE	684	23.8	4.5342	3.8491	274.6	4.8921	3.9800	260.2	55.821
1,2,4-TRIMETHYL-3-ETHYLBENZENE	697.3	27.95	4.0652	3.8555	291.7	4.5349	3.9119	272.3	44.191
1,2,4-TRIMETHYL-5-ETHYLBENZENE	687.3	26.78	4.2714	3.7980	281.8	4.5906	3.9302	267.3	49.470
1,2,4-TRIMETHYLBENZENE	649.1	32.32	3.5699	3.7581	285.5	3.9106	3.8525	267.8	38.606
1,2-BENZENE DICARBOXYLIC ACID, HEPTYL, UNDECYL ESTER	878	10.7	8.8166	4.1068	286.8	9.2871	4.2961	277.6	155.962
1,2-BENZENEDICARBOXYLIC ACID, HEPTYL, NONYL ESTER	841	11.6	9.6136	3.8582	267.2	9.9405	3.9958	261.7	104.484
1,2-BENZENEDIOL	764	74.9	6.0694	2.7193	268.9	6.4791	2.5113	265.8	-18.759
1,2-BUTADIENE	452	43.6	2.2166	3.5813	244.3	2.2535	3.7663	236.7	18.198
1,2-BUTANEDIOL	680	52.1	6.1258	2.6962	242.0	5.9521	2.8249	242.7	16.728
1,2-DIBROMOETHANE	650.15	54.77	2.4118	3.6829	337.0	2.5667	3.7668	320.4	17.996
1,2-DIBROMOPROPANE	647.9	46.53	2.8020	3.7238	312.1	2.9424	3.7855	300.3	16.317
1,2-DIBROMOTETRAFLUOROETHANE	487.8	33.93	2.7337	3.7990	237.5	2.8476	3.8710	229.4	17.548
1,2-DICHLORO-1,1,2-TRIFLUOROETHANE	461.6	36.1	2.6052	3.6607	231.6	2.8314	3.7302	217.6	20.887
1,2-DICHLORO-4-NITROBENZENE	758	36	4.8851	3.3293	296.9	5.1956	3.5025	282.5	47.331
1,2-DICHLOROBUTANE	600	36.8	2.9664	3.7260	286.2	3.2812	3.8361	265.5	36.674
1,2-DICHLOROETHANE	561.6	53.7	2.8672	3.3308	269.6	3.1858	3.3440	251.6	15.647
1,2-DICHLOROHEXAFLUOROCYCLOBUTANE	497	27.3	2.4797	4.1175	257.4	2.7691	4.2296	236.6	39.528
1,2-DICHLOROPROPANE	572	42.4	2.6970	3.6544	283.3	2.9506	3.7421	264.8	24.906
1,2-DICHLOROTETRAFLUOROETHANE	418.85	32.6	2.7777	3.6479	202.4	2.9169	3.6969	194.9	14.408
1,2-DIETHOXYETHANE	561	29.3	4.5057	3.4235	224.1	4.7357	3.5211	215.8	32.265
1,2-DIFLUOROBENZENE	566	42.99	2.8489	3.5877	273.0	3.1280	3.6348	255.6	20.894
1,2-DIFLUOROETHANE	445	43.4	2.0106	3.4525	264.2	2.6877	3.5299	214.7	25.401
1,2-DIMETHOXYETHANE	536.15	38.71	3.5684	3.3503	233.8	3.6636	3.4884	226.9	23.877

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
1,2-DIMETHOXYPROPANE	543	34.46	3.5841	3.5320	235.6	3.7010	3.6277	228.9	20.867
1,2-DIMETHYL-3-PROPYLBENZENE	687.7	27.24	4.2282	3.8227	282.0	4.5044	3.9378	269.2	40.830
1,2-DIPHENYLETHANE	785.1	26.5	4.0922	4.0307	328.8	4.5143	4.1499	307.1	61.144
1,2-EPOXY-2-METHYLPROPANE	521	46.6	2.1191	3.7963	287.2	2.2921	3.8399	270.7	15.558
1,2-EPOXY-3-PHENOXYPROPANE	720	29.5	5.0878	3.3575	281.5	5.6531	3.5551	261.1	54.582
1,2-EPOXYBUTANE	526	43.9	2.5754	3.5438	266.8	2.7812	3.6734	250.0	24.613
1,2-ETHANEDITHIOL	663	53.6	2.7196	3.5190	328.0	2.9557	3.6332	306.7	24.552
1,2-HEXADIENE	526	33.5	2.8726	3.7355	253.8	3.1049	3.8649	238.2	32.027
1,2-PENTADIENE	500	38	2.3188	3.7906	264.0	2.1640	4.1349	267.0	26.461
1,2-PROPANEDIAMINE	587	52.7	4.6772	2.8979	227.9	4.6713	2.9553	226.9	6.593
1,2-PROPYLENE GLYCOL	676.4	59.41	5.6894	2.5866	249.3	5.7683	2.7344	243.8	23.324
1,2-PROPYLENE OXIDE	482.25	49.2	2.5051	3.2918	251.6	3.0432	3.3271	220.3	24.083
1,3,5,7-CYCLOOCTATETRAENE	641.4	44.2	3.0529	3.7191	295.6	3.1889	3.7285	287.2	8.125
1,3,5-TRICHLOROBENZENE	718	37.2	3.4751	3.7323	318.8	3.7590	3.8589	300.8	38.210
1,3,5-TRIETHYLBENZENE	678	23	4.6295	3.8344	270.1	4.9452	3.9966	256.9	61.429
1,3,5-TRIISOPROPYLBENZENE	696.6	19.5	5.0568	4.0239	266.2	5.1463	4.1935	260.5	56.384
1,3,5-TRI-tert-BUTYLBENZENE	717.8	16.56	4.6755	4.3301	283.9	4.7740	4.6087	275.3	93.696
1,3-BENZENEDIOL	810	74.9	6.6711	2.6064	275.6	6.3366	2.5848	283.7	-9.070
1,3-BUTADIENE	425	43.2	2.2263	3.5911	228.8	2.4768	3.5824	212.9	12.283
1,3-CYCLOHEXADIENE	558	47.3	2.5503	3.6802	279.9	2.7526	3.6678	266.4	8.478
1,3-DIBROMOPROPANE	680.6	46.48	2.9020	3.6776	326.0	3.1978	3.7359	304.4	24.361
1,3-DICHLOROHEXAFLUOROPROPANE	449	25.7	3.3094	3.7134	202.8	3.5145	3.8276	193.2	32.324
1,3-DICHLOROPROPANE	603	41.5	2.8059	3.6055	297.3	3.2251	3.7148	268.8	35.527

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1,3-DIFLUOROBENZENE	548.4	42.99	2.9080	3.5634	261.0	3.1829	3.5741	245.8	15.746
1,3-DIMETHYL UREA	787.1	48.7	5.2873	2.9358	300.3	5.6179	3.1067	286.0	36.197
1,3-DIMETHYL-2-IMIDAZOLIDINONE	749.9	42.75	3.4579	3.5686	336.7	3.8421	3.7073	311.5	41.877
1,3-DIMETHYL-5-NITROBENZENE	787.7	33.13	4.2094	3.5418	330.9	4.6771	3.8033	304.3	55.291
1,3-DIMETHYLADAMANTANE	708	30	3.1316	4.3284	322.7	3.2394	4.3597	315.0	17.930
1,3-DIOXANE	590	51.5	3.0795	3.3491	273.2	3.2053	3.4395	263.7	15.045
1,3-DIPHENYLTRIAZENE	845	28.3	5.7591	3.6344	308.3	5.8428	3.7509	303.3	35.925
1,3-DI-TERT-BUTYL GLYCERIN	667.1	21.86	6.1828	3.6635	235.4	6.1162	3.7072	236.1	10.601
1,3-PROPANEDIAMINE	632	55.9	3.9166	3.0932	262.7	3.8538	3.1987	262.2	8.264
1,3-PROPYLENE GLYCOL	718.2	65.5	5.8711	2.5395	261.6	5.9003	2.6752	257.0	21.225
1,3-PROPYLENE OXIDE	520	57.5	2.1877	3.3913	287.0	2.5189	3.4629	258.5	20.441
1,4-BENZENEDICARBOXYLIC ACID, 2-HYDROXYETHYL METHYL ESTER	832	26.75	7.3613	3.3583	281.0	7.4050	3.4389	278.7	26.207
1,4-BIS(3-AMINOPROPYL)PIPERAZINE	750.3	22.66	7.4718	3.3752	253.5	7.6450	3.4629	249.2	32.817
1,4-BUTANEDIISOCYANATE	724.3	29.47	3.5686	3.7383	329.2	4.2860	3.9788	288.7	58.010
1,4-BUTANEDIOL	723.8	55.2	6.5403	2.6085	252.7	6.2610	2.7702	254.4	20.532
1,4-CYCLOHEXANEDICARBOXYLIC ACID	819.8	37.36	9.0045	2.7464	262.4	9.1504	2.7866	260.1	12.244
1,4-CYCLOHEXANEDIMETHANOL	800.3	40	5.8465	3.1941	288.1	5.5759	3.3460	291.5	19.510
1,4-DIBROMOBENZENE	738.15	44.72	3.8561	3.5500	311.5	4.2845	3.4848	294.3	13.206
1,4-DICHLOROBUTANE	641	36.1	3.1597	3.6628	300.0	3.4947	3.8564	276.4	43.067
1,4-DICHLORO-cis-2-BUTENE	640	37.8	3.1727	3.5938	299.3	3.5253	3.7835	275.0	41.028
1,4-DICHLORO-trans-2-BUTENE	646	37.8	3.1309	3.6224	304.1	3.5115	3.8008	278.0	41.430
1,4-DICYANO-2-BUTENE	755	29.5	5.2693	3.1158	299.8	6.2541	3.4636	265.4	55.838
1,4-DIFLUOROBENZENE	556.9	44	2.9784	3.5220	262.5	3.2790	3.5264	246.5	15.389

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1,4-DIOXANE	587	52.08	2.9644	3.3803	276.3	3.1286	3.4511	265.0	15.519
1,4-DI-tert-BUTYLBENZENE	708	23	4.6809	4.0306	277.5	4.9019	4.0689	269.1	28.166
1,4-HEXADIENE	510	33.5	2.8208	3.7720	247.4	3.1339	3.8125	230.1	25.022
1,4-PENTADIENE	479	37.4	1.9394	4.0645	273.3	1.6289	4.5161	294.7	12.771
1,4-PENTANEDIOL	708.4	43.54	5.8898	2.9080	256.7	5.8086	3.0711	254.7	25.291
1,5,9-CYCLODODECATRIENE	745	29.9	3.8302	4.0584	314.2	4.1042	4.0641	301.8	24.307
1,5-CYCLOOCTADIENE	645	39	3.1114	3.8097	296.0	3.1797	3.8987	289.2	14.137
1,5-DICHLOROPENTANE	668	31.9	3.5727	3.6940	296.6	3.8937	3.9129	276.0	50.126
1,5-HEXADIENE	508	33.5	2.5277	3.9250	258.1	2.7143	4.0078	244.0	24.997
1,5-NAPHTHALENE DIISOCYANATE	818	27.2	6.6313	3.4301	286.2	6.7843	3.5312	280.8	35.549
1,5-PENTANEDIAMINE	642	37.35	5.1583	3.1421	245.0	5.5969	3.1760	233.6	20.828
1,6-DIMETHYLINDAN	717.3	30.98	3.2204	4.1110	328.5	3.4933	4.2137	309.4	41.710
1,6-HEXANEDIOL DIACRYLATE	765	19.3	7.5543	3.4657	260.6	7.9808	3.6081	251.2	68.720
1,9-DECADIENE	606.8	22.67	4.7286	3.7210	238.8	4.9722	3.8617	229.5	47.507
1-AMINO-2-PROPANOL	614	56.7	7.0486	2.4220	210.0	7.2658	2.4393	206.8	7.841
1-BROMOBUTANE	570.4	40.41	2.8521	3.7007	276.2	3.3791	3.6170	249.4	18.827
1-BROMODODECANE	727.9	18.37	6.1312	3.7959	262.8	6.3835	3.9725	254.3	71.699
1-BROMOHEPTANE	646.1	28.97	4.0838	3.7609	268.5	4.5015	3.7793	253.0	29.333
1-BROMONAPHTHALENE	824	37	3.5827	3.8578	362.1	3.8356	4.0168	342.5	45.813
1-BROMOPROPANE	535.5	45.78	2.4622	3.6570	279.2	3.1426	3.4884	241.3	17.661
1-BUTANOL	563.1	44.14	5.9827	2.6867	201.4	5.6038	2.8741	204.8	19.367
1-BUTENE	419.5	40.2	2.4122	3.5822	215.3	2.3960	3.6957	213.4	11.145
1-CHLORO-1,1-DIFLUOROETHANE	410.29	40.41	2.5438	3.4381	207.6	2.7514	3.4894	195.9	15.110

Name	T_c (K)	P_c (bar)	PC-SAFT parameter values			I-PC-SAFT parameter values			
			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
1-CHLORO-2,4-DINITROBENZENE	813.77	34.9	6.4202	3.0586	291.8	6.8001	3.2409	279.2	49.738
1-CHLORONAPHTHALENE	785	34	3.2954	3.9616	362.9	3.9424	4.0234	322.8	55.174
1-CHLOROPENTANE	571.2	33.52	2.9279	3.8150	274.0	3.2532	3.9051	253.7	34.581
1-cis-2-trans-3-TRIMETHYLCYCLOPENTANE	579.82	28.98	2.9507	4.0469	275.2	3.1342	4.1759	261.6	36.712
1-cis-2-trans-4-TRIMETHYLCYCLOPENTANE	579.26	28.78	2.8765	4.0974	278.4	3.1148	4.1936	262.0	36.751
1-CYCLOHEXYLETHANONE	673.7	33.61	3.5413	3.7790	294.9	3.5488	3.9926	288.7	36.636
1-DECANOL	688	23.08	5.7798	3.5603	251.7	5.7579	3.7716	248.1	53.144
1-DECENE	616.6	22.23	4.4384	3.8638	248.5	4.7249	3.9877	237.4	48.440
1-DECYNE	619.85	23.7	4.6684	3.7387	245.3	5.0277	3.8151	233.6	40.226
1-DOCOSANOL	824.4	10.35	7.7692	4.1783	279.4	8.2141	4.4954	268.7	160.346
1-DODECANOL	718.7	19.54	5.7898	3.7840	265.6	6.1605	3.9334	253.8	70.205
1-DODECENE	657.1	18.88	5.1128	3.9067	252.3	5.3878	4.0809	242.0	67.266
1-EICOSANOL	807.7	11.54	7.5300	4.1006	276.6	8.0530	4.3437	264.6	141.820
1-EICOSENE	771	12.2	7.7033	4.0249	260.6	8.0657	4.1954	252.5	102.349
1-ETHOXY-2-PROPANOL	560.4	37.48	6.4870	2.8330	197.0	7.0214	2.7566	190.5	3.773
1-ETHYL-2-ISOPROPYLBENZENE	666	26.7	4.0128	3.8682	278.5	4.2204	4.0223	267.0	46.356
1-ETHYLCYCLOHEXENE	614.9	33.05	3.0265	3.9287	288.6	3.2296	4.0318	273.9	31.205
1-ETHYL-DECALIN	708.8	24.69	3.9277	4.0669	299.8	4.1723	4.2339	285.4	57.173
1-ETHYLNAPHTHALENE	776	33.2	3.7658	3.8914	334.2	4.1382	3.9659	313.4	42.451
1-ETHYLTETRALIN	733	27.52	4.0305	3.9051	307.7	4.3131	4.0769	291.5	56.933
1-HEPTADECANOL	779.2	13.77	6.9977	3.9909	272.2	7.4818	4.1794	260.3	107.077
1-HEPTADECENE	736	14.1	6.4691	4.0532	262.9	6.9552	4.1988	250.9	93.842
1-HEPTANOL	632.3	30.85	5.7031	3.2161	230.1	5.3889	3.4203	232.9	24.447

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1-HEPTENE	537.4	29.2	3.2797	3.8260	243.9	3.6297	3.8482	228.2	27.350
1-HEPTYNE	547	32.1	3.5731	3.6342	238.8	3.9033	3.6497	225.8	21.484
1-HEXADECANOL	768.6	14.68	6.6096	3.9791	274.0	7.1963	4.1419	259.5	106.341
1-HEXADECENE	722	14.8	6.3216	3.9983	259.4	6.7351	4.1620	248.4	90.162
1-HEXANOL	611.3	34.46	5.6799	3.0511	223.0	5.3602	3.2666	225.5	28.800
1-HEXATRIACONTENE	894	7.16	11.8173	4.2195	270.5	12.1852	4.3507	266.1	127.538
1-HEXENE	504	32.1	3.1210	3.7046	231.4	3.1743	3.8341	226.2	22.231
1-HEXYNE	516.2	36.2	3.2588	3.5594	233.4	3.5471	3.5649	221.3	17.330
1H-PERFLUORO-N-HEXANE	471.75	19.35	4.6253	3.6785	185.6	4.6354	3.8488	182.8	36.649
1-METHOXY-2-PROPANOL PROPANOATE	611.7	26.02	4.8723	3.4866	238.2	4.9631	3.7009	231.5	48.200
1-METHYL-1-ETHYLCYCLOPENTANE	582	30.2	3.0872	3.9766	271.7	3.5244	3.9508	250.1	28.311
1-METHYL-2-n-PROPYLBENZENE	662	29.4	3.6680	3.8836	288.7	4.1356	3.9178	267.4	38.577
1-METHYL-3-(METHYLETHOXY)BENZENE	670	28.4	4.1108	3.7946	278.0	4.4429	3.8705	263.6	37.404
1-METHYL-3-HYDROXY-5-ISOPROPYL BENZENE	726.8	34.08	5.9462	3.3355	257.5	5.5876	3.4151	264.6	2.162
1-METHYL-3-HYDROXY-6-ISOPROPYL BENZENE	722.5	34.08	5.6021	3.4123	262.4	5.5750	3.4115	263.2	-0.338
1-METHYL-3-n-PROPYLBENZENE	654	28.1	3.8156	3.8540	280.3	4.1817	3.9444	263.1	40.503
1-METHYL-4-n-PROPYLBENZENE	656	28.1	3.8099	3.8690	281.2	4.1869	3.9466	263.8	37.317
1-METHYL-4-VINYLCYCLOHEXENE	626	31.2	3.4927	3.8237	275.8	3.6400	3.9564	265.6	33.199
1-METHYLCYCLOPENTENE	542	41.3	2.6740	3.7238	266.0	2.7600	3.7968	258.4	14.847
1-METHYL-DECALIN	707.2	27.7	3.7840	4.0039	301.9	3.9095	4.1738	291.8	44.908
1-METHYLINDAN	694.1	34.37	3.1808	3.9662	318.6	3.3994	4.0667	302.7	33.580
1-METHYLINDENE	703	34.6	3.3023	3.8645	319.5	3.5641	4.0043	300.8	41.460
1-METHYLNAPHTHALENE	772	36	3.4822	3.8645	341.5	3.6172	4.0546	328.3	42.900

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
1-METHYLTETRALIN	719.3	30.57	3.7169	3.8805	311.1	3.9491	4.0463	295.6	48.303
1-METHYLVINYL ACETATE	552.2	41.81	3.8557	3.3253	231.7	4.1014	3.2900	223.7	6.810
1-n-BUTYLNAPHTHALENE	792	26.8	4.6064	3.8883	314.6	4.8436	4.0331	302.3	52.224
1-n-DECYLNAPHTHALENE	844	15.23	6.4163	4.0169	304.5	6.9151	4.2941	288.2	117.651
1-n-HEXYL-1,2,3,4-TETRAHYDRONAPHTHALENE	779	18.9	5.2614	4.0118	298.1	5.6080	4.2476	283.2	92.346
1-n-HEXYLNAPHTHALENE	813	22.5	5.4118	3.9039	304.7	5.5964	4.0687	295.8	59.720
1-NITROBUTANE	623	37.6	3.5097	3.4813	282.9	4.5164	3.4185	243.7	37.954
1-NITROPROPANE	605	43.5	3.7634	3.2015	262.5	4.1816	3.3224	243.4	32.953
1-n-NONYLNAPHTHALENE	835.1	16.43	6.2196	3.9779	303.8	6.7127	4.2254	287.6	108.814
1-NONADECANOL	798.8	12.2	7.2940	4.0806	276.3	7.8752	4.2903	263.2	133.634
1-NONADECENE	760	12.8	7.1522	4.0631	263.2	7.6540	4.2049	252.3	99.773
1-NONANOL	670.9	25.27	5.6314	3.4621	247.5	5.5692	3.6787	244.5	49.083
1-NONENE	593.1	24.28	4.0921	3.8398	246.1	4.3732	3.9398	234.7	40.242
1-NONYNE	598.05	26.1	4.5041	3.6472	238.1	4.6484	3.7658	231.5	32.717
1-n-PENTYLNAPHTHALENE	803	24.4	4.9263	3.9125	311.8	5.1706	4.0727	299.8	60.418
1-OCTADECANOL	789.3	12.95	7.0633	4.0480	275.8	7.6520	4.2423	262.1	125.536
1-OCTADECENE	748	13.4	6.8619	4.0492	262.2	7.3280	4.1982	251.3	96.338
1-OCTANOL	652.3	27.83	5.7253	3.3260	237.7	5.4511	3.5601	239.3	36.724
1-OCTENE	566.9	26.63	3.6316	3.8545	247.2	4.0173	3.8881	231.5	32.785
1-OCTYNE	574	28.8	3.9684	3.6653	240.4	4.2656	3.7172	229.2	27.461
1-PENTADECANOL	757.3	15.69	6.4049	3.9262	272.4	6.9582	4.0899	258.1	99.701
1-PENTADECENE	708	15.7	5.9608	3.9954	259.2	6.3768	4.1494	247.5	83.629
1-PENTANOL	588.1	38.97	5.7447	2.8915	213.6	5.4932	3.0645	215.3	22.359

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1-PENTENE	464.8	35.6	2.5925	3.7386	232.6	2.8020	3.7701	220.1	16.720
1-PENTENE-4-YNE	503	44	2.0245	3.8728	285.2	2.3511	3.8347	258.2	16.905
1-PENTYNE	481.2	41.7	2.9334	3.4739	227.0	3.2118	3.4453	214.9	5.843
1-PHENYLNAPHTHALENE	849	26.3	4.8024	3.8560	334.9	5.1338	4.0582	317.7	73.015
1-PROPANOL	536.8	51.69	6.0994	2.4830	191.4	5.8729	2.6323	192.4	17.118
1-tert-BUTOXY-2-[2-(HYDROXY)PROPOXY]PROPANE	689.9	23	8.6477	3.1647	221.4	8.5389	3.1906	222.7	6.765
1-tert-BUTOXY-2-[2-(tert-BUTOXY)PROPOXY]PROPANE	729.4	15.27	5.1827	3.9692	288.3	5.9980	4.3395	259.7	105.322
1-tert-BUTYL GLYCERIN	690	29.59	6.9139	3.0766	238.6	7.0198	3.1971	234.6	33.205
1-TETRADECENE	691	16.27	5.8129	3.9345	254.7	6.1167	4.1389	244.6	86.958
1-TRIACONTENE	857	8.47	10.3576	4.1523	267.6	10.7217	4.3107	262.2	134.077
1-TRIDECANOL	732.4	18.1	6.0175	3.8276	267.7	6.4320	3.9876	255.3	79.228
1-TRIDECENE	674.8	17.49	5.4528	3.9252	253.8	5.7609	4.1094	243.3	76.734
1-UNDECANOL	703.9	21.19	5.5399	3.7354	263.8	5.8954	3.8723	252.0	60.342
1-UNDECENE	637.8	20.44	4.7826	3.8852	250.4	5.0654	4.0342	239.7	57.593
2-(2-ETHOXYETHOXY)ETHANOL	670	31.67	5.2677	3.2839	253.7	5.4207	3.4484	246.3	39.124
2-(2-HEXOXYETHOXY)ETHANOL	684	24.1	10.4991	2.9350	207.7	10.0883	2.9031	212.1	-17.071
2-(2-METHOXYETHOXY)ETHANOL	672	36.7	4.8328	3.2270	262.7	5.0214	3.3893	253.3	36.469
2-(2-PENTOXYETHOXY)ETHANOL	705.3	25.03	6.7791	3.3439	243.1	6.5711	3.5027	244.4	31.556
2-(5H)-FURANONE	754.8	49.98	2.9900	3.2917	370.5	3.3223	3.7224	332.3	36.822
2-(alpha-METHYLBENZYLOXY)-1-PROPANOL	722.7	24.92	5.6249	3.4484	271.2	6.0486	3.6617	256.7	63.811
2-(DIFLUOROMETHOXY)-1,1,1-TRIFLUOROETHANE	444.03	34.2	3.8589	3.2072	187.4	3.9900	3.3058	181.8	19.088
2-(N-MORPHOLINO)-2'-HYDROXYDIETHYLETHER	728.4	28.93	6.8236	3.1944	252.6	6.9699	3.2900	248.1	29.690
2,2,3,3-TETRAMETHYLBUTANE	568	28.7	2.7343	4.2454	275.8	2.8619	4.2985	266.5	20.557

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2,2,3,3-TETRAMETHYLHEXANE	623	25.1	3.4887	4.1706	274.4	3.8089	4.1756	259.6	29.466
2,2,3,3-TETRAMETHYLPENTANE	607.5	27.41	3.1068	4.1919	280.3	3.3302	4.2265	267.2	26.483
2,2,3,4-TETRAMETHYLPENTANE	592.6	26	3.1821	4.1858	270.8	3.3986	4.2344	258.5	29.790
2,2,3-TRIMETHYLBUTANE	531.1	29.5	2.7345	4.0939	258.8	2.9014	4.1447	247.7	21.917
2,2,3-TRIMETHYLPENTANE	563.5	27.3	3.0851	4.0827	260.8	3.2677	4.1561	249.8	30.717
2,2,4,4,6,8,8-HEPTAMETHYLNONANE	692	15.7	4.9805	4.3100	267.5	5.2749	4.4532	256.6	81.447
2,2,4,4-TETRAFLUOROPENTANE	515.5	32.01	3.4312	3.6235	227.5	3.5346	3.7172	221.3	20.275
2,2,4,4-TETRAMETHYL-1,3-CYCLOBUTANEDIOL	699.5	31.72	5.4505	3.2785	261.3	5.4629	3.4854	256.5	42.183
2,2,4,4-TETRAMETHYLPENTANE	574.6	24.9	3.1721	4.2106	262.9	3.3971	4.2526	250.7	28.807
2,2,4-TRIMETHYL-1,3-PENTANEDIOL	697.9	27.04	5.7097	3.3185	257.9	5.6655	3.6188	252.9	57.691
2,2,4-TRIMETHYLPENTANE	543.8	25.7	3.1298	4.0951	250.2	3.3176	4.1675	239.5	29.206
2,2,5,5-TETRAMETHYLHEXANE	581.4	21.9	3.8867	4.0638	243.7	3.8943	4.2347	240.2	37.401
2,2,5-TRIMETHYLHEXANE	569.8	23.3	3.5273	4.0824	249.4	3.6412	4.2257	241.7	38.339
2,2-DICHLORO-1,1,1-TRIFLUOROETHANE	456.94	36.76	2.9813	3.4842	214.8	3.1537	3.5552	205.6	17.512
2,2-DICHLORO-1,1,2-TRIFLUOROETHANE	462	36.1	2.7748	3.5531	225.9	2.9960	3.6569	212.5	23.907
2,2-DIMETHYL-1-PROPANOL	552.7	40.78	6.3086	2.8478	190.4	5.6592	2.9208	200.4	-8.081
2,2-DIMETHYL-3-ETHYLPENTANE	590	25.7	3.4689	4.0655	259.1	3.5673	4.1693	252.3	28.893
2,2-DIMETHYLBUTANE	489	31	2.5969	4.0074	243.7	2.7776	4.0279	232.5	17.105
2,2-DIMETHYLHEPTANE	576.7	23.5	3.6809	4.0282	249.5	4.0086	4.0801	235.7	37.393
2,2-DIMETHYLHEXANE	549.8	25.3	3.4029	3.9844	244.6	3.5873	4.0852	234.6	33.574
2,2-DIMETHYLOCTANE	602	21.6	4.1450	3.9879	248.0	4.3093	4.1404	239.5	47.882
2,2-DIMETHYLPENTANE	520.5	27.7	2.9913	3.9950	244.4	3.1897	4.0635	233.1	27.248
2,2'-IMINOBIS-ACETONITRILE	731	35.4	5.8669	2.8484	276.8	6.6928	3.1334	251.9	44.244

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2,3,3,3-TETRAFLUOROPROPENE	367.85	33.82	2.9411	3.3271	174.5	3.1502	3.4018	165.6	17.306
2,3,3,4-TETRAMETHYLPENTANE	607.5	27.2	3.2512	4.1327	274.1	3.4033	4.2037	264.8	27.184
2,3,3-TRIMETHYL-1-BUTENE	531	31.4	2.7251	4.0492	258.0	2.8142	4.1034	251.0	15.130
2,3,3-TRIMETHYLPENTANE	573.5	28.2	3.0285	4.1010	267.3	3.2147	4.1602	256.0	27.101
2,3,4,5,2',3',4',5'-OCTAHYDRO-BIFURYL-(3,3')	738	37	3.4684	3.7010	331.6	3.8538	3.8650	306.2	47.811
2,3,4-TRIMETHYLPENTANE	566.4	27.3	3.2249	4.0202	257.3	3.4104	4.0985	246.7	30.308
2,3,5-TRIMETHYLTHIOPHENE	656.8	36.3	3.2721	3.7990	297.3	3.4771	3.8879	283.8	27.815
2,3-BUTANEDIOL	611	51.3	9.9434	2.2539	189.3	10.0396	2.1784	189.7	-9.174
2,3-DICHLOROBUTANE	599	37.4	2.7961	3.8307	291.7	3.0421	3.9192	273.7	26.518
2,3-DICHLOROPROPENE	578	43.8	2.4349	3.7306	300.7	2.4726	3.9532	289.8	24.456
2,3-DIHYDROFURAN	524	55	2.5505	3.3786	264.1	2.7117	3.4337	251.8	13.184
2,3-DIMETHYL-1,3-BUTADIENE	526	35.2	2.5758	3.8511	264.6	2.6246	4.0356	256.6	26.725
2,3-DIMETHYL-1-BUTENE	501	33.2	2.6366	3.9170	248.1	2.7717	3.9718	238.4	17.290
2,3-DIMETHYL-1-HEXENE	561	27.6	3.4276	3.9067	247.6	3.4860	4.0378	242.2	28.091
2,3-DIMETHYL-2,3-DIPHENYLBUTANE	805	19.9	4.5465	4.1349	327.8	5.0517	4.4036	302.9	92.693
2,3-DIMETHYL-2-BUTENE	528	33.2	2.7114	3.8486	259.4	2.6976	4.0807	254.4	30.181
2,3-DIMETHYLBENZOTHIOPHENE	786	34.64	4.0745	3.7254	326.7	4.2436	3.8891	314.5	42.344
2,3-DIMETHYLBUTANE	500	31.5	2.7090	3.9398	244.8	2.8952	3.9773	233.4	19.776
2,3-DIMETHYLDECANE	653.5	18.8	4.7763	4.0188	256.7	5.0116	4.1999	246.5	67.633
2,3-DIMETHYLDODECANE	689.7	16.56	5.4277	4.0424	259.6	5.7138	4.2297	249.3	81.644
2,3-DIMETHYLHEPTANE	588.8	23.9	3.6378	4.0294	256.8	4.0115	4.0843	240.6	40.996
2,3-DIMETHYLHEXANE	563.5	26.3	3.4498	3.9425	249.4	3.6482	4.0406	238.9	34.464
2,3-DIMETHYLNONANE	633.9	20.16	4.4071	4.0199	256.3	4.6430	4.1867	245.5	60.451

Name	T_c (K)	P_c (bar)	PC-SAFT parameter values			I-PC-SAFT parameter values			
			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
2,3-DIMETHYLOCTANE	613.1	21.73	3.9976	4.0329	257.5	4.2754	4.1701	244.6	53.300
2,3-DIMETHYLPENTANE	537.3	29.1	3.0654	3.9390	249.6	3.2624	4.0069	238.3	28.104
2,3-DIMETHYLTHIOPHENE	637	40.5	2.8491	3.7799	307.4	3.0631	3.8860	290.2	29.561
2,3-DIMETHYLUNDECANE	671.4	17.61	5.0775	4.0346	258.5	5.3633	4.2146	247.7	75.243
2,3-PENTADIENE	497	38	2.6327	3.6234	248.1	2.6563	3.8440	241.1	26.423
2,3-XYLENOL	722.95	49	4.9973	3.2212	271.5	5.0106	3.1566	272.8	-8.538
2,4,4-TRIMETHYL-1-PENTENE	550	26.8	2.9789	4.1120	260.1	3.2988	4.1338	242.8	30.278
2,4,4-TRIMETHYL-2-PENTENE	555	26.8	3.1774	4.0096	254.0	3.2676	4.1607	246.0	33.539
2,4,4-TRIMETHYLHEXANE	581	24.6	3.4178	4.1077	258.4	3.7008	4.1517	244.9	33.045
2,4,6-TRIMETHYLPYRIDINE	653	33.3	3.6851	3.6598	283.0	3.8805	3.8332	270.2	42.882
2,4-DIAMINOTOLUENE	804	43.8	5.3455	3.0925	303.6	5.5311	3.2621	293.6	36.836
2,4-DICHLOROBENZOTRIFLUORIDE	646	28.1	4.0147	3.6764	273.1	4.3542	3.8675	256.0	54.123
2,4-DICHLOROTOLUENE	705	35.9	3.5082	3.7327	312.2	3.7546	3.8829	295.5	40.343
2,4-DIMETHYL-1,3-DIOXOLANE-2-METHANOL	621.3	35.4	5.0481	3.1244	239.5	5.2958	3.2709	230.1	34.445
2,4-DIMETHYL-3-ETHYLPENTANE	591	25.3	3.4908	4.0591	260.1	3.7072	4.1338	248.9	33.024
2,4-DIMETHYLHEXANE	553.5	25.6	3.4541	3.9650	244.5	3.6329	4.0592	235.0	31.052
2,4-DIMETHYLOCTANE	600	21.7	4.2347	3.9646	244.6	4.3551	4.1126	237.8	40.479
2,4-DIMETHYLPENTANE	519.8	27.4	3.1224	3.9434	239.6	3.3081	4.0227	229.2	28.611
2,4-DINITROPHENOL	766.9	38.88	7.3395	2.8227	261.3	7.5133	2.9360	255.9	28.450
2,4-DIPHENYL-4-METHYLPENTENE-1	835	20	4.8352	4.1719	329.7	5.2628	4.3775	309.9	94.860
2,4-TOLUENE DIISOCYANATE	725	30.4	5.6554	3.2988	270.4	6.1826	3.3993	255.8	44.219
2,4-XYLENOL	707.65	44	4.8109	3.2303	273.6	4.9933	3.2531	267.3	13.677
2,5-DIHYDROFURAN	542	55	2.6274	3.3337	269.7	2.6667	3.4931	262.5	17.561

Name	T_c (K)	P_c (bar)	PC-SAFT parameter values			I-PC-SAFT parameter values			
			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
2,5-DIMETHYL-1,5-HEXADIENE	567	27.4	3.3029	3.9122	256.5	3.4769	4.0660	245.0	38.724
2,5-DIMETHYL-2,4-HEXADIENE	597	27.4	3.3414	3.8758	270.8	3.4617	4.1431	258.4	52.902
2,5-DIMETHYLFURAN	558.6	41.25	3.3615	3.4616	247.5	3.3377	3.5834	245.5	15.364
2,5-DIMETHYLHEXANE	550	24.9	3.5094	3.9455	242.2	3.7433	4.0427	230.8	36.114
2,5-DIMETHYLOCTANE	603	21.7	4.1217	3.9934	249.8	4.4021	4.1023	238.0	46.721
2,5-DIMETHYLTETRAHYDROFURAN	551.1	36.43	3.0440	3.7257	255.9	3.2345	3.7611	245.3	17.416
2,5-DIMETHYLTHIOPHENE	629.9	44.62	3.1446	3.6620	286.7	3.3570	3.6258	276.1	8.254
2,5-XYLENOL	707.05	49	5.3213	3.1089	260.5	5.4026	3.0395	260.2	-6.511
2,6,8-TRIMETHYL-4-NONANONE	658	19.7	5.9606	3.7050	237.9	6.1058	3.8232	233.0	45.964
2,6-DIETHYLNAPHTHALENE	807	25.8	4.6405	3.8454	322.7	4.9790	4.0653	305.1	71.882
2,6-DIMETHYL-4-HEPTANOL	603	25.5	7.5381	3.1157	200.4	7.3955	3.1405	202.1	3.496
2,6-DIMETHYLHEPTANE	579	23	3.9285	3.9357	243.0	4.0219	4.1098	236.3	43.918
2,6-DIMETHYLNAPHTHALENE	777	31.7	4.0157	3.8471	324.7	4.2207	3.9988	311.5	41.724
2,6-DIMETHYLOCTANE	606	21.7	4.2445	3.9633	247.1	4.3880	4.1142	239.5	43.377
2,6-DIMETHYLPYRIDINE	623.75	37.5	3.5140	3.5520	274.6	3.6466	3.7142	264.4	32.288
2,6-DINITROPHENOL	770.1	39.05	7.4550	2.7740	261.5	7.5645	2.9271	256.5	33.457
2,6-DI-tert-BUTYL-p-CRESOL	724	21.1	6.0756	3.7448	260.3	6.3540	3.7938	253.3	37.475
2,6-NAPHTHALENEDICARBOXYLIC ACID	904	30.5	10.3094	2.8115	281.2	10.5280	2.8874	277.7	27.048
2,6-TOLUENE DIISOCYANATE	749	29	4.2018	3.6713	311.9	4.3495	4.0221	297.0	60.815
2,6-XYLENOL	701.05	43	4.4294	3.4485	276.2	4.5230	3.3982	274.1	-2.026
2,7-DIMETHYLBENZOTHIOPHENE	772.4	34.64	4.0109	3.7421	323.0	4.2550	3.8626	308.7	38.832
2,7-DIMETHYLNAPHTHALENE	775	32.3	4.2629	3.7683	315.4	4.4612	3.8861	304.5	33.360
2,7-DIMETHYLOCTANE	604	21.3	4.2460	3.9606	246.7	4.4153	4.1253	238.2	50.696

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
2-ACETOACETOXY ETHYL METHACRYLATE	724.2	22.57	7.3121	3.3013	247.3	7.5097	3.4537	241.7	53.196
2-AMINO-2-METHYL-1-PROPANOL	619.8	38.62	5.9680	2.7790	226.6	6.0857	2.9986	219.7	35.258
2-AMINODIPHENYL	838	39.33	4.5221	3.7984	326.0	4.5308	3.7128	327.4	-16.806
2-AMINOETHOXYETHANOL	735	59	5.6530	2.8876	264.2	5.3698	2.9014	271.0	-5.561
2-BROMOBUTANE	567	46.3	3.1352	3.5548	255.0	3.0436	3.5832	259.0	2.184
2-BROMOPROPANE	532	55.1	2.7339	3.5658	251.9	2.8483	3.3896	250.1	-17.586
2-BUTANOL	535.9	41.88	5.8564	2.7012	193.6	5.5425	2.8898	195.6	20.455
2-BUTOXIME	608.5	42.04	5.6138	2.8066	225.9	5.7588	2.9642	219.4	29.508
2-BUTOXYETHANOL	633.9	32.7	4.7901	3.3335	248.2	4.9990	3.4605	239.3	34.054
2-BUTYL-2-ETHYL-1,3-PROPANEDIOL	732	25.97	6.3600	3.3263	261.0	6.4540	3.5298	255.0	53.918
2-BUTYLBENZOTHIOPHENE	818.7	28.41	5.0460	3.8080	311.5	5.1104	3.9147	306.8	31.313
2-BUTYL-NONAN-1-OL	681.5	18.26	9.7950	3.1854	212.9	9.7790	3.2267	212.9	15.593
2-BUTYNE-1,4-DIOL	695	58.6	10.2954	2.1251	214.8	10.2561	2.1539	214.7	4.185
2-CHLORO-1,1,1,2-TETRAFLUOROETHANE	395.65	36.6	3.0553	3.3255	183.3	3.1948	3.3776	177.1	13.787
2-CHLORO-1,1,1-TRIFLUOROETHANE	430	38.4	2.4693	3.5058	223.8	2.8738	3.5500	201.4	24.178
2-CHLORO-1,1-DIFLUOROETHYLENE	400.55	44.58	2.5854	3.2690	200.2	2.6039	3.4155	196.1	13.960
2-CHLORO-1,3-PROPANEDIOL	669.7	50.65	9.6544	2.2564	210.5	9.6722	2.2947	209.7	7.060
2-CHLOROETHANOL	585	59.2	5.5182	2.5044	219.8	6.1791	2.5349	206.4	18.904
2-CHLOROPROPENE	478	47.1	2.0251	3.7565	268.4	2.1440	3.8042	256.4	9.126
2-CYCLOHEXENE-1-ONE	684.2	45.35	2.9985	3.5855	326.2	3.3400	3.7139	300.6	35.238
2-CYCLOHEXENYL CYCLOHEXANONE	792.8	29.33	4.1647	3.9411	325.9	4.3061	4.0996	315.5	45.736
2-ETHOXY-1-PROPANOL	592.3	36.4	4.9769	3.1309	227.8	5.1816	3.2177	221.0	22.103
2-ETHOXYETHYL ACETATE	607.3	31.66	4.9468	3.3291	234.8	5.3077	3.3662	224.8	23.011

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
2-ETHYL BUTYRIC ACID	655	34.1	5.8430	3.0842	238.8	5.9696	3.2093	233.6	27.850
2-ETHYL HEXANOIC ACID	674.6	27.78	7.3484	3.0734	228.3	7.3878	3.1698	226.1	29.431
2-ETHYL-1-BUTANOL	591.2	35.35	6.3439	2.9162	206.9	5.9732	3.0638	210.8	15.105
2-ETHYL-1-BUTENE	511	33	2.8980	3.7790	242.4	2.9191	3.9331	237.7	22.319
2-ETHYL-1-HEXANOL	640.4	27.56	5.4852	3.3699	237.0	5.2878	3.5939	237.3	37.642
2-ETHYL-1-HEXENE	569	26.7	3.5660	3.8582	248.7	3.7445	3.9942	238.7	36.851
2-ETHYL-1-PENTENE	543	29.5	2.9692	3.9501	258.2	3.3478	3.9651	238.3	29.159
2-ETHYL-2-HEXENAL	636	26.4	4.0572	3.6032	270.9	4.5080	3.8756	248.9	56.388
2-ETHYLBENZOTHIOPHENE	774	35.26	4.1742	3.7040	317.0	4.3060	3.8248	308.0	32.073
2-ETHYLHEXANAL	619.2	26.79	4.3452	3.6643	250.9	4.5106	3.8216	242.3	38.877
2-ETHYLHEXYL ACRYLATE	655	20.7	6.0765	3.5949	235.9	6.3061	3.7045	229.7	44.717
2-ETHYLHEXYL BENZOATE	755.6	18.68	6.1526	3.8205	272.5	6.4129	3.9922	263.7	73.052
2-ETHYL-m-XYLENE	671	30.2	3.8358	3.8014	285.9	4.1324	3.9016	271.1	38.000
2-ETHYLNAPHTHALENE	771	31.7	3.7399	3.9224	334.5	4.2496	3.9780	308.3	49.145
2-ETHYL-p-XYLENE	663	28.8	3.9545	3.7748	279.1	4.1708	3.9340	266.9	44.390
2-ETHYL-TETRAHYDROTHIOPHENE	657.8	38.1	2.9260	3.8831	311.4	2.9124	4.0818	306.3	28.067
2-ETHYLTHIOPHENE	626.6	44.09	3.1653	3.6421	284.0	3.2363	3.6828	278.9	10.678
2-FORMYL BENZOIC ACID	772	38.3	7.0532	2.7375	270.8	7.5373	2.9531	257.4	41.711
2-HEPTANOL	608.3	30	5.8651	3.1572	218.7	5.4350	3.3963	223.4	29.836
2-HEPTANONE	611.4	29.7	3.8930	3.6585	260.0	4.2172	3.7740	245.2	39.858
2-HEXANOL	585.3	33.11	5.9550	2.9956	208.4	5.3144	3.2742	216.5	26.771
2-HEXANONE	587.1	33	3.6301	3.5730	257.2	3.9997	3.6684	240.1	36.229
2-HEXYNE	549	35.3	2.6521	3.8391	273.0	2.6797	4.0600	265.3	28.264

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
2-HYDROXYPROPYL METHACRYLATE	663	31.4	6.9270	3.0053	228.3	6.9901	3.0986	225.7	23.413
2-MERCAPTOBENZOTHAZOLE	749	40	3.3360	3.7926	337.0	3.5422	3.9057	321.2	32.427
2-METHOXY PROPANOL-1	588.4	39.4	4.2179	3.1324	244.3	4.6621	3.2613	227.6	34.749
2-METHOXYETHANOL	597.6	52.85	4.1417	2.9378	247.9	4.5139	3.0104	233.8	22.062
2-METHYL BENZOTHIOPHENE	768.7	35	3.1747	3.9514	358.6	3.5275	4.1254	330.2	53.217
2-METHYL OCTANAL	638.3	25	5.1515	3.5641	242.7	5.2758	3.7119	236.7	40.421
2-METHYL THIAINDAN	788.6	37.09	3.0364	4.0530	371.5	3.3085	4.1784	347.8	42.449
2-METHYL-, 3-HYDROXY-2,2,4-TRIMETHYLPENTYL PROPANOATE	687.9	17.57	7.0286	3.5496	239.4	7.4365	3.7063	230.2	72.651
2-METHYL-1,3-PROPANEDIOL	697	53.5	6.7334	2.6273	240.5	6.6525	2.6943	240.6	8.503
2-METHYL-1-BUTANOL	575.4	39.4	5.8205	2.8637	208.0	5.5993	3.0076	209.3	19.450
2-METHYL-1-BUTENE	465	34.47	2.6454	3.6948	231.2	2.7775	3.8233	221.1	23.669
2-METHYL-1-BUTENE-3-YNE	492	43.8	1.9859	3.9217	277.7	2.0338	4.0067	270.8	10.979
2-METHYL-1-HEPTANOL	608.5	28.57	7.2015	3.0711	204.7	7.0565	3.0950	206.6	2.447
2-METHYL-1-HEPTENE	567	26	3.4481	3.9188	252.5	3.7239	4.0334	238.4	40.251
2-METHYL-1-HEXANOL	595	30.3	7.1827	2.9240	201.8	7.1498	2.9953	201.3	16.533
2-METHYL-1-HEXENE	538	28.7	3.2045	3.8471	245.9	3.3639	3.9823	235.6	32.558
2-METHYL-1-NONENE	616	21.9	4.2704	3.9136	252.2	4.5009	4.0835	241.2	54.541
2-METHYL-1-OCTENE	593	23.8	3.8596	3.9092	252.4	4.1205	4.0580	239.8	50.165
2-METHYL-1-PENTANOL	604.4	34.5	5.2815	3.1261	225.7	4.9644	3.3549	228.7	28.614
2-METHYL-1-PENTENE	505	31.9	2.8397	3.8206	242.9	2.9875	3.9295	232.6	25.428
2-METHYL-1-PROPANOL	547.8	42.95	6.1396	2.6590	193.8	5.5826	2.8783	199.5	20.811
2-METHYL-2-AMINOBUTANE	526	36.6	3.4293	3.5384	230.5	3.4486	3.6115	228.0	10.055
2-METHYL-2-BUTANOL	543.7	37.1	5.3968	2.9309	200.0	4.7371	3.2205	209.1	21.772

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
2-METHYL-2-BUTENE	470	34.2	2.7309	3.6523	233.1	3.1891	3.6613	210.5	28.453
2-METHYL-2-PENTENAL	605	32.6	3.3107	3.6279	278.3	3.6786	3.8397	255.6	44.749
2-METHYL-2-PENTENE	514	31.6	2.8421	3.8183	247.1	2.8582	4.0283	241.3	29.843
2-METHYL-2-PROPANOL	506.2	39.72	6.2820	2.6273	178.2	5.8258	2.8276	181.9	17.585
2-METHYL-3-ETHYLPENTANE	567.1	27	3.3129	3.9808	255.3	3.5232	4.0662	243.8	34.507
2-METHYLBENZOFURAN	697	36.4	3.4943	3.7089	310.3	3.8826	3.8021	288.3	39.349
2-METHYLBUTYRALDEHYDE	543.2	38.29	3.5830	3.3869	237.4	3.9039	3.4332	224.2	21.498
2-METHYLBUTYRIC ACID	643	38.9	5.4507	3.0048	240.3	5.6133	3.1311	233.7	27.329
2-METHYLDECANE	631.8	19.82	4.9061	3.8838	245.0	5.0694	4.0617	237.4	57.242
2-METHYL-DODECAN-1-OL	682.5	18.26	9.7796	3.1839	213.3	9.7436	3.2337	213.4	17.599
2-METHYLDODECANE	668	17.17	5.5511	3.9283	249.4	5.8559	4.0931	239.6	72.373
2-METHYLHEPTANAL	605.7	26.82	4.8110	3.5104	235.2	4.7768	3.7076	232.3	37.668
2-METHYLHEPTANE	559.7	25	3.6800	3.8811	242.0	3.9171	3.9920	230.8	39.244
2-METHYLHEXANAL	592	28.5	4.3586	3.5184	240.1	4.5672	3.6699	230.6	39.231
2-METHYLHEXANE	530.4	27.4	3.3059	3.8687	239.1	3.5102	3.9625	228.3	31.070
2-METHYLHEXANOIC ACID	666	31.1	6.4230	3.1047	234.8	6.4954	3.2122	231.5	26.204
2-METHYLINDENE	711	34.6	3.4245	3.8156	318.5	3.6898	3.9679	300.0	43.485
2-METHYLNAPHTHALENE	761	35	3.5152	3.8866	337.9	3.9058	3.9577	314.1	42.989
2-METHYLNONANE	610	21.2	4.3884	3.9213	247.0	4.6594	4.0591	236.0	52.034
2-METHYLOCTANE	582.87	23.1	4.3420	3.8003	236.0	4.5617	3.9177	227.2	40.558
2-METHYLOCTANOIC ACID	694	25.4	7.2040	3.2110	236.6	7.3025	3.3136	233.4	31.514
2-METHYLPENTANE	497.7	30.4	2.9510	3.8440	234.8	3.1277	3.9088	224.7	22.128
2-METHYLPROPANAL	519	42.1	2.8383	3.4666	252.1	3.0996	3.5676	235.2	24.427

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
2-METHYLPYRIDINE	621	46	3.0699	3.5321	288.8	3.2827	3.6016	274.8	19.752
2-METHYLtetrahydrofuran	537	37.58	2.7943	3.6246	264.0	3.1470	3.7273	241.8	34.142
2-METHYLthiacyclopentane	628.4	41.83	2.7165	3.7918	309.4	2.8927	3.9062	293.5	26.276
2-METHYLthiophene	609	49.1	2.6775	3.6655	298.8	2.8154	3.7000	287.8	11.127
2-METHYLtridecane	684.1	16.04	5.9065	3.9384	250.6	6.2382	4.1107	240.7	80.846
2-METHYLundecane	650.7	18.42	5.2202	3.9103	247.6	5.4687	4.0764	238.5	64.612
2-NITROPROPANE	594	44.5	3.0605	3.4359	284.4	3.9491	3.3496	244.1	28.631
2-NONANOL	649.5	25.41	5.9229	3.4120	233.9	5.7762	3.5786	234.0	30.377
2-NONANONE	651.9	24.82	4.6293	3.7232	259.2	4.9557	3.8425	246.9	46.654
2-NORBORNENE	583	39.3	2.1082	4.2124	320.5	2.2010	4.2786	308.8	16.283
2-n-PROPYLthiophene	649.2	38.97	3.5182	3.6926	281.8	3.6102	3.7300	276.3	12.895
2-OCTANOL	629.8	27.49	5.8362	3.2891	227.8	5.6026	3.4938	229.1	35.230
2-OCTANONE	632.7	27.09	4.2394	3.7048	259.9	4.5465	3.8230	246.9	41.692
2-PENTANETHIOL	584.3	35.36	2.9870	3.8351	273.5	3.0450	3.9589	266.9	21.384
2-PENTANOL	561	37	5.9408	2.8463	200.3	5.3306	3.1070	207.3	24.372
2-PENTANONE	561.19	36.72	3.2605	3.5232	257.5	3.6459	3.6111	237.9	31.803
2-PENTOXYETHANOL	641.2	30.36	5.8284	3.2379	232.6	5.8887	3.3313	229.6	23.099
2-PENTYNE	519	40.3	2.2635	3.8172	278.5	2.3248	4.0057	267.8	22.803
2-PHENYL-1-PROPANOL	685	34.9	7.1251	2.9473	232.5	7.0733	3.0088	232.4	11.811
2-PHENYL-2-PROPANOL	660	34.9	6.2162	3.0785	234.5	6.4682	3.0872	229.7	12.625
2-PHENYLBUTENE-1	666	30.1	3.5593	3.8746	292.3	3.7116	4.0579	280.4	43.634
2-PHENYLETHANOL	684	39.2	6.2616	2.9471	245.3	6.8928	2.9253	233.8	19.668
2-PROPYLBENZOTHIOPHENE	807.5	31.56	4.7290	3.8099	312.4	4.7063	3.8879	311.3	17.269

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
2-PYRROLIDONE	802	61.7	3.9095	3.0746	343.3	4.3387	3.2024	318.3	30.620
3-(METHYLMERCAPTO)PROPANAL	650	40.2	3.8618	3.3065	279.4	4.2136	3.4833	260.7	38.266
3-(N,N-DIMETHYLAMINO) PROPYLAMINE	593.3	35.86	4.3454	3.3614	238.5	4.5150	3.4173	232.1	18.068
3-(TRIETHOXSILYL)PROPIONITRILE	672.1	17.61	6.1633	3.6882	244.5	6.6818	3.8480	231.7	80.291
3,3,3-TRIFLUOROPROPENE	378.59	36.09	2.3530	3.4008	204.5	3.0199	3.4126	173.5	25.790
3,3,5-TRIMETHYLHEPTANE	609.5	23.2	3.7074	4.1199	262.1	3.9578	4.1942	250.3	38.086
3,3-DIETHYLPENTANE	610.05	26.75	3.2759	4.1228	276.4	3.5895	4.1505	260.3	32.755
3,3-DIMETHYL-1-BUTENE	480	32.9	2.4912	4.0148	243.5	2.7343	3.9463	229.8	9.255
3,3-DIMETHYL-1-BUTYNE	488.5	36.75	2.2573	4.0797	255.8	2.2203	4.1126	257.7	1.796
3,3-DIMETHYL-2-BUTANONE	570.9	34.3	3.0486	3.7936	266.3	3.2160	3.8909	254.8	24.533
3,3-DIMETHYLHEXANE	562	26.5	3.2228	4.0319	256.1	3.4491	4.1115	243.6	36.673
3,3-DIMETHYLPENTANE	536.4	29.5	2.8805	4.0376	255.1	3.0398	4.0897	245.2	19.629
3,4-DICHLORO-1-BUTENE	589	38.5	3.1907	3.5803	270.3	3.2584	3.7651	261.4	29.115
3,4-DICHLOROANILINE	800	41.1	4.2846	3.4088	329.3	4.6228	3.5743	310.3	45.081
3,4-DICHLOROPHENYL ISOCYANATE	730.3	34.09	4.8954	3.3563	284.1	4.9235	3.5995	277.2	47.457
3,4-DIMETHYLHEXANE	568.8	26.9	3.3899	3.9559	253.5	3.5898	4.0471	242.6	33.250
3,4-DIMETHYLTHIOPHENE	642.8	41.89	2.9694	3.7299	303.0	3.1233	3.8272	290.4	23.087
3,4-XYLENOL	729.95	50	5.4459	3.0748	267.4	5.5054	3.0281	267.0	-3.099
3,5-DIISOPROPYLTOLUENE	681.4	22.39	4.6042	3.9451	270.0	4.7912	4.0904	261.0	50.805
3,5-DIMETHYLBENZOFURAN	713.7	32.16	3.8356	3.7415	306.5	4.2569	3.8558	285.2	47.606
3,5-DIMETHYLBENZOTHIOPHENE	784.8	34.64	3.7742	3.8435	338.8	4.2766	3.8756	313.1	40.223
3,5-XYLENOL	715.65	36	4.5474	3.3262	288.4	4.7633	3.5573	274.7	46.073
3-AMINO-1-PROPANOL	649	55	7.5618	2.3750	218.2	7.6096	2.4601	215.8	13.516

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3-BUTEN-2-ONE	540	44.03	3.0689	3.2861	255.6	3.4099	3.4399	235.2	29.825
3-CHLORO- <i>o</i> -XYLENE	685.1	33.88	3.3912	3.8158	307.8	3.6238	3.9734	291.2	41.939
3-CHLOROPROPENE	514.15	47.1	1.9776	3.7851	295.6	2.1160	3.9153	277.6	20.138
3-CHLOROPROPYLDIMETHYLCHLOROSILANE	640.7	25.99	4.1538	3.7822	265.6	4.4765	3.9161	251.4	48.901
3-CHLOROPROPYLTRIMETHOXYSILANE	647.3	21.34	4.6402	3.8062	260.0	5.1666	3.9647	241.7	69.187
3-ETHYL-1-HEPTANOL	636.7	25.46	7.9778	3.0475	209.5	7.9394	3.1017	209.4	14.096
3-ETHYL-1-HEXENE	553.9	26.04	3.5439	3.8731	243.0	3.7625	3.9846	231.9	36.209
3-ETHYL-1-PENTENE	530	30.3	3.2448	3.8291	238.6	3.3050	3.9166	233.8	18.433
3-ETHYL-2,5-DIMETHYLTHIOPHENE	669	32.6	3.5858	3.7072	295.6	3.9157	3.8784	275.9	49.086
3-ETHYLBENZOTHIOPHENE	776.5	35.26	4.0825	3.7252	321.8	4.3129	3.8266	308.8	34.533
3-ETHYLDODECANE	691.4	16.22	5.4436	4.0952	259.3	5.6964	4.2679	250.1	76.622
3-ETHYLHEPTANE	590	23.9	3.8959	3.9284	249.4	4.1434	4.0369	238.1	42.392
3-ETHYLHEXANE	565.5	26.1	3.5438	3.9016	248.0	3.7664	4.0076	236.7	38.280
3-ETHYL- <i>o</i> -XYLENE	680	28.8	3.6262	3.8845	297.3	3.7791	4.1188	284.3	53.451
3-ETHYLPENTANE	540.6	28.9	3.1889	3.8875	247.0	3.3614	3.9805	236.8	27.120
3-HEPTANOL	605.4	30.73	5.3441	3.2706	226.2	5.2989	3.3986	224.2	23.532
3-HEPTANONE	606.6	29.2	3.9571	3.6243	255.9	4.1400	3.8124	244.9	44.827
3-HEXANONE	582.82	33.2	3.5526	3.5955	257.4	3.9215	3.6796	240.2	34.131
3-HEXYNE	544	35.3	2.7744	3.7765	263.4	2.6559	4.0603	263.9	28.483
3-HYDROXY-2-METHYL PROPIONALDEHYDE	615	45.9	7.2541	2.5276	209.1	7.3152	2.6110	206.7	15.037
3-HYDROXYBUTYROLACTONE	830.6	53.97	5.2597	2.8430	320.5	5.8053	3.0154	298.7	34.204
3-MERCAPTOPROPIONIC ACID	729	50.2	5.3832	2.8855	273.6	5.6059	3.0005	265.1	19.427
3-METHOXY-3-BUTEN-2-ONE	610	41.02	3.5213	3.4359	269.6	3.9076	3.4863	251.7	25.792

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3-METHOXYISOPROPYLAMINE	548	40.9	4.2604	3.1795	220.6	4.2607	3.2577	218.9	10.547
3-METHOXYPROPIONITRILE	638	36.3	4.1018	3.1480	272.5	4.5575	3.4740	248.7	41.061
3-METHYL SULFOLANE	817	42.4	3.8608	3.5037	351.5	4.2323	3.6867	327.2	45.570
3-METHYL-1,2-BUTADIENE	490	38.3	2.4859	3.7019	249.8	2.4185	3.9426	248.2	21.294
3-METHYL-1,4-PENTADIENE	497	34.9	2.7683	3.7818	240.2	2.8766	3.8449	232.7	15.840
3-METHYL-1-BUTANOL	577.2	39.3	6.1178	2.8238	203.9	5.6181	3.0091	209.7	19.142
3-METHYL-1-BUTENE	452.7	35.3	2.4275	3.8332	232.6	2.5900	3.8529	222.2	13.324
3-METHYL-1-BUTYNE	463.2	42	3.0184	3.4684	214.7	3.3538	3.3405	203.1	0.862
3-METHYL-1-HEXENE	528	29.5	3.2370	3.8390	238.6	3.3354	3.9336	232.1	23.093
3-METHYL-1-PENTANOL	588	34	6.5565	2.8897	206.3	6.7252	2.9475	202.4	20.207
3-METHYL-1-PENTENE	495	32.9	2.7090	3.8960	242.6	3.0100	3.8531	227.2	15.519
3-METHYL-2-BUTANOL	556.1	38.7	5.5737	2.8979	201.9	4.8957	3.1580	211.5	18.975
3-METHYL-2-PENTANONE	574.7	32.95	3.4656	3.6279	256.3	3.8551	3.6955	238.4	32.728
3-METHYL-3-ETHYLPENTANE	576.5	28.1	3.1147	4.0641	265.9	3.3299	4.1192	253.6	27.712
3-METHYL-3-PENTANOL	575.6	35.2	4.2116	3.3750	235.0	4.3340	3.4585	228.5	20.300
3-METHYLBUTYRALDEHYDE	543.2	38.29	3.7646	3.3354	231.6	3.9369	3.4223	223.5	20.139
3-METHYL-cis-2-PENTENE	515	32.9	2.9043	3.7746	244.5	2.9668	3.9245	237.9	25.048
3-METHYLCYCLOPENTANONE	633.2	38.96	3.1110	3.6321	295.6	3.2727	3.8356	280.5	37.423
3-METHYLCYCLOPENTENE	526	41.3	2.7032	3.7130	255.5	2.7431	3.7672	251.5	10.398
3-METHYLDECANE	634.1	19.89	4.7339	3.9292	250.1	5.0486	4.0685	238.6	59.136
3-METHYLDODECANE	669	17.19	5.4638	3.9448	251.6	5.8289	4.1014	240.3	74.774
3-METHYLHEPTANE	563.6	25.5	3.6051	3.8975	245.8	3.8596	3.9972	233.7	39.671
3-METHYLHEXANAL	595	28.5	4.1941	3.5477	246.0	4.5359	3.6861	232.4	44.508

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
3-METHYLHEXANE	535.2	28.1	3.2529	3.8695	242.9	3.4506	3.9662	232.0	32.720
3-METHYLNONANE	613	21.6	4.3864	3.9055	247.8	4.5996	4.0610	238.2	52.629
3-METHYLOCTANE	590.15	23.4	3.8815	3.9490	250.5	4.1782	4.0528	237.5	44.298
3-METHYLPENTANE	504.6	31.2	2.8517	3.8751	242.0	3.0581	3.9246	230.0	23.134
3-METHYLPYRIDINE	645	46.6	2.9704	3.5709	306.1	3.2731	3.6355	285.7	24.545
3-METHYLTHIOPHENE	613	49.1	2.7044	3.6469	299.5	2.8209	3.7055	289.5	13.415
3-METHYL-trans-2-PENTENE	517	31.9	2.8860	3.7812	247.8	2.9993	3.9548	237.7	32.335
3-METHYLTRIDECANE	684.7	16.06	5.9237	3.9272	250.7	6.2537	4.1059	240.7	82.396
3-METHYLUNDECANE	652.3	18.47	5.0885	3.9398	251.1	5.4454	4.0831	239.4	66.684
3-NITROBENZOTRIFLUORIDE	667	28	4.6610	3.4378	269.1	5.1789	3.6544	248.9	54.308
3-NONANONE	648.1	24.53	4.4900	3.7514	259.8	4.5833	3.9709	252.2	53.213
3-OCTANONE	627.7	27.04	4.1617	3.7038	259.6	4.4039	3.8630	247.7	47.416
3-PENTANOL	559.6	37.14	5.7606	2.8634	201.2	4.9987	3.1818	211.3	26.025
3-PENTANONE	560.95	37.4	3.4118	3.4569	250.8	3.6428	3.5897	237.9	29.272
3-PHENYL-1-PROPANOL	694	34.3	7.3694	2.9222	233.8	7.4047	2.9798	232.5	14.427
4-((2-HYDROXYETHOXY)CARBONYL) BENZOIC ACID	871.4	29.6	8.7969	3.0580	280.4	8.8173	3.1254	279.0	20.181
4-(2-METHOXYETHYL)MORPHOLINE	669.8	31.33	4.4990	3.4764	268.9	4.6376	3.6832	259.5	45.672
4,4'-DIISOPROPYLBIPHENYL	813.6	18.41	5.4491	4.0482	307.8	5.8360	4.2767	292.1	98.095
4,4'-DINITRODIPHENYLAMINE	926	26.2	9.1545	3.1433	296.6	9.3237	3.2387	292.5	37.058
4,4'-DINITROTRIPHENYLAMINE	946	20	9.6776	3.3513	299.5	9.9019	3.4718	294.6	56.978
4,6-DIMETHYLDIBENZOTHIOPHENE	939.4	29.81	4.3506	3.8957	387.8	4.8034	4.1340	359.6	72.922
4-[2-(2-AMINOETHOXY)ETHYL]MORPHOLINE	706.9	28.5	6.6204	3.3448	243.7	6.4759	3.3777	246.0	3.581
4-CHLORO-3-NITROBENZOTRIFLUORIDE	686	27.4	5.1583	3.4368	265.3	5.7314	3.5652	247.7	55.812

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4-CHLORO- <i>o</i> -XYLENE	689.1	33.22	3.3518	3.8219	312.9	3.6604	3.9923	291.7	50.048
4-ETHYL- <i>m</i> -XYLENE	665	28.8	3.8900	3.8017	282.5	4.1910	3.9306	267.3	44.364
4-ETHYL- <i>o</i> -XYLENE	667	28.8	3.9139	3.7936	282.3	4.1703	3.9421	268.6	45.700
4-HEPTANONE	602	29.2	3.8698	3.6628	256.4	4.1752	3.7904	242.3	40.246
4-HYDROXYACETOPHENONE	860	44.5	5.2209	3.1943	331.5	6.0388	3.2005	305.6	33.927
4-HYDROXYBUTYRALDEHYDE	599	44.8	7.4530	2.4277	204.1	7.7217	2.5484	198.4	23.520
4-HYDROXYMETHYL BENZOIC ACID	814.4	45.1	11.7279	2.4378	240.1	11.1395	2.3836	247.1	-22.864
4-HYDROXYSTYRENE	736	45.2	5.0287	3.2182	277.9	4.9559	3.2764	278.7	7.823
4-ISOBUTYLSTYRENE	735	23.8	4.1902	3.9673	306.5	4.5852	4.1822	285.9	72.071
4-METHOXYPHENYLACETIC ACID	768	39	8.7038	2.8750	242.2	8.2217	2.8203	250.3	-24.497
4-METHYL DIBENZOTHIOPHENE	904.1	33.78	4.1799	3.8865	372.9	4.4102	4.0484	356.7	51.630
4-METHYL-1-HEPTENE	557.3	26.04	3.5255	3.8814	245.3	3.7553	3.9956	233.5	37.678
4-METHYL-1-HEXENE	534	30.4	3.2445	3.8286	240.5	3.3094	3.9203	235.5	20.165
4-METHYL-1-OCTANOL	631.7	24.84	7.8379	3.0788	209.7	7.9736	3.1132	207.5	16.094
4-METHYL-1-PENTENE	496	32.2	2.7127	3.8996	242.0	2.8152	3.9772	234.4	18.442
4-METHYL-2-PENTANOL	574.4	34.7	5.6851	3.0535	208.1	5.4780	3.1640	210.4	13.950
4-METHYL- <i>cis</i> -2-PENTENE	499	32.2	2.7725	3.8624	241.4	2.8559	3.9649	234.4	20.154
4-METHYL-CYCLOHEXANE-METHANOL	647.6	32.43	6.2465	3.1391	227.4	5.9441	3.2569	231.2	6.440
4-METHYLCYCLOPENTENE	527	41.3	2.7461	3.7011	254.0	2.7906	3.7468	250.1	8.976
4-METHYLGUAIACOL	707.8	40.56	5.4329	3.1678	261.6	5.4614	3.2242	259.5	12.031
4-METHYLHEPTANE	561.7	25.4	3.6177	3.8923	244.5	3.8467	4.0030	233.2	39.255
4-METHYLNONANE	610	21.6	4.3564	3.9232	247.2	4.6008	4.0539	237.0	47.556
4-METHYLOCTANE	587.65	23.4	3.8841	3.9455	249.3	4.1828	4.0453	236.4	44.038

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4-METHYLPHENANTHRENE	895.3	27.21	4.0347	4.0364	380.5	4.4000	4.3407	353.5	77.329
4-METHYLPYRIDINE	646.15	46.6	2.9979	3.5662	305.3	3.2983	3.6275	285.3	23.737
4-METHYL-trans-2-PENTENE	501	32.2	2.8518	3.8287	239.3	2.9417	3.9286	232.3	20.364
4-NONANONE	643.7	24.53	4.7167	3.6976	253.2	4.8736	3.8670	245.2	44.896
4-OCTANONE	623.8	27.04	4.2400	3.6879	254.5	4.2426	3.9110	249.6	43.187
5-(HYDROXYMETHYL) FURFURAL	794.9	49.5	6.1753	2.8330	285.0	6.3099	2.9542	278.7	24.769
5-ETHYLIDENE-2-NORBORNENE	629	34	3.2430	3.8414	285.3	3.4006	3.9490	274.3	27.808
5-ETHYL-m-XYLENE	655	27.5	3.8668	3.8225	279.8	4.2148	3.9629	262.7	50.863
5-HEXEN-2-ONE	586.8	34.13	3.7595	3.4660	254.2	4.2185	3.5537	235.3	37.515
5-METHYL FURFURAL	687.8	47.03	4.0870	3.2356	285.5	4.3635	3.3234	272.4	24.444
5-METHYL-1-HEXANOL	605	30.3	7.3528	2.9401	203.0	7.2128	3.0006	204.1	6.479
5-METHYL-1-HEXENE	528	28.7	3.2518	3.8350	239.0	3.3724	3.9538	231.0	28.236
5-METHYL-2-HEXANONE	604.1	29.81	3.8022	3.6832	259.3	4.1734	3.7694	243.2	37.933
5-METHYLINDAN	711.2	35.22	3.1106	3.9954	330.9	3.4963	4.0246	306.6	33.706
5-METHYLNONANE	610	21.6	4.1504	3.9889	253.0	4.5292	4.0789	238.3	50.261
5-NONANONE	640	23.2	4.5516	3.7357	258.3	4.9937	3.8940	241.7	63.358
5-o-TOLYL-2-PENTENE	702.6	25.16	4.4714	3.8359	282.7	4.7163	3.9996	270.6	54.186
6-AMINOHEXANAMIDE	807.8	34.56	6.3133	3.1697	288.2	6.5110	3.3039	280.6	37.674
6-AMINOHEXANOL	665	34.4	9.2275	2.7139	208.2	8.8346	2.7141	212.8	-9.032
6-HYDROXYHEXANOIC ACID	730	35.8	10.9389	2.5323	220.9	10.6847	2.5314	223.5	-3.447
6-METHYL-1-HEPTENE	558	26	3.5158	3.8936	245.7	3.7271	4.0106	234.5	37.447
6-METHYL-1-OCTANOL	633.4	24.84	7.8883	3.0640	210.0	8.0154	3.1088	207.8	17.781
7-METHYL-1-OCTENE	579	23.8	3.8552	3.8489	247.4	4.1158	4.0275	234.3	52.982

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8-HYDROXYQUINOLINE	788	43.6	4.9769	3.2517	302.2	5.0640	3.3632	296.2	22.473
8-METHYL-1-NONANOL	676.7	23.93	6.1161	3.4612	240.7	5.7883	3.6978	243.6	40.884
8-METHYL-1-NONENE	619	21.9	4.1053	3.8643	260.5	4.4981	4.0911	242.5	66.182
8-METHYLQUINOLINE	787	43	3.4692	3.8079	346.3	3.7483	3.7952	330.0	17.378
ACENAPHTHALENE	792	32	4.0258	3.9127	328.2	4.0694	4.0683	321.8	35.657
ACENAPHTHENE	803.15	31	3.6564	3.8528	354.8	3.9299	4.1860	330.7	61.941
ACETAL	539.7	32.2	4.4670	3.4443	213.3	4.7767	3.3569	207.0	1.583
ACETALDEHYDE	466	55.7	2.4978	3.0542	245.3	2.9980	3.1730	214.3	20.579
ACETALDOL	620	45.9	6.7977	2.4695	219.3	7.3477	2.6131	208.1	28.170
ACETALDOXIME	568	60.4	5.6043	2.4345	211.9	6.0182	2.5209	202.0	17.224
ACETAMIDE	761	66	3.8229	2.7985	335.2	4.2476	3.1023	304.3	27.253
ACETAMINOPHEN	736	42.6	8.1533	2.9336	232.8	7.3744	2.8320	246.8	-47.522
ACETANILIDE	825	37.3	5.0013	3.3009	322.3	5.4091	3.5029	303.5	49.958
ACETIC ACID	591.95	57.86	3.2601	2.8898	284.1	4.6125	2.8871	229.8	23.851
ACETIC ANHYDRIDE	606	40	4.0714	3.1705	255.6	4.5224	3.3163	236.9	35.441
ACETOACETANILIDE	879	30.3	6.9655	3.1873	307.2	7.3311	3.3747	295.3	60.542
ACETOACETIC ACID	678.5	46.97	6.3819	2.6514	242.2	6.5932	2.7993	234.8	28.170
ACETOIN	607.4	44.63	4.8686	2.8962	237.5	5.0964	3.0519	227.9	29.003
ACETONE	508.1	47	3.0103	3.1689	242.5	3.3448	3.3216	223.1	26.341
ACETONE CYANOHYDRIN	620	42.5	6.9176	2.5988	215.3	7.0985	2.7212	210.1	23.989
ACETONITRILE	545.5	48.5	3.2578	2.9421	256.4	3.6197	3.2690	231.9	27.173
ACETOPHENONE	709.6	40.1	3.6211	3.5810	310.4	3.9445	3.6813	291.8	33.503
ACETOVANILLONE	786	36.5	7.3191	3.0018	264.9	7.2541	3.0696	264.8	13.460

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ACETOXYACETIC ACID	764	43.2	5.8648	2.7317	288.4	6.6193	2.9897	264.1	38.008
ACETYL CHLORIDE	508	57.4	2.8298	3.1843	247.6	3.5575	3.0375	217.5	12.509
ACETYLENE	308.3	61.38	2.2345	2.8701	165.4	2.4473	2.8751	155.3	6.211
ACETYLSALICYLIC ACID	765	32.7	7.4774	2.9404	259.7	7.6560	3.0823	254.0	37.889
ACRIDINE	905	36.4	4.0041	3.8669	380.4	4.3995	3.9539	357.3	46.999
ACROLEIN	506	50	2.7528	3.1705	254.4	3.4459	3.2140	219.4	24.583
ACROLEIN CYANOHYDRIN	639	45.1	7.4083	2.4676	218.5	7.7485	2.5942	211.5	26.729
ACRYLIC ACID	615	56.6	4.7717	2.6952	243.0	5.1945	2.8096	229.2	23.974
ACRYLONITRILE	540	46.6	2.6393	3.2437	281.5	3.3740	3.3886	236.2	28.211
ACRYLOXY PROPIONIC ACID	729.5	34.41	6.9281	2.8971	255.4	7.3918	3.0288	244.5	41.472
ADAMANTANE	703	29.2	2.1619	4.6557	392.4	2.4021	4.8790	357.2	59.948
ADIPIC ACID	841	37	7.0149	2.9274	292.7	7.1876	3.1378	284.0	47.717
ADIPONITRILE	781	28.3	5.3351	3.1532	308.6	6.1871	3.5678	275.5	60.377
AGATHADIOL	790	16.1	11.7030	3.2780	236.0	11.6185	3.2603	237.5	-8.518
AIR	132.45	37.74	0.8927	3.6879	109.0	0.9525	3.5938	106.1	-0.371
ALLYL ACETATE	559	36.8	3.5390	3.4350	247.0	3.9832	3.4857	229.0	28.697
ALLYL ACRYLATE	575.5	33.96	4.2185	3.3386	235.5	4.2905	3.5136	229.3	31.300
ALLYL ALCOHOL	545.1	56.2	5.2538	2.5530	206.4	5.4508	2.6530	200.0	17.613
ALLYL ETHER	550.6	31.99	2.9573	3.7970	262.1	3.1049	3.9850	249.4	36.459
ALLYL GLYCIDYL ETHER	629	36.8	3.9205	3.4522	265.5	4.1489	3.5695	253.8	30.245
ALLYL METHACRYLATE	600	30.2	3.8004	3.6380	257.2	3.9852	3.8112	245.7	40.438
ALLYLAMINE	505	51.7	3.2952	3.0617	228.6	3.4984	3.1586	217.7	18.947
ALLYLIDENE DIACETATE	639.1	28.64	5.3401	3.3438	240.3	5.4555	3.5011	234.4	37.792

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ALLYL-TERT-BUTYLPEROXIDE	563	28.8	4.0074	3.7029	232.4	4.0953	3.7515	228.2	15.614
alpha-EPICHLOROHYDRIN	615	49	2.5013	3.5336	322.2	2.9190	3.6672	286.1	30.934
alpha-HYDROXYISOBUTYRAMIDE	771.7	53.42	6.0286	2.8391	276.3	6.0755	2.8973	273.7	11.441
alpha-HYDROXYISOBUTYRIC ACID	664	49.2	9.2368	2.3932	208.6	8.9603	2.3924	211.8	-4.430
alpha-METHYLBENZYL ALCOHOL	699	37.7	4.4023	3.3655	281.5	4.3848	3.5902	276.3	37.290
alpha-METHYLBENZYL ALCOHOL FORMATE	690	32.3	4.1857	3.6210	283.7	4.3807	3.7651	272.9	38.869
alpha-METHYLSTYRENE	654	33.6	3.2604	3.8288	298.3	3.4706	3.9865	282.8	38.226
alpha-PHELLANDRENE	649	28.2	3.9479	3.8395	270.5	3.9264	4.0253	267.3	31.410
alpha-PINENE	644	27.6	2.6784	4.3450	319.7	2.6763	4.6499	311.4	51.852
alpha-TERPINENE	649	28	3.6473	3.9305	281.6	3.8580	4.0618	269.1	42.921
alpha-TERPINEOL	675	29.5	6.4605	3.2381	236.2	6.5250	3.2776	234.3	13.083
alpha-TOCOPHEROL	964.3	10.8	9.0127	4.2110	312.3	9.3834	4.3981	304.1	142.707
AMINOACETONITRILE	638	54.4	4.1452	2.8416	268.8	4.6058	3.0233	247.8	27.348
AMINOCAPRONITRILE	697	30.5	5.6599	3.1629	261.5	6.1406	3.3609	246.4	50.093
AMMONIA	405.65	112.8	2.6291	2.3153	204.9	2.9213	2.4170	188.6	8.863
AMMONIUM CHLORIDE	1155.2	1640	4.8193	1.9395	366.9	4.4098	1.2043	455.7	-41.508
AMMONIUM SULFIDE	479	31.54	1.7927	3.8505	306.4	2.2523	4.2783	250.9	37.900
ANETHOLE	723	29	4.3994	3.6488	295.1	4.7586	3.8376	277.6	57.793
ANILINE	705	56.3	3.7248	3.2469	300.2	3.8020	3.3264	294.0	13.559
ANISOLE	645.6	42.5	3.4906	3.4979	284.2	3.6847	3.5896	272.6	23.343
ANTHRACENE	873	29	4.2903	3.8386	363.2	4.7670	4.0837	335.0	69.760
ANTHRAQUINONE	900	31.5	5.7333	3.4495	335.0	6.3703	3.5653	314.7	62.038
ANTIMONY TRICHLORIDE	794	48.2	1.9776	4.0202	471.7	2.2896	4.3711	412.7	41.089

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ARGON	150.86	48.98	0.9319	3.4758	122.0	0.9525	3.4408	120.8	-0.346
ARSENIC (III) CHLORIDE	629	52.6	2.9996	3.3803	297.4	3.3062	3.4499	277.5	21.941
ARSINE	373	65.5	1.0246	4.0041	292.7	1.0490	4.0530	286.0	3.702
AZELAIC ACID	844	27.2	8.1569	3.0918	279.1	8.1687	3.2913	275.5	55.388
BENZALDEHYDE	695	46.5	3.1438	3.5763	321.5	3.3903	3.6821	303.4	27.572
BENZAMIDE	824	50.5	5.2027	3.0551	312.6	5.3594	3.1770	304.0	26.036
BENZENE	562.05	48.95	2.4521	3.6459	288.4	2.5942	3.7113	275.6	15.134
BENZENE-1,2,4-TRICARBOXYLIC ACID TRIMETHYL ESTER	821.7	23.34	7.5934	3.3499	279.5	8.1014	3.4453	268.8	54.214
BENZIDINE	929	33	6.7489	3.3408	322.6	6.8235	3.4459	318.4	31.303
BENZO[b]FLUORANTHENE	1026	21.86	5.2631	3.8706	406.4	6.2965	4.2275	360.0	102.222
BENZOIC ACID	751	44.7	6.1052	2.8640	268.0	5.7233	3.1232	271.3	31.291
BENZONITRILE	702.3	42.15	3.2669	3.5624	323.3	3.6299	3.7227	298.3	40.240
BENZOPHENONE	830	33.52	4.5307	3.7479	331.4	4.8987	3.7851	315.6	32.194
BENZOTHIOPHENE	764	47.6	3.0229	3.8193	357.2	3.3462	3.7887	335.3	11.977
BENZOTRICHLORIDE	737	33.4	2.6860	4.2541	368.2	2.9778	4.3946	339.9	49.039
BENZOTRIFLUORIDE	559.9	32.1	3.0683	3.7613	262.8	3.2891	3.9199	247.5	38.341
BENZOYL CHLORIDE	697	40.6	3.9017	3.4739	294.5	4.2067	3.5558	279.7	27.936
BENZYL ACETATE	699	31.8	4.4245	3.5754	282.0	4.6670	3.7082	270.2	36.631
BENZYL ALCOHOL	720.15	43.74	4.0028	3.3044	301.2	3.7871	3.6495	300.8	39.556
BENZYL CHLORIDE	686	39.1	3.1954	3.7063	316.2	3.3967	3.8815	299.3	38.166
BENZYL DICHLORIDE	731	36.5	3.0210	3.9626	347.1	3.4975	4.0131	315.1	40.569
BENZYL ETHYL ETHER	662	31.1	4.1201	3.6187	274.3	4.3452	3.7725	262.6	43.448
BENZYL FORMATE	698	35.9	4.0048	3.5445	292.9	4.2416	3.6946	279.3	37.723

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BENZYL MERCAPTAN	718	40.6	3.1553	3.7766	331.9	3.3892	3.8949	313.5	31.106
BENZYLAMINE	684	43.2	3.8529	3.4070	290.1	4.0882	3.4993	277.5	25.332
beta-PHELLANDRENE	648	28.2	3.8303	3.8806	274.0	3.8939	4.0359	267.8	33.072
beta-PINENE	643	27.6	3.0322	4.1653	305.3	3.4860	4.2257	277.6	48.823
beta-TERPINEOL	665.2	30.12	6.5954	3.2216	229.5	6.4245	3.2604	232.0	3.076
BICYCLO[2.2.1]HEPTANE	594	36.96	2.0352	4.3075	335.5	2.2361	4.3706	312.3	26.804
BICYCLO[2.2.2]OCTANE	625	34.2	2.3010	4.1825	337.7	2.5567	4.3553	308.5	45.387
BICYCLOHEXYL	727	25.6	3.8181	4.1158	312.2	4.2997	4.1700	289.4	53.036
BIPHENYL	773	33.8	3.8342	3.8244	329.9	4.1026	3.9502	313.2	43.436
BIS-(2-AMINOETHYL)ETHER	655.8	44.21	6.8529	2.9837	216.2	5.8253	2.9744	235.6	-34.069
BIS(alpha-METHYLBENZYL) ETHER	770.6	19.92	4.5683	4.1468	309.4	4.7486	4.4466	296.1	89.709
BIS(CHLOROMETHYL)ETHER	579	45.8	3.2105	3.3215	266.7	3.4776	3.4498	250.2	27.073
BIS(CYANOETHYL)ETHER	783	28.3	6.1226	3.0491	294.4	7.1859	3.3507	264.5	58.088
BIS(DIFLUOROMETHYL)ETHER	420.25	42.28	3.6882	2.9846	180.6	3.8222	3.0738	174.9	14.782
BIS(TRIFLUOROMETHYL)SULFIDE	376.75	30.58	2.7741	3.6525	181.4	3.0083	3.6055	173.0	7.900
BIS[3-(TRIMETHOXYSILYL)PROPYL]DISULFIDE	736.2	13.09	10.4303	3.5529	226.8	10.4826	3.5820	226.3	23.765
BORON TRIBROMIDE	573.15	48.7	2.5263	3.6927	290.7	2.9780	3.5638	264.3	10.475
BORON TRICHLORIDE	451.95	38.71	1.9385	3.8307	264.8	2.1363	3.9911	242.9	29.060
BORON TRIFLUORIDE	260.9	49.9	3.9381	2.3442	110.1	4.3488	2.3618	103.4	8.309
BROMINE	584.15	103	1.8871	3.3201	332.7	1.9727	3.2239	326.4	-3.103
BROMOBENZENE	670.15	45.19	2.5756	3.8601	339.6	2.9055	3.8833	312.4	25.021
BROMOCHLORODIFLUOROMETHANE	426.15	42.54	2.2254	3.6405	228.4	2.4156	3.6354	216.0	10.274
BROMOCHLOROMETHANE	557	64.7	2.4509	3.3146	285.5	2.5641	3.3854	274.6	10.496

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BROMODIFLUOROMETHANE	411.98	51.32	2.4481	3.2407	211.1	2.5536	3.3122	203.5	11.189
BROMOETHANE	503.8	55.65	2.3000	3.4755	266.6	2.5555	3.4467	248.7	9.497
BROMOMETHANE	464	69.29	1.9194	3.3291	268.7	2.1585	3.3042	248.1	7.923
BROMOTRICHLOROMETHANE	606	49.7	2.3755	3.8336	312.6	2.4534	3.8607	304.9	8.488
BROMOTRIFLUOROETHYLENE	432	44.8	2.2333	3.5873	230.5	2.3260	3.6367	222.9	7.642
BROMOTRIFLUOROMETHANE	340.15	39.7	2.1570	3.5004	184.6	2.2878	3.5162	176.9	7.928
BUTANAL	537.2	44.1	2.8410	3.4653	260.4	3.1542	3.5311	241.7	23.029
BUTYL VINYL ETHER	536	31.2	3.7340	3.5467	229.9	3.9222	3.6530	220.9	27.370
BUTYRONITRILE	585.4	38.8	3.3152	3.3240	271.2	3.7632	3.5533	245.1	36.278
CAMPHENE	638	27.5	2.9937	4.1680	302.9	3.2572	4.3262	283.2	51.902
CAMPHOR	709	29.9	3.1467	4.1533	329.0	3.4391	4.2720	307.7	48.314
CARBAMYL CHLORIDE	517	73.8	5.0353	2.6907	186.9	4.4362	2.5837	203.5	-26.892
CARBON DIOXIDE	304.21	73.83	2.5332	2.5750	153.3	2.6969	2.6017	146.6	4.876
CARBON DISULFIDE	552.49	73.29	1.5277	3.7636	356.9	1.6327	3.7816	339.6	7.201
CARBON MONOXIDE	132.92	34.99	1.3740	3.2000	89.2	1.3571	3.2110	89.8	-0.245
CARBON TETRACHLORIDE	556.35	45.6	2.3007	3.8227	293.8	2.4578	3.8591	279.7	14.247
CARBON TETRAFLUORIDE	227.51	37.45	2.2384	3.1088	120.8	2.3537	3.1049	116.7	3.823
CARBONYL FLUORIDE	297	57.6	3.7724	2.6396	120.1	3.1573	2.6504	133.6	-12.792
CARBONYL SULFIDE	378.8	63.49	1.6053	3.4566	237.9	1.7105	3.4425	227.4	2.661
CHLORINE	417.15	77.1	1.5648	3.3617	264.1	1.5160	3.4740	266.3	3.834
CHLORINE TRIFLUORIDE	433.7	45.78	2.8920	2.7894	220.1	3.5819	3.0993	185.2	22.915
CHLOROACETALDEHYDE	555	53.7	3.0489	3.0475	266.4	3.5235	3.2101	238.5	25.046
CHLOROACETIC ACID	686	57.8	4.7813	2.6977	274.0	5.2580	2.8794	254.7	26.972

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CHLOROACETYL CHLORIDE	581	51.1	3.5299	3.1179	256.0	3.7148	3.2492	244.5	22.083
CHLOROCYCLOHEXANE	638	38.27	2.6814	3.9521	316.7	2.9875	3.9979	293.8	28.159
CHLORODIFLUOROMETHANE	369.3	49.71	2.4712	3.1329	189.3	2.6632	3.1806	178.9	10.668
CHLOROFLUOROMETHANE	427	56.2	1.9410	3.2901	253.8	2.5981	3.2324	209.2	18.855
CHLOROFORM	536.4	54.72	2.4971	3.4749	271.9	2.6837	3.4792	259.0	9.395
CHLOROMETHYL METHYL ETHER	521	50.3	2.8378	3.2707	252.5	3.0545	3.3843	237.6	17.949
CHLOROPENTAFLUOROETHANE	353.15	31.57	2.7803	3.4985	170.2	2.9120	3.5322	164.4	10.605
CHLOROPRENE	525	42.6	2.2457	3.7839	283.0	2.4952	3.8518	262.1	22.729
CHLOROTRIFLUOROETHYLENE	379.15	40.53	2.6382	3.3221	188.4	2.8562	3.3508	178.1	11.082
CHLOROTRIFLUOROMETHANE	302	38.7	2.1975	3.3770	162.1	2.2977	3.4033	156.7	6.656
CHRYSENE	979	23.9	5.0740	3.8885	386.4	5.7251	4.2030	353.6	91.338
CINNAMIC ACID	797	35.4	6.4651	3.0297	284.0	6.6328	3.2374	275.4	48.359
cis,trans-2,4-HEXADIENE	538	33.5	2.8319	3.7565	262.2	3.0982	3.8971	243.9	35.633
cis-1,2-DICHLOROETHYLENE	544	51.9	2.0709	3.6582	304.3	2.0172	3.9263	300.7	19.872
cis-1,2-DIMETHYLCYCLOHEXANE	606.15	29.38	2.6553	4.1791	302.9	2.7651	4.4118	288.8	45.550
cis-1,2-DIMETHYLCYCLOPENTANE	565.15	34.45	2.8127	3.9168	272.6	3.0272	3.9577	258.8	21.172
cis-1,3-DICHLOROPROPENE	594.4	47.04	2.5896	3.6345	299.2	2.7288	3.7643	284.9	22.531
cis-1,3-DIMETHYLCYCLOHEXANE	591.15	29.38	2.7417	4.1696	288.7	2.7970	4.3573	280.2	33.826
cis-1,3-DIMETHYLCYCLOPENTANE	551	34.45	3.0177	3.8554	254.7	3.0896	3.8957	250.1	10.615
cis-1,3-PENTADIENE	499	37.4	2.2705	3.8214	266.4	2.1095	4.1906	269.8	27.827
cis-1,4-DIMETHYLCYCLOHEXANE	598.15	29.38	2.7028	4.1701	295.0	2.7550	4.3979	285.4	39.240
cis-1,8-TERPIN	694.8	29.49	10.4122	2.8247	209.8	9.8134	2.7635	216.8	-32.195
cis-1-PROPENYLBENZENE	671	33.6	3.3450	3.8094	303.3	3.6132	3.9612	285.5	40.255

Name	T_c (K)	P_c (bar)	PC-SAFT parameter values			I-PC-SAFT parameter values			
			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
cis-2-BUTENE	435.5	42.1	2.3766	3.5667	226.6	2.5294	3.6163	216.0	13.219
cis-2-DECENE	621	21.8	4.4509	3.8640	250.3	4.6823	4.0377	239.8	56.616
cis-2-DODECENE	663	18.9	5.2141	3.8882	252.6	5.4472	4.0734	243.3	67.635
cis-2-HEPTENE	543.7	28.4	3.2226	3.8424	249.7	3.5757	3.9210	232.3	37.018
cis-2-HEXENE	511.4	31.6	2.9421	3.7728	243.5	3.1918	3.8652	228.9	29.413
cis-2-METHYLCYCLOHEXANOL	614	37.9	5.8580	3.0070	223.4	6.3684	2.9514	214.7	9.100
cis-2-NONENE	598.1	23.7	4.0305	3.8530	250.7	4.3223	4.0009	237.7	51.094
cis-2-OCTENE	572	25.9	3.5926	3.8622	251.3	3.9917	3.9456	234.1	43.296
cis-2-PENTENE	475	36.4	2.7052	3.6677	233.1	2.8651	3.7398	222.8	16.790
cis-2-PHENYLBUTENE-2	685	30.1	3.4079	3.9086	309.3	3.7339	4.0870	287.7	54.773
cis-3-HEPTENE	545	28.4	3.0610	3.9202	254.9	3.2507	4.0640	242.1	36.628
cis-3-HEXENE	509	31.7	2.9549	3.7744	240.8	3.1242	3.8851	229.9	26.614
cis-3-METHYLCYCLOHEXANOL	625	37.9	6.7064	2.8824	214.7	6.4837	2.9465	217.4	6.600
cis-3-OCTENE	569	25.9	3.5444	3.8825	251.2	3.9208	3.9656	234.5	42.710
cis-4-METHYLCYCLOHEXANOL	622	37.9	6.4658	2.9201	216.8	6.4312	2.9519	216.9	6.101
cis-4-OCTENE	568	25.9	3.5913	3.8631	249.3	3.9637	3.9469	233.1	42.362
cis-CROTONALDEHYDE	554	45.9	3.2346	3.2721	253.9	3.4795	3.3963	239.3	24.819
cis-CROTONIC ACID	647	47	5.1356	2.8193	249.4	5.4723	2.9767	237.1	31.014
cis-CROTONITRILE	568	38.8	3.5195	3.1796	256.9	3.9106	3.4671	234.3	35.022
cis-DECAHYDRONAPHTHALENE	703.6	32	2.9176	4.2147	335.2	3.1270	4.3129	317.7	35.669
cis-STILBENE	784	27.4	4.2552	3.9249	323.4	4.6873	4.0420	302.6	58.433
CITRACONIC ACID	829	42.4	7.8594	2.5597	283.1	8.4682	2.7767	268.1	38.957
CROTYL GLYCOL ETHER	643.9	33.87	5.2142	3.1878	244.3	5.3160	3.3541	238.2	34.232

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
CUMENE	631	32.09	3.2968	3.8748	285.2	3.5054	3.9853	271.8	32.846
CYANOGEN	400.15	59.24	2.8873	2.8534	191.4	3.1000	2.9192	181.4	11.393
CYANOGEN CHLORIDE	449	59.9	3.0383	2.7655	214.6	3.4639	2.9024	194.3	18.199
CYCLOBUTANE	459.93	49.8	2.1613	3.5823	250.1	2.3978	3.5473	233.9	10.447
CYCLOHEPTANE	604.2	38.2	2.6783	3.9484	297.1	2.8301	4.0049	284.9	18.519
CYCLOHEPTENE	598	40.1	2.9277	3.7747	280.3	2.9143	3.8864	278.4	12.967
CYCLOHEXANE	553.8	40.8	2.4799	3.8637	281.6	2.5769	3.9334	272.4	15.198
CYCLOHEXANECARBOXALDEHYDE	639.4	35.79	3.5228	3.6195	283.6	3.9421	3.6938	263.0	35.380
CYCLOHEXANOL	650.1	42.6	4.3951	3.1830	258.7	3.8340	3.5419	270.2	28.080
CYCLOHEXANONE	653	40	2.8504	3.7165	320.1	3.2827	3.8370	288.9	39.849
CYCLOHEXANONE OXIME	715	46.9	4.7837	3.2885	271.9	4.5762	3.3079	278.4	-4.961
CYCLOHEXENE	560.4	43.5	2.4433	3.8096	287.7	2.6096	3.8485	274.1	15.192
CYCLOHEXYL ACETATE	648	31.2	4.1517	3.6425	265.7	4.2465	3.7751	259.2	30.901
CYCLOHEXYL FORMATE	645	35.2	3.5144	3.7025	284.4	3.8248	3.7680	268.4	29.035
CYCLOHEXYL HYDROPEROXIDE	685	42.1	7.1386	2.7752	232.0	7.0123	2.8370	233.0	9.374
CYCLOHEXYL ISOCYANATE	633	34.7	4.7996	3.2080	249.1	5.0839	3.3683	237.7	37.032
CYCLOHEXYL MERCAPTAN	664	39.7	2.7770	3.9517	322.4	3.0108	3.9911	304.7	22.147
CYCLOHEXYLAMINE	615	42	3.3703	3.5820	274.0	3.7654	3.5172	257.5	11.973
CYCLOHEXYLBENZENE	744	28.8	3.9617	3.9581	310.4	3.9073	4.1911	307.0	40.588
CYCLOOCTANE	647.2	35.6	2.8210	4.0438	310.9	2.9193	4.1491	301.0	23.299
CYCLOOCTENE	632	36.8	3.1232	3.8400	289.1	3.1376	3.9670	285.0	20.670
CYCLOPENTADIENE	507	51.5	2.2773	3.6044	267.6	2.5304	3.5566	251.5	10.069
CYCLOPENTANE	511.7	45.1	2.3356	3.7211	267.8	2.4756	3.7574	256.4	13.914

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CYCLOPENTANONE	624.5	46	2.8746	3.5016	303.6	3.1940	3.6445	279.5	33.222
CYCLOPENTENE	507	48	2.3311	3.6512	265.2	2.4851	3.6640	253.6	9.992
CYCLOPENTYLACETIC ACID	708	36.2	5.8062	3.1024	258.5	5.8193	3.2630	254.4	31.362
CYCLOPENTYLAMINE	584	46.4	3.4884	3.3398	254.7	3.5208	3.4290	251.1	14.474
CYCLOPROPANE	398	55.4	1.8237	3.5083	234.7	1.9638	3.4936	222.9	5.666
CYCLOPROPANE CARBOXYLIC ACID	671	59.95	5.6038	2.6727	246.6	5.7403	2.7244	242.2	10.605
CYCLOPROPANECARBOXAMIDE	779.1	57.39	4.9273	2.7368	309.7	5.4748	2.9623	285.5	30.582
CYCLOPROPYL CYANIDE	621.9	44.62	2.9820	3.2962	305.2	3.6162	3.5126	264.5	33.676
CYCLOPROPYLAMINE	508.6	57.48	2.9883	3.1043	239.7	3.3203	3.1155	224.0	13.185
DECAFLUOROBUTANE	386.35	23.23	3.7288	3.5720	164.5	3.8134	3.6523	160.9	18.098
DECAMETHYLCYCLOPENTASILOXANE	617.4	10.35	5.7974	4.4655	225.7	5.8842	4.7104	221.1	106.632
DECAMETHYLTETRAASILOXANE	599.4	11.9	6.1820	4.2531	212.7	6.1943	4.3580	211.3	44.047
DECANAL	674	26	5.2008	3.6722	251.9	5.0458	3.7983	253.7	21.050
DEHYDROABIETIC ACID	828	17.5	8.2267	3.6535	272.1	8.3683	3.7478	268.6	45.117
DEHYDROABIETYLAMINE	863	17	6.6202	3.9869	304.4	6.8810	4.1792	295.1	91.780
DEUTERIUM OXIDE	643.89	216.71	3.3667	1.9329	294.9	3.8085	2.0580	268.4	7.133
DI-(2-CHLOROETHOXY)METHANE	696.2	30.66	4.7010	3.4756	276.6	5.0696	3.6274	261.6	49.025
DI(2-CHLOROETHYL)ETHER	666	35.9	3.7037	3.5415	290.4	4.0317	3.7087	271.6	44.194
DI-(2-ETHYLHEXYL) MALEATE	778.6	10.68	8.0362	4.0002	262.6	8.5844	4.2796	251.0	144.582
DI-2-ETHYLHEXYLAMINE	702	14.7	8.2793	3.6544	230.0	8.3904	3.7549	227.6	46.449
DIACETYL	546.9	43.84	3.6660	3.1528	237.5	3.7949	3.3245	228.3	26.300
DIALLYL MALEATE	693	23.3	7.0976	3.2743	238.5	7.2798	3.4132	233.2	45.446
DIALLYL PHTHALATE	790.2	20.96	6.5760	3.6210	279.2	6.8215	3.7987	270.8	69.167

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DIALLYL SULFIDE	653.53	33.59	1.8857	4.5787	383.8	1.6192	5.2022	403.4	45.160
DIALLYLAMINE	556	33.2	4.3964	3.3374	222.6	4.4663	3.4456	218.3	15.870
DIAMYL KETONE	678.5	20.52	5.4367	3.7441	254.8	5.6408	3.9373	246.2	63.845
DIAMYLAMINE	639	21.2	6.1626	3.5245	228.9	6.3366	3.6376	223.8	41.472
DIBENZOFURAN	824	36.4	3.5940	3.9257	362.3	4.0703	3.9488	334.8	36.559
DIBENZOTHIOPHENE	897	38.6	3.8036	3.9210	381.4	4.0661	3.9850	364.6	32.137
DIBENZYL ETHER	777	25.6	6.2740	3.4749	272.6	5.6242	3.8311	282.3	51.947
DIBORANE	289.8	40.53	1.9075	3.4818	166.0	1.9886	3.4731	161.3	3.065
DIBROMODIFLUOROMETHANE	478	40.7	1.7014	4.0877	296.4	1.8169	4.2262	278.3	25.140
DIBROMOMETHANE	611	71.7	2.4490	3.3880	310.5	2.5877	3.3632	300.0	3.519
DIBUTYL MALEATE	716	19	8.1027	3.3865	236.5	8.2300	3.4998	233.3	44.783
DIBUTYL SEBACATE	768	13.2	10.0888	3.5675	239.6	10.2088	3.6677	237.5	54.750
DIBUTYL TEREPHTHALATE	787.2	16.94	8.5025	3.5147	258.2	8.7937	3.6434	252.2	67.046
DICHLOROACETALDEHYDE	555	49.5	3.3565	3.1558	250.5	3.6336	3.2610	235.6	22.391
DICHLOROACETIC ACID	686	51.7	5.1164	2.8362	262.9	5.3307	2.9719	253.5	24.083
DICHLOROACETYL CHLORIDE	585	46.1	3.2476	3.4096	264.4	3.3604	3.4980	256.3	16.704
DICHLORODIETHYLSILANE	595.75	30.6	3.5613	3.8269	257.2	3.4389	4.0003	258.6	21.204
DICHLORODIFLUOROMETHANE	384.95	41.25	2.2249	3.5623	205.8	2.3594	3.5796	197.3	8.625
DICHLOROFLUOROMETHANE	451.58	51.84	2.4418	3.3389	231.7	2.5522	3.4043	223.1	10.728
DICHLOROMETHANE	510	60.8	2.2464	3.3365	275.6	2.5044	3.3839	254.2	14.471
DICHLOROSILANE	451.5	45.99	2.2029	3.6304	242.0	2.2315	3.7111	237.6	8.612
DICYANDIAMIDE	834	53.4	6.3617	2.7912	295.6	6.4678	2.8966	290.3	20.976
DICYCLOHEXYL SULFIDE	802	26.5	3.9025	4.2373	337.0	4.0441	4.3608	326.7	40.625

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DICYCLOPENTADIENE	660	30.6	2.9855	4.0583	313.6	3.1968	4.2512	295.3	41.974
DIETHANOLAMINE	736.6	42.7	8.1332	2.5029	247.1	8.6946	2.6319	236.7	34.061
DIETHYL CARBONATE	576	33.9	4.2905	3.3556	235.9	4.7672	3.3748	221.0	27.553
DIETHYL DISULFIDE	642	38.7	3.2932	3.7274	290.1	3.6592	3.7061	271.8	20.052
DIETHYL ETHER	466.7	36.4	2.9526	3.5133	220.9	3.1426	3.5967	210.3	20.362
DIETHYL MALEATE	680	26.1	6.0291	3.4319	244.5	6.2458	3.4862	239.2	24.240
DIETHYL MALONATE	653	27.8	5.7113	3.3088	239.9	5.8280	3.4663	234.6	38.418
DIETHYL PHTHALATE	776	22.6	5.4770	3.7350	293.1	5.9062	3.9123	277.6	75.539
DIETHYL SUCCINATE	663	25.3	5.9159	3.3931	243.5	6.5275	3.4286	230.2	37.786
DIETHYL SULFIDE	557.15	39.6	3.0539	3.5968	258.7	3.2125	3.6804	248.7	20.367
DIETHYLALUMINUM CHLORIDE	723.15	30	3.0093	3.9455	352.2	3.4292	4.3000	314.2	58.585
DIETHYLAMINE	496.6	37.1	3.1744	3.4513	227.8	3.3207	3.5763	218.7	23.355
DIETHYLENE GLYCOL	744.6	46	5.4226	2.8940	283.5	5.8829	3.0498	266.7	35.861
DIETHYLENE GLYCOL DIETHYL ETHER	624	23.7	6.1265	3.3855	224.0	6.3699	3.4696	218.2	33.142
DIETHYLENE GLYCOL DIMETHYL ETHER	608	28.6	5.2232	3.3218	231.0	5.5151	3.4297	222.3	33.535
DIETHYLENE GLYCOL DI-n-BUTYL ETHER	680	17.6	7.3364	3.5771	232.4	7.7661	3.6207	224.9	42.225
DIETHYLENE GLYCOL ETHYL ETHER ACETATE	680.2	25.9	5.3619	3.5422	254.2	5.3251	3.7329	251.5	41.663
DIETHYLENE GLYCOL MONOBUTYL ETHER ACETATE	679	20.6	7.7398	3.3093	226.4	7.7354	3.4399	224.8	38.686
DIETHYLENE GLYCOL MONOPROPYL ETHER	679.8	30.02	5.5870	3.3536	251.1	5.7940	3.4325	244.6	26.623
DIETHYLENETRIAMINE	709.8	43.8	4.5177	3.2333	281.7	4.5289	3.3897	277.4	24.201
DIETHYLSULFITE	624	37.7	4.7305	3.3039	242.1	4.9357	3.2997	236.6	9.065
DIFLUOROMETHANE	351.26	57.84	2.6797	2.7220	177.2	3.1120	2.8136	158.9	14.894
DIFLUOROMETHYL TRIFLUOROMETHYL ETHER	354.49	33.76	3.3564	3.1729	157.9	3.4891	3.2388	153.0	14.454

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DIGLYCOLIC ACID	820	44.2	9.2992	2.3713	266.2	9.8187	2.5513	255.9	35.037
DIHEXYL ADIPATE	767	13.2	9.7141	3.6333	241.9	9.9328	3.7129	238.7	48.979
DIIODOMETHANE	747	54.7	1.8539	4.0130	451.9	2.0598	4.2577	408.6	34.164
DIISOBUTYL ETHER	562	25.3	4.1903	3.7733	228.3	4.2737	3.8512	224.3	22.612
DIISOBUTYL KETONE	615	24.8	4.4820	3.7533	247.6	4.9771	3.7631	232.6	35.889
DIISOBUTYL PHTHALATE	762	17.8	8.2627	3.5454	249.7	8.3725	3.6240	247.2	37.623
DIISOBUTYLAMINE	580	25.7	4.7103	3.6305	225.3	4.7645	3.7105	222.6	21.525
DIISONONYL PHTHALATE	852.7	10.84	9.7837	3.9758	267.5	9.8231	4.1285	266.1	79.426
DIISOCTYL PHTHALATE	851	11.8	9.6211	3.8789	269.6	9.8837	3.9993	265.1	84.307
DIISOPENTYLSULFIDE	664.4	21.81	5.4999	3.7239	246.6	5.6764	3.8213	240.6	39.109
DIISOPROPYL ETHER	500.05	28.8	3.5494	3.6761	216.8	3.5942	3.7881	213.2	20.849
DIISOPROPYL KETONE	576	30.2	4.0348	3.5867	238.2	4.1150	3.7140	233.1	27.646
DIISOPROPYL SULFIDE	585.2	32.25	3.2541	3.9029	263.1	3.4036	3.9224	255.1	14.098
DIISOPROPYLAMINE	523.1	32	3.4811	3.7403	230.1	3.9868	3.5708	214.2	4.958
DIKETENE	616	59.6	3.9238	3.0021	255.7	3.9373	3.0793	253.5	9.723
DILACTIC ACID	660	34.8	8.6151	2.7911	210.2	8.2943	2.7743	214.6	-12.461
DIMERCAPTOETHYL ETHER	720	36.9	3.8497	3.5370	309.9	4.2337	3.7017	288.3	46.143
DIMETHYL CARBONATE	548	45	3.4200	3.1939	247.6	3.9575	3.2461	225.0	27.544
DIMETHYL DISULFIDE	615	53.6	2.4775	3.6617	312.5	2.5605	3.7275	303.4	11.480
DIMETHYL ETHER	400.1	53.7	2.2997	3.2483	211.7	2.5167	3.2473	198.9	8.284
DIMETHYL GLUTARATE	682	27.7	4.8904	3.4774	266.8	5.0383	3.7358	256.8	56.447
DIMETHYL ISOPHTHALATE	766	26.5	5.5653	3.4651	288.8	6.0528	3.6566	272.0	63.591
DIMETHYL MALEATE	675	32.2	4.9871	3.2683	263.6	5.3910	3.4455	248.6	47.384

Name	T_c (K)	P_c (bar)	PC-SAFT parameter values			I-PC-SAFT parameter values			
			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
DIMETHYL PEROXIDE	448.3	52.68	3.2384	3.0103	201.8	3.2356	3.1044	199.5	9.244
DIMETHYL PHTHALATE	772	27.7	5.3560	3.5194	293.1	5.7101	3.7006	279.1	61.266
DIMETHYL SILANE	402	35.6	1.6791	4.1426	250.6	1.9800	4.0507	224.2	14.040
DIMETHYL SUCCINATE	657	32.8	5.2422	3.2453	251.7	5.8843	3.2740	235.3	33.247
DIMETHYL SULFIDE	503.04	55.3	2.2238	3.4862	271.4	2.4708	3.4929	252.3	13.185
DIMETHYL SULFOXIDE	729	56.5	2.9836	3.2809	351.1	3.1386	3.6060	328.7	31.622
DIMETHYL TEREPHTHALATE	777.4	27.6	4.9555	3.6066	305.5	5.5414	3.7597	283.7	63.279
DIMETHYL-1,4-CYCLOHEXANEDICARBOXYLATE	748.4	25.13	4.9940	3.7165	290.4	5.2724	3.9084	277.6	63.666
DIMETHYL-2,6-NAPHTHALENEDICARBOXYLATE	883	24.85	6.0095	3.6174	323.4	6.4088	3.8244	308.2	77.032
DIMETHYLACETYLENE	473.2	48.7	2.6340	3.3343	235.6	2.8123	3.4122	223.8	15.501
DIMETHYLALUMINUM CHLORIDE	619	36.2	2.2493	3.8974	343.6	2.3877	4.3623	315.4	42.589
DIMETHYLAMINE	437.2	53.4	3.1552	2.9571	201.0	3.2896	3.0462	193.3	13.416
DIMETHYLCHLOROSILANE	472	36.2	2.6241	3.7242	235.2	2.9209	3.7132	219.5	17.526
DIMETHYLDICHLOROSILANE	520.35	34.9	3.0184	3.7165	241.4	3.0367	3.8293	237.9	15.634
DIMETHYLDIMETHOXSILANE	524	26.6	3.1419	3.8534	241.7	3.0014	4.2196	240.8	47.496
DIMETHYLETHANOLAMINE	571.82	41.4	6.6033	2.6909	199.1	6.6236	2.7524	197.7	11.327
DIMETHYLKETENE	470.2	42.35	3.0528	3.4071	217.6	3.3784	3.3390	205.6	7.370
DIMETHYLMALONATE	622.4	40.74	6.9972	2.7775	214.4	7.6239	2.6791	206.9	2.105
DIMETHYLMERCURY	601	66.1	2.3020	3.5345	315.7	2.5930	3.4342	294.8	5.080
DI-n-BUTYL DISULFIDE	711	24.7	4.7154	3.8386	279.4	4.9169	3.9741	270.0	47.563
DI-n-BUTYL ETHER	584.1	24.6	4.2886	3.7430	237.4	4.4607	3.8728	229.5	38.438
DI-n-BUTYL PHTHALATE	797	16.6	6.9259	3.8015	277.8	7.1805	4.0278	269.3	97.274
DI-n-BUTYL SULFIDE	652	25.79	4.3345	3.8025	264.6	4.6121	3.9033	253.1	42.479

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DI-n-BUTYL SULFONE	767	25.4	6.1419	3.4432	277.4	6.4289	3.6177	267.5	59.254
DI-n-BUTYLAMINE	602.3	25.7	4.6341	3.6570	238.9	5.1236	3.6502	225.5	29.150
DI-n-DECYL PHTHALATE	870	9.4	11.3542	3.8776	265.8	11.7234	4.0110	261.1	114.562
DI-n-HEPTYL PHTHALATE	830	12.4	9.4026	3.8069	264.5	9.6566	3.9431	260.0	84.585
DI-n-HEXYL ETHER	658	18.16	6.4668	3.6560	232.4	6.6198	3.7970	227.5	53.241
DI-n-HEXYL PHTHALATE	817	13.4	8.5703	3.8069	267.5	8.8617	3.9748	261.3	94.987
DI-n-NONYL PHTHALATE	858	10.2	10.1495	3.9305	269.7	10.5805	4.0786	263.2	119.675
DI-n-OCTYL ETHER	707	14.4	8.3575	3.6488	231.7	8.5269	3.7625	228.3	57.545
DI-n-OCTYL TEREPHTHALATE	855	11.6	9.6231	3.8792	271.4	9.8974	4.0259	266.3	96.182
DI-n-OCTYLAMINE	734	12.6	7.0604	3.9269	257.0	7.5360	4.2068	244.7	120.555
DINONYL ETHER	736	13	8.9612	3.7135	236.8	9.1249	3.8268	233.7	59.045
DINONYLPHENOL	902	12.4	9.3760	3.6103	295.2	10.2097	3.9510	279.0	135.305
DI-n-PENTYL ETHER	622	20.9	5.3819	3.6913	233.7	5.7100	3.7825	224.9	45.111
DI-n-PROPYL DISULFIDE	675	30.3	4.1979	3.7254	275.4	4.3752	3.8200	267.0	29.638
DI-n-PROPYL ETHER	530.6	30.28	3.5362	3.6827	232.5	3.8317	3.7098	220.6	23.873
DI-n-PROPYL PHTHALATE	784	19	6.2885	3.7504	281.7	6.5159	3.9918	272.3	89.059
DI-n-PROPYL SULFIDE	608	30.8	3.5511	3.7785	267.3	3.8736	3.8442	251.7	33.137
DI-n-PROPYL SULFONE	763	31.1	5.2807	3.3864	290.6	5.5526	3.5875	278.3	55.091
DI-n-PROPYLAMINE	550	31.4	4.1704	3.4851	225.1	4.4771	3.4943	215.8	18.221
DI-n-UNDECYL PHTHALATE	886	8.9	12.3021	3.8495	265.5	12.6400	3.9631	261.8	102.674
DIPHENYL CARBONATE	796.5	26.18	5.9172	3.5325	290.8	6.1706	3.6898	281.2	54.570
DIPHENYL DISULFIDE	829.8	35.69	6.3753	3.4805	281.6	5.4513	3.5504	304.5	-29.860
DIPHENYL ETHER	766.8	30.8	3.8474	3.9171	329.0	4.3905	3.9588	303.0	46.300

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
DIPHENYLACETYLENE	832	29	3.7139	4.1638	359.5	3.9493	4.3226	341.9	55.466
DIPHENYLAMINE	817	31.8	4.6926	3.6446	324.5	5.1239	3.7637	305.9	51.383
DIPHENYLDICHLOROSILANE	814	23.3	4.0785	4.2030	341.6	4.3056	4.4658	323.9	82.397
DIPHENYLMETHANE	778	29.23	3.8024	3.9966	334.1	4.0382	4.1804	317.1	56.376
DIPROPYL MALEATE	691	22	7.0106	3.3648	238.6	7.2198	3.4883	233.1	44.764
DIPROPYLENE GLYCOL MONOMETHYL ETHER ACETATE	647	22.7	6.2487	3.4672	230.9	6.5461	3.5217	224.4	31.121
DIPROPYLENE GLYCOL n-BUTYL ETHER	647.1	20.96	8.9491	3.1314	207.6	9.1264	3.1262	205.5	9.789
DI-sec-BUTYL ETHER	559	25.3	4.0347	3.8098	232.2	4.3347	3.8233	221.9	24.148
DISILANE	432	51.3	1.8096	3.9765	245.8	1.7069	3.8642	259.6	-15.221
DI-t-BUTYL PEROXIDE	547	24.8	4.1015	3.8545	222.7	4.1048	3.9021	221.6	11.322
DI-tert-BUTYL DISULFIDE	689.7	31.59	4.0832	3.9822	277.9	4.0957	3.8921	279.6	-12.836
DI-tert-BUTYL ETHER	550	23.23	3.2646	4.0929	249.4	3.2785	4.3453	243.5	48.185
DI-tert-BUTYL SULFIDE	623.2	25.91	3.2120	4.2218	283.2	3.2964	4.3595	275.2	34.943
DIVINYL ETHER	463	42.5	3.0505	3.3622	214.3	3.2208	3.3764	206.5	9.775
DODECAMETHYLCYCLOHEXASILOXANE	645.8	9.01	6.4631	4.5723	228.0	6.6115	4.7698	223.3	110.003
DODECAMETHYLPENTASILOXANE	628.4	9.45	6.5605	4.4787	220.3	6.7009	4.6248	216.5	78.978
DODECANAL	705.1	23.2	6.3939	3.5648	247.3	6.3713	3.6393	246.5	20.447
DODECANEDIOIC ACID	847	21.5	9.2089	3.2181	271.7	9.4747	3.3334	266.5	52.349
D-XYLOSE	955.7	58.42	7.5290	2.6679	322.3	7.7738	2.7176	316.0	15.768
EICOSAMETHYLNONASILOXANE	707.2	5.75	9.2871	4.7598	225.1	9.5472	4.8549	222.1	112.704
ERUCIC ACID	809.9	10.21	10.8143	3.6982	251.4	11.2642	3.8833	245.1	122.345
ETHANE	305.32	48.72	1.6241	3.5143	190.1	1.7490	3.4727	181.2	3.237
ETHANESULFONYL CHLORIDE	682	47.4	3.4485	3.3879	305.3	3.8317	3.4738	283.6	29.833

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ETHANOL	514	61.37	5.8651	2.3092	187.7	6.0607	2.4184	182.4	17.074
ETHYL ACETATE	523.3	38.8	3.5268	3.2982	231.4	3.8131	3.4060	218.0	26.884
ETHYL ACETOACETATE	642.9	32.7	4.9203	3.2724	251.0	5.3324	3.3876	237.6	40.100
ETHYL ACRYLATE	553	36.8	3.7025	3.3697	238.4	3.8558	3.5162	229.4	29.139
ETHYL BENZOATE	698	31.8	4.4469	3.5669	280.5	4.6974	3.6970	269.2	38.068
ETHYL CAPRATE	688.1	17.88	5.7881	3.8125	253.0	5.9095	4.0629	246.1	81.062
ETHYL CAPRYLATE	649	21.18	5.5663	3.6467	241.3	5.7946	3.7964	233.6	52.538
ETHYL CHLORIDE	460.35	52.7	2.2401	3.4137	247.5	2.4274	3.4674	232.8	13.185
ETHYL CHLOROFORMATE	508.15	45	8.0341	2.4231	164.6	7.6754	2.4152	168.6	-6.445
ETHYL CYANOACETATE	679	33.4	4.7303	3.1641	274.8	5.3588	3.4188	250.5	46.012
ETHYL FLUORIDE	375.31	50.28	2.3107	3.1752	200.3	2.6528	3.1900	182.2	13.559
ETHYL FORMATE	508.4	47.4	2.9316	3.2778	242.7	3.1712	3.3779	228.2	20.819
ETHYL HYDROPEROXIDE	560	65.81	4.9296	2.5865	212.6	4.6054	2.7167	217.5	7.727
ETHYL IODIDE	554	47.11	2.0928	3.7350	311.8	2.2649	3.9212	289.5	28.427
ETHYL ISOAMYL KETONE	617	27.27	4.3524	3.6388	248.6	4.2729	3.8751	246.2	40.872
ETHYL ISOBUTYL ETHER	519.2	30.41	3.6662	3.6330	222.2	3.7243	3.7172	218.3	17.952
ETHYL ISOBUTYRATE	553.15	30.4	4.0649	3.5059	229.3	4.2902	3.5980	220.4	26.970
ETHYL ISOPROPYL ETHER	489	34.1	3.2821	3.5933	218.5	3.3346	3.6538	215.0	10.996
ETHYL ISOPROPYL KETONE	567	33.2	3.8958	3.4805	238.5	3.9928	3.6212	232.1	25.240
ETHYL ISOVALERATE	587.95	28.4	4.2430	3.6069	237.4	4.0797	3.8295	238.7	30.711
ETHYL LACTATE	606.95	37.4	5.4667	3.0276	226.0	5.7269	3.0865	219.2	19.439
ETHYL LAURATE	716.3	15.29	6.3314	3.8830	256.8	6.5249	4.1619	248.7	101.074
ETHYL LEVULINATE	666.1	29.24	5.3498	3.3234	252.6	5.7587	3.4480	240.2	44.476

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ETHYL LINOLEATE	777.8	11.27	8.1395	3.9547	260.6	8.6200	4.1943	250.4	136.676
ETHYL LINOLENATE	779.8	11.5	8.0558	3.9491	261.9	8.5249	4.1905	251.8	134.802
ETHYL MERCAPTAN	499.15	54.9	2.2752	3.4688	265.1	2.4209	3.5172	252.7	11.709
ETHYL METHACRYLATE	577	32.5	3.3732	3.6625	259.8	3.6301	3.8022	245.1	38.728
ETHYL METHYL DISULFIDE	628.9	46.15	2.9861	3.6485	294.6	3.2983	3.6066	277.7	12.705
ETHYL MYRISTATE	738.7	13.23	6.7171	3.9752	261.3	7.0731	4.2633	250.6	117.770
ETHYL n-BUTYRATE	571	29.5	3.6716	3.6364	249.6	4.0883	3.7416	231.6	42.295
ETHYL n-HEXYL ETHER	583	24.6	4.6733	3.6238	229.4	4.8374	3.7489	222.6	36.994
ETHYL n-OCTYL SULFIDE	700	24	4.9118	3.8930	269.4	5.1645	3.9139	261.4	22.839
ETHYL n-PENTYL SULFIDE	633.2	27.97	4.1813	3.7133	260.0	4.3587	3.8462	250.9	37.567
ETHYL OLEATE	772.1	10.98	8.0731	3.9772	260.0	8.6054	4.2238	248.7	139.339
ETHYL PHENYL ACETATE	702.1	28.53	4.8361	3.5795	274.3	5.0867	3.7210	263.5	44.665
ETHYL PHENYL CARBONATE	710.1	30.49	4.7050	3.5548	279.7	4.8866	3.7122	270.2	42.346
ETHYL PROPIONATE	546	33.62	3.7692	3.4174	234.9	4.0350	3.5467	222.6	32.649
ETHYL PROPYL DISULFIDE	660	36.12	3.7988	3.6958	278.6	4.0082	3.6983	269.7	15.135
ETHYL PROPYL ETHER	500.23	33.7	3.2961	3.6078	225.9	3.6623	3.5701	211.7	16.282
ETHYL PROPYL SULFIDE	583.9	34.46	3.2476	3.7379	265.7	3.5501	3.7746	250.2	24.892
ETHYL STEARATE	777.9	10.19	7.6087	4.0999	267.4	8.2220	4.4303	253.5	153.628
ETHYL t-BUTYL SULFIDE	588	31.3	3.0899	3.9653	271.1	3.1822	4.0667	263.6	24.275
ETHYL TERT-BUTYL DISULFIDE	659.9	30.76	3.4744	3.9779	290.0	3.6604	4.0373	279.3	25.904
ETHYL tert-PENTYL ETHER	546	27.4	3.5374	3.8204	237.9	3.5903	3.9676	232.9	29.313
ETHYL THIOLACETATE	590.55	40.75	3.2038	3.5490	269.7	3.3675	3.6535	258.5	22.984
ETHYL VANILLIN	748	32.7	9.7536	2.6801	234.6	9.7489	2.7448	233.8	15.958

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ETHYL VINYL ETHER	475.15	40.7	2.8111	3.4807	229.7	3.0291	3.5327	217.5	15.921
ETHYL-3-ETHOXYPROPIONATE	621	26.6	4.6611	3.5630	245.7	4.8627	3.7225	236.7	40.950
ETHYLACETYLENE	440	46	2.7507	3.3005	213.8	2.8776	3.3668	206.0	12.091
ETHYLAL	524	32.8	3.9303	3.4405	220.1	4.3166	3.4371	208.3	19.252
ETHYLAMINE	456.15	56.2	3.1103	2.9559	210.4	3.1717	3.0780	204.8	12.679
ETHYLBENZENE	617.15	36.09	3.0598	3.7988	288.5	3.3177	3.8818	271.9	29.246
ETHYLBENZENE HYDROPEROXIDE	737	37.9	7.4731	2.8630	247.6	7.4874	2.9265	246.2	14.861
ETHYLCHLOROACETATE	618	37.9	3.7892	3.3747	266.1	4.0259	3.5546	252.1	38.021
ETHYLCYCLOHEXANE	609.15	30.4	2.7982	4.1116	295.5	2.8663	4.3139	285.6	38.203
ETHYLCYCLOPENTANE	569.5	34	2.8687	3.9059	272.3	3.0571	3.9712	259.7	24.038
ETHYLDIETHANOLAMINE	734.8	36.94	6.2908	3.0596	260.1	6.2183	3.1922	258.8	25.943
ETHYLENE	282.34	50.41	1.5577	3.4373	179.4	1.6486	3.4136	172.7	2.561
ETHYLENE CARBONATE	806	67.7	3.5604	3.0102	364.8	4.4176	3.0884	317.8	27.962
ETHYLENE GLYCOL	719	82	4.9288	2.4853	279.6	5.0541	2.6447	270.5	20.090
ETHYLENE GLYCOL DIACETATE	654.2	30.67	5.0712	3.2983	252.3	5.2800	3.4949	242.5	46.827
ETHYLENE GLYCOL DIACRYLATE	689	27	5.8563	3.3255	253.1	6.2121	3.4700	242.7	49.156
ETHYLENE GLYCOL DINITRATE	654	40.4	7.1319	2.6837	224.4	7.2948	2.7843	220.0	21.653
ETHYLENE GLYCOL MONOPROPYL ETHER	615.2	36.51	4.2982	3.3120	253.3	4.7758	3.3631	235.9	34.095
ETHYLENE OXIDE	469.15	71.9	2.2314	3.0505	254.7	2.4953	3.1160	234.2	13.304
ETHYLENEDIAMINE	593	62.9	4.1460	2.7753	246.4	4.6596	2.7983	229.4	16.633
ETHYLENEIMINE	537	68.5	2.5714	2.9800	274.4	2.5206	3.3010	266.8	19.483
ETHYLIDENE DIACETATE	627	31.4	4.9083	3.3372	243.0	5.0966	3.4679	235.2	33.886
ETHYLNORBORNENE	625	30.6	2.6846	4.1756	311.7	2.9829	4.2802	288.0	41.544

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ETHYLTRIACETOXSILANE	672.1	16.89	4.8388	3.9211	268.8	5.2903	4.2989	249.0	90.313
ETHYLTRICHLOROSILANE	559.95	33.3	3.0497	3.8647	258.6	3.0547	3.9775	255.4	14.605
ETHYNYLBENZENE	650	42.8	2.6255	3.8933	323.0	2.7181	4.0078	312.1	19.552
EUGENOL	740.6	29.62	4.9819	3.5211	287.3	5.2535	3.6925	275.0	52.041
FLUORANTHENE	905	26.1	4.5933	3.8776	372.0	5.5976	4.0128	329.3	77.720
FLUORENE	826	30	3.5820	3.9270	371.6	4.1129	4.1983	334.3	65.399
FLUORINE	144.12	51.72	1.3352	2.9071	98.5	1.3949	2.8675	96.0	0.220
FLUOROBENZENE	560.09	45.51	2.6815	3.5941	276.7	2.8792	3.6613	262.1	18.832
FORMANILIDE	787	41.1	4.8869	3.1976	309.3	5.2485	3.3795	292.4	43.532
FUMARIC ACID	771	49.8	8.5635	2.3909	253.5	9.0056	2.4988	245.6	27.035
FUMARONITRILE	657	37.3	4.3463	2.9467	281.4	5.3438	3.2629	242.6	39.890
FURAN	490.15	55	2.5089	3.3187	247.9	2.5268	3.4422	243.3	11.916
FURAN 2,5-DICARBOXYLIC ACID	894.5	44.66	8.1942	2.4186	306.7	9.2243	2.6932	283.3	38.721
FURFURAL	670.15	56.6	3.6419	3.1629	289.8	3.8240	3.2578	278.9	18.402
FURFURYL ALCOHOL	632	53.5	6.7018	2.5528	218.9	6.8185	2.5806	216.6	8.821
GALLIUM TRICHLORIDE	694	38.2	3.5654	3.2461	321.6	4.5412	3.5175	270.9	42.470
gamma-AMINOPROPYLTRIETHOXSILANE	634.6	19.11	7.8787	3.4109	210.5	8.1449	3.3709	207.3	3.572
gamma-BUTYROLACTONE	731	51.3	3.1783	3.2839	346.7	3.7647	3.4857	306.0	34.261
gamma-TERPINENE	661	28	3.7508	3.9124	283.2	3.8904	4.0738	273.2	39.388
gamma-VALEROLACTONE	727	48.4	3.4168	3.4367	329.1	4.1040	3.4333	294.5	30.005
GERMANIUM TETRACHLORIDE	550	38.5	2.5957	3.8802	275.0	2.8318	3.8703	259.3	14.185
GERMANIUM TETRAFLUORIDE	352	46.04	2.4238	3.1635	182.6	2.6931	3.1986	169.7	13.210
GERMANIUM TETRAHYDRIDE	308	55.5	1.6630	3.4965	187.8	2.1367	3.1144	165.5	-4.076

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
GLUTARALDEHYDE	660	35.9	4.6673	3.1033	267.3	5.1859	3.3502	246.2	41.901
GLUTARIC ACID	840	42.7	6.7638	2.8009	296.3	6.9746	3.0293	286.1	41.662
GLUTARIC ANHYDRIDE	838	58	4.5155	3.0861	338.2	5.1855	3.0917	312.5	23.549
GLUTARONITRILE	782	31.5	4.0146	3.3080	354.2	5.7273	3.5562	282.4	55.350
GLYCERYL TRIACETATE	701.4	23.33	7.8628	3.1854	233.8	8.0265	3.2822	230.0	35.464
GLYCOL ALDEHYDE	609.3	66.44	6.2940	2.1030	225.6	7.1080	2.3298	206.4	19.315
GLYCOLIC ACID	616	73.1	9.7677	1.9416	192.4	9.6283	1.9789	193.1	3.344
GUAIACOL	697	47.3	4.5457	3.2227	279.7	5.4593	3.0479	255.6	8.297
HALOTHANE	496	39.2	2.6829	3.6827	245.6	3.0957	3.6004	224.9	13.040
HEPTAFLUOROPROPYL METHYL ETHER	437.7	24.81	3.8796	3.5047	185.4	4.1077	3.6212	177.2	30.975
HEPTANAL	620	31.6	3.7467	3.6856	267.0	4.1256	3.7455	250.6	32.621
HEXACHLOROBENZENE	825	28.5	4.8885	3.4972	326.7	4.8597	4.0001	314.5	66.837
HEXACHLOROCYCLOPENTADIENE	746	30.1	3.6578	3.9709	325.1	3.9478	4.1174	306.6	50.760
HEXACHLORODISILOXANE	597.4	26.76	3.7443	3.9919	250.8	3.5188	4.1516	256.9	14.130
HEXACHLOROETHANE	695	33.4	2.4114	4.2153	369.8	2.8128	4.3979	328.6	51.411
HEXACHLOROSILANE	599.7	27.86	4.3877	3.7193	237.4	4.2379	3.8234	240.0	12.235
HEXACOSAMETHYLDODECASILOXANE	751.3	4.7	11.6993	4.8203	225.1	11.8819	4.7815	224.8	11.595
HEXADECAMETHYLCYCLOOCTASILOXANE	689.2	6.92	7.8049	4.7296	230.8	8.0847	4.8772	225.6	128.832
HEXADECAMETHYLHEPTASILOXANE	671.8	6.77	7.9268	4.6569	223.4	8.1174	4.8629	219.6	148.530
HEXAETHYLBENZENE	746	17.3	6.8351	3.8044	258.7	6.9809	3.9336	254.0	53.932
HEXAFLUORO-1,3-BUTADIENE	409.9	31.31	3.8115	3.2274	172.8	3.6913	3.4137	172.9	19.603
HEXAFLUROACETONE	357.14	28.37	3.7506	3.2202	152.0	3.7907	3.3360	149.1	17.728
HEXAFLUROBENZENE	516.73	32.73	3.7544	3.3998	222.5	4.0425	3.5110	210.5	30.858

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HEXAFLUOROETHANE	293.03	30.43	2.8209	3.3233	140.0	2.9394	3.3489	135.9	7.891
HEXAMETHYLBENZENE	758	27.7	4.6185	3.7542	301.5	4.8471	3.9299	289.2	56.266
HEXAMETHYLCYCLOTRISILOXANE	554.2	17.8	5.1223	3.8962	207.8	4.8520	4.1010	211.4	32.117
HEXAMETHYLDISILAZANE	544	19.2	4.5848	3.8851	216.4	4.9649	3.9379	205.9	40.648
HEXAMETHYLDISILOXANE	519	19.2	4.1679	4.0056	211.3	4.1927	4.1420	208.6	32.996
HEXAMETHYLENEDIAMINE	685	35.9	4.5746	3.4400	269.7	4.5732	3.5657	266.7	22.230
HEXAMETHYLENEIMINE	624	42.7	3.3955	3.5589	276.6	3.6472	3.5571	264.5	13.385
HEXANAL	594	34.6	3.4960	3.6118	262.7	3.7768	3.7046	248.4	29.849
HEXANENITRILE	633.8	33	3.7120	3.5615	278.4	4.3539	3.6426	251.2	45.216
HMX	1030	25	9.0720	2.9335	343.9	10.2740	3.2594	318.1	76.446
HYDRACRYLONITRILE	692.3	48.3	5.9298	2.5177	263.7	7.3274	2.6685	232.6	29.918
HYDRAZINE	653.15	147	3.2242	2.3879	297.1	3.4024	2.4542	284.7	6.999
HYDRAZOBENZENE	939	30.9	5.8141	3.4199	349.9	6.2957	3.6574	329.5	66.186
HYDROGEN BROMIDE	363.15	85.52	1.6078	3.1054	225.6	1.5510	3.1790	229.1	1.538
HYDROGEN CHLORIDE	324.65	83.1	1.7928	2.8284	194.4	1.9920	2.8377	180.5	5.575
HYDROGEN CYANIDE	457	54	3.2958	2.5414	219.0	4.1144	2.8329	184.9	20.101
HYDROGEN IODIDE	423.85	83.1	1.3433	3.5508	287.5	1.2779	3.6208	295.1	0.119
HYDROGEN PEROXIDE	730.15	217	3.3143	2.1664	329.7	3.7484	2.1580	306.2	4.497
HYDROGEN SELENIDE	411.15	89.2	1.5049	3.2900	263.6	1.4041	3.3833	272.9	0.454
HYDROGEN SULFIDE	373.53	89.63	1.6855	3.0277	227.5	1.7086	3.0555	224.3	1.999
HYDROXYACETONITRILE	664	59.3	6.6923	2.2181	239.7	7.3829	2.4496	222.6	23.319
HYDROXYCAPROIC ACID	683	36.4	10.5748	2.4966	208.2	10.3257	2.5019	210.7	-2.884
IBUPROFEN	765	29.8	9.8250	3.0385	233.0	9.1958	2.9296	242.4	-53.557

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
IMIDAZOLE	844.8	105.5	4.5183	2.6863	328.1	4.1899	2.7619	339.6	0.599
INDANE	684.9	39.5	3.0971	3.8267	317.7	3.3626	3.8806	300.0	24.670
INDENE	687	38.2	3.1999	3.7468	317.2	3.5555	3.8482	294.2	37.834
INDOLE	790	43	3.5413	3.5192	353.3	3.8913	3.7468	326.5	43.982
IODINE	819.15	116.54	1.8134	3.6247	474.9	1.8398	3.5462	473.9	-4.084
IODOBENZENE	721.15	45.19	2.7059	3.8927	354.9	2.8745	3.9946	337.7	25.330
IRON PENTACARBONYL	559.65	31.53	3.5318	3.6760	242.7	3.2421	3.9635	248.9	26.002
ISOBUTANE	407.8	36.4	2.2366	3.7752	217.7	2.3885	3.7883	207.8	11.478
ISOBUTENE	417.9	40	2.2591	3.6583	222.9	2.4753	3.6556	209.4	12.013
ISOBUTYL ACETATE	560.8	30.1	4.2426	3.4455	228.7	4.3516	3.6066	222.3	34.568
ISOBUTYL ACRYLATE	587	29.5	4.3207	3.5361	237.7	4.5209	3.6322	229.5	28.978
ISOBUTYL CHLORIDE	528	39	2.6230	3.7407	263.7	2.8357	3.7999	248.8	22.239
ISOBUTYL FORMATE	551.35	38.81	4.0012	3.3436	226.4	3.9969	3.4043	225.6	9.650
ISOBUTYL ISOBUTYRATE	601.89	26.1	4.1312	3.7967	246.2	4.0846	3.9679	244.2	29.539
ISOBUTYL MERCAPTAN	559	40.6	2.6727	3.7784	276.1	2.9225	3.7805	259.9	16.129
ISOBUTYL METHACRYLATE	612	26.7	4.0274	3.7773	255.2	4.2435	3.9023	244.8	38.836
ISOBUTYLAMINE	513.73	42.15	3.5514	3.2867	223.8	3.7840	3.3024	214.6	13.431
ISOBUTYLBENZENE	650	30.5	3.8243	3.8404	273.8	3.9342	3.9205	267.5	21.436
iso-BUTYLCYCLOHEXANE	642.1	25.85	3.5908	4.0814	279.0	3.7119	4.2173	270.3	35.319
ISOBUTYLENE GLYCOL	626.3	50.33	8.1733	2.4316	203.7	8.0328	2.4452	205.3	0.708
ISOBUTYL-tert-BUTYL ETHER	558.3	25.61	3.6756	3.9520	238.1	3.6785	4.0515	235.9	17.570
ISOBUTYRIC ACID	605	37	5.1806	2.8876	236.1	5.8162	3.0746	217.5	36.324
ISOBUTYRIC ANHYDRIDE	631.5	27.19	5.3246	3.4898	236.7	5.6392	3.5004	229.2	16.505

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ISOBUTYRONITRILE	565	37.6	3.2326	3.3604	263.8	3.5918	3.6108	241.0	36.335
ISOPENTANE	460.4	33.8	2.5414	3.8319	232.0	2.7298	3.8592	220.6	16.502
ISOPENTYL ACETATE	586.1	27.6	3.9709	3.6989	250.0	4.7904	3.6282	224.5	35.576
ISOPENTYL BUTYRATE	618.83	23.55	5.0576	3.6424	238.0	5.4764	3.6914	226.7	39.920
ISOPENTYL ISOVALERATE	637	22	5.0864	3.7472	244.4	5.5236	3.7994	232.7	46.472
ISOPHORONE	707.6	30.9	3.6789	3.8661	309.0	4.2111	3.9126	283.9	45.006
ISOPHTHALIC ACID	1007	39.5	8.8437	2.5925	335.3	9.6474	2.8595	315.5	48.470
ISOPHTHALOYL CHLORIDE	768	33.3	5.9178	3.2428	279.3	6.0768	3.3859	272.4	37.666
ISOPIMARIC ACID	807.1	16.48	7.0995	3.8643	277.8	7.2987	4.0260	271.4	74.520
ISOPRENE	484	38.5	2.2669	3.8207	257.3	2.1958	4.0522	256.7	19.836
ISOPROPANOL	508.3	47.65	6.4918	2.4283	177.9	6.2224	2.5927	179.0	17.806
ISOPROPYL ACETATE	532	32.9	3.7523	3.4250	227.8	3.8239	3.6145	221.4	31.830
ISOPROPYL ACRYLATE	560	33.1	3.8673	3.5141	236.0	4.1202	3.5668	226.5	22.185
ISOPROPYL BUTYL ETHER	549	27.4	4.0526	3.6735	226.2	4.1055	3.7789	222.4	22.252
ISOPROPYL CHLORIDE	489	45.4	2.4797	3.5887	247.8	2.5038	3.6783	243.7	11.349
ISOPROPYL IODIDE	578	51.2	2.5069	3.7643	289.5	2.8080	3.5890	273.5	-3.173
ISOPROPYL ISOBUTYL ETHER	537	27.9	3.9094	3.7228	223.1	3.9086	3.7990	221.6	13.296
ISOPROPYL MERCAPTAN	517	47.5	2.4342	3.6758	264.5	2.6213	3.6326	252.3	6.175
ISOPROPYL PALMITATE	766.2	10.9	7.4407	4.0690	264.2	7.9657	4.3710	251.7	142.941
ISOPROPYLAMINE	471.85	45.4	3.1589	3.2175	215.0	3.1024	3.3692	213.8	14.295
ISOPROPYLCYCLOHEXANE	627	28.5	3.2572	4.0489	285.1	3.5220	4.1301	269.5	35.704
ISOPROPYLCYCLOPENTANE	593	30.4	3.0432	4.0017	277.5	3.3140	4.0576	261.3	31.114
ISOQUINOLINE	803.15	51	3.2284	3.7495	360.8	3.3178	3.7766	353.8	9.178

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ISOSORBIDE	824.7	51.33	6.6395	2.8163	286.7	6.6331	2.8929	285.0	14.215
ISOVALERIC ACID	629.09	36.88	6.1848	2.8618	226.2	6.3789	3.0004	219.9	31.990
ISOXAZOLE	590	61	2.4493	3.3061	311.1	2.9538	3.3479	273.0	23.818
ITACONIC ACID	821	42.4	7.8830	2.5643	279.5	8.4496	2.7705	265.7	38.610
KETENE	370	58.1	2.0475	3.1989	205.3	1.9473	3.3656	208.1	7.131
KRYPTON	209.35	55.02	0.9349	3.7064	169.5	0.9525	3.6920	167.7	0.321
LACTIC ACID	675	59.6	9.2243	2.1763	215.0	9.3011	2.2187	213.3	9.226
LACTONITRILE	643	50.3	6.8711	2.4038	226.5	7.2796	2.5759	216.4	26.735
L-ARABINOSE	955.7	58.42	7.5316	2.6673	322.3	7.7743	2.7176	316.0	15.765
LEVOGLUCOSAN	905.7	47.97	7.4929	2.8679	302.6	7.4087	2.9112	303.4	7.151
LEVULINIC ACID	738	40.2	6.4812	2.7715	265.5	7.0011	2.9555	251.1	38.837
L-GLUTAMIC ACID	782	41.3	11.0823	2.4961	234.9	10.7377	2.4639	239.1	-15.087
LINOLEIC ACID	775	14.1	10.4513	3.4241	240.5	10.7074	3.5195	237.1	62.331
LINOLENIC ACID	780	14.4	10.5821	3.4091	241.0	10.7693	3.4929	238.4	47.741
L-MENTHOL	658	27.1	6.8937	3.2032	227.1	7.2034	3.2046	222.1	16.944
L-PHENYLALANINE	854	34.7	7.6189	3.0077	287.6	7.8177	3.1063	282.0	30.560
LYSINE	821	35.3	9.3847	2.8055	258.1	9.2184	2.8316	260.0	1.408
MALEIC ACID	773	49.9	8.8111	2.3631	251.9	9.0856	2.4892	245.7	26.670
MALEIC ANHYDRIDE	721	72.8	4.3919	2.8748	291.3	5.2595	2.7105	267.7	1.895
MALONIC ACID	834	61	6.8553	2.5573	289.4	6.8535	2.7035	285.5	22.467
MALTOL	748.5	48.53	4.8573	2.9919	293.8	5.0797	3.1861	281.1	35.303
m-CHLOROANILINE	751	45.9	4.0014	3.3777	314.2	4.2379	3.4893	300.6	24.837
m-CHLOROBENZOYL CHLORIDE	724	36.8	4.1761	3.4645	300.3	4.5136	3.6208	283.2	44.077

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m-CHLORONITROBENZENE	742	39.8	4.2028	3.3907	308.9	4.8174	3.4664	283.7	42.243
m-CHLOROPHENOL	729	53.2	4.2896	3.2206	294.6	4.7663	3.1416	279.8	6.454
m-CRESOL	705.85	45.6	4.3576	3.2044	285.8	4.4638	3.3571	277.2	29.452
m-CYMENE	649	28.1	3.6855	3.8804	281.1	3.9051	4.0384	267.9	45.702
m-DIBROMOBENZENE	761	46.6	2.9810	3.8665	356.5	3.2376	3.8569	338.6	16.383
m-DICHLOROBENZENE	683.95	40.7	2.9110	3.8242	327.1	3.1264	3.9435	308.9	29.840
m-DIETHYLBENZENE	663	28.8	3.5349	3.9461	291.9	3.7151	4.1104	279.0	43.412
m-DIISOPROPYLBENZENE	684	24.5	4.0196	4.0828	281.1	3.7520	4.3672	286.7	24.616
m-DIVINYLBENZENE	692	31.2	3.5773	3.8174	305.2	3.8682	3.9986	286.7	51.263
MELAMINE	1008	58.58	5.6180	2.7666	386.6	6.5092	2.9836	350.2	37.149
MERCURY DICHLORIDE	972	115.21	2.6483	3.1257	487.4	2.9501	3.2002	450.0	17.808
MESITYL OXIDE	600	34.1	3.2772	3.6277	274.9	3.4893	3.8469	258.9	42.685
MESITYLENE	637.3	31.27	3.7508	3.7037	274.5	4.0682	3.8137	259.0	39.364
METHACROLEIN	530	42.5	2.4780	3.5572	277.5	2.8671	3.6828	248.5	30.773
METHACRYLONITRILE	554	38.8	2.2999	3.7034	309.1	3.3005	3.6622	244.6	34.835
METHANE	190.56	45.99	1.0116	3.6912	149.1	1.0581	3.6329	145.5	0.102
METHANOL	512.5	80.84	4.6613	2.2241	207.1	5.4194	2.3078	188.4	14.314
METHOXYACETIC ACID	691	49.8	5.3150	2.7234	266.4	5.9055	2.8925	247.2	30.711
METHOXYACETONE	584.1	42.13	3.4777	3.3003	261.5	3.9247	3.4002	240.6	32.179
METHOXYDIHYDROPYRAN	599	39.3	3.7087	3.4478	256.3	3.8170	3.5464	249.4	20.603
METHYL ACETATE	506.55	47.5	3.1795	3.1737	234.3	3.5357	3.2397	217.4	20.973
METHYL ACRYLATE	536	42.5	3.2361	3.3110	246.5	3.6227	3.3952	227.8	28.285
METHYL alpha-HYDROXYISOBUTYRATE	585.1	34.88	4.9175	3.1373	227.4	5.2443	3.2347	217.4	28.916

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METHYL alpha-METHOXYISOBUTYRATE	589.3	29.35	3.8971	3.5610	252.0	4.2491	3.7319	235.6	47.454
METHYL BENZOATE	693	35.9	3.6947	3.6447	303.0	4.2436	3.6851	277.2	37.129
METHYL CAPRYLATE	650.7	23.84	4.9317	3.6846	250.3	4.8402	3.9287	248.4	47.776
METHYL CHLORIDE	416.25	66.8	1.9331	3.2212	240.5	2.1400	3.2354	223.5	8.542
METHYL CHLOROACETATE	600	45	4.0002	3.1073	253.3	4.3516	3.2260	237.8	27.874
METHYL CHLOROFORMATE	525	53.6	3.9470	2.9214	218.7	4.0167	3.0018	214.4	11.743
METHYL CHLOROSILANE	442	41.7	2.4382	3.5664	227.6	2.7091	3.5592	212.5	15.009
METHYL CYANOACETATE	687	38.1	4.4987	3.0794	284.5	5.2187	3.3202	255.7	41.043
METHYL DECANOATE	686.9	19.42	5.2077	3.8490	261.8	5.2828	4.1358	254.6	80.302
METHYL DICHLOROSILANE	483	39.5	2.5964	3.6813	242.7	3.1012	3.5573	218.9	15.834
METHYL DIETHANOLAMINE	741.9	41.6	5.7978	3.0107	271.4	5.9364	3.1382	265.0	29.591
METHYL DODECANOATE	712	16.5	5.9571	3.8731	260.8	6.2340	4.1280	250.6	94.225
METHYL EICOSANOATE	797.9	9.59	7.5619	4.1801	275.7	8.2538	4.5513	259.7	167.203
METHYL ERUCATE	806.2	9.38	9.3932	3.9606	260.7	9.9765	4.2227	250.7	161.411
METHYL ETHYL ETHER	437.8	44	2.8435	3.2981	208.5	2.7568	3.4636	208.9	13.577
METHYL ETHYL KETONE	536.7	42.07	3.1337	3.3568	250.4	3.4819	3.4587	231.8	27.987
METHYL ETHYL SULFIDE	533	42.6	2.4429	3.6556	276.9	2.5850	3.8239	261.8	26.584
METHYL FLUORIDE	317.42	58.75	1.9678	2.9386	186.3	2.4744	2.9346	159.1	13.438
METHYL FORMATE	487.2	60	2.7035	3.0685	241.5	2.9441	3.1620	225.8	16.314
METHYL GLYOXAL	534.9	55.05	3.3246	3.0098	242.5	3.5814	3.1258	228.4	20.437
METHYL HYDROPEROXIDE	566.1	92.44	4.6823	2.3739	220.2	4.7433	2.4065	217.6	4.394
METHYL IODIDE	528.2	66	1.7651	3.6110	321.8	2.1831	3.4929	280.9	11.648
METHYL ISOBUTYL ETHER	497	34.1	3.2492	3.5941	224.0	3.3515	3.6668	218.0	16.859

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METHYL ISOBUTYL KETONE	574.6	32.7	3.3921	3.6674	258.1	3.7055	3.7602	242.1	33.085
METHYL ISOBUTYRATE	540.7	34.32	3.5898	3.4686	236.4	3.7914	3.5948	225.7	29.055
METHYL ISOCYANATE	488	54.8	2.9188	2.9967	236.8	3.2959	3.1305	215.5	21.729
METHYL ISOPROPENYL KETONE	566	38.9	2.8808	3.5917	274.5	3.1826	3.7345	253.7	34.434
METHYL ISOPROPYL ETHER	464.48	37.62	2.8940	3.5302	220.6	3.0218	3.6023	212.8	15.572
METHYL ISOPROPYL KETONE	552.8	38	3.1968	3.5366	254.4	3.5519	3.5868	236.8	25.736
METHYL ISOPROPYL SULFIDE	553.1	40.21	2.7589	3.7306	268.1	2.8709	3.8034	259.2	16.823
METHYL LACTATE	607.3	42.35	4.7811	2.9886	239.0	5.1244	3.0988	227.4	28.734
METHYL LINOLENATE	769.4	13.29	9.0787	3.6838	248.1	9.3723	3.8087	242.7	75.582
METHYL MERCAPTAN	469.95	72.3	1.8766	3.3375	275.8	2.1947	3.2530	249.3	7.235
METHYL METHACRYLATE	566	36.8	3.0597	3.5998	265.3	3.1361	3.8245	255.3	33.424
METHYL MYRISTATE	741.2	14.21	6.3827	3.9704	265.2	6.5139	4.3167	257.5	112.588
METHYL n-BUTYL ETHER	512.74	33.71	3.2099	3.6127	233.9	3.3924	3.7028	223.8	24.381
METHYL n-BUTYL SULFIDE	593	34.7	3.2196	3.7297	271.1	3.4700	3.8175	256.5	29.298
METHYL n-BUTYRATE	554.5	34.73	3.6316	3.4523	242.1	3.9011	3.5721	229.0	32.329
METHYL NONAFLUORO-N-BUTYL ETHER	468.45	22.3	3.8807	3.7293	199.1	4.3368	3.7588	185.9	34.074
METHYL n-PENTYL ETHER	546.49	30.42	3.4751	3.6981	241.2	3.6377	3.8142	231.9	28.454
METHYL n-PROPYL ETHER	476.25	38.01	2.7895	3.5774	231.9	3.1109	3.5823	215.5	17.094
METHYL n-PROPYL SULFIDE	565	39.7	2.9067	3.6640	268.9	3.0850	3.7490	256.6	20.994
METHYL OLEATE	777	12.1	7.7402	3.9617	263.0	8.1187	4.2056	254.0	129.770
METHYL PALMITATE	762.2	12.35	6.9453	4.0138	266.6	7.1766	4.3805	257.5	129.621
METHYL PALMITOLEATE	744.4	14.15	8.8583	3.6214	240.8	9.0843	3.7418	236.6	63.676
METHYL para-TOLUATE	718.4	31.78	3.9954	3.7510	298.7	3.8114	4.0465	299.3	42.679

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METHYL PENTYL SULFIDE	611.9	30.81	3.7510	3.6979	261.6	3.8047	3.8782	255.1	34.922
METHYL PHENYL SULFIDE	712.8	42.06	3.2788	3.7075	321.7	3.3531	3.8551	312.6	25.778
METHYL PROPIONATE	530.6	40.04	3.4084	3.3242	237.7	3.6565	3.4397	224.7	26.208
METHYL RICINOLEATE	800.3	11.84	9.0319	3.7559	260.3	9.5076	3.9843	251.6	129.219
METHYL <i>sec</i> -BUTYL ETHER	498	34.1	3.2303	3.5877	225.4	3.3394	3.6741	218.8	19.576
METHYL SILANE	352.5	47	1.9376	3.6402	197.0	1.9913	3.5273	196.1	-6.440
METHYL SILICATE	562.8	28.73	4.2398	3.5721	228.8	4.4331	3.6411	221.6	23.401
METHYL STEARATE	781.1	10.84	7.5496	4.0357	267.4	7.8858	4.4269	257.3	147.004
METHYL <i>t</i> -BUTYL SULFIDE	570	35.4	2.7308	3.9473	277.0	2.7722	4.0584	271.3	18.793
METHYL <i>tert</i> -BUTYL ETHER	497.1	32.86	2.8513	3.7527	238.1	2.8742	3.9243	232.8	24.474
METHYL <i>tert</i> -PENTYL ETHER	534	30.4	3.0553	3.8370	249.7	3.2754	3.9351	236.5	30.644
METHYL <i>t</i> -PENTYL SULFIDE	632	31.3	2.9041	4.0639	303.2	3.1620	4.1753	284.0	38.316
METHYL TRICHLOROSILANE	517	35.3	2.7157	3.8204	253.4	3.0050	3.8209	237.5	18.580
METHYL VINYL DICHLOROSILANE	544.1	29.4	2.9503	3.8769	260.6	3.2344	4.0226	242.2	42.932
METHYL VINYL ETHER	437	46.7	2.6458	3.2742	217.8	2.8356	3.3597	205.9	16.740
METHYL-3-MERCAPTOPROPIONATE	644	39.26	3.8608	3.3955	274.1	4.0721	3.5462	261.6	32.943
METHYL-4-FORMYLBENZOATE	759.5	31.69	5.2096	3.3368	293.6	5.7885	3.4994	273.4	53.302
METHYLACETYLENE	402.4	56.3	2.4703	3.1091	205.6	2.6037	3.1648	197.0	9.096
METHYLAL	480.6	39.5	2.9643	3.3459	229.7	3.1777	3.5203	215.6	29.788
METHYLAMINE	430.05	74.6	3.0659	2.6248	200.4	3.1454	2.7545	193.7	11.034
METHYLCYCLOHEXANE	572.1	34.8	2.6219	4.0259	284.4	2.7930	4.0758	271.3	20.152
METHYLCYCLOPENTADIENE	541	44.3	2.7390	3.6114	262.3	2.8046	3.6858	256.1	12.676
METHYLCYCLOPENTADIENE DIMER	675	26.4	4.0171	3.8821	282.9	4.2621	4.0403	269.6	50.349

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METHYLCYCLOPENTANE	532.7	37.9	2.6462	3.8125	262.8	2.7366	3.8964	255.0	17.188
METHYLCYCLOPROPANE	440.5	45.14	2.0206	3.7381	247.0	2.1621	3.7440	235.4	9.743
METHYLETHANOLAMINE	630	52.2	5.3937	2.7138	236.5	5.5809	2.8262	229.4	20.160
METHYLGERMANIUM TRICHLORIDE	595.4	39.51	2.7213	3.8364	290.3	2.7025	4.0055	286.6	20.997
METHYLGLUTARONITRILE	742	28.8	5.1811	3.2050	294.1	6.0151	3.5282	264.0	56.768
METHYLNORBORNENE	600	34.4	2.3656	4.1635	316.3	2.5978	4.2643	294.0	32.828
m-ETHYLPHENOL	716.45	42.9	4.9286	3.2382	274.5	5.0367	3.2829	269.8	12.835
m-ETHYLSTYRENE	670.7	29.36	3.7826	3.8022	288.6	4.0437	3.9706	273.2	47.979
m-ETHYLTOLUENE	637.15	31.5	3.6024	3.7609	277.9	3.8013	3.9032	265.7	37.135
METHYLTRIACETOXSILANE	663.5	16.49	4.1308	4.0617	287.1	5.0031	4.4127	250.4	92.377
m-METHYLSTYRENE	657	32.9	3.3710	3.7770	297.3	3.6734	3.9368	277.7	45.851
m-NITROANILINE	815	44.2	6.1028	3.0796	294.7	6.7809	3.0006	279.8	10.078
MONOCHLOROBENZENE	632.35	45.19	2.6873	3.7386	312.5	2.8999	3.8114	295.0	22.502
MONOCHLOROSILANE	399.2	53.01	2.0285	3.4434	221.8	2.0011	3.5261	221.5	5.177
MONOMETHYL TEREPHTHALATE	797.8	31.08	7.5364	2.8976	274.3	8.0365	3.1120	261.5	52.048
MONOMETHYL UREA	836.5	63.53	5.7847	2.6934	304.8	5.4454	2.9387	307.0	25.782
MONOOLEIN	856.9	12.01	9.6469	3.8118	272.4	9.9771	3.9678	266.4	101.358
MONOPALMITIN	832.2	13.4	10.3806	3.5992	258.2	10.5676	3.6884	255.4	54.359
MONO-TERT-BUTYLHYDROQUINONE	805.5	37.65	6.8506	3.2247	273.5	6.8011	3.1490	276.3	-17.021
MORPHOLINE	618	53.4	3.4642	3.2401	272.8	3.7461	3.2582	259.2	13.925
m-PHENYLENEDIAMINE	824	51.8	4.7926	3.0702	325.0	5.2604	3.1741	305.9	32.699
m-TERPHENYL	883	24.8	5.7890	3.7554	325.2	6.1215	3.9013	312.4	65.346
m-tert-BUTYLPHENOL	725.1	33.39	5.5913	3.3136	266.2	5.5250	3.4516	264.9	25.884

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m-TOLUALCOHOL	681	39.1	7.1759	2.9026	228.6	6.9594	2.9115	232.1	-1.567
m-TOLUALDEHYDE	691	36.7	4.0695	3.4386	289.7	4.3452	3.6213	274.1	44.342
m-TOLUIC ACID	754	39.01	6.4733	2.9511	265.5	6.3721	3.1295	263.6	30.931
m-TOLUIDINE	707	42.8	3.9588	3.3804	299.2	4.3575	3.4630	280.1	31.809
m-XYLENE	617	35.41	3.2610	3.7196	280.8	3.4775	3.8392	266.6	31.556
N-(2-HYDROXYETHYL)PIPERAZINE	780	49.37	4.7309	3.3038	296.6	4.2420	3.4475	312.1	1.949
N,N'-BIS(2-HYDROXYETHYL)ETHYLENEDIAMINE	781.8	38.04	10.6447	2.5699	237.8	10.3476	2.5764	241.1	-3.767
N,N'-DI(2-HYDROXYETHYL)PIPERAZINE	825.3	38.8	6.2667	3.2682	287.9	5.9509	3.3247	294.6	-0.767
N,N-DIETHYLANILINE	702	28.5	4.3698	3.7054	282.8	4.2887	3.9807	279.8	50.758
N,N-DIETHYLHYDROXYLAMINE	567	41.3	6.8210	2.6799	194.4	6.6610	2.7403	195.7	5.653
N,N-DIETHYLMETHYLAMINE	506.1	33.43	3.1692	3.6803	230.7	3.3306	3.7221	222.6	16.554
N,N-DIMETHYLACETAMIDE	658	40.3	3.3860	3.3850	301.7	3.7902	3.6383	274.8	39.223
N,N-DIMETHYLANILINE	687.15	36.3	3.9305	3.5473	289.3	4.0969	3.7109	278.5	37.557
N,N-DIMETHYLFORMAMIDE	649.6	44.2	2.4816	3.5450	352.9	3.4293	3.6462	282.3	35.719
N,N-DIMETHYL-n-BUTYLAMINE	538	29.3	3.4663	3.7475	237.2	3.6067	3.8544	229.1	26.252
N,N'-DIPHENYL-p-PHENYLENEDIAMINE	1017	23.1	7.2017	3.5342	355.8	7.8826	3.7571	335.0	89.829
N,N'-DI-tert-BUTYLETHYLENEDIAMINE	625	21.6	6.0408	3.7106	220.7	5.9301	3.6891	223.3	-10.858
N-AMINOETHYL ETHANOLAMINE	698	44.6	9.6521	2.4059	218.5	9.5230	2.4448	219.4	6.321
N-AMINOETHYL PIPERAZINE	710.7	37.87	4.8746	3.3371	274.8	5.1032	3.3951	266.5	22.953
NAPHTHALENE	748.4	40.5	3.0083	3.9116	353.4	3.3064	3.9884	330.1	33.285
n-BUTANE	425.12	37.96	2.3279	3.7065	223.2	2.5162	3.7200	211.4	12.467
n-BUTYL ACETATE	575.4	30.9	4.1001	3.4949	238.9	4.3945	3.5923	227.3	32.192
n-BUTYL ACRYLATE	598	29.1	4.2871	3.5596	244.5	4.7350	3.6053	230.0	30.621

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n-BUTYL BENZOATE	724	25.9	5.2293	3.6248	275.1	5.5087	3.7592	264.8	48.128
n-BUTYL CHLORIDE	539.2	37.21	2.6186	3.7531	272.1	2.8796	3.8658	252.3	30.224
n-BUTYL ETHYL ETHER	531	29.9	3.7981	3.5858	225.4	3.9637	3.6789	217.9	25.614
n-BUTYL FORMATE	559	35.1	3.7524	3.4226	240.0	3.9827	3.5412	229.0	29.840
n-BUTYL ISOCYANATE	568	34.4	3.8824	3.3635	242.5	4.1954	3.5135	228.2	39.102
n-BUTYL MERCAPTAN	570.1	39.7	2.7084	3.7607	282.2	3.0670	3.7682	259.6	23.687
n-BUTYL METHACRYLATE	619	26.3	4.4122	3.6460	248.9	4.4531	3.8640	243.3	46.772
n-BUTYL n-BUTYRATE	616	25.4	4.4670	3.6853	247.5	4.7335	3.8105	237.0	43.882
n-BUTYL PROPIONATE	594.6	28	4.4647	3.5374	238.1	4.5951	3.6883	231.1	36.864
n-BUTYL STEARATE	764	11.1	9.1983	3.9436	243.9	9.3228	4.0446	241.3	51.263
n-BUTYL VALERATE	629	23.3	5.5376	3.5357	233.0	5.6635	3.6739	228.0	41.024
n-BUTYLAMINE	531.9	42	3.4175	3.3359	235.5	3.5193	3.4366	228.7	18.390
n-BUTYLBENZENE	660.5	28.9	3.7637	3.8656	283.4	4.0332	3.9752	269.3	38.943
n-BUTYLCYCLOHEXANE	667	25.7	3.2444	4.2265	302.0	3.0901	4.5776	302.7	51.522
n-BUTYLCYCLOPENTANE	621	27.2	3.5556	3.9541	273.0	3.8564	4.0420	257.6	39.894
n-BUTYLHYDROPEROXIDE	565	52.1	8.6356	2.4141	177.1	7.9405	2.3476	185.8	-21.264
n-BUTYRIC ACID	615.7	40.6	5.7437	2.7696	229.8	6.3225	2.8959	215.8	32.993
n-CROTYL ACETATE	585.4	33.14	4.2010	3.4047	240.1	4.3856	3.5324	231.4	30.336
n-DECANE	617.7	21.1	4.5342	3.8737	247.5	4.8208	4.0280	236.1	56.776
n-DECYL FORMATE	672	19.9	6.4506	3.5567	237.8	6.6309	3.7062	232.2	52.897
n-DECYL MERCAPTAN	696	21.3	5.0434	3.8368	270.5	5.5967	3.9344	253.2	68.014
n-DECYLAMINE	663	21.8	5.8144	3.5850	243.9	6.2505	3.6695	233.1	49.381
n-DECYLBENZENE	753	17.7	5.8154	3.9739	278.5	6.3619	4.0735	263.4	73.862

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n-DECYLCYCLOHEXANE	751.25	16.5	5.9130	4.0395	274.7	6.2196	4.2065	264.6	80.198
n-DODECANE	658	18.2	5.2157	3.9122	251.2	5.5060	4.0966	240.7	72.857
n-DODECANOIC ACID	743	19.3	8.1557	3.3604	245.2	8.2204	3.5267	242.1	56.090
n-DODECYLAMINE	696	18.8	6.3874	3.6844	250.0	7.0691	3.7185	236.2	56.530
n-DODECYLBENZENE	780	15.6	6.5442	3.9847	276.2	6.8116	4.1762	267.5	87.135
n-DOTRIACONTANE	855	7.5	12.0643	4.0333	259.0	12.4964	4.1693	253.2	134.981
n-EICOSANE	768	11.6	7.9984	3.9922	257.0	8.2948	4.2084	249.7	121.343
NEOABIETIC ACID	812	16.7	7.6995	3.7602	272.5	7.8883	3.8823	267.5	59.270
NEOHEXANOIC ACID	653	34.1	5.2181	3.1671	248.8	5.4301	3.3334	239.9	41.915
NEON	44.4	26.53	0.6563	3.3342	40.2	0.6668	3.4365	39.3	2.533
NEOPENTANE	433.8	31.96	2.3538	3.9538	225.8	2.4816	3.9854	217.1	13.130
N-ETHYL-2-METHYLLALLYLAMINE	556	31.8	3.5914	3.6357	241.5	3.7227	3.7474	233.8	24.681
N-ETHYLANILINE	698.55	35.8	4.0508	3.5234	291.6	4.1988	3.7135	280.6	40.869
N-ETHYLMORPHOLINE	617	36.83	3.4329	3.6757	272.2	3.5472	3.7615	264.5	20.688
n-HENEICOSANE	778	11.1	8.0921	4.0362	260.5	8.5998	4.2204	250.6	129.231
n-HEPTACOSANE	826	8.83	10.5001	3.9999	257.9	11.0091	4.1474	251.2	130.746
n-HEPTADECANE	736	13.4	6.8444	3.9907	257.6	7.1192	4.2281	249.2	112.802
n-HEPTADECANOIC ACID	792	13.7	8.6803	3.6777	260.3	9.2708	3.8258	250.5	101.002
n-HEPTADECYLBENZENE	826	12.1	8.0502	4.0497	275.7	8.4039	4.2268	267.7	108.716
n-HEPTANE	540.2	27.4	3.4532	3.8072	239.7	3.6792	3.9177	228.2	34.179
n-HEPTANOIC ACID	677.3	30.43	7.1044	2.9957	231.5	7.0365	3.1446	230.1	30.232
n-HEPTYL ACETATE	637	23.3	5.4339	3.5672	238.3	5.6534	3.6921	231.0	41.357
n-HEPTYL FORMATE	628	25.4	4.7119	3.6212	248.5	5.1569	3.7063	234.7	44.031

Name	T_c (K)	P_c (bar)	PC-SAFT parameter values			I-PC-SAFT parameter values			
			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
n-HEPTYL MERCAPTAN	645	27.7	3.8042	3.8478	277.8	4.2598	3.9170	257.7	45.294
n-HEPTYLAMINE	607	28.5	4.5269	3.5262	243.1	4.9455	3.5861	230.0	35.167
n-HEPTYLBENZENE	714	21.8	4.4447	4.0413	291.4	5.1036	4.0875	267.7	63.382
n-HEXACOSANE	819	9.1	9.9645	4.0265	259.3	10.4770	4.1907	251.8	138.164
n-HEXADECANE	723	14	6.4136	4.0022	258.4	6.6778	4.2573	249.3	110.719
n-HEXADECANOIC ACID	785	14.9	8.6176	3.6172	257.2	9.0358	3.7528	249.8	79.823
n-HEXADECYLBENZENE	818	12.7	8.0507	3.9915	271.8	8.2314	4.1842	266.5	94.821
n-HEXANE	507.6	30.25	3.0262	3.8065	238.2	3.3004	3.8648	224.1	27.047
n-HEXANOIC ACID	660.2	33.08	6.8406	2.8962	229.0	6.8092	3.0753	226.4	36.333
n-HEXATRIACONTANE	874	6.8	13.7720	4.0065	257.2	13.8850	4.1208	253.6	107.197
n-HEXYL ACETATE	618	25.4	4.9099	3.5668	239.9	5.2048	3.6728	230.2	39.627
n-HEXYL FORMATE	607	28	4.5393	3.5166	242.5	4.7454	3.6669	233.3	41.928
n-HEXYL MERCAPTAN	623	30.8	3.4483	3.8199	278.4	3.8265	3.8935	259.2	38.646
n-HEXYLAMINE	584	31.8	4.2146	3.4581	239.6	4.5413	3.5302	228.0	30.285
n-HEXYLBENZENE	698	23.8	4.2722	3.9658	287.3	4.7128	4.0666	268.9	57.185
NIACIN	760	46.4	5.4503	3.0168	283.5	5.6653	3.1098	275.4	23.478
NICKEL CARBONYL	452.55	30.4	4.0555	3.3698	187.5	4.5848	3.2793	176.1	10.446
NICOTINONITRILE	703	41.2	3.7226	3.3120	311.0	4.2511	3.5342	281.1	40.325
NITRIC OXIDE	180.15	64.8	5.5935	1.6738	66.1	5.5599	1.7351	65.7	3.187
NITROBENZENE	719	44	4.0256	3.3359	303.1	4.4728	3.4156	282.2	35.199
NITROETHANE	593	51.6	3.2601	3.1320	276.2	3.9234	3.1944	244.3	27.482
NITROGEN	126.2	34	1.2481	3.2913	89.0	1.2751	3.2594	88.0	-0.368
NITROGEN TRIFLUORIDE	234	44.61	1.8539	3.1410	136.3	1.9043	3.1791	133.1	3.990

Name	T_c (K)	P_c (bar)	PC-SAFT parameter values			I-PC-SAFT parameter values			
			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
NITROMETHANE	588.15	63.1	2.9063	2.9711	291.0	3.6678	3.0555	248.8	22.483
NITROSYL CHLORIDE	440.65	91.2	2.9876	2.7195	202.1	3.2942	2.5538	194.7	-4.509
NITROUS OXIDE	309.57	72.45	2.1335	2.7771	168.2	2.0631	2.8890	169.2	4.096
N-METHYL-2-PYRROLIDONE	721.6	45.2	3.2719	3.4870	335.1	3.8672	3.5838	299.0	38.251
N-METHYLACETAMIDE	718	49.8	3.7663	3.0877	317.7	4.3602	3.3087	284.4	33.935
N-METHYLANILINE	701.55	52	4.3603	3.2485	279.4	4.6807	3.1477	271.0	-0.707
N-METHYLCYCLOHEXYLAMINE	622	34.9	3.8221	3.5841	263.4	3.9645	3.6830	255.3	24.640
N-METHYLFORMAMIDE	721	56.2	3.4432	2.9410	336.6	4.1598	3.2407	290.6	30.421
N-METHYLPYRROLIDINE	581.5	36.6	2.6488	3.9593	288.8	2.9431	3.9554	269.5	21.055
N-METHYLPYRROLE	610	47.7	2.7132	3.5869	298.6	2.6137	3.8370	298.1	18.961
N-METHYLPYRROLIDINE	550	42	2.6352	3.7562	271.2	2.7134	3.8170	264.3	12.735
N-NITROSODIETHANOLAMINE	887.1	48.36	8.8241	2.5647	286.8	8.9600	2.6502	282.9	20.879
N-NITROSODIMETHYLAMINE	661	48.9	2.6278	3.4406	342.3	3.0858	3.6849	300.2	33.176
n-NONADECANE	758	12.1	7.4803	4.0123	258.8	7.8236	4.2398	250.2	124.719
n-NONANE	594.6	22.9	4.2054	3.8423	244.5	4.4271	4.0017	234.2	49.318
n-NONANOIC ACID	710.7	25.14	7.3553	3.1955	240.0	7.1957	3.3728	240.0	36.931
n-NONYL ACETATE	661	19.9	6.4325	3.5749	233.4	6.5616	3.7024	229.1	41.392
n-NONYL FORMATE	656	21.4	5.9311	3.5679	238.3	6.1177	3.7124	232.2	48.673
n-NONYL MERCAPTAN	681	23.1	4.5190	3.8848	275.5	5.0944	3.9494	255.5	57.233
n-NONYL n-UNDECYL PHTHALATE	914.6	9.95	7.5039	4.3020	318.6	8.3042	4.6923	297.3	184.347
n-NONYLAMINE	648	23.6	5.4012	3.5771	244.1	5.8411	3.6480	232.6	42.503
n-OCTACOSANE	832	8.5	10.7773	4.0157	258.4	11.2258	4.1719	252.0	135.339
n-OCTADECANE	747	12.7	7.1291	4.0092	258.7	7.4736	4.2357	249.6	119.394

Name	T_c (K)	P_c (bar)	PC-SAFT parameter values			I-PC-SAFT parameter values			
			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
n-OCTADECYLBENZENE	834	11.6	8.2668	4.0670	276.7	8.6735	4.2401	268.1	116.851
n-OCTANE	568.7	24.9	3.8078	3.8332	243.2	4.0762	3.9583	230.9	42.232
n-OCTANOIC ACID	694.26	27.79	7.1998	3.0934	236.5	7.1509	3.2454	234.8	35.226
n-OCTYL ACETATE	652	21.5	5.9537	3.5620	236.5	6.1623	3.6879	230.2	44.606
n-OCTYL FORMATE	645	23.3	4.8344	3.7254	254.9	5.5939	3.7236	234.7	46.546
n-OCTYL MERCAPTAN	667.3	25.2	4.0923	3.8923	278.9	4.4776	4.0103	261.8	53.655
n-OCTYLAMINE	627	25.8	5.0599	3.5308	241.1	5.4483	3.6040	230.1	37.586
n-OCTYLBENZENE	729	20.2	4.8922	4.0158	286.4	5.4293	4.1176	267.8	70.293
NONANAL	658.5	26.8	4.6138	3.7062	259.3	4.6672	3.8484	254.6	33.859
NONYLPHENOL	770	20.7	7.8503	3.4290	256.9	8.0586	3.5174	252.2	43.632
n-PENTACOSANE	812	9.5	9.4778	4.0436	260.6	10.0375	4.2022	252.1	135.840
n-PENTADECANE	708	14.8	6.1403	3.9784	256.5	6.4171	4.2206	247.0	103.671
n-PENTADECANOIC ACID	774	15.7	8.3077	3.5860	256.6	8.7905	3.7165	248.0	78.791
n-PENTADECYLBENZENE	809	13.3	7.6280	3.9999	273.3	7.8621	4.1893	266.7	94.520
n-PENTANE	469.7	33.7	2.6993	3.7545	231.0	2.9127	3.8005	218.7	19.520
n-PENTANOIC ACID	639.16	36.3	6.3542	2.8341	228.5	6.5873	2.9914	221.3	36.961
n-PENTASILANE	628.6	27.75	3.2605	4.2389	280.1	3.2441	4.2982	279.5	11.973
n-PENTYL ACETATE	599.9	27.7	4.0997	3.6559	250.0	4.4617	3.7555	235.7	40.751
n-PENTYL FORMATE	576	31.25	4.5076	3.3918	231.5	5.0084	3.4003	217.3	25.655
n-PENTYL MERCAPTAN	598	34.7	3.1414	3.7722	277.0	3.4528	3.8352	259.1	28.858
n-PENTYLAMINE	555	35.8	3.8861	3.3819	234.5	4.1356	3.4595	224.2	24.488
n-PENTYLBENZENE	679.9	26.04	3.9434	3.9454	288.6	4.3816	4.0253	268.8	50.710
n-PENTYLCYCLOHEXANE	669.2	23.85	4.2772	3.9570	273.0	4.5693	4.0561	260.7	45.407

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
n-PROPYL ACETATE	549.73	33.6	3.7365	3.4325	237.4	3.9915	3.5702	225.0	33.727
n-PROPYL ACRYLATE	569	32.5	4.1767	3.4143	233.6	4.3316	3.5389	225.9	28.422
n-PROPYL BENZOATE	710	28.5	4.5292	3.6840	285.8	5.0524	3.7463	267.1	45.570
n-PROPYL FORMATE	538	40.2	3.1856	3.4192	247.5	3.3592	3.5610	235.8	26.515
n-PROPYL IODIDE	586.3	41.52	2.3556	3.8379	312.0	2.6919	3.9251	282.7	32.381
n-PROPYL ISOBUTYRATE	579.4	28.4	4.6857	3.4815	226.5	4.7519	3.5915	222.6	24.805
n-PROPYL MERCAPTAN	536.6	46.3	2.4655	3.6465	276.3	2.7600	3.6427	255.9	15.834
n-PROPYL METHACRYLATE	599	29.1	3.7286	3.7285	258.9	4.0526	3.8319	243.8	37.545
n-PROPYL n-BUTYRATE	593.7	27.2	4.1953	3.6250	243.9	4.3470	3.8036	235.4	42.656
n-PROPYL PROPIONATE	568.6	30.6	4.2378	3.4464	232.6	4.4690	3.5663	223.2	32.556
n-PROPYLAMINE	496.95	47.4	3.2726	3.1583	223.1	3.1331	3.3671	224.2	17.199
n-PROPYLBENZENE	638.35	32	3.4015	3.8442	285.0	3.6392	3.9492	270.8	32.782
n-PROPYLCYCLOHEXANE	639.15	28.07	3.0292	4.1719	298.3	2.9750	4.4423	294.9	41.676
n-PROPYLCYCLOPENTANE	596	30.2	3.2649	3.9084	270.3	3.4994	3.9926	256.9	32.165
n-TETRACOSANE	804	9.8	9.3442	4.0087	258.4	9.7333	4.2045	251.4	136.613
n-TETRADECANE	693	15.7	5.7850	3.9713	255.9	6.0562	4.2098	246.0	97.092
n-TETRADECANOIC ACID	763	16.4	8.2574	3.5176	253.3	8.7003	3.6624	245.1	77.955
n-TETRADECYLAMINE	722	16.6	7.2603	3.6878	249.3	7.8979	3.7387	237.7	61.855
n-TETRADECYLBENZENE	800	14	7.2320	4.0015	274.7	7.4873	4.1917	267.2	93.003
n-TETRASILANE	570.6	31.81	3.1518	4.0033	257.4	3.1908	4.0006	255.5	4.622
n-TRICOSANE	796	10.2	8.9371	4.0141	258.9	9.3369	4.2146	251.3	135.563
n-TRIDECANE	675	16.8	5.5659	3.9304	252.2	5.8439	4.1408	242.3	84.080
n-TRIDECANOIC ACID	754	17.9	8.0886	3.4576	250.6	8.3511	3.6086	244.7	65.439

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n-TRIDECYLBENZENE	790	14.8	6.8746	3.9976	275.8	7.2055	4.1663	266.6	87.967
n-UNDECANE	639	19.5	4.8478	3.9029	250.1	5.1293	4.0800	239.2	66.020
n-UNDECANOIC ACID	732	20.9	7.8250	3.3172	244.0	7.8309	3.4913	241.6	51.827
n-UNDECYLBENZENE	764	16.72	6.1389	3.9907	278.1	6.7731	4.0625	262.4	73.585
o-ANISIDINE	736	42.4	4.0727	3.4036	307.9	4.4372	3.4960	289.7	32.623
o-CHLOROANILINE	722	45.9	3.6423	3.4536	316.9	4.2499	3.4400	288.7	27.653
o-CHLOROBENZOIC ACID	792	40.3	5.7369	2.9656	296.7	6.2285	3.1771	278.8	42.923
o-CHLORONITROBENZENE	757	39.8	4.2957	3.3946	311.3	4.7730	3.5025	290.4	41.224
o-CHLOROPHENOL	675	50	3.6732	3.3790	291.8	4.3768	3.2321	267.0	10.549
o-CHLOROTOLUENE	656	39.1	3.0642	3.7569	306.9	3.3252	3.8540	288.7	31.152
o-CRESOL	697.55	50.1	4.2630	3.2110	281.6	4.3501	3.2733	276.5	13.910
OCTADECAMETHYLOCTASILOXANE	688.9	6.24	8.8467	4.6977	221.4	8.9636	4.8193	219.7	80.836
OCTAFLUORO-2-BUTENE	392	23.3	2.8919	3.7568	190.1	3.2292	3.8991	174.6	41.130
OCTAFLUOROCYCLOBUTANE	388.37	27.77	3.6686	3.3904	166.2	3.7289	3.4763	163.2	15.022
OCTAFLUOROPROPANE	345.05	26.8	3.4143	3.4260	151.4	3.5102	3.4589	148.5	9.550
OCTAHYDRO-PENTALENE-1-CARBOXYLIC ACID	799.5	33.37	5.8983	3.1731	296.2	6.4717	3.3398	278.2	51.805
OCTAMETHYLCYCLOTETRAILOXANE	586.5	13.17	5.5558	4.1817	216.4	5.5664	4.3716	213.8	63.278
OCTAMETHYLTRISILOXANE	564.4	14.6	5.0279	4.2109	215.5	5.1897	4.2908	210.4	39.646
OCTANAL	638.9	29.6	4.3547	3.6478	256.6	4.4153	3.7666	251.9	26.726
o-CYMENE	657	29	3.6663	3.8683	284.3	3.8116	4.0494	273.7	43.822
o-DICHLOROBENZENE	705	40.7	2.6767	3.9259	350.0	2.6627	4.2178	341.6	37.713
o-DIETHYLBENZENE	668	28.8	3.4496	3.9569	297.8	3.6010	4.1690	284.6	50.051
o-ETHYLANILINE	704	37.4	4.4308	3.4007	282.9	4.5763	3.5487	274.1	31.583

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o-ETHYLPHENOL	703	42.9	4.4800	3.3480	279.0	4.6913	3.3555	271.3	10.095
o-ETHYLSTYRENE	666.7	29.36	3.7417	3.7937	288.8	4.0496	3.9605	271.4	51.227
o-ETHYLTOLUENE	650	32.9	3.3793	3.8277	291.1	3.5676	3.9657	278.0	35.235
OLEIC ACID	781	13.9	10.5897	3.4503	240.8	10.7265	3.5424	238.9	50.903
o-METHYLSTYRENE	659	34.7	3.4783	3.7302	291.4	3.6137	3.8951	280.4	34.886
o-NITROANISOLE	782	37.6	5.0719	3.2666	302.2	5.3826	3.4386	288.1	45.624
o-NITRODIPHENYLAMINE	835	28.7	7.0110	3.3535	285.9	7.0955	3.4260	283.0	24.741
o-NITROTOLUENE	720	38	4.0321	3.4855	305.6	4.7844	3.4947	276.0	37.622
o-PHENYLENEDIAMINE	781	51.8	4.9619	3.0024	302.4	5.1992	3.1326	291.0	28.198
o-TERPHENYL	857	29.9	5.0991	3.9292	323.0	5.3002	3.8506	317.3	-4.939
o-tert-BUTYLPHENOL	703.6	33.39	5.2600	3.4128	263.6	5.4279	3.4420	258.5	15.817
o-TOLUALDEHYDE	694	36.7	3.8419	3.5023	299.5	4.3562	3.6230	275.0	44.516
o-TOLUIC ACID	751	38.6	5.9542	3.0374	273.5	6.1744	3.1781	265.0	34.766
o-TOLUIDINE	716.5	47	3.6631	3.4648	309.7	3.9543	3.4995	294.3	19.133
OXAZOLE	554	63.2	3.1885	3.3427	240.2	2.7539	3.3216	264.4	-19.033
OXYGEN	154.58	50.43	1.1272	3.2030	114.7	1.1492	3.1797	113.5	-0.140
o-XYLENE	630.3	37.63	3.1059	3.7625	292.8	3.3940	3.8231	275.1	27.803
OZONE	261	55.7	2.3459	2.6799	138.2	2.6065	2.7483	127.7	10.640
p.alpha-DIMETHYLBENZYL ALCOHOL	695.9	34.92	5.5787	3.2302	256.2	5.6550	3.3224	252.4	22.451
PALUSTRIC ACID	789	17.2	8.3678	3.6725	256.3	8.3858	3.7058	255.8	14.640
p-AMINOAZOBENZENE	877	29	5.8546	3.5993	319.2	5.9854	3.7294	312.5	41.940
p-AMINODIPHENYL	867	32.9	5.0519	3.6687	330.8	5.2236	3.7664	322.6	33.863
p-AMINODIPHENYLAMINE	867	31.9	6.5244	3.4039	302.2	6.4815	3.4809	301.6	19.123

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PARALDEHYDE	579	35	4.4286	3.3963	228.8	4.3737	3.4597	229.1	8.153
p-BROMOTOLUENE	699	43.7	3.4390	3.6718	305.0	3.4310	3.7498	303.7	10.460
p-CHLOROANILINE	754	45.9	3.9741	3.3626	317.6	4.2472	3.4910	301.6	31.780
p-CHLOROBENZOTRIFLUORIDE	601	30.1	3.5701	3.7088	265.0	3.8534	3.8665	249.3	44.905
p-CHLORONITROBENZENE	751	39.8	4.4445	3.3198	305.1	4.7810	3.4909	287.9	43.703
p-CHLOROPHENOL	738	53.2	4.2094	3.2260	302.1	4.7606	3.1559	283.4	10.832
p-CHLOROTOLUENE	660	39.1	3.1234	3.7521	305.9	3.3865	3.8361	288.3	29.224
p-CRESOL	704.65	51.5	4.5649	3.1445	279.1	4.9414	3.0953	267.1	9.002
p-CUMYLPHENOL	834	28.6	6.4182	3.5100	292.4	6.4382	3.5737	290.7	18.196
p-CYMENE	652	28	3.5524	3.9447	287.6	3.8715	4.0627	270.0	45.637
p-DICHLOROBENZENE	684.75	40.7	2.9665	3.7986	324.7	3.1705	3.9251	307.4	30.993
p-DIETHYLBENZENE	657.9	28.03	3.7850	3.8560	282.8	4.1020	3.9848	266.5	46.297
p-DIISOPROPYLBENZENE	689	24.5	4.0513	4.0203	285.3	4.0004	4.2730	281.8	51.216
p-DIISOPROPYLBENZENE HYDROPEROXIDE	810	24.9	8.3920	3.1924	264.7	8.4774	3.2887	261.9	33.180
p-DIMETHYLAMINOBENZALDEHYDE	832	30.7	4.1741	3.6750	354.7	5.1035	3.8375	312.0	61.971
p-DIVINYLBENZENE	691.5	30.77	3.5611	3.8280	306.9	3.9443	3.9866	284.3	53.700
PENTACHLOROETHANE	665	36.8	2.5795	4.0420	338.3	2.8661	4.1680	311.8	40.966
PENTACHLOROFLUOROETHANE	624	33.4	2.6277	4.0605	314.5	2.8625	4.2164	292.8	42.628
PENTAETHYLBENZENE	731	18.9	5.9965	3.8452	265.3	6.2786	3.9682	256.7	59.601
PENTAETHYLENE GLYCOL DIMETHYL ETHER	769.8	16.67	10.2146	3.2865	239.6	10.3368	3.3762	237.4	36.946
PENTAETHYLENE GLYCOL MONOMETHYL ETHER	776.6	18.8	8.8536	3.3297	251.3	9.0496	3.4581	247.1	53.937
PENTAFLURO(TRIFLUOROMETHYL)SULFUR	381.3	33.71	3.1552	3.4759	170.7	3.1314	3.4540	172.1	-3.610
PENTAFLUROETHANE	339.17	36.2	3.1624	3.1030	155.4	3.3317	3.1715	149.1	13.226

Name	T_c (K)	P_c (bar)	PC-SAFT parameter values			I-PC-SAFT parameter values			
			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
PENTAFLUOROETHYL METHYL ETHER	406.83	28.87	3.4426	3.3807	181.5	3.7110	3.4915	171.3	27.298
PENTAFLUOROETHYL TRIFLUOROVINYL ETHER	401	28	4.7931	3.2853	151.0	4.4740	3.2684	157.4	-12.972
PENTAFLUOROPHENOL	609	40	4.5772	3.1711	242.2	4.9073	3.2164	231.4	20.205
PENTAMETHYLBENZENE	719.15	28.7	4.3289	3.7576	292.5	4.5895	3.8993	279.7	45.616
PENTANAL	566.1	38.45	3.4955	3.4188	247.7	3.3935	3.6624	247.1	28.597
PERCHLORYL FLUORIDE	368.4	53.7	2.1903	3.2564	197.6	2.3047	3.2568	190.9	4.249
PERFLUOROBUTANOIC ACID	530	26.5	7.1488	2.8355	182.2	7.3130	2.9844	178.2	34.506
PERFLUOROMETHYLCYCLOPENTANE	451.44	21.72	4.0968	3.6887	185.5	4.1681	3.8034	181.8	26.158
PERFLUORO-n-DODECANE	570.5	9.72	5.2116	4.3571	222.7	5.8729	4.6883	204.4	130.043
PERFLUORO-n-HEPTANE	475.65	16.1	5.2076	3.7262	179.6	5.2318	3.9102	176.9	47.052
PERFLUORO-n-HEXADECANE	620.8	6.35	5.4737	4.7950	241.9	6.0819	5.4767	220.1	214.684
PERFLUORO-n-HEXANE	449.55	18.02	4.7838	3.6715	174.7	4.8549	3.8081	171.4	33.670
PERFLUORO-n-NONANE	523.9	12.96	4.7409	4.1865	207.5	5.0887	4.3897	196.6	90.871
PERFLUORO-n-OCTANE	502.2	14.78	4.7201	4.0291	197.7	4.9509	4.1885	190.2	60.985
PERFLUORO-n-PENTANE	423.1	20.47	4.1510	3.6622	172.5	4.0929	3.8230	171.6	26.837
p-ETHYLPHENOL	716.45	42.9	5.2821	3.1441	265.7	5.0080	3.2903	270.3	14.628
p-ETHYLSTYRENE	674	29.36	3.7572	3.8104	291.2	4.0517	3.9741	274.3	48.799
p-ETHYLTOLUENE	640.2	32.3	3.4665	3.8288	284.0	3.8144	3.8719	266.7	28.461
PHENANTHRENE	869	29	3.8247	3.9458	383.1	4.6463	4.1189	336.5	69.766
PHENETOLE	647.15	34.2	3.8470	3.5725	276.9	4.2221	3.6679	259.4	36.710
PHENOL	694.25	61.3	4.1725	3.0611	283.2	4.4271	3.0348	273.5	6.446
PHENOTHIAZINE	923	40.01	5.7185	3.4892	331.8	5.5326	3.5199	337.1	-1.461
PHENYL ISOCYANATE	653	40.6	3.5223	3.5157	290.6	4.1780	3.4885	262.8	27.209

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PHENYL MERCAPTAN	689	47.4	3.0236	3.6317	321.5	3.0003	3.8134	316.7	21.666
PHENYLACETONITRILE	732	34.6	4.1701	3.4122	308.4	4.6526	3.6657	283.3	49.244
PHENYLHYDRAZINE	761	49.1	4.6516	3.1391	302.7	5.1684	3.1692	284.1	25.590
PHENYLMETHYLDICHLOROSILANE	689	28.7	3.9077	3.8928	290.2	4.0975	4.0166	279.3	34.651
PHENYLTRICHLOROSILANE	688	29.6	3.8295	3.8874	292.1	4.0448	3.9932	280.2	35.164
PHOSGENE	455	56.74	2.3780	3.3303	235.0	2.5250	3.3240	225.9	6.132
PHOSPHINE	324.75	65.4	1.2003	3.7104	233.4	1.3337	3.5331	221.3	-2.742
PHOSPHORUS PENTAFLUORIDE	295.7	37.15	2.3071	3.3560	154.3	2.2903	3.4296	153.7	5.452
PHOSPHORUS TRICHLORIDE	563.15	56.7	2.5012	3.6014	282.0	2.7805	3.4511	267.6	-1.473
PHOSPHORUS TRIFLUORIDE	271.1	43.27	2.3622	3.0765	140.8	2.6080	3.0272	132.6	4.438
PHTHALAN	700	42.85	3.6092	3.5098	305.4	3.8535	3.6162	290.4	28.652
PHTHALIC ACID	800	39.5	9.7262	2.6048	250.2	9.6223	2.6515	250.8	8.048
PHTHALIDE	830.9	50.95	4.3976	3.3120	337.4	5.1760	3.2215	310.1	17.634
p-HYDROQUINONE	838.8	58.91	4.9631	2.9066	323.7	4.7684	3.1814	321.9	32.840
p-HYDROXYBENZALDEHYDE	844	49.9	5.4541	2.9703	317.9	5.8426	3.1036	302.9	36.732
PIMARIC ACID	807.1	16.48	7.0966	3.8656	277.9	7.3057	4.0243	271.4	74.409
PIMELIC ACID	842	32.8	7.5103	3.0043	284.9	7.4740	3.2128	281.4	42.609
PIPERAZINE	638	55.3	4.6404	3.1777	240.2	4.1895	3.1195	256.5	-26.291
PIPERIDINE	594.05	46.51	2.8717	3.5877	281.6	2.8453	3.7224	279.4	14.702
p-ISOPROPENYL PHENOL	742.7	39.36	4.7681	3.1730	295.3	5.0748	3.4089	279.0	43.198
p-MENTHANE HYDROPEROXIDE	711	29.5	8.6260	3.0475	225.7	8.2417	3.0135	231.5	-18.862
p-METHYLSTYRENE	665	33.6	3.2786	3.8421	302.0	3.4279	4.0270	289.0	34.073
p-NITROANILINE	851	44.2	7.0830	2.8883	291.9	7.2268	2.9620	287.0	19.970

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
p-NITROTOLUENE	743	32.07	3.8529	3.5802	324.9	4.2810	3.9030	296.3	54.693
p-PHENETIDINE	754	35.7	4.9228	3.3696	292.8	5.1684	3.5135	281.5	35.988
p-PHENYLENEDIAMINE	796	51.8	4.9291	3.0111	309.8	5.1971	3.1531	296.7	31.318
PROPADIENE	394	52.5	1.8780	3.4478	229.3	1.7840	3.6629	231.5	10.087
PROPANAL	503.6	50.38	2.8297	3.2162	245.4	3.1441	3.3097	226.9	21.434
PROPANE	369.83	42.48	2.0078	3.6122	207.9	2.1498	3.6112	198.1	7.421
PROPARGYL ALCOHOL	588.8	61.9	3.8328	2.7605	256.3	4.5332	2.8370	230.0	22.243
PROPARGYL CHLORIDE	541	53	1.8109	3.7611	328.8	2.1321	3.8188	291.0	25.514
PROPENYL CYCLOHEXENE	636	31.2	3.4816	3.8472	280.5	3.6201	3.9855	270.4	34.274
PROPIONIC ACID	600.81	46.68	4.9823	2.7184	236.6	5.5322	2.8978	219.4	28.926
PROPIONIC ANHYDRIDE	623	32.7	4.9786	3.2778	241.1	5.3711	3.3425	229.7	27.855
PROPIONITRILE	561.3	42.6	2.7534	3.2916	289.5	3.6839	3.4236	237.0	31.765
PROPYL CHLORIDE	503.15	44.25	2.3902	3.6229	263.5	2.6308	3.6812	245.2	19.641
PROPYLENE	364.85	46	1.9988	3.5088	204.9	2.0379	3.5654	200.6	6.344
PROPYLENE GLYCOL 1-tert-BUTYL ETHER	600.7	27.2	4.5744	3.5408	238.9	4.7724	3.6814	230.4	38.627
PROPYLENE GLYCOL 2-tert-BUTYL ETHER	600.6	27.2	4.5756	3.5403	238.9	4.7751	3.6804	230.4	38.582
PROPYLENE GLYCOL alpha-METHYLBENZYL ETHER	719	24.79	5.6907	3.5260	266.3	6.0067	3.6724	255.9	53.590
PROPYLENE GLYCOL ETHYL ETHER ACETATE	613	27.6	5.0624	3.4381	234.5	5.2285	3.5563	228.0	33.931
PROPYLENE GLYCOL MONOALLYL ETHER	616.6	33.76	4.7398	3.2915	240.8	4.7184	3.4712	237.5	30.439
PROPYLENE GLYCOL MONOMETHYL ETHER	579.8	41.13	4.4036	3.0813	233.0	4.4210	3.2663	228.5	27.724
PROPYLENE GLYCOL MONOMETHYL ETHER ACETATE	597.9	30.09	4.7308	3.3709	233.7	4.7271	3.5675	230.1	35.609
PROPYLENE GLYCOL n-BUTYL ETHER	624.9	27.39	4.7731	3.4903	245.0	4.8894	3.6860	237.7	46.455
PROPYLENE GLYCOL n-PROPYL ETHER	605.1	30.51	4.6064	3.3849	239.3	4.5317	3.6249	236.4	39.115

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PROPYLENEIMINE	539.9	54.79	2.8396	3.2058	260.1	2.7423	3.4588	258.2	20.183
p-TERPHENYL	908	29.9	6.0926	3.6757	322.2	6.0527	3.7173	322.4	9.026
p-tert-AMYLPHENOL	752	29.8	5.2706	3.5533	282.9	5.4006	3.6626	276.8	32.480
p-tert-BUTYL ETHYLBENZENE	684	23.8	4.1216	3.9933	283.8	4.3569	4.1652	271.0	57.024
p-tert-BUTYL CATECHOL	776	37.7	7.0391	3.1059	261.7	6.8208	3.1049	266.0	-7.493
p-tert-BUTYLPHENOL	734	33.4	4.8764	3.5249	283.2	4.9591	3.6198	277.9	24.641
p-tert-BUTYLSTYRENE	709	24.8	3.8118	4.0734	305.7	4.2519	4.1973	283.4	63.046
p-tert-OCTYLPHENOL	765	22.8	5.7844	3.7257	280.1	5.9694	3.8652	272.8	50.681
p-TOLUALDEHYDE	715.8	39.22	3.5720	3.6170	315.8	3.9423	3.7202	294.4	37.456
p-TOLUIC ACID	775	38	5.6532	3.0535	289.9	5.9408	3.2807	276.7	45.075
p-TOLUIDINE	718	43.02	3.7918	3.4353	304.1	3.4947	3.7776	309.6	34.006
p-XYLENE	616.2	35.31	3.1377	3.7751	286.0	3.4694	3.8445	266.5	31.962
PYRAZINE	626	54.9	2.3331	3.5597	335.0	2.5379	3.7312	310.1	28.329
PYRAZOLE	734	66	2.7113	3.2568	371.7	3.1874	3.4126	328.8	27.220
PYRENE	936	26.1	3.9292	4.0800	412.0	4.9431	4.2672	354.8	82.531
PYRIDAZINE	774	54.9	2.0204	3.7977	458.6	2.5418	4.0026	383.1	35.024
PYRIDINE	619.95	56.3	2.6917	3.4590	305.0	2.8128	3.5572	293.1	15.473
PYRIMIDINE	638	54.9	2.2265	3.6257	351.0	2.5959	3.7254	312.8	28.841
PYRROLE	639.75	65.3	3.1907	3.0946	292.8	3.2721	3.2404	283.4	18.442
PYRROLIDINE	568.55	56.1	3.1146	3.2590	258.9	3.0316	3.3689	260.2	8.930
QUATERPHENYL	989.3	19.06	6.8579	3.8929	347.0	7.1866	4.1323	334.2	108.968
QUINALDINE	769	33.5	3.6822	3.7636	335.1	3.7552	4.0900	322.3	55.209
QUINOLINE	782.15	48.6	3.4099	3.6780	345.6	3.6556	3.6702	331.3	13.358

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QUINONE	683	59.6	4.7958	2.9340	262.0	4.8385	2.9422	260.8	3.051
RADON	377.5	62.8	0.8484	4.4092	318.4	0.9525	4.2999	302.3	4.072
RDX	895.2	41.6	9.6613	2.8012	276.2	9.2109	2.7602	283.6	-21.578
SACCHARIN	968	57.25	6.8427	3.2989	314.6	5.8296	3.1062	347.7	-85.140
SALICYLIC ACID	739	51.8	8.0544	2.5942	240.4	7.8146	2.5905	244.0	-5.636
SALICYLIC ACID PHENYL ESTER	804.9	26.46	5.7809	3.5396	296.7	6.0340	3.7242	286.1	60.647
sec-BUTENYL ACETATE	563.5	33.07	3.9906	3.4640	234.3	4.0177	3.6099	230.1	25.144
sec-BUTYL ACETATE	561	31.7	4.0743	3.4968	230.4	4.0431	3.6470	228.5	22.850
sec-BUTYL ACRYLATE	580	29.7	4.4700	3.4807	230.2	4.4138	3.6435	228.7	26.859
sec-BUTYL CHLORIDE	520.6	39	2.8957	3.6193	248.3	3.2175	3.6144	232.3	17.956
sec-BUTYL FORMATE	546	35.8	3.6516	3.4520	234.8	3.6747	3.5980	230.8	23.313
sec-BUTYL MERCAPTAN	554	40.6	2.6570	3.7886	274.0	2.9056	3.7770	258.2	14.441
sec-BUTYLAMINE	514.3	40	3.0102	3.5015	240.8	3.1462	3.5986	231.6	20.078
sec-BUTYLBENZENE	664.54	29.5	3.0575	4.1458	310.0	3.1277	4.3475	300.1	41.389
sec-BUTYLCYCLOHEXANE	654	25.85	3.5025	4.0928	288.9	3.6961	4.2500	275.8	46.496
sec-BUTYL-tert-BUTYL ETHER	559.4	25.61	3.6074	3.9594	241.2	3.6751	4.0555	236.4	22.946
SILANE	269.7	48.4	1.3038	3.8065	186.1	1.7055	3.3683	162.1	-6.831
SITOSTEROL	953	11.2	8.8068	3.9235	316.7	9.5852	4.2861	299.1	162.173
STIGMASTEROL	953.6	11.38	8.8790	3.9045	316.0	9.6631	4.2484	298.7	159.220
STYRENE	636	38.4	2.9410	3.7947	303.8	3.2678	3.8620	281.9	29.799
STYRENE GLYCOL	776.4	39.24	5.6078	3.1276	288.4	5.8316	3.2728	278.8	36.278
SUBERIC ACID	843	29.7	7.8750	3.0216	281.7	7.8166	3.2577	278.3	57.040
SUCCINIC ANHYDRIDE	811	67.3	4.6300	2.7074	328.8	5.1445	2.9196	303.3	27.511

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SUCCINIMIDE	858	59.7	4.2501	2.9668	360.0	4.7483	3.1966	329.7	33.328
SUCROSE	1086	26.9	3.4236	4.5984	494.3	3.8040	4.9131	452.8	96.937
SULFOLANE	853	50.3	3.3472	3.4888	393.2	3.9394	3.6312	350.9	40.530
SULFUR DIOXIDE	430.75	78.84	2.8507	2.6781	206.0	2.8652	2.7977	202.0	8.227
SULFUR HEXAFLUORIDE	318.69	37.6	2.6049	3.2766	157.2	2.6315	3.3374	155.3	6.530
SULFUR TRIOXIDE	490.85	82.1	5.1403	2.1942	184.0	4.2709	2.4871	195.9	9.138
SULFURYL CHLORIDE	545	46.1	2.3353	3.5928	289.8	2.3342	3.8876	280.7	29.232
SYRINGALDEHYDE	809	38.29	7.6978	2.9198	270.2	7.9221	2.9350	266.2	11.768
SYRINGOL	752.2	37.85	6.0145	3.1131	271.1	6.1566	3.2045	265.7	24.153
t-BUTYL ACETOACETATE	636.5	27.73	5.4664	3.4170	235.9	5.5619	3.5064	232.0	25.203
t-BUTYL HYDROPEROXIDE	552	43.4	6.4251	2.6937	192.0	6.2167	2.7504	194.4	4.006
TEREPHTHALDEHYDE	739	36.7	5.0522	3.1362	289.7	5.5620	3.3566	269.4	45.200
TEREPHTHALIC ACID	883.6	34.86	7.5482	2.7130	310.4	8.6429	3.0001	284.3	50.151
TEREPHTHALOYL CHLORIDE	755.4	38.2	6.3093	3.1343	265.5	6.3058	3.1673	264.9	7.917
TERPINOLENE	667	28.2	3.7611	3.8868	285.9	3.8903	4.0764	275.7	44.939
tert-BUTYL ACETATE	545	31.7	3.7241	3.5895	231.6	3.6013	3.7729	232.2	23.023
tert-BUTYL CHLORIDE	507	39	2.3665	3.9070	262.6	2.4493	3.9463	255.3	10.080
tert-BUTYL ETHYL ETHER	509.4	29.34	3.3294	3.7479	227.8	3.4177	3.8592	221.7	22.932
tert-BUTYL FORMATE	537	35.8	3.1487	3.6527	245.7	3.2467	3.7453	238.7	17.007
tert-BUTYL MERCAPTAN	530	40.6	2.4986	3.8852	265.5	2.4489	3.9520	266.9	4.155
tert-BUTYL METHACRYLATE	588.3	27.27	4.0986	3.7377	241.1	4.0617	3.8890	239.2	27.027
tert-BUTYLAMINE	483.9	38.4	3.1177	3.4684	221.1	3.0941	3.5962	219.5	15.705
tert-BUTYLBENZENE	660	29.7	3.1247	4.1119	303.1	3.0362	4.3744	301.8	35.439

Name	T_c (K)	P_c (bar)	PC-SAFT parameter values			I-PC-SAFT parameter values			
			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
tert-BUTYLCYCLOHEXANE	652	26.6	3.2116	4.2207	296.9	3.2837	4.3932	288.4	36.938
tert-BUTYLFORMAMIDE	692	35.6	4.0258	3.4145	294.5	4.4721	3.6193	271.6	45.560
tert-DODECYL MERCAPTAN	691	18.6	5.5348	3.8918	257.6	5.7808	4.0521	248.9	65.048
tert-NONYL MERCAPTAN	659	23.4	4.2353	3.8809	271.6	4.4910	4.0887	258.3	63.891
tert-OCTYL MERCAPTAN	627	25.9	3.1151	4.2436	290.1	3.2910	4.3716	277.1	40.317
TETRACHLOROETHYLENE	620	44.9	2.6554	3.7445	305.6	2.6209	3.9326	302.6	20.957
TETRACHLOROSILANE	507	35.9	2.7147	3.7772	247.0	2.7598	3.8909	241.8	17.499
TETRADECAMETHYLHEXASILOXANE	653.2	8.04	6.9669	4.6381	225.4	7.1804	4.8007	220.7	112.917
TETRADECANEDIOIC ACID	849	19	10.3287	3.2312	264.2	10.5906	3.3017	260.4	41.788
TETRAETHYL LEAD	655	21.25	4.2421	3.9889	271.7	4.7308	4.1285	252.0	71.530
TETRAETHYL SILANE	606	24	3.9347	4.0014	253.0	4.0815	4.0909	246.0	31.691
TETRAETHYLENE GLYCOL	795	25.9	7.9872	3.1051	266.5	8.3864	3.2412	257.8	56.398
TETRAETHYLENE GLYCOL DIMETHYL ETHER	705	19.4	8.8170	3.2515	227.0	8.8021	3.3553	225.8	29.497
TETRAETHYLENE GLYCOL MONOETHYL ETHER	732	23.6	8.3929	3.2451	236.7	8.2742	3.2721	238.1	5.563
TETRAETHYLENE GLYCOL MONOMETHYL ETHER	720	26.01	9.0734	3.0557	227.4	8.8588	3.0554	230.3	-4.943
TETRAETHYLENEPENTAMINE	774	25.3	11.3419	2.8275	233.0	11.2168	2.8323	234.5	1.451
TETRAFLUROETHYLENE	306.45	39.44	2.6029	3.1363	152.7	2.7190	3.2051	147.1	10.034
TETRAFLUROHYDRAZINE	309.35	37.1	2.4253	3.3603	157.9	2.6948	3.2917	149.1	7.037
TETRAHYDROFURAN	540.15	51.9	2.5012	3.4996	275.3	2.7103	3.5370	259.7	14.598
TETRAHYDROFURFURYL ALCOHOL	639	46.6	5.4545	2.8725	242.2	6.5682	2.7556	221.4	16.881
TETRAHYDROPYRAN	572.04	47.71	2.5583	3.6929	285.8	2.6398	3.7423	278.3	11.496
TETRAHYDROTHIOPHENE	631.95	51.6	2.3452	3.7337	333.2	2.5115	3.8351	314.5	22.186
TETRAMETHYLETHYLENEDIAMINE	569	28.2	3.8752	3.7083	239.8	4.0118	3.8213	232.5	29.154

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TETRAMETHYLSILANE	450.4	28.14	2.7007	3.9468	219.7	2.6998	4.0883	216.9	19.026
TETRANITROMETHANE	540	26.8	5.9177	2.9658	201.3	6.5752	3.1314	187.1	43.382
TETRAPHENYLETHYLENE	996	17.1	5.9808	4.0193	373.8	6.7708	4.4054	342.1	124.395
TETRAPHENYLMETHANE	983	17.9	5.7232	4.0337	373.1	6.3591	4.4362	343.9	119.295
TETRYL	828	26.1	11.7745	2.8271	246.8	11.5942	2.8220	249.1	-5.316
THIACYCLOPROPANE	547	67.8	1.9945	3.4215	313.1	2.2161	3.4843	288.8	14.896
THIAINDAN	759.8	37.07	2.9943	3.8975	366.9	3.5472	4.0231	325.7	49.631
THIOGLYCOLIC ACID	733	61	4.8797	2.7312	288.8	5.3701	2.8667	270.3	27.185
THIONYL CHLORIDE	567	44.3	1.6008	3.9843	374.3	1.7116	4.4388	340.2	32.165
THIOPHENE	579.35	56.9	2.3329	3.5780	304.2	2.4917	3.6161	289.4	11.960
THIOUREA	854	82.3	3.8641	3.0979	353.4	3.7512	3.1402	358.0	1.376
THYMOL	698.25	34.08	6.5357	3.1411	243.4	6.7217	3.1195	240.3	6.522
TIN(IV) CHLORIDE	591.85	37.44	2.8470	3.8203	284.3	2.9888	3.9271	272.5	23.770
TITANIUM TETRACHLORIDE	638	46.61	2.7456	3.8152	309.3	3.1634	3.6672	286.7	7.204
TOLUENE	591.75	41.08	2.7745	3.7292	288.4	3.0098	3.7977	271.6	23.255
trans,trans-2,4-HEXADIENE	535	33.5	2.8625	3.7510	259.2	3.1507	3.8662	240.8	34.203
trans-1,2-DICHLOROETHYLENE	516.5	55.1	2.2545	3.5496	277.2	2.6952	3.4225	248.9	9.084
trans-1,2-DIMETHYLCYCLOHEXANE	596.15	29.38	2.6680	4.1947	296.2	2.8070	4.3641	282.1	39.088
trans-1,2-DIMETHYLCYCLOPENTANE	553.15	34.45	2.8825	3.9100	262.2	3.0547	3.9167	252.3	12.772
trans-1,3,3,3-TETRAFLUOROPROPENE	382.51	36.62	3.3534	3.1478	171.0	3.4768	3.2374	165.3	14.926
trans-1,3-DICHLOROPROPENE	606.5	47.04	2.6442	3.6160	302.2	2.6950	3.8063	292.3	24.610
trans-1,3-DIMETHYLCYCLOHEXANE	598	29.38	2.7217	4.1575	294.1	2.7729	4.3875	284.5	39.389
trans-1,3-DIMETHYLCYCLOPENTANE	553	34.45	2.8887	3.9109	261.7	3.0560	3.9158	252.2	12.853

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			m	σ (Å)	ϵ/k_B (K)	m	σ (Å)	ϵ/k_B (K)	C (cm ³ mol ⁻¹)
trans-1,3-HEXADIENE	521.1	33.54	2.8668	3.7498	251.2	3.1209	3.8442	235.5	28.838
trans-1,3-PENTADIENE	500	37.4	2.1539	3.9181	272.3	1.8753	4.3653	286.5	24.648
trans-1,4-DIETHYLCYCLOHEXANE	649.9	28.17	3.9570	3.9181	269.1	3.9573	4.0166	266.9	21.497
trans-1,4-DIMETHYLCYCLOHEXANE	587.7	29.4	2.7807	4.1523	285.7	2.9383	4.2726	272.6	32.330
trans-1,8-TERPIN	702.7	29.49	10.2852	2.8261	213.6	9.8293	2.7719	219.2	-28.337
trans-1-PROPENYLBENZENE	670	33.6	3.3435	3.8064	303.3	3.5991	3.9649	285.5	41.752
trans-2,2,4,6,6-PENTAMETHYL-3-HEPTENE	637.8	19.64	3.4184	4.3838	288.0	3.7776	4.5812	266.7	78.046
trans-2,n-HEXYL-DECAHYDRONAPHTHALENE	777.2	18.14	4.0348	4.3558	333.3	4.6151	4.6526	301.7	99.873
trans-2-BUTENE	428.6	41	2.3854	3.5867	223.0	2.6504	3.5701	208.1	12.318
trans-2-DECENE	619	21.8	4.5013	3.8383	248.6	4.7370	4.0149	238.1	56.932
trans-2-DODECENE	663	18.9	5.1899	3.8786	253.4	5.4477	4.0732	243.3	71.083
trans-2-HEPTENE	543.1	28.5	3.3146	3.8116	245.6	3.5781	3.9140	232.0	34.834
trans-2-HEXENE	509.8	31.68	2.9902	3.7628	240.3	3.2017	3.8536	227.9	26.985
trans-2-METHYL-1,3-PENTADIENE	530.3	33.8	2.7032	3.8157	262.7	2.8831	3.9679	248.0	31.762
trans-2-METHYLCYCLOHEXANOL	617	37.9	6.1267	2.9598	219.9	6.3562	2.9585	215.9	9.991
trans-2-NONENE	597.1	23.7	4.1037	3.8332	247.8	4.3221	3.9988	237.3	49.669
trans-2-OCTENE	571.6	25.89	3.5841	3.8712	251.2	3.9528	3.9599	234.8	42.434
trans-2-PENTADECENE	701.6	15.67	6.1281	3.9350	254.0	6.4425	4.1216	244.5	84.352
trans-2-PENTENE	474.2	36.6	2.7123	3.6757	232.0	2.8884	3.7202	221.6	16.051
trans-2-PHENYLBUTENE-2	654	30.1	3.5540	3.8624	287.5	3.7705	4.0097	273.6	41.609
trans-3,5-DIMETHOXYSTILBENE	885	21.6	6.6403	3.6465	314.7	7.1184	3.8348	299.7	85.085
trans-3-HEPTENE	540	28.5	3.2660	3.8369	245.8	3.5578	3.9148	231.2	33.044
trans-3-HEXENE	509	31.7	3.0608	3.7317	236.6	3.1761	3.8620	228.3	25.156

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trans-3-METHYLCYCLOHEXANOL	627	37.9	6.3916	2.9169	219.9	6.3689	2.9719	219.2	12.289
trans-3-OCTENE	574	25.8	3.3207	3.9883	260.4	3.6349	4.0972	243.7	43.404
trans-4-METHYLCYCLOHEXANOL	622	37.9	6.5933	2.9009	215.2	6.4813	2.9422	216.4	6.357
trans-4-OCTENE	573	25.8	3.2799	4.0066	261.4	3.5992	4.1099	244.2	42.970
trans-CROTONIC ACID	666	47	5.3221	2.8286	252.2	5.4601	3.0082	244.2	28.396
trans-CROTONITRILE	586	38.8	3.1198	3.3354	283.8	4.0611	3.4534	238.3	35.941
trans-DECAHYDRONAPHTHALENE	687	32	3.0751	4.1646	318.0	3.2850	4.2028	303.9	25.148
trans-STILBENE	820	27.4	4.7343	3.7740	323.1	4.7812	4.0709	314.4	69.313
TRIALLYLAMINE	592	24.6	4.6500	3.6639	233.5	4.8721	3.7574	225.5	34.215
TRIAMYLAMINE	660	15	7.7430	3.6622	220.1	7.8271	3.7680	217.8	46.379
TRIBROMOMETHANE	696	60.9	2.2704	3.8089	365.6	2.1790	3.9359	370.5	5.860
TRICAPRIN	876.6	4.55	11.4073	4.2772	278.2	12.6886	4.9310	258.8	326.893
TRICAPRYLIN	850.7	5.93	9.9396	4.1977	278.2	11.0440	4.7750	258.6	258.378
TRICHLOROACETALDEHYDE	565	44.1	3.4350	3.3453	249.6	3.5442	3.4409	242.3	17.669
TRICHLOROACETIC ACID	688	48.1	5.3452	2.9327	256.5	5.2819	3.0586	255.0	17.167
TRICHLOROACETYL CHLORIDE	604	43.2	2.8959	3.7472	286.0	3.1529	3.6977	271.8	8.804
TRICHLOROETHYLENE	571	49.1	2.6056	3.5830	283.6	2.6429	3.7029	277.6	14.852
TRICHLOROFLUOROMETHANE	471.2	44.08	2.2779	3.6942	249.3	2.4333	3.7056	238.0	10.084
TRICHLOROSILANE	479	41.7	2.5033	3.6862	240.8	2.5386	3.7400	237.2	8.949
TRIDECAFLUOROHEPTANOIC ACID	583	20.75	9.0689	3.0329	184.1	8.7239	3.0919	187.2	4.094
TRIDECANAL	720	22.38	6.7828	3.5421	248.9	6.9122	3.5828	245.9	20.517
TRIETHYL ALUMINUM	678.15	89.3	8.6913	2.6052	202.1	7.7339	2.1090	224.5	-99.024
TRIETHYL ESTER PHOSPHOROUS ACID	664.4	53.77	4.3486	3.6510	246.1	3.5322	3.4039	285.3	-76.180

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TRIETHYL GALLIUM	581.2	25	4.3979	3.5515	238.0	4.8479	3.7218	221.8	53.702
TRIETHYL ORTHOFORMATE	585	26.76	5.1595	3.4789	220.3	5.2468	3.5326	217.3	16.078
TRIETHYLAMINE	535.15	30.4	3.2733	3.8020	241.0	3.4174	3.8772	232.9	22.290
TRIETHYLENE GLYCOL BIS(2-ETHYLHEXANOATE)	820.7	10.94	9.0915	3.9911	264.6	9.4333	4.1400	258.5	116.984
TRIETHYLENE GLYCOL DIMETHYL ETHER	651	23.1	7.3028	3.2453	220.4	7.3047	3.3475	218.9	19.140
TRIETHYLENEDIAMINE	655	39.1	4.4795	3.3693	259.0	4.5616	3.4177	255.3	12.008
TRIETHYLENETETRAMINE	718	31.7	8.9186	2.8182	229.5	8.8744	2.8555	229.5	9.330
TRIFLUOROACETIC ACID	491.25	32.58	3.9899	2.9201	217.5	5.0762	3.1630	184.5	34.517
TRIFLUOROIODOMETHANE	396.44	39.53	2.1376	3.6793	216.9	2.3332	3.6807	204.2	10.346
TRIFLUOROMETHANE	299.01	48.16	2.6701	2.8205	149.4	3.0109	2.8683	137.2	12.439
TRIFLUOROMETHYL TRIFLUOROVINYL ETHER	363	31.1	3.8922	3.2849	148.3	3.6811	3.2890	153.3	-6.146
TRISOBUTYL ALUMINUM	690.1	17.59	3.8436	4.5319	296.3	4.3227	4.6347	274.2	81.377
TRIMETHYL BORATE	501.7	35.87	3.8275	3.3040	213.4	4.2085	3.3204	201.3	21.562
TRIMETHYL SILANE	432	31.9	2.2060	4.0149	232.6	2.3242	4.0737	223.0	15.029
TRIMETHYL SILANOL	526.5	38.09	6.5983	2.7360	180.5	5.9821	2.8735	187.6	4.927
TRIMETHYLALUMINUM	620	40	2.6933	3.6536	310.5	2.6529	4.0697	300.9	38.424
TRIMETHYLAMINE	433.25	40.7	2.3199	3.6358	228.6	2.5630	3.6342	213.6	13.159
TRIMETHYLCHLOROSILANE	497.75	32	2.8977	3.8153	236.3	3.0574	3.8743	226.9	17.352
TRIMETHYLENE SULFIDE	602	58.6	2.1138	3.6106	335.6	2.3091	3.7236	311.7	22.045
TRIMETHYLGALLIUM	510	40.4	3.0600	3.4197	234.4	2.5744	3.8408	251.0	24.524
TRIMETHYLOLPROPANE	708.6	39.09	14.8920	2.1658	201.6	14.5306	2.0969	203.8	-17.476
TRI-n-BUTYL BORATE	743.15	19.89	2.3814	5.5323	383.4	2.4283	5.6277	375.7	11.097
TRI-n-BUTYL PHOSPHATE	716.7	15.23	7.6266	3.6830	242.5	7.9459	3.8279	235.6	70.185

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TRI-n-BUTYLAMINE	644	18	6.3185	3.6890	228.9	6.4839	3.8144	224.0	51.890
TRI-n-OCTYLAMINE	782	10.1	8.4311	4.1942	257.0	8.8335	4.3105	250.3	91.440
TRIOXANE	604	58.2	3.3399	3.1036	272.1	3.5551	3.2039	258.7	18.900
TRIPHENYLENE	990.8	28.7	5.8504	3.6506	365.8	6.3084	3.8131	347.4	73.012
TRIPHENYLETHYLENE	908	21	5.3179	4.0556	346.5	5.6990	4.2875	328.5	96.514
TRIPHENYLMETHANE	865	22	5.2309	3.9966	330.1	5.4822	4.2203	316.8	86.033
TRIPROPYLAMINE	577.5	22.3	6.5521	3.3223	201.3	6.5270	3.4152	200.5	27.437
TRIPROPYLENE GLYCOL MONOETHYL ETHER	664	20.2	11.0374	2.9975	199.3	10.5358	2.9878	203.9	-15.588
TRIPROPYLENE GLYCOL MONOMETHYL ETHER	657	21.8	10.5959	2.9565	199.5	10.2173	2.9444	203.2	-11.579
TRIS(2-METHOXYETHOXY)VINYLSILANE	723.9	17.79	6.5544	3.8512	253.2	6.6575	3.9372	249.9	42.817
TRISILANE	495.9	36.67	3.0038	3.7529	227.8	3.1403	3.6622	223.5	-1.894
UNDECANAL	690	23.93	5.9952	3.5906	247.0	5.9913	3.6692	245.8	21.588
UNDECYL MERCAPTAN	710	19.8	5.4189	3.8468	269.5	6.0210	3.9377	252.5	72.204
UNDECYLAMINE	682	20.2	5.8138	3.6960	253.1	6.5674	3.7212	236.3	57.500
VALERONITRILE	610.3	35.8	3.3773	3.5032	281.0	4.1347	3.5711	246.5	40.461
VANADIUM OXYTRICHLORIDE	636	37.4	1.7859	4.3871	390.7	1.9843	4.6395	354.4	42.581
VANADIUM TETRACHLORIDE	697	60.3	2.3741	3.9294	352.5	2.4061	3.8182	353.9	-8.784
VANILLIC ACID	825.1	37.98	7.7126	2.8845	276.2	7.8069	2.9815	272.5	24.445
VANILLIN	777	40.1	6.9872	2.9309	266.4	7.0143	3.0067	264.2	16.994
VINYL ACETATE	519.13	39.58	3.4249	3.2650	233.0	3.6937	3.4150	219.0	30.684
VINYL CHLORIDE	432	56.7	1.9504	3.4768	244.5	1.7536	3.7030	256.0	6.971
VINYL FLUORIDE	327.8	52.4	2.1489	3.1557	177.7	2.0780	3.2724	178.6	6.248
VINYL FORMATE	498	50.2	3.1998	3.0971	227.3	3.1724	3.2907	223.5	18.080

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VINYL PIVALATE	556	29.5	3.9465	3.6425	231.3	4.0106	3.7358	227.2	20.934
VINYL PROPIONATE	546	36.8	3.7450	3.3616	234.1	3.9220	3.4788	225.0	24.971
VINYLCETONITRILE	584	38.8	3.3905	3.2148	270.4	3.9063	3.5008	241.0	36.014
VINYLCACETYLENE	454	48.6	2.1498	3.5150	246.2	1.8047	3.9246	265.2	14.051
VINYLCYCLOHEXANE	599.4	32.7	3.1376	3.8928	275.0	3.2139	4.0190	267.6	26.182
VINYLETHYLENE CARBONATE	759.1	48	4.4270	3.1341	308.2	4.6674	3.3227	293.5	36.790
VINYLNORBORNENE	626	32.1	2.7622	4.1268	304.9	2.8909	4.2621	292.4	20.191
VINYLTRICHLOROSILANE	543.15	30.6	2.8611	3.8853	263.2	3.1463	4.0069	244.6	38.665
VINYLTRIMETHOXYSILANE	553.7	26.85	4.9022	3.4295	214.7	5.3010	3.4502	205.0	25.570
WATER	647.1	220.64	3.2786	1.9589	298.2	3.6429	2.0835	274.4	7.080
XENON	289.74	58.4	0.9337	4.0364	235.9	0.9525	4.0333	232.1	1.217

Appendix A7 – Compound-by-compound results for the 2 investigated SAFT-type EoS described in Chapters 2 and 3.

Table S3. Compound-by-compound analysis of the performance of the PC-SAFT EoS for 1 800 compounds.

PC-SAFT EoS

Average MAPE (%) on:						
p^{sat}	ρ_{liq}^{sat}	$\Delta_{vap}H$	$C_{P,liq}^{sat}$	v_c	T_c	P_c
1.18	0.95	3.25	4.17	4.38	2.28	20.8
Global average deviation: 2.2%						

Name	MAPE on p^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on v_c	MAPE on T_c	MAPE on P_c
(3,3,3-TRIFLUOROPROPYL)METHYLDICHLOROSILANE	0.72%	0.19%	1.12%		1.66%	15.23%	26.34%
(3-GLYCIDOXYPROPYL)METHYLDIETHOXSILANE	0.87%	0.55%	1.95%		2.25%	26.36%	40.09%
(3-METHYLACRYLOXYPROPYL)TRICHLOROSILANE	1.34%	0.49%	1.86%		1.99%	22.24%	39.87%
[3-(2,3-EPOXYPROXY)PROPYL]TRIMETHOXSILANE	1.18%	0.81%	2.31%	2.65%	2.47%	29.01%	46.56%
[3-(MERCAPTO)PROPYL]TRIETHOXSILANE	0.33%	1.36%			0.54%	5.08%	30.88%
1-(4-ETHYLPHENYL)-2-(4-ETHYLPHENYL)ETHANE	0.62%	1.29%	1.56%		3.53%	36.25%	41.30%
1-(4-ETHYLPHENYL)-2-PHENYLETHANE	0.90%	1.14%	2.93%	4.74%	3.32%	34.46%	39.87%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
1,1,1,2,2,3,4,5,5,5-DECAFLUOROPENTANE	2.18%	0.39%	4.23%		0.80%	14.71%	27.95%
1,1,1,2,2-PENTAFLUOROPROPANE	0.52%	0.34%	2.64%		2.03%	16.24%	22.91%
1,1,1,2,3,3,3-HEPTAFLUOROPROPANE	0.68%	0.16%	2.03%		1.72%	15.45%	30.22%
1,1,1,2,3,3-HEXAFLUOROPROPANE	0.51%	0.17%	1.65%		1.76%	15.10%	24.08%
1,1,1,2-TETRACHLORODIFLUOROETHANE	1.27%	0.31%	3.25%		2.36%	19.11%	30.50%
1,1,1,2-TETRACHLOROETHANE	1.26%	1.23%	3.79%	9.39%	3.05%	21.73%	32.37%
1,1,1,2-TETRAFLUROETHANE	0.07%	0.46%	3.17%	0.73%	2.65%	20.94%	28.61%
1,1,1,3,3,3-HEXAFLUOROPROPANE	1.05%	0.32%	0.83%		1.51%	14.40%	28.84%
1,1,1,3,3-PENTACHLOROPROPANE	1.58%	0.70%	3.39%		2.47%	23.19%	29.69%
1,1,1,3,3-PENTAFLUROBUTANE	3.03%	0.74%			0.10%	10.28%	24.85%
1,1,1,3,3-PENTAFLUROPROPANE	1.75%	0.27%	2.19%		1.48%	15.80%	25.59%
1,1,1-TRICHLOROETHANE	0.26%	0.51%	1.69%	4.54%	2.02%	13.57%	25.01%
1,1,1-TRICHLOROFLUROETHANE	0.43%	1.47%	4.63%		4.04%	31.28%	33.49%
1,1,1-TRICHLOROTRIFLUOROETHANE	2.45%	0.47%	3.71%	0.45%	2.56%	14.95%	25.61%
1,1,1-TRIFLUOROETHANE	0.43%	1.04%	3.58%	1.26%	3.42%	24.40%	30.60%
1,1,2,2,3-PENTAFLUROPROPANE	0.37%	0.12%	1.10%		1.73%	14.46%	23.45%
1,1,2,2-TETRACHLORODIFLUOROETHANE	0.29%	0.13%	3.01%		2.59%	19.80%	30.26%
1,1,2,2-TETRACHLOROETHANE	2.61%	0.83%			2.17%	26.02%	34.48%
1,1,2,2-TETRAFLUROETHANE	3.74%	1.17%	1.77%	3.12%	1.94%	13.00%	22.52%
1,1,2,2-TETRAPHENYLETHANE	1.16%	0.11%	1.66%	1.29%	1.56%	18.53%	34.29%
1,1,2-TRICHLOROETHANE	0.73%	1.71%	4.05%	9.32%	3.08%	24.58%	32.53%
1,1,2-TRICHLOROTRIFLUOROETHANE	0.66%	0.09%	1.75%	2.41%	1.48%	12.05%	21.85%
1,1,2-TRIFLUOROETHANE	1.06%	0.19%	2.97%	6.94%	1.92%	18.12%	26.97%
1,1,2-TRIMETHYLCYCLOPENTANE	0.73%	0.34%	2.01%		2.54%	19.38%	31.08%
1,1,2-TRIPHENYLETHANE	0.88%	1.17%	2.83%	2.12%	3.33%	35.28%	41.24%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
1,1,3-TRIMETHYLCYCLOHEXANE	0.52%	0.25%	1.10%		1.33%	8.39%	21.30%
1,1,3-TRIMETHYLCYCLOPENTANE	1.75%	0.87%	3.70%		1.95%	18.29%	33.91%
1,1,5-TRIMETHYLINDAN	0.13%	0.57%	2.29%		2.81%	22.46%	31.06%
1,1-DIBROMOETHANE	4.37%	0.77%	4.57%	2.75%	2.30%	4.67%	4.58%
1,1-DICHLORO-1-FLUOROETHANE	0.19%	0.27%	1.54%	2.21%	1.51%	10.14%	20.86%
1,1-DICHLOROETHANE	0.30%	0.30%	2.52%	1.94%	1.23%	10.69%	19.12%
1,1-DICHLOROETHYLENE	5.87%	1.92%	6.35%	6.99%	1.60%	6.80%	14.91%
1,1-DICHLOROPROPANE	0.35%	1.18%	3.02%	5.07%	2.48%	18.91%	25.79%
1,1-DICHLOROTETRAFLUOROETHANE	0.20%	0.09%	0.82%	4.70%	1.46%	10.28%	19.56%
1,1-DIETHYLCYCLOHEXANE	0.94%	0.63%	3.29%	6.44%	2.29%	21.44%	29.85%
1,1-DIFLUOROETHANE	0.40%	1.09%	5.15%	1.90%	3.68%	27.02%	32.38%
1,1-DIFLUOROETHYLENE	2.58%	1.12%		2.05%	1.84%	13.36%	22.18%
1,1-DIMETHOXYETHANE	0.24%	0.42%	2.88%	6.64%	2.16%	15.97%	25.59%
1,1-DIMETHYLCYCLOHEXANE	0.83%	0.90%	4.36%	2.41%	2.60%	21.62%	23.90%
1,1-DIMETHYLCYCLOPENTANE	0.84%	0.28%	2.58%	2.02%	1.45%	8.41%	22.24%
1,1-DIPHENYLETHANE	0.70%	1.06%	4.17%		2.48%	23.13%	32.69%
1,2,3,4-TETRAHYDRONAPHTHALENE	0.04%	0.33%	5.80%	0.79%	2.54%	19.40%	34.00%
1,2,3,4-TETRAMETHYLBENZENE	0.94%	0.85%	1.32%	5.33%	3.30%	22.98%	30.01%
1,2,3,4-TETRAMETHYLCYCLOHEXANE	0.83%	0.49%	2.78%	2.98%	2.38%	21.57%	31.12%
1,2,3,5-TETRAETHYLBENZENE	1.83%	0.33%	3.81%	7.66%	2.01%	22.12%	34.84%
1,2,3,5-TETRAMETHYLBENZENE	0.31%	0.76%	1.92%	4.47%	2.98%	24.13%	31.45%
1,2,3,6-TETRAHYDROBENZALDEHYDE	0.49%	0.60%	2.24%	4.36%	2.12%	17.97%	30.57%
1,2,3,6-TETRAHYDROBENZYL ALCOHOL	0.94%	0.67%	1.37%		3.02%	21.12%	29.45%
1,2,3-TRICHLOROBENZENE	0.95%	0.38%	3.71%	5.60%	0.45%	3.86%	14.19%
1,2,3-TRICHLOROPROPANE	0.73%	0.52%	4.47%	6.72%	4.20%	35.87%	39.80%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
1,2,3-TRIETHYLBENZENE	0.92%	0.65%	3.08%	5.82%	2.62%	25.81%	34.12%
1,2,3-TRIMETHYL-4-ETHYLBENZENE	0.68%	0.51%	1.31%		2.42%	22.55%	31.22%
1,2,3-TRIMETHYLBENZENE	0.33%	0.52%	2.56%	5.10%	2.51%	20.51%	28.79%
1,2,3-TRIMETHYLINDENE	0.82%	1.28%	5.87%	11.51%	3.52%	33.93%	37.31%
1,2,4,5-TETRAISOPROPYLBENZENE	1.45%	0.24%	2.44%		1.65%	19.87%	37.19%
1,2,4,5-TETRAMETHYLBENZENE	0.28%	0.25%	3.26%	5.99%	2.97%	26.90%	34.03%
1,2,4-TRICHLOROBENZENE	0.93%	0.98%	3.65%	1.37%	3.02%	27.01%	36.74%
1,2,4-TRIETHYLBENZENE	0.26%	0.70%	1.91%	4.46%	2.77%	24.29%	32.75%
1,2,4-TRIMETHYL-3-ETHYLBENZENE	1.18%	0.66%			2.92%	22.02%	30.21%
1,2,4-TRIMETHYL-5-ETHYLBENZENE	0.13%	0.65%	1.56%		2.71%	23.80%	31.72%
1,2,4-TRIMETHYLBENZENE	0.27%	0.47%	3.01%	3.49%	2.86%	22.77%	29.44%
1,2-BENZENE DICARBOXYLIC ACID, HEPTYL, UNDECYL ESTER	0.86%	1.56%	3.04%		2.04%	25.37%	66.00%
1,2-BENZENEDICARBOXYLIC ACID, HEPTYL, NONYL ESTER	1.07%	1.65%	3.79%		1.31%	17.87%	58.21%
1,2-BENZENEDIOL	4.22%	1.27%	11.17%		0.78%	15.16%	5.77%
1,2-BUTADIENE	1.09%	1.35%	6.39%	4.66%	2.36%	21.10%	30.60%
1,2-BUTANEDIOL	2.68%	1.66%	1.96%		0.62%	11.65%	19.38%
1,2-DIBROMOETHANE	0.83%	0.60%	5.00%	3.07%	2.19%	16.66%	25.76%
1,2-DIBROMOPROPANE	0.27%	0.43%	1.73%		1.70%	12.56%	19.85%
1,2-DIBROMOTETRAFLUOROETHANE	0.63%	0.34%	3.12%		1.67%	12.33%	16.85%
1,2-DICHLORO-1,1,2-TRIFLUOROETHANE	0.05%	0.75%	2.75%	5.89%	2.51%	18.43%	27.47%
1,2-DICHLORO-4-NITROBENZENE	0.74%	0.63%	2.34%		2.92%	29.03%	33.84%
1,2-DICHLOROBUTANE	0.11%	0.48%	3.40%		3.28%	25.72%	31.74%
1,2-DICHLOROETHANE	2.22%	0.91%	1.96%	0.99%	2.38%	16.05%	31.75%
1,2-DICHLOROHEXAFLUOROCYCLOBUTANE	0.26%	1.24%	4.22%		3.44%	25.90%	30.71%
1,2-DICHLOROPROPANE	0.24%	0.77%	3.41%	4.56%	2.80%	21.44%	28.48%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
1,2-DICHLOROTETRAFLUROETHANE	0.40%	0.11%	1.09%	3.83%	1.62%	11.41%	21.12%
1,2-DIETHOXYETHANE	0.53%	1.31%	3.22%	11.19%	2.05%	17.73%	32.00%
1,2-DIFLUOROBENZENE	0.32%	0.66%	1.02%		2.59%	17.94%	25.82%
1,2-DIFLUOROETHANE	0.73%	3.20%	6.92%	9.43%	7.26%	54.84%	45.73%
1,2-DIMETHOXYETHANE	0.86%	0.37%	2.58%		1.97%	18.54%	41.85%
1,2-DIMETHOXYPROPANE	0.59%	0.13%	1.17%		1.65%	14.16%	24.77%
1,2-DIMETHYL-3-PROPYLBENZENE	0.14%	1.35%	1.99%		2.37%	20.44%	19.40%
1,2-DIPHENYLETHANE	0.72%	0.95%	1.20%		3.29%	26.31%	32.65%
1,2-EPOXY-2-METHYLPROPANE	0.26%	0.25%	3.36%	1.90%	2.17%	14.62%	28.04%
1,2-EPOXY-3-PHENOXYPROPANE	0.40%	1.39%	3.31%		4.15%	40.56%	45.78%
1,2-EPOXYBUTANE	0.71%	0.96%	4.54%	4.02%	3.08%	24.50%	28.71%
1,2-ETHANEDITHIOL	0.58%	1.09%	3.68%		3.06%	23.93%	64.03%
1,2-HEXADIENE	0.62%	0.77%	3.81%	2.12%	3.01%	24.03%	31.47%
1,2-PENTADIENE	2.68%	0.66%	7.97%	1.75%	2.18%	23.51%	32.13%
1,2-PROPANEDIAMINE	0.50%	0.44%	1.71%		0.50%	6.43%	2.31%
1,2-PROPYLENE GLYCOL	1.62%	1.80%	2.54%		1.84%	22.38%	27.75%
1,2-PROPYLENE OXIDE	0.83%	1.04%	3.47%	2.62%	4.70%	32.86%	46.05%
1,3,5,7-CYCLOOCTATETRAENE	0.33%	0.93%	2.02%	1.08%	1.02%	6.70%	22.61%
1,3,5-TRICHLOROBENZENE	0.92%	1.03%	6.13%	8.13%	2.73%	23.95%	25.86%
1,3,5-TRIETHYLBENZENE	0.39%	0.50%	1.92%	4.62%	2.76%	25.84%	37.77%
1,3,5-TRIISOPROPYLBENZENE	1.53%	0.40%	2.24%		1.61%	17.46%	33.97%
1,3,5-TRI-tert-BUTYLBENZENE	2.27%	0.65%			2.36%	26.51%	34.37%
1,3-BENZENEDIOL	1.22%	2.47%	6.44%	4.33%	1.35%	9.87%	0.09%
1,3-BUTADIENE	0.36%	0.50%	1.90%	1.97%	2.21%	13.30%	23.37%
1,3-CYCLOHEXADIENE	0.48%	1.26%	1.00%	3.11%	1.51%	8.90%	18.03%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
1,3-DIBROMOPROPANE	0.30%	0.96%	1.58%		2.70%	19.54%	23.73%
1,3-DICHLOROHEXAFLUOROPROPANE	0.54%	0.71%	2.73%		2.43%	19.87%	31.22%
1,3-DICHLOROPROPANE	1.29%	1.05%	3.57%	4.57%	4.17%	32.35%	38.38%
1,3-DIFLUOROBENZENE	0.42%	0.53%	0.96%		2.15%	13.61%	21.08%
1,3-DIMETHYL UREA	0.78%	0.96%	1.69%		2.96%	31.38%	38.68%
1,3-DIMETHYL-2-IMIDAZOLIDINONE	0.28%	1.28%	3.05%		3.67%	30.77%	34.30%
1,3-DIMETHYL-5-NITROBENZENE	0.89%	2.03%	3.43%		4.68%	46.59%	44.82%
1,3-DIMETHYLADAMANTANE	0.14%	0.51%	1.99%	0.74%	1.00%	7.07%	14.75%
1,3-DIOXANE	0.59%	1.11%	1.96%	2.94%	1.88%	15.26%	32.85%
1,3-DIPHENYLTRIAZENE	0.99%	0.33%	1.41%		1.18%	13.23%	28.90%
1,3-DI-TERT-BUTYL GLYCERIN	1.02%	1.28%	3.87%		0.03%	2.25%	22.58%
1,3-PROPANEDIAMINE	1.25%	1.95%	0.84%		0.80%	9.43%	0.84%
1,3-PROPYLENE GLYCOL	2.25%	2.75%	1.88%		1.62%	19.52%	27.15%
1,3-PROPYLENE OXIDE	0.25%	1.51%	4.32%	6.74%	3.90%	28.00%	33.32%
1,4-BENZENEDICARBOXYLIC ACID, 2-HYDROXYETHYL METHYL ESTER	1.20%	0.75%	3.27%		0.67%	8.93%	30.02%
1,4-BIS(3-AMINOPROPYL)PIPERAZINE	0.41%	0.42%	4.01%	2.02%	1.10%	12.52%	23.34%
1,4-BUTANEDISOCYANATE	0.28%	2.67%	4.95%	2.57%	6.30%	57.81%	48.40%
1,4-BUTANEDIOL	3.94%	2.87%	2.57%		0.63%	14.07%	25.31%
1,4-CYCLOHEXANEDICARBOXYLIC ACID	1.09%	0.80%	8.04%		0.47%	7.27%	32.49%
1,4-CYCLOHEXANEDIMETHANOL	3.25%	0.90%			0.30%	8.77%	26.02%
1,4-DIBROMOBENZENE	3.35%	0.79%			1.75%	8.59%	23.30%
1,4-DICHLOROBUTANE	0.91%	0.85%	5.09%	5.24%	4.12%	35.72%	43.47%
1,4-DICHLORO-cis-2-BUTENE	0.73%	1.66%	4.66%	2.37%	4.20%	36.51%	36.81%
1,4-DICHLORO-trans-2-BUTENE	0.64%	1.70%	4.46%	2.51%	4.31%	36.65%	36.89%
1,4-DICYANO-2-BUTENE	0.50%	3.36%	5.37%		7.03%	81.66%	66.50%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
1,4-DIFLUOROBENZENE	0.55%	0.98%	0.97%		2.22%	13.87%	16.97%
1,4-DIOXANE	0.63%	0.34%	1.54%	10.79%	1.88%	14.90%	31.25%
1,4-DI-tert-BUTYLBENZENE	0.86%	0.16%	1.08%	0.46%	1.47%	10.26%	16.55%
1,4-HEXADIENE	0.26%	0.73%	1.98%	6.43%	2.72%	18.74%	27.47%
1,4-PENTADIENE	4.15%	3.45%	10.95%	14.45%	1.24%	16.09%	17.15%
1,4-PENTANEDIOL	2.64%	0.30%	2.52%		1.21%	17.17%	31.85%
1,5,9-CYCLODODECATRIENE	1.58%	0.41%			1.41%	10.18%	22.66%
1,5-CYCLOOCTADIENE	0.88%	1.87%	1.60%	4.93%	1.41%	11.27%	25.23%
1,5-DICHLOROPENTANE	0.99%	0.91%	5.00%	6.12%	3.89%	36.02%	46.56%
1,5-HEXADIENE	0.42%	0.56%	3.42%		2.39%	17.47%	23.97%
1,5-NAPHTHALENE DIISOCYANATE	0.48%	0.31%	2.46%		1.25%	13.73%	31.26%
1,5-PENTANEDIAMINE	1.46%	1.60%			2.14%	16.50%	12.89%
1,6-DIMETHYLINDAN	0.15%	0.69%	2.81%		2.69%	20.92%	28.34%
1,6-HEXANEDIOL DIACRYLATE	0.41%	0.40%			2.24%	24.01%	40.48%
1,9-DECADIENE	0.55%	0.43%	1.79%		2.25%	21.34%	31.30%
1-AMINO-2-PROPANOL	1.66%	1.69%	7.65%		0.71%	7.00%	7.96%
1-BROMOBUTANE	1.45%	0.80%	1.67%		3.06%	15.61%	24.98%
1-BROMODECANE	0.99%	0.39%	1.58%		2.09%	23.11%	36.08%
1-BROMOHEPTANE	1.07%	0.86%			2.39%	16.32%	28.24%
1-BROMONAPHTHALENE	0.68%	1.03%	3.24%		2.93%	25.44%	36.25%
1-BROMOPROPANE	2.00%	0.55%	2.36%		3.79%	16.71%	23.26%
1-BUTANOL	4.23%	2.07%	3.56%	18.44%	0.38%	13.32%	29.51%
1-BUTENE	1.17%	1.56%	6.67%	2.22%	1.20%	10.35%	20.00%
1-CHLORO-1,1-DIFLUOROETHANE	0.07%	0.41%	2.68%	1.05%	2.27%	16.12%	25.06%
1-CHLORO-2,4-DINITROBENZENE	0.89%	0.47%	1.79%		2.80%	31.58%	35.19%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
1-CHLORONAPHTHALENE	1.35%	1.67%	4.28%		4.66%	33.92%	47.44%
1-CHLOROPENTANE	0.51%	0.74%	1.86%		3.26%	24.12%	32.66%
1-cis-2-trans-3-TRIMETHYLCYCLOPENTANE	0.66%	0.50%	2.54%		2.52%	20.21%	32.98%
1-cis-2-trans-4-TRIMETHYLCYCLOPENTANE	0.48%	0.67%	2.12%		2.67%	19.90%	33.77%
1-CYCLOHEXYLETHANONE	1.93%	0.43%	3.17%		2.04%	20.63%	28.60%
1-DECANOL	3.61%	0.48%		12.27%	1.58%	20.20%	28.09%
1-DECENE	0.14%	0.54%	2.54%	0.81%	2.40%	21.16%	31.63%
1-DECYNE	0.53%	0.50%	1.64%	7.16%	2.35%	18.79%	31.31%
1-DOCOSANOL	3.54%	1.37%			2.47%	37.39%	44.39%
1-DODECANOL	2.48%	0.29%		12.59%	2.66%	24.58%	29.53%
1-DODECENE	0.64%	0.60%	1.55%	3.23%	2.45%	24.42%	33.05%
1-EICOSANOL	2.05%	1.70%		8.39%	2.68%	33.34%	40.56%
1-EICOSENE	0.60%	0.82%	1.21%	1.27%	1.97%	22.72%	34.73%
1-ETHOXY-2-PROPANOL	3.83%	1.06%			1.10%	3.06%	24.44%
1-ETHYL-2-ISOPROPYLBENZENE	0.43%	0.51%	2.50%	1.32%	2.37%	21.96%	30.44%
1-ETHYLCYCLOHEXENE	0.92%	0.67%	1.85%		2.51%	18.88%	26.69%
1-ETHYL-DECALIN	0.61%	0.66%	1.82%		2.69%	24.16%	31.29%
1-ETHYLNAPHTHALENE	0.65%	0.42%	1.14%	2.03%	2.88%	21.24%	24.57%
1-ETHYLTETRALIN	0.61%	0.81%	2.57%		2.94%	26.65%	33.01%
1-HEPTADECANOL	1.41%	2.04%		9.41%	2.66%	28.60%	35.20%
1-HEPTADECENE	0.75%	0.98%	1.98%	1.75%	2.64%	25.16%	33.95%
1-HEPTANOL	5.26%	0.63%		10.40%	0.62%	12.91%	27.94%
1-HEPTENE	0.60%	0.55%	1.06%	1.27%	2.55%	16.73%	26.88%
1-HEPTYNE	0.69%	0.40%	2.19%	3.14%	2.14%	14.27%	22.03%
1-HEXADECANOL	1.58%	1.14%		10.48%	3.05%	29.64%	34.36%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
1-HEXADECENE	0.50%	0.90%	2.57%	0.91%	2.53%	25.33%	34.13%
1-HEXANOL	4.63%	1.85%		10.89%	0.73%	15.16%	28.70%
1-HEXATRIACONTENE	1.15%	0.43%	4.39%		0.99%	15.71%	38.53%
1-HEXENE	0.86%	0.50%	3.44%	1.21%	1.60%	14.72%	25.04%
1-HEXYNE	0.96%	0.73%	1.45%	2.59%	1.88%	12.38%	22.73%
1H-PERFLUORO-N-HEXANE	1.85%	0.16%	2.39%		1.45%	16.49%	27.25%
1-METHOXY-2-PROPANOL PROPANOATE	2.03%	0.49%	3.64%		2.22%	24.97%	33.79%
1-METHYL-1-ETHYLCYCLOPENTANE	0.96%	0.84%		3.02%	2.81%	16.56%	24.79%
1-METHYL-2-n-PROPYLBENZENE	0.94%	0.89%	1.33%	1.80%	3.11%	21.29%	29.47%
1-METHYL-3-(METHYLETHOXY)BENZENE	1.08%	0.66%	2.51%		2.51%	19.04%	32.09%
1-METHYL-3-HYDROXY-5-ISOPROPYL BENZENE	2.26%	1.66%	4.93%		0.75%	1.36%	19.40%
1-METHYL-3-HYDROXY-6-ISOPROPYL BENZENE	0.36%	1.33%	5.15%		0.14%	0.80%	18.70%
1-METHYL-3-n-PROPYLBENZENE	0.43%	1.45%	2.05%	1.54%	2.90%	22.47%	33.82%
1-METHYL-4-n-PROPYLBENZENE	0.54%	2.07%	1.85%	1.56%	2.85%	21.56%	34.23%
1-METHYL-4-VINYLCYCLOHEXENE	0.77%	0.51%	2.45%	5.59%	2.13%	18.47%	27.25%
1-METHYLCYCLOPENTENE	0.56%	0.52%	2.50%	2.55%	1.48%	11.22%	20.04%
1-METHYL-DECALIN	1.11%	0.45%	1.78%		2.16%	20.07%	28.65%
1-METHYLINDAN	0.28%	0.64%	2.77%		2.38%	18.68%	26.92%
1-METHYLINDENE	0.47%	0.90%	2.89%	1.70%	2.97%	24.63%	29.15%
1-METHYLNAPHTHALENE	0.88%	0.60%	5.55%	2.33%	2.43%	23.42%	27.81%
1-METHYLTETRALIN	0.75%	0.78%	2.64%		2.79%	24.79%	31.21%
1-METHYLVINYL ACETATE	0.78%	0.51%	2.50%		1.17%	5.12%	16.95%
1-n-BUTYLNAPHTHALENE	0.53%	0.46%	1.71%	2.39%	2.26%	21.10%	29.80%
1-n-DECYLNAPHTHALENE	0.63%	0.39%	1.79%		3.40%	38.96%	59.82%
1-n-HEXYL-1,2,3,4-TETRAHYDRONAPHTHALENE	0.95%	1.03%	3.04%	1.19%	3.08%	32.24%	48.16%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
1-n-HEXYLNAPHTHALENE	0.87%	0.52%	1.29%	1.32%	1.90%	20.19%	35.15%
1-NITROBUTANE	2.69%	1.73%	2.10%		5.50%	33.17%	34.67%
1-NITROPROPANE	4.96%	1.83%	5.58%	4.12%	3.63%	30.60%	33.84%
1-n-NONYLNAPHTHALENE	0.65%	0.42%	1.77%		3.32%	36.39%	55.48%
1-NONADECANOL	1.69%	2.02%			2.84%	32.16%	38.52%
1-NONADECENE	0.79%	0.96%	1.65%	1.70%	2.41%	24.01%	34.22%
1-NONANOL	4.02%	0.95%		14.82%	1.59%	20.23%	27.74%
1-NONENE	0.10%	0.48%	2.58%	1.30%	2.32%	19.35%	29.20%
1-NONYNE	0.36%	0.27%	1.07%	6.13%	1.68%	16.16%	27.78%
1-n-PENTYLNAPHTHALENE	0.74%	0.48%	1.60%	1.88%	2.32%	22.30%	32.96%
1-OCTADECANOL	1.40%	1.46%		9.99%	2.96%	31.52%	37.33%
1-OCTADECENE	0.70%	0.95%	1.73%	1.74%	2.43%	24.27%	34.18%
1-OCTANOL	4.57%	0.42%	7.49%	10.93%	0.88%	16.48%	27.62%
1-OCTENE	0.74%	0.61%	1.09%	0.46%	2.69%	18.12%	27.15%
1-OCTYNE	0.37%	0.37%	1.97%	3.57%	2.11%	15.71%	24.97%
1-PENTADECANOL	1.73%	0.89%		10.79%	3.06%	29.47%	32.44%
1-PENTADECENE	0.56%	0.88%	1.53%	0.96%	2.61%	25.08%	33.53%
1-PENTANOL	3.62%	1.90%	4.45%	11.58%	0.67%	13.43%	28.30%
1-PENTENE	0.20%	0.65%	4.76%	0.60%	2.00%	13.54%	23.33%
1-PENTENE-4-YNE	0.68%	0.85%	2.90%	3.80%	2.78%	16.38%	23.76%
1-PENTYNE	1.16%	3.08%	1.64%	2.43%	1.62%	9.34%	15.46%
1-PHENYLNAPHTHALENE	0.66%	1.14%	2.53%		3.06%	30.13%	36.38%
1-PROPANOL	3.06%	2.91%	2.58%	33.72%	0.64%	14.37%	31.42%
1-tert-BUTOXY-2-[2-(HYDROXY)PROPOXY]PROPANE	1.44%	1.98%	5.03%		0.25%	0.50%	32.38%
1-tert-BUTOXY-2-[2-(tert-BUTOXY)PROPOXY]PROPANE	0.45%	2.78%	3.99%		5.95%	65.65%	57.60%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
1-tert-BUTYL GLYCERIN	1.44%	0.97%	2.37%		1.26%	15.87%	38.39%
1-TETRADECENE	0.92%	0.75%	1.53%	0.56%	2.51%	27.15%	36.08%
1-TRIACONTENE	1.03%	0.17%	3.64%		1.30%	18.97%	36.79%
1-TRIDECANOL	2.06%	0.67%		12.27%	2.75%	26.34%	30.40%
1-TRIDECENE	0.61%	0.70%	1.52%	0.82%	2.53%	25.87%	34.50%
1-UNDECANOL	2.58%	0.68%		13.73%	2.68%	23.52%	28.76%
1-UNDECENE	0.33%	0.54%	2.05%	2.85%	2.43%	22.81%	31.63%
2-(2-ETHOXYETHOXY)ETHANOL	1.37%	0.40%	1.34%		2.07%	22.36%	33.26%
2-(2-HEXOXYETHOXY)ETHANOL	1.02%	2.50%		9.11%	1.22%	9.58%	24.66%
2-(2-METHOXYETHOXY)ETHANOL	1.16%	0.47%	1.55%		2.36%	24.14%	32.85%
2-(2-PENTOXYETHOXY)ETHANOL	3.78%	0.93%			0.39%	10.88%	30.16%
2-(5H)-FURANONE	5.73%	2.85%	9.03%		6.64%	72.91%	81.98%
2-(alpha-METHYLBENZYLOXY)-1-PROPANOL	0.69%	1.19%	1.54%	16.42%	3.32%	35.36%	42.01%
2-(DIFLUOROMETHOXY)-1,1,1-TRIFLUOROETHANE	0.69%	0.33%	2.01%		1.78%	15.78%	24.51%
2-(N-MORPHOLINO)-2'-HYDROXYDIETHYLETHER	0.74%	0.37%	2.72%	6.38%	1.19%	13.59%	31.66%
2,2,3,3-TETRAMETHYLBUTANE	0.40%	0.17%	1.65%	0.16%	1.42%	10.50%	18.98%
2,2,3,3-TETRAMETHYLHEXANE	0.64%	0.26%	1.51%	1.15%	2.07%	13.01%	23.50%
2,2,3,3-TETRAMETHYLPENTANE	0.44%	0.11%	0.74%	0.88%	1.91%	12.66%	28.50%
2,2,3,4-TETRAMETHYLPENTANE	0.40%	0.69%	1.58%	4.14%	1.94%	13.42%	28.91%
2,2,3-TRIMETHYLBUTANE	0.06%	0.12%	1.62%	1.12%	1.76%	12.45%	25.37%
2,2,3-TRIMETHYLPENTANE	0.19%	1.19%	1.37%	2.84%	1.92%	14.45%	31.21%
2,2,4,4,6,8,8-HEPTAMETHYLNONANE	0.14%	1.28%	1.56%	5.79%	2.26%	20.88%	41.55%
2,2,4,4-TETRAFLUOROPENTANE	0.61%	0.10%	0.52%		1.57%	13.33%	23.98%
2,2,4,4-TETRAMETHYL-1,3-CYCLOBUTANEDIOL	2.45%	0.27%	2.53%		1.81%	22.66%	34.03%
2,2,4,4-TETRAMETHYLPENTANE	0.41%	0.20%	1.00%	1.65%	1.94%	13.20%	26.90%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
2,2,4-TRIMETHYL-1,3-PENTANEDIOL	3.92%	0.68%			2.21%	31.27%	42.21%
2,2,4-TRIMETHYLPENTANE	0.23%	0.41%	1.40%	2.66%	1.93%	14.48%	25.31%
2,2,5,5-TETRAMETHYLHEXANE	1.21%	0.10%	2.64%	1.46%	1.38%	14.97%	25.99%
2,2,5-TRIMETHYLHEXANE	0.48%	0.39%	2.47%	3.01%	1.87%	17.06%	30.59%
2,2-DICHLORO-1,1,1-TRIFLUOROETHANE	0.24%	0.28%	2.27%	1.87%	1.99%	15.14%	23.92%
2,2-DICHLORO-1,1,2-TRIFLUOROETHANE	0.46%	0.86%	2.99%	5.88%	2.79%	21.62%	28.05%
2,2-DIMETHYL-1-PROPANOL	3.29%	2.33%	8.50%		1.73%	7.40%	14.87%
2,2-DIMETHYL-3-ETHYLPENTANE	0.66%	0.46%	2.23%	4.70%	1.52%	12.95%	24.51%
2,2-DIMETHYLBUTANE	0.50%	0.26%	1.78%	1.48%	1.67%	10.82%	22.12%
2,2-DIMETHYLHEPTANE	0.50%	0.53%	1.15%	0.96%	2.43%	17.22%	31.05%
2,2-DIMETHYLHEXANE	0.29%	0.52%	1.73%	1.24%	2.05%	16.62%	26.00%
2,2-DIMETHYLOCTANE	0.73%	0.23%	2.32%	1.18%	2.06%	19.47%	34.57%
2,2-DIMETHYLPENTANE	0.10%	0.53%	1.70%	1.55%	2.04%	15.10%	25.19%
2,2'-IMINOBIS-ACETONITRILE	0.55%	2.64%	4.17%		5.64%	65.99%	60.31%
2,3,3,3-TETRAFLUOROPROPENE	0.21%	0.51%	2.45%		2.33%	17.79%	26.34%
2,3,3,4-TETRAMETHYLPENTANE	0.12%	0.53%	1.58%	1.09%	1.59%	12.42%	25.56%
2,3,3-TRIMETHYL-1-BUTENE	0.72%	0.30%	1.18%	7.37%	1.31%	9.09%	23.01%
2,3,3-TRIMETHYLPENTANE	0.08%	0.65%	1.57%	2.13%	1.83%	13.40%	23.87%
2,3,4,5,2',3',4',5'-OCTAHYDRO-BIFURYL-(3,3')	0.71%	1.37%	2.60%		3.89%	33.12%	35.49%
2,3,4-TRIMETHYLPENTANE	0.17%	0.81%	1.81%	1.83%	1.91%	14.82%	25.00%
2,3,5-TRIMETHYLTHIOPHENE	0.25%	0.42%	2.01%		2.17%	17.09%	26.00%
2,3-BUTANEDIOL	2.85%	1.94%	13.30%		0.42%	8.89%	23.63%
2,3-DICHLOROBUTANE	0.22%	1.60%	3.96%		2.71%	20.38%	29.41%
2,3-DICHLOROPROPENE	3.06%	2.69%		0.79%	3.02%	24.55%	32.03%
2,3-DIHYDROFURAN	0.24%	0.33%	2.51%		1.97%	14.17%	28.80%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
2,3-DIMETHYL-1,3-BUTADIENE	1.19%	0.44%	4.58%	0.74%	2.25%	19.99%	31.47%
2,3-DIMETHYL-1-BUTENE	0.65%	0.57%	1.80%	3.47%	1.72%	11.79%	24.84%
2,3-DIMETHYL-1-HEXENE	1.00%	0.44%	2.44%	5.55%	1.56%	14.25%	26.59%
2,3-DIMETHYL-2,3-DIPHENYLBUTANE	0.46%	1.75%	4.30%		4.35%	42.85%	43.55%
2,3-DIMETHYL-2-BUTENE	1.89%	0.32%	5.13%	1.79%	2.22%	21.19%	31.57%
2,3-DIMETHYLBENZOTHIOPHENE	0.98%	0.49%	1.83%		2.34%	22.01%	37.87%
2,3-DIMETHYLBUTANE	0.05%	0.57%	1.86%	2.83%	1.81%	12.41%	21.86%
2,3-DIMETHYLDECANE	0.87%	0.62%	2.02%		2.41%	23.79%	33.06%
2,3-DIMETHYLDODECANE	0.74%	0.55%	1.72%		2.42%	24.96%	35.32%
2,3-DIMETHYLHEPTANE	0.77%	0.71%	1.15%	3.66%	2.79%	19.56%	28.10%
2,3-DIMETHYLHEXANE	0.16%	0.72%	1.90%	1.20%	2.09%	16.96%	26.88%
2,3-DIMETHYLNONANE	0.73%	0.76%	2.45%		2.46%	23.05%	31.84%
2,3-DIMETHYLOCTANE	0.52%	0.72%	1.63%		2.65%	22.61%	30.54%
2,3-DIMETHYLPENTANE	0.31%	1.24%	2.02%	2.74%	2.00%	14.87%	30.21%
2,3-DIMETHYLTHIOPHENE	0.46%	0.35%	2.25%		2.65%	20.54%	25.26%
2,3-DIMETHYLUDECANE	0.65%	0.60%	1.90%		2.51%	24.86%	34.26%
2,3-PENTADIENE	1.56%	0.76%	5.38%	1.79%	2.51%	23.54%	22.87%
2,3-XYLENOL	0.80%	1.73%	4.86%	3.51%	0.57%	6.13%	13.58%
2,4,4-TRIMETHYL-1-PENTENE	0.71%	0.43%	2.00%	1.97%	2.57%	16.40%	30.45%
2,4,4-TRIMETHYL-2-PENTENE	1.20%	0.38%	3.35%	3.22%	2.03%	17.54%	31.64%
2,4,4-TRIMETHYLHEXANE	0.39%	0.50%	1.63%	2.45%	2.21%	15.30%	28.09%
2,4,6-TRIMETHYLPYRIDINE	0.70%	0.52%	3.84%		2.65%	25.01%	30.33%
2,4-DIAMINOTOLUENE	1.32%	0.53%	3.24%		2.25%	25.11%	35.30%
2,4-DICHLOROBENZOTRIFLUORIDE	0.69%	1.20%	3.49%		3.49%	32.30%	43.82%
2,4-DICHLOROTOLUENE	0.80%	0.81%	3.79%		2.87%	24.92%	34.72%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
2,4-DIMETHYL-1,3-DIOXOLANE-2-METHANOL	0.78%	0.57%	1.07%		2.44%	24.54%	34.00%
2,4-DIMETHYL-3-ETHYLPENTANE	0.35%	0.59%	2.20%		2.02%	15.23%	26.45%
2,4-DIMETHYLHEXANE	0.28%	0.48%	1.94%	0.60%	1.93%	15.68%	26.95%
2,4-DIMETHYLOCTANE	0.96%	0.84%	2.15%	3.18%	1.81%	17.39%	33.27%
2,4-DIMETHYLPENTANE	0.26%	0.80%	1.61%	0.69%	2.00%	15.32%	25.78%
2,4-DINITROPHENOL	1.07%	0.33%	2.55%		1.45%	17.70%	38.75%
2,4-DIPHENYL-4-METHYLPENTENE-1	0.14%	1.09%	2.60%		3.38%	32.23%	37.91%
2,4-TOLUENE DIISOCYANATE	1.94%	1.29%			2.85%	25.74%	25.90%
2,4-XYLENOL	0.53%	1.29%	2.16%	2.32%	1.07%	7.91%	14.29%
2,5-DIHYDROFURAN	0.97%	0.30%	6.50%	1.15%	2.06%	19.25%	32.58%
2,5-DIMETHYL-1,5-HEXADIENE	0.74%	0.61%	4.11%	1.33%	2.51%	21.77%	28.88%
2,5-DIMETHYL-2,4-HEXADIENE	2.30%	0.28%	5.64%	1.00%	3.27%	31.16%	42.08%
2,5-DIMETHYLFURAN	1.31%	0.24%	1.05%		1.14%	11.32%	22.65%
2,5-DIMETHYLHEXANE	0.22%	0.35%	1.91%	1.32%	2.29%	18.26%	27.01%
2,5-DIMETHYLOCTANE	0.48%	0.48%	1.41%	3.08%	2.41%	19.81%	33.94%
2,5-DIMETHYLTETRAHYDROFURAN	0.19%	0.26%	1.19%		1.67%	11.71%	25.90%
2,5-DIMETHYLTHIOPHENE	0.89%	0.61%			1.03%	5.32%	19.28%
2,5-XYLENOL	1.13%	2.06%	6.49%	6.48%	0.37%	5.15%	14.26%
2,6,8-TRIMETHYL-4-NONANONE	0.93%	0.99%	2.50%		1.37%	14.78%	36.13%
2,6-DIETHYLNAPHTHALENE	0.68%	1.10%	4.74%	1.40%	3.23%	32.61%	37.60%
2,6-DIMETHYL-4-HEPTANOL	1.56%	1.70%	5.74%		0.32%	0.44%	21.82%
2,6-DIMETHYLHEPTANE	1.02%	0.44%	2.54%	0.91%	1.91%	19.18%	34.17%
2,6-DIMETHYLNAPHTHALENE	0.50%	1.69%	3.07%	2.64%	2.31%	21.66%	30.64%
2,6-DIMETHYLOCTANE	0.76%	0.83%	2.46%	2.18%	1.92%	18.49%	34.60%
2,6-DIMETHYLPYRIDINE	0.70%	0.16%	3.27%	1.15%	2.31%	21.90%	23.59%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
2,6-DINITROPHENOL	2.03%	0.16%	2.65%		1.56%	21.61%	38.72%
2,6-DI-tert-BUTYL-p-CRESOL	0.97%	1.52%			1.36%	11.49%	25.62%
2,6-NAPHTHALENEDICARBOXYLIC ACID	1.21%	0.56%	5.74%		0.81%	12.46%	40.18%
2,6-TOLUENE DIISOCYANATE	2.54%	2.03%	7.69%		3.70%	41.93%	36.34%
2,6-XYLENOL	0.79%	1.23%	3.61%	2.92%	0.02%	1.92%	15.86%
2,7-DIMETHYLBENZOTHIOPHENE	0.31%	0.49%	1.04%		2.36%	20.48%	29.28%
2,7-DIMETHYLNAPHTHALENE	0.61%	1.78%	4.38%	3.96%	1.89%	17.82%	10.83%
2,7-DIMETHYLOCTANE	0.47%	0.31%	1.95%	1.16%	2.13%	20.77%	36.68%
2-ACETOACETOXY ETHYL METHACRYLATE	1.08%	0.52%	3.69%		1.60%	20.44%	43.20%
2-AMINO-2-METHYL-1-PROPANOL	2.66%	0.80%	4.13%		2.51%	31.96%	41.20%
2-AMINODIPHENYL	0.91%	0.39%	5.71%		0.48%	6.85%	0.59%
2-AMINOETHOXYETHANOL	1.87%	1.10%	4.55%	10.55%	0.89%	5.60%	1.79%
2-BROMOBUTANE	0.77%	2.47%	2.38%	1.13%	0.29%	1.09%	6.06%
2-BROMOPROPANE	1.56%	2.36%	5.58%	1.52%	1.11%	11.28%	0.60%
2-BUTANOL	4.27%	1.48%	6.06%		0.71%	15.22%	31.33%
2-BUTOXIME	1.64%	0.65%	1.78%	4.32%	2.12%	24.16%	32.39%
2-BUTOXYETHANOL	1.18%	0.43%	3.11%	10.03%	2.19%	20.29%	26.84%
2-BUTYL-2-ETHYL-1,3-PROPANEDIOL	3.01%	0.34%			1.91%	24.06%	37.29%
2-BUTYLBENZOTHIOPHENE	0.91%	0.36%	1.98%		1.10%	11.53%	25.77%
2-BUTYL-NONAN-1-OL	1.41%	1.25%	4.94%		0.07%	3.77%	32.95%
2-BUTYNE-1,4-DIOL	0.99%	0.73%	4.45%		0.12%	3.69%	28.40%
2-CHLORO-1,1,1,2-TETRAFLUOROETHANE	0.27%	2.97%	11.05%	2.44%	1.58%	11.70%	22.88%
2-CHLORO-1,1,1-TRIFLUOROETHANE	0.69%	1.36%	3.13%	3.05%	3.77%	26.42%	30.40%
2-CHLORO-1,1-DIFLUOROETHYLENE	0.96%	0.42%	5.53%	1.93%	1.79%	16.97%	26.40%
2-CHLORO-1,3-PROPANEDIOL	0.99%	0.68%	5.17%		0.32%	5.80%	29.49%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
2-CHLOROETHANOL	2.73%	2.00%			2.79%	22.64%	29.18%
2-CHLOROPROPENE	0.41%	2.16%	3.02%	1.20%	1.77%	12.06%	20.20%
2-CYCLOHEXENE-1-ONE	0.31%	1.23%	3.30%		3.69%	29.56%	32.74%
2-CYCLOHEXENYL CYCLOHEXANONE	0.97%	0.34%	1.26%		2.04%	19.37%	28.94%
2-ETHOXY-1-PROPANOL	0.29%	0.42%	2.57%		1.72%	15.89%	24.23%
2-ETHOXYETHYL ACETATE	0.67%	0.60%	1.09%		2.04%	14.83%	17.36%
2-ETHYL BUTYRIC ACID	1.13%	0.47%	1.33%		1.56%	17.52%	36.85%
2-ETHYL HEXANOIC ACID	1.77%	2.21%	3.45%		0.81%	11.37%	27.46%
2-ETHYL-1-BUTANOL	3.65%	1.15%			0.05%	7.47%	26.64%
2-ETHYL-1-BUTENE	1.12%	0.50%	4.65%	2.79%	1.67%	15.51%	25.12%
2-ETHYL-1-HEXANOL	3.67%	0.39%			1.07%	17.24%	30.89%
2-ETHYL-1-HEXENE	0.51%	0.46%	5.15%		2.20%	19.77%	30.38%
2-ETHYL-1-PENTENE	1.00%	0.83%	2.56%	7.43%	2.97%	18.64%	28.18%
2-ETHYL-2-HEXENAL	1.82%	2.19%	5.55%	4.14%	4.71%	47.22%	44.83%
2-ETHYLBENZOTHIOPHENE	0.73%	0.20%	1.13%	2.16%	1.75%	16.12%	31.11%
2-ETHYLHEXANAL	0.93%	1.21%	2.08%		2.18%	21.08%	32.62%
2-ETHYLHEXYL ACRYLATE	0.88%	0.61%		9.34%	1.55%	16.42%	32.07%
2-ETHYLHEXYL BENZOATE	0.86%	0.57%	2.19%		2.08%	22.70%	36.05%
2-ETHYL-m-XYLENE	0.11%	0.85%	1.96%	1.21%	2.53%	20.67%	27.76%
2-ETHYLNAPHTHALENE	1.30%	0.47%	1.75%	1.61%	3.36%	24.73%	29.63%
2-ETHYL-p-XYLENE	0.54%	0.70%	4.40%	1.08%	2.49%	23.31%	32.37%
2-ETHYL-TETRAHYDROTHIOPHENE	1.78%	0.45%	2.83%		1.87%	17.73%	26.25%
2-ETHYLTHIOPHENE	0.28%	0.58%	1.79%		0.90%	6.87%	20.08%
2-FORMYL BENZOIC ACID	1.05%	1.33%	4.13%	6.79%	3.30%	41.38%	50.17%
2-HEPTANOL	4.65%	1.29%			0.26%	13.63%	25.72%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
2-HEPTANONE	0.46%	0.80%	1.32%		2.89%	23.79%	30.86%
2-HEXANOL	5.33%	1.56%	7.04%		0.22%	13.26%	27.25%
2-HEXANONE	0.44%	0.47%	1.23%		3.15%	24.55%	30.79%
2-HEXYNE	1.56%	1.80%	6.23%		2.44%	22.48%	30.22%
2-HYDROXYPROPYL METHACRYLATE	1.47%	0.75%	2.27%	3.64%	0.92%	11.92%	31.21%
2-MERCAPTOBENZOTHAZOLE	0.48%	0.47%	2.43%		2.37%	19.46%	27.82%
2-METHOXY PROPANOL-1	0.19%	1.15%	2.67%		3.55%	31.35%	35.70%
2-METHOXYETHANOL	0.23%	0.93%	1.98%		2.76%	22.18%	19.16%
2-METHYL BENZOTHIOPHENE	1.35%	1.59%	2.28%	3.39%	3.96%	32.82%	35.27%
2-METHYL OCTANAL	1.18%	0.17%	1.25%		1.72%	18.27%	30.56%
2-METHYL THIAINDAN	0.31%	0.88%	3.05%		3.02%	23.90%	29.51%
2-METHYL-, 3-HYDROXY-2,2,4-TRIMETHYLPENTYL PROPANOATE	1.14%	0.53%			2.39%	25.40%	39.83%
2-METHYL-1,3-PROPANEDIOL	1.43%	0.50%	2.71%	4.96%	0.29%	6.51%	23.65%
2-METHYL-1-BUTANOL	4.13%	2.47%	4.93%		0.60%	11.09%	23.02%
2-METHYL-1-BUTENE	0.41%	0.49%	3.14%	1.74%	2.32%	19.36%	28.04%
2-METHYL-1-BUTENE-3-YNE	0.15%	0.67%	2.82%	1.03%	1.34%	10.74%	25.53%
2-METHYL-1-HEPTANOL	1.31%	1.64%	4.66%		0.33%	0.63%	22.98%
2-METHYL-1-HEPTENE	0.16%	0.71%	3.85%	2.92%	2.70%	22.00%	33.42%
2-METHYL-1-HEXANOL	1.29%	1.77%	2.80%	8.88%	0.42%	7.31%	25.98%
2-METHYL-1-HEXENE	0.46%	0.50%	3.08%	1.42%	2.27%	19.62%	30.54%
2-METHYL-1-NONENE	0.79%	0.73%	2.36%	1.19%	2.55%	23.85%	40.97%
2-METHYL-1-OCTENE	0.39%	0.39%	4.29%	1.98%	2.67%	23.74%	35.93%
2-METHYL-1-PENTANOL	3.66%	1.40%			0.74%	15.57%	27.77%
2-METHYL-1-PENTENE	0.47%	0.50%	3.15%	2.03%	2.17%	17.36%	27.91%
2-METHYL-1-PROPANOL	4.92%	2.96%	5.25%	7.30%	0.05%	12.78%	29.01%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
2-METHYL-2-AMINOBUTANE	0.62%	0.72%	1.48%		0.86%	7.92%	8.53%
2-METHYL-2-BUTANOL	5.74%	1.23%	6.40%	14.90%	0.06%	13.36%	25.36%
2-METHYL-2-BUTENE	0.76%	0.65%	2.12%	1.62%	3.52%	23.16%	30.44%
2-METHYL-2-PENTENAL	0.73%	1.61%	4.98%	4.86%	4.35%	39.04%	44.88%
2-METHYL-2-PENTENE	1.44%	0.64%	4.33%	4.37%	2.15%	20.67%	24.19%
2-METHYL-2-PROPANOL	4.92%	0.86%	5.59%	11.30%	0.27%	13.75%	28.44%
2-METHYL-3-ETHYLPENTANE	0.20%	1.25%	1.85%	2.57%	2.12%	16.48%	31.70%
2-METHYLBENZOFURAN	0.90%	1.04%	2.67%		3.22%	25.15%	30.39%
2-METHYLBUTYRALDEHYDE	0.54%	0.40%	2.24%	2.07%	2.35%	17.41%	26.42%
2-METHYLBUTYRIC ACID	0.97%	0.37%	2.13%		1.83%	19.45%	32.02%
2-METHYLDECANE	1.08%	0.35%	1.80%		2.05%	21.39%	31.86%
2-METHYL-DODECAN-1-OL	1.33%	1.23%	4.94%		0.08%	4.31%	33.49%
2-METHYLDODECANE	0.43%	0.45%	1.68%		2.35%	23.66%	34.78%
2-METHYLHEPTANAL	2.33%	0.15%	3.52%		1.53%	18.61%	29.86%
2-METHYLHEPTANE	0.35%	0.52%	2.19%	0.81%	2.35%	19.51%	27.15%
2-METHYLHEXANAL	0.75%	0.50%	2.47%	1.77%	2.38%	22.71%	31.14%
2-METHYLHEXANE	0.36%	0.48%	2.68%	1.09%	2.20%	17.33%	27.43%
2-METHYLHEXANOIC ACID	1.54%	0.46%	2.81%		1.09%	13.54%	30.73%
2-METHYLINDENE	0.40%	0.93%	3.18%	1.63%	3.02%	25.88%	30.62%
2-METHYLNAPHTHALENE	3.89%	1.33%	4.65%	2.70%	3.20%	22.66%	29.59%
2-METHYLNONANE	0.33%	0.56%	1.20%	1.72%	2.47%	21.93%	36.78%
2-METHYLOCTANE	0.38%	0.33%	1.98%	3.01%	2.07%	18.46%	29.26%
2-METHYLOCTANOIC ACID	1.11%	0.56%	2.97%		1.02%	12.99%	32.39%
2-METHYLPENTANE	0.22%	0.62%	2.44%	0.71%	1.91%	14.07%	23.30%
2-METHYLPROPANAL	0.91%	1.00%	2.36%		3.13%	23.56%	29.42%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
2-METHYLPYRIDINE	0.10%	0.66%	1.93%	0.85%	2.18%	16.51%	11.69%
2-METHYLTETRAHYDROFURAN	0.20%	0.64%	3.72%		3.68%	28.09%	48.34%
2-METHYLTHIACYCLOPENTANE	0.63%	0.69%	2.45%		2.54%	19.85%	26.94%
2-METHYLTHIOPHENE	0.42%	0.81%	1.34%	3.08%	1.50%	10.08%	25.00%
2-METHYLTRIDECANE	0.43%	0.49%	1.84%		2.39%	24.66%	36.33%
2-METHYLUNDECANE	0.71%	0.42%	1.48%		2.24%	22.57%	33.20%
2-NITROPROPANE	2.41%	1.53%	2.52%	4.92%	5.06%	29.11%	28.45%
2-NONANOL	2.81%	0.21%			0.75%	12.67%	22.78%
2-NONANONE	0.37%	0.86%	1.40%		2.56%	22.24%	29.99%
2-NORBORNENE	0.62%	0.30%	2.23%	1.25%	1.64%	11.32%	22.00%
2-n-PROPYLTHIOPHENE	0.21%	0.72%	2.46%		0.92%	7.05%	21.18%
2-OCTANOL	3.57%	1.57%			0.73%	14.80%	24.01%
2-OCTANONE	0.43%	1.10%	1.36%		2.64%	22.35%	30.24%
2-PENTANETHIOL	0.96%	0.64%	2.06%		1.65%	14.15%	18.95%
2-PENTANOL	5.52%	2.01%			0.00%	13.84%	28.90%
2-PENTANONE	0.49%	1.14%	1.96%		3.42%	26.00%	31.95%
2-PENTOXYETHANOL	1.03%	0.61%	2.08%	6.84%	1.00%	11.40%	27.80%
2-PENTYNE	1.66%	1.79%	7.00%	1.00%	2.65%	21.93%	29.32%
2-PHENYL-1-PROPANOL	1.14%	0.76%	2.30%	14.12%	0.27%	5.67%	23.63%
2-PHENYL-2-PROPANOL	1.45%	1.01%	5.94%		0.90%	6.99%	19.12%
2-PHENYLBUTENE-1	1.10%	0.70%	4.12%		2.53%	23.43%	35.07%
2-PHENYLETHANOL	2.66%	1.63%	9.15%		2.06%	12.79%	24.96%
2-PROPYLBENZOTHIOPHENE	0.95%	0.75%	2.48%		0.52%	6.21%	21.84%
2-PYRROLIDONE	0.52%	1.84%	1.59%	13.51%	3.76%	32.15%	36.46%
3-(METHYLMERCAPTO)PROPANAL	0.61%	0.83%	3.95%	4.33%	3.69%	33.93%	42.71%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
3-(N,N-DIMETHYLAMINO) PROPYLAMINE	0.15%	0.47%	2.97%		1.37%	11.37%	24.26%
3-(TRIETHOXSILYL)PROPIONITRILE	0.40%	0.81%	1.35%	3.85%	3.04%	29.62%	42.36%
3,3,3-TRIFLUOROPROPENE	3.04%	2.31%			5.29%	38.39%	37.79%
3,3,5-TRIMETHYLHEPTANE	0.31%	0.54%	2.91%	2.86%	2.11%	15.99%	26.19%
3,3-DIETHYLPENTANE	0.46%	0.23%	1.05%	1.64%	2.33%	15.51%	33.63%
3,3-DIMETHYL-1-BUTENE	1.11%	0.25%	2.24%	6.08%	1.55%	6.34%	21.43%
3,3-DIMETHYL-1-BUTYNE	0.51%	0.75%	1.49%		0.05%	0.76%	15.49%
3,3-DIMETHYL-2-BUTANONE	0.76%	0.86%	2.03%	1.92%	2.19%	16.83%	20.76%
3,3-DIMETHYLHEXANE	0.19%	1.77%	1.54%	0.46%	2.21%	16.77%	32.68%
3,3-DIMETHYLPENTANE	0.14%	0.68%	2.14%	1.16%	1.65%	11.90%	21.72%
3,4-DICHLORO-1-BUTENE	2.10%	0.64%			2.50%	21.96%	28.48%
3,4-DICHLOROANILINE	0.58%	1.06%	2.47%		3.25%	30.08%	31.90%
3,4-DICHLOROPHENYL ISOCYANATE	2.57%	0.46%			2.30%	27.05%	34.63%
3,4-DIMETHYLHEXANE	0.13%	0.74%	1.61%	1.06%	2.07%	16.46%	25.76%
3,4-DIMETHYLTHIOPHENE	0.51%	0.41%	1.91%		2.09%	16.47%	24.72%
3,4-XYLENOL	0.81%	2.22%	4.51%	2.66%	0.21%	3.41%	15.60%
3,5-DIISOPROPYLTOLUENE	0.73%	0.35%	1.65%		2.01%	19.18%	30.97%
3,5-DIMETHYLBENZOFURAN	0.38%	0.98%	2.88%		3.34%	27.41%	32.84%
3,5-DIMETHYLBENZOTHIOPHENE	0.97%	0.74%			3.23%	22.08%	29.46%
3,5-XYLENOL	2.16%	0.22%	6.25%	5.68%	3.27%	33.44%	14.78%
3-AMINO-1-PROPANOL	1.28%	0.48%	1.88%		0.94%	13.12%	33.48%
3-BUTEN-2-ONE	0.56%	1.11%	3.28%		4.00%	33.84%	40.46%
3-CHLORO- <i>o</i> -XYLENE	0.72%	0.88%	2.03%		2.92%	25.07%	30.94%
3-CHLOROPROPENE	1.40%	1.31%		2.63%	3.02%	22.19%	29.29%
3-CHLOROPROPYLDIMETHYLCHLOROSILANE	0.16%	0.72%	2.57%		2.81%	24.47%	31.90%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
3-CHLOROPROPYLTRIMETHOXSILANE	0.51%	1.31%		10.01%	3.70%	33.24%	37.59%
3-ETHYL-1-HEPTANOL	1.14%	1.14%	4.28%	10.84%	0.21%	4.98%	29.07%
3-ETHYL-1-HEXENE	0.36%	0.38%	2.06%	4.54%	2.32%	19.13%	30.14%
3-ETHYL-1-PENTENE	0.71%	0.47%	1.81%	3.83%	1.26%	10.57%	21.80%
3-ETHYL-2,5-DIMETHYLTHIOPHENE	0.55%	1.10%	3.41%		3.53%	30.89%	34.14%
3-ETHYLBENZOTHIOPHENE	0.21%	0.38%	2.10%		2.10%	17.89%	27.95%
3-ETHYLDODECANE	0.74%	0.38%	1.46%		2.18%	22.28%	33.64%
3-ETHYLHEPTANE	0.38%	0.65%	2.28%	5.73%	2.32%	19.12%	29.58%
3-ETHYLHEXANE	0.23%	0.94%	1.91%	0.83%	2.28%	18.67%	31.97%
3-ETHYL- <i>o</i> -XYLENE	1.19%	1.21%	4.04%	1.00%	2.89%	28.48%	29.07%
3-ETHYLPENTANE	0.16%	0.54%	2.43%	0.88%	2.00%	16.00%	24.62%
3-HEPTANOL	3.18%	0.40%			1.16%	12.33%	25.81%
3-HEPTANONE	1.36%	0.43%	3.66%	0.95%	2.74%	25.93%	32.97%
3-HEXANONE	0.60%	0.63%	2.20%	1.28%	3.11%	23.50%	28.71%
3-HEXYNE	1.99%	0.51%			1.77%	20.78%	29.03%
3-HYDROXY-2-METHYL PROPIONALDEHYDE	1.21%	0.56%	2.05%	5.69%	0.95%	12.50%	32.15%
3-HYDROXYBUTYROLACTONE	0.17%	1.35%	3.27%		3.96%	39.99%	43.61%
3-MERCAPTOPROPIONIC ACID	0.84%	3.48%	4.65%	2.57%	1.88%	20.37%	43.23%
3-METHOXY-3-BUTEN-2-ONE	0.71%	0.63%			2.80%	20.71%	28.39%
3-METHOXYISOPROPYLAMINE	0.82%	0.50%	0.67%		0.79%	8.41%	11.51%
3-METHOXYPROPIONITRILE	2.58%	2.07%	9.50%		5.41%	60.11%	50.34%
3-METHYL SULFOLANE	0.61%	1.18%	3.79%		3.78%	34.31%	51.28%
3-METHYL-1,2-BUTADIENE	1.79%	1.23%	5.50%	4.97%	1.95%	19.68%	21.85%
3-METHYL-1,4-PENTADIENE	0.36%	0.52%	1.66%	4.22%	1.48%	11.09%	22.19%
3-METHYL-1-BUTANOL	4.52%	3.29%	5.99%		0.17%	8.68%	23.72%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
3-METHYL-1-BUTENE	0.13%	0.58%	1.48%	6.58%	1.60%	10.39%	16.53%
3-METHYL-1-BUTYNE	3.55%	1.09%	5.96%	2.78%	1.08%	1.28%	11.15%
3-METHYL-1-HEXENE	0.50%	0.70%	1.97%	1.14%	1.55%	12.88%	24.63%
3-METHYL-1-PENTANOL	0.84%	2.33%	8.20%		1.18%	10.90%	26.13%
3-METHYL-1-PENTENE	0.61%	0.64%	0.98%	3.68%	1.92%	10.30%	21.46%
3-METHYL-2-BUTANOL	5.56%	1.82%	6.61%		0.36%	10.21%	21.79%
3-METHYL-2-PENTANONE	0.54%	0.78%	1.11%	2.45%	3.07%	22.73%	29.59%
3-METHYL-3-ETHYLPENTANE	0.09%	0.37%	1.83%	1.82%	1.96%	14.18%	24.97%
3-METHYL-3-PENTANOL	2.21%	0.17%			1.75%	13.19%	19.26%
3-METHYLBUTYRALDEHYDE	0.33%	0.29%	1.26%		1.86%	15.74%	24.42%
3-METHYL-cis-2-PENTENE	0.54%	0.49%	3.07%	2.46%	1.86%	17.11%	26.47%
3-METHYLCYCLOPENTANONE	1.44%	1.06%	3.48%		3.17%	28.39%	32.48%
3-METHYLCYCLOPENTENE	0.56%	0.88%	1.57%	2.38%	0.93%	7.06%	16.49%
3-METHYLDECANE	0.15%	0.56%	2.65%		2.51%	22.89%	32.27%
3-METHYLDODECANE	0.08%	0.58%			2.57%	24.83%	35.16%
3-METHYLHEPTANE	0.21%	0.98%	1.58%	0.92%	2.39%	19.26%	32.01%
3-METHYLHEXANAL	0.57%	0.45%	5.22%	2.09%	2.90%	26.42%	37.44%
3-METHYLHEXANE	0.42%	1.19%	1.80%	0.62%	2.20%	17.43%	30.66%
3-METHYLNONANE	0.40%	0.38%	2.05%	0.74%	2.26%	21.53%	34.91%
3-METHYLOCTANE	0.54%	0.60%	1.72%	0.65%	2.59%	20.63%	32.13%
3-METHYLPENTANE	0.38%	1.05%	1.88%	1.18%	2.07%	14.27%	21.80%
3-METHYLPYRIDINE	0.24%	0.70%	2.22%	0.93%	2.80%	20.51%	19.88%
3-METHYLTHIOPHENE	0.31%	0.38%	1.74%	3.01%	1.55%	11.38%	25.37%
3-METHYL-trans-2-PENTENE	1.00%	0.59%	3.47%	7.61%	2.52%	22.24%	30.95%
3-METHYLTRIDECANE	0.49%	0.52%	1.85%		2.43%	25.27%	36.76%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
3-METHYLUNDECANE	0.09%	0.56%			2.58%	23.97%	33.71%
3-NITROBENZOTRIFLUORIDE	1.96%	1.87%	3.41%		4.29%	42.06%	43.52%
3-NONANONE	1.87%	0.61%	0.0410622	0.00%	2.26%	24.24%	40.24%
3-OCTANONE	0.72%	0.25%	2.27%		2.64%	24.33%	29.46%
3-PENTANOL	6.07%	1.77%			0.26%	15.14%	28.49%
3-PENTANONE	0.79%	1.11%	3.89%	0.58%	2.67%	23.64%	23.72%
3-PHENYL-1-PROPANOL	1.08%	0.82%		19.72%	0.45%	7.17%	27.45%
4-((2-HYDROXYETHOXY)CARBONYL) BENZOIC ACID	1.36%	0.89%	4.71%		0.44%	7.57%	32.67%
4-(2-METHOXYETHYL)MORPHOLINE	1.67%	0.64%	2.99%		2.52%	26.34%	33.75%
4,4'-DIISOPROPYLBIPHENYL	0.67%	1.02%	1.50%		3.10%	32.27%	39.66%
4,4'-DINITRODIPHENYLAMINE	1.25%	0.48%	3.22%		0.96%	13.23%	37.96%
4,4'-DINITROTRIPHENYLAMINE	1.20%	0.33%	3.01%		1.12%	16.05%	41.11%
4,6-DIMETHYLDIBENZOTHIOPHENE	0.59%	1.61%	2.74%		4.13%	39.78%	41.32%
4-[2-(2-AMINOETHOXY)ETHYL]MORPHOLINE	1.28%	1.54%	4.39%	3.43%	0.29%	0.17%	21.88%
4-CHLORO-3-NITROBENZOTRIFLUORIDE	1.06%	1.13%	1.95%		3.52%	31.43%	41.61%
4-CHLORO- <i>o</i> -XYLENE	0.63%	0.75%	2.77%		3.52%	30.10%	39.20%
4-ETHYL- <i>m</i> -XYLENE	0.39%	0.82%	4.08%	1.29%	2.76%	23.69%	32.77%
4-ETHYL- <i>o</i> -XYLENE	0.14%	0.66%	2.33%	1.17%	2.63%	23.83%	30.99%
4-HEPTANONE	0.09%	1.07%	2.25%	2.66%	2.82%	24.28%	31.65%
4-HYDROXYACETOPHENONE	2.66%	0.90%			3.58%	24.59%	35.94%
4-HYDROXYBUTYRALDEHYDE	0.86%	0.29%	3.57%	3.51%	1.88%	23.44%	39.83%
4-HYDROXYMETHYL BENZOIC ACID	2.50%	2.86%	10.98%		1.76%	14.67%	22.06%
4-HYDROXYSTYRENE	1.08%	1.00%	2.10%	3.49%	0.22%	3.91%	20.66%
4-ISOBUTYLSTYRENE	0.52%	1.29%	3.56%	1.26%	3.73%	34.95%	37.83%
4-METHOXYPHENYLACETIC ACID	1.41%	2.95%	8.42%		1.83%	14.14%	16.12%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
4-METHYL DIBENZOTHIOPHENE	0.68%	0.58%			2.53%	23.32%	31.29%
4-METHYL-1-HEPTENE	0.33%	0.45%	2.35%		2.41%	19.90%	30.94%
4-METHYL-1-HEXENE	0.71%	0.82%	2.71%	2.00%	1.31%	11.14%	22.32%
4-METHYL-1-OCTANOL	0.30%	1.02%			0.63%	6.42%	31.00%
4-METHYL-1-PENTENE	0.23%	0.60%	2.31%	3.17%	1.53%	12.03%	23.74%
4-METHYL-2-PENTANOL	2.03%	1.65%	2.29%		0.08%	6.39%	20.73%
4-METHYL-cis-2-PENTENE	0.58%	0.42%	2.24%	4.56%	1.66%	13.49%	24.13%
4-METHYL-CYCLOHEXANE-METHANOL	2.67%	1.79%	3.98%		0.16%	4.80%	32.40%
4-METHYLCYCLOPENTENE	0.39%	1.58%	6.50%	2.39%	0.86%	6.44%	16.72%
4-METHYLGUAIACOL	0.66%	0.49%	3.15%		0.61%	6.76%	20.31%
4-METHYLHEPTANE	0.28%	0.81%	1.95%	0.93%	2.33%	19.27%	28.76%
4-METHYLNONANE	0.34%	0.68%	2.02%	2.36%	2.26%	20.27%	34.25%
4-METHYLOCTANE	0.47%	0.57%	1.74%	1.99%	2.56%	20.31%	33.08%
4-METHYLPHENANTHRENE	1.02%	1.76%	5.09%		4.26%	43.32%	42.26%
4-METHYLPYRIDINE	0.14%	0.89%	2.75%	0.73%	2.74%	19.94%	17.88%
4-METHYL-trans-2-PENTENE	0.55%	0.47%	1.90%	3.06%	1.66%	13.52%	24.63%
4-NONANONE	1.09%	1.25%	2.01%		2.10%	21.41%	29.77%
4-OCTANONE	2.21%	0.51%	4.63%		1.96%	21.69%	28.66%
5-(HYDROXYMETHYL) FURFURAL	1.13%	0.15%	1.59%		1.60%	18.36%	33.25%
5-ETHYLIDENE-2-NORBORNENE	0.31%	0.53%	2.22%		2.01%	16.75%	25.64%
5-ETHYL-m-XYLENE	0.36%	0.83%	2.23%	1.48%	3.09%	26.77%	36.95%
5-HEXEN-2-ONE	0.62%	0.48%			3.42%	27.12%	39.33%
5-METHYL FURFURAL	0.14%	0.44%	2.11%		2.33%	19.61%	28.67%
5-METHYL-1-HEXANOL	1.60%	0.42%	3.31%		0.02%	3.66%	28.10%
5-METHYL-1-HEXENE	0.76%	0.50%	2.82%	4.99%	1.92%	16.23%	28.11%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
5-METHYL-2-HEXANONE	0.45%	0.61%	1.16%		2.92%	22.68%	31.22%
5-METHYLINDAN	0.85%	0.66%			2.81%	19.44%	27.19%
5-METHYLNONANE	0.81%	0.61%	1.59%	3.14%	2.83%	21.70%	34.25%
5-NONANONE	0.48%	0.59%	1.45%	0.75%	3.45%	30.79%	36.53%
5-o-TOLYL-2-PENTENE	0.68%	0.56%	1.65%		2.51%	23.73%	35.07%
6-AMINOHEXANAMIDE	0.96%	0.17%	1.51%	4.41%	1.77%	19.84%	34.40%
6-AMINOHEXANOL	2.41%	2.21%	7.12%		1.13%	6.78%	22.88%
6-HYDROXYHEXANOIC ACID	1.15%	1.90%			0.64%	3.98%	29.92%
6-METHYL-1-HEPTENE	0.55%	0.42%	2.18%	3.03%	2.37%	19.41%	31.30%
6-METHYL-1-OCTANOL	0.41%	0.85%			0.67%	7.39%	31.36%
7-METHYL-1-OCTENE	0.77%	0.83%	3.23%	1.96%	2.99%	27.15%	32.72%
8-HYDROXYQUINOLINE	0.92%	0.78%	1.07%		1.40%	14.56%	20.99%
8-METHYL-1-NONANOL	4.95%	0.75%			0.50%	14.44%	31.06%
8-METHYL-1-NONENE	0.76%	1.39%	3.83%	1.27%	3.92%	37.10%	39.14%
8-METHYLQUINOLINE	0.72%	0.45%	1.70%	3.77%	1.74%	9.81%	15.52%
ACENAPHTHALENE	1.30%	0.10%	1.96%	3.47%	1.56%	15.58%	26.09%
ACENAPHTHENE	1.07%	1.20%	3.87%	3.04%	4.31%	45.12%	29.84%
ACETAL	2.20%	0.83%	6.07%	3.92%	0.67%	0.85%	15.55%
ACETALDEHYDE	0.30%	1.42%	20.00%		5.51%	43.51%	50.56%
ACETALDOL	1.06%	2.97%			3.10%	35.06%	34.66%
ACETALDOXIME	0.36%	1.55%	1.21%		2.59%	24.42%	22.36%
ACETAMIDE	1.98%	2.20%	8.01%	5.56%	5.83%	62.64%	48.63%
ACETAMINOPHEN	1.85%	3.92%	11.17%	1.83%	3.15%	23.66%	5.94%
ACETANILIDE	0.56%	1.17%	3.56%		3.49%	35.98%	42.56%
ACETIC ACID	2.65%	1.19%		5.52%	8.15%	59.85%	60.19%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
ACETIC ANHYDRIDE	0.16%	1.70%	3.05%	4.76%	3.83%	34.20%	38.12%
ACETOACETANILIDE	0.86%	0.75%	1.49%		2.56%	30.06%	42.55%
ACETOACETIC ACID	1.31%	0.47%	1.32%		2.15%	25.29%	38.05%
ACETOIN	1.09%	0.73%	1.61%		2.63%	26.85%	35.19%
ACETONE	2.05%	1.67%	5.06%	5.02%	3.97%	34.27%	40.66%
ACETONE CYANOHYDRIN	1.22%	0.16%	1.59%		1.70%	20.71%	36.59%
ACETONITRILE	9.31%	17.26%	12.02%		5.89%	63.18%	61.51%
ACETOPHENONE	0.19%	0.95%	2.52%		2.88%	23.08%	27.06%
ACETOVANILLONE	1.33%	0.99%	3.13%		0.28%	5.99%	27.80%
ACETOXYACETIC ACID	0.59%	2.48%	2.61%		5.30%	60.72%	57.60%
ACETYL CHLORIDE	3.16%	0.74%	4.10%	6.75%	3.36%	15.07%	25.14%
ACETYLENE	0.17%	0.30%	2.34%	2.10%	2.04%	12.69%	24.29%
ACETYLSALICYLIC ACID	1.06%	0.14%	1.54%	3.21%	1.60%	20.71%	38.25%
ACRIDINE	0.93%	0.22%	1.87%	1.18%	2.80%	22.50%	26.90%
ACROLEIN	4.25%	1.35%	5.31%	6.53%	5.30%	39.84%	42.37%
ACROLEIN CYANOHYDRIN	1.00%	0.49%			2.11%	25.82%	41.25%
ACRYLIC ACID	1.27%	0.99%		5.13%	2.99%	29.16%	44.78%
ACRYLONITRILE	1.32%	3.31%			7.15%	59.06%	48.68%
ACRYLOXY PROPIONIC ACID	0.28%	0.65%			2.59%	27.49%	40.90%
ADAMANTANE	0.89%	1.02%		0.73%	4.46%	34.04%	37.58%
ADIPIC ACID	2.66%	0.97%			2.34%	30.05%	44.15%
ADIPONITRILE	2.53%	2.46%			6.93%	86.02%	88.39%
AGATHADIOL	1.62%	1.73%	7.13%		0.48%	3.10%	32.03%
AIR	0.52%	0.82%	5.45%	6.97%	0.05%	1.22%	6.34%
ALLYL ACETATE	1.62%	0.87%	6.15%		3.01%	22.95%	30.34%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
ALLYL ACRYLATE	1.63%	0.41%	2.52%		2.07%	21.32%	30.10%
ALLYL ALCOHOL	0.85%	1.52%	2.10%	6.60%	1.97%	19.67%	29.24%
ALLYL ETHER	1.29%	0.89%	3.44%		2.92%	25.39%	30.33%
ALLYL GLYCIDYL ETHER	0.41%	0.48%	1.40%		2.40%	20.76%	29.43%
ALLYL METHACRYLATE	1.45%	0.79%	3.34%		2.75%	24.68%	32.68%
ALLYLAMINE	0.58%	1.28%	2.58%		2.47%	20.18%	9.60%
ALLYLIDENE DIACETATE	1.42%	0.23%	1.49%		1.80%	19.94%	31.87%
ALLYL-TERT-BUTYLPEROXIDE	0.69%	0.54%	1.97%		0.99%	7.66%	21.20%
alpha-EPOCHLOROHYDRIN	2.09%	1.77%	6.91%		5.08%	38.25%	49.29%
alpha-HYDROXYISOBUTYRAMIDE	0.69%	0.70%	3.10%		0.71%	8.07%	25.90%
alpha-HYDROXYISOBUTYRIC ACID	1.54%	1.92%	6.56%		0.77%	4.89%	24.26%
alpha-METHYLBENZYL ALCOHOL	2.46%	0.28%	4.16%		2.03%	23.28%	31.42%
alpha-METHYLBENZYL ALCOHOL FORMATE	0.52%	0.34%	2.40%		2.24%	21.17%	31.86%
alpha-METHYLSTYRENE	0.71%	1.46%	3.77%	0.83%	2.81%	24.29%	35.20%
alpha-PHELLANDRENE	1.25%	1.11%	4.49%	0.52%	1.39%	16.10%	30.44%
alpha-PINENE	2.20%	0.43%			2.71%	25.77%	42.44%
alpha-TERPINENE	0.49%	0.63%	2.24%	0.85%	2.36%	20.34%	31.37%
alpha-TERPINEOL	0.41%	0.90%	4.76%		0.49%	5.54%	25.08%
alpha-TOCOPHEROL	0.92%	0.37%	3.10%		1.71%	22.43%	43.87%
AMINOACETONITRILE	0.63%	1.76%	4.04%	6.67%	4.40%	42.13%	41.94%
AMINOCAPRONITRILE	0.32%	1.23%	3.08%	0.49%	3.50%	37.41%	43.62%
AMMONIA	2.92%	1.76%	9.57%	6.37%	3.64%	31.83%	37.53%
AMMONIUM CHLORIDE	7.63%	9.09%			16.93%	82.09%	82.41%
AMMONIUM SULFIDE	8.05%	10.65%			9.14%	89.16%	75.38%
ANETHOLE	0.58%	0.96%	2.84%		3.37%	31.90%	43.35%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
ANILINE	0.62%	0.23%	4.22%	5.14%	1.30%	11.47%	18.45%
ANISOLE	0.20%	0.34%	1.98%		2.04%	17.13%	24.93%
ANTHRACENE	4.60%	1.73%	4.15%	2.24%	4.42%	42.26%	50.60%
ANTHRAQUINONE	4.02%	0.47%	7.68%		3.09%	29.83%	36.53%
ANTIMONY TRICHLORIDE	4.89%	3.38%			6.45%	59.03%	69.09%
ARGON	0.42%	0.47%	2.11%	5.41%	0.00%	0.11%	14.44%
ARSENIC (III) CHLORIDE	0.20%	0.82%	1.97%	2.73%	2.87%	21.54%	28.46%
ARSINE	0.98%	1.08%	3.29%	13.93%	1.21%	8.07%	61.38%
AZELAIC ACID	3.80%	0.69%			1.26%	22.39%	49.82%
BENZALDEHYDE	0.17%	0.76%	2.88%	1.20%	2.67%	21.69%	27.85%
BENZAMIDE	0.89%	0.18%	0.91%		1.82%	18.69%	30.70%
BENZENE	0.50%	0.47%	3.00%	2.55%	1.96%	14.07%	24.31%
BENZENE-1,2,4-TRICARBOXYLIC ACID TRIMETHYL ESTER	1.65%	0.39%			2.24%	21.16%	38.79%
BENZIDINE	1.14%	0.47%	1.69%		1.00%	12.41%	30.91%
BENZO[b]FLUORANTHENE	0.77%	3.15%			6.74%	73.56%	61.79%
BENZOIC ACID	4.43%	0.36%	7.48%	11.79%	0.77%	20.59%	35.36%
BENZONITRILE	0.44%	1.53%	3.28%		3.85%	33.15%	47.44%
BENZOPHENONE	0.72%	0.36%	1.03%		2.19%	15.45%	20.88%
BENZOTHIOPHENE	0.95%	2.78%	1.55%		2.05%	11.26%	17.37%
BENZOTRICHLORIDE	0.44%	1.24%	3.96%		3.51%	27.35%	36.81%
BENZOTRIFLUORIDE	0.88%	0.42%	3.52%	1.44%	3.11%	25.86%	35.79%
BENZOYL CHLORIDE	0.81%	0.84%	4.87%		2.33%	19.61%	29.64%
BENZYL ACETATE	0.53%	1.51%	1.72%		2.37%	21.60%	35.68%
BENZYL ALCOHOL	4.35%	0.34%			2.28%	29.39%	19.45%
BENZYL CHLORIDE	1.20%	0.93%	4.81%	12.03%	3.02%	26.52%	35.07%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
BENZYL DICHLORIDE	1.10%	1.83%	5.36%		3.62%	26.31%	37.39%
BENZYL ETHYL ETHER	0.62%	0.46%	2.82%		2.43%	23.41%	33.47%
BENZYL FORMATE	0.61%	1.14%	2.74%	3.59%	2.66%	24.19%	35.73%
BENZYL MERCAPTAN	0.60%	1.59%	4.93%	1.02%	2.75%	21.88%	33.55%
BENZYLAMINE	0.22%	0.54%	1.81%		2.24%	18.51%	17.65%
beta-PHELLANDRENE	1.21%	0.73%	3.38%	0.50%	1.69%	16.54%	30.77%
beta-PINENE	0.92%	1.14%	2.13%		3.78%	26.20%	30.70%
beta-TERPINEOL	1.34%	1.51%	4.53%		0.33%	0.07%	21.69%
BICYCLO[2.2.1]HEPTANE	0.39%	0.75%	3.09%		2.64%	18.09%	26.54%
BICYCLO[2.2.2]OCTANE	0.96%	0.39%		1.61%	4.19%	31.26%	25.06%
BICYCLOHEXYL	1.00%	0.50%	1.63%		3.13%	22.89%	31.61%
BIPHENYL	0.58%	0.25%	1.72%	1.48%	2.66%	22.20%	27.53%
BIS-(2-AMINOETHYL)ETHER	3.56%	4.47%			3.67%	22.24%	5.41%
BIS(alpha-METHYLBENZYL) ETHER	2.25%	0.96%			3.06%	33.00%	37.81%
BIS(CHLOROMETHYL)ETHER	0.56%	1.02%	3.28%		3.15%	26.16%	35.80%
BIS(CYANOETHYL)ETHER	0.68%	1.80%	3.31%		6.27%	72.94%	103.40%
BIS(DIFLUOROMETHYL)ETHER	0.69%	0.36%	1.93%		1.83%	15.78%	23.53%
BIS(TRIFLUOROMETHYL)SULFIDE	0.96%	0.25%			1.23%	6.17%	18.97%
BIS[3-(TRIMETHOXSILYL)PROPYL]DISULFIDE	1.15%	1.86%	5.62%		0.11%	3.31%	40.42%
BORON TRIBROMIDE	1.87%	0.26%			2.17%	9.30%	20.36%
BORON TRICHLORIDE	1.40%	0.46%	7.45%		3.94%	29.84%	118.21%
BORON TRIFLUORIDE	1.16%	0.93%	2.89%	2.48%	2.61%	17.62%	17.23%
BROMINE	0.57%	0.33%	2.56%	4.43%	0.30%	4.49%	16.43%
BROMOBENZENE	0.80%	0.64%	1.87%	1.10%	3.00%	19.13%	26.85%
BROMOCHLORODIFLUOROMETHANE	0.16%	0.46%	1.47%	7.81%	1.71%	10.24%	12.86%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
BROMOCHLOROMETHANE	0.50%	0.91%	3.00%		1.83%	13.73%	16.96%
BROMODIFLUOROMETHANE	0.38%	0.81%	5.07%		1.75%	13.51%	33.22%
BROMOETHANE	1.71%	0.90%	1.60%		2.01%	11.00%	22.99%
BROMOMETHANE	0.34%	0.72%	1.39%	4.12%	2.24%	12.73%	22.10%
BROMOTRICHLOROMETHANE	0.25%	0.20%	1.32%	1.93%	0.98%	6.65%	18.99%
BROMOTRIFLUOROETHYLENE	0.39%	1.65%	2.84%	2.32%	1.45%	10.23%	11.82%
BROMOTRIFLUOROMETHANE	0.23%	0.29%	2.87%	12.81%	1.46%	9.26%	18.73%
BUTANAL	0.22%	0.63%	2.80%		2.99%	21.94%	30.85%
BUTYL VINYL ETHER	0.53%	0.38%	1.70%		2.13%	17.97%	30.80%
BUTYRONITRILE	4.64%	2.65%	6.50%		5.13%	47.83%	43.69%
CAMPHENE	0.42%	0.55%	4.10%		3.21%	26.46%	28.85%
CAMPHOR	0.57%	0.75%	4.27%		3.04%	23.58%	30.13%
CARBAMYL CHLORIDE	1.33%	4.29%	13.46%		4.05%	26.87%	3.41%
CARBON DIOXIDE	0.16%	0.29%	4.08%	2.61%	1.66%	11.98%	21.49%
CARBON DISULFIDE	0.42%	0.61%	3.10%	5.58%	1.61%	10.44%	20.77%
CARBON MONOXIDE	0.38%	0.26%	1.59%	11.63%	0.03%	0.35%	11.53%
CARBON TETRACHLORIDE	0.29%	0.34%	2.08%	6.26%	1.83%	12.20%	22.51%
CARBON TETRAFLUORIDE	0.19%	0.16%	0.46%	0.76%	1.01%	5.99%	17.74%
CARBONYL FLUORIDE	3.02%	3.52%	8.16%	11.67%	3.32%	19.63%	1.35%
CARBONYL SULFIDE	1.12%	2.09%	1.95%	7.97%	1.33%	6.86%	22.39%
CHLORINE	0.65%	0.37%	0.77%	6.70%	0.82%	7.63%	20.93%
CHLORINE TRIFLUORIDE	2.03%	4.05%	10.81%	2.47%	8.67%	88.24%	63.08%
CHLOROACETALDEHYDE	0.65%	2.04%	5.80%		5.16%	43.98%	42.51%
CHLOROACETIC ACID	0.82%	1.27%	3.42%		4.18%	41.98%	48.84%
CHLOROACETYL CHLORIDE	0.88%	0.71%			2.59%	22.92%	28.62%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
CHLOROCYCLOHEXANE	0.38%	0.74%	1.97%		2.78%	19.36%	26.58%
CHLORODIFLUOROMETHANE	0.23%	0.53%	3.00%	1.98%	2.20%	15.66%	24.03%
CHLOROFLUOROMETHANE	1.59%	2.81%	4.10%	10.78%	5.52%	35.21%	36.74%
CHLOROFORM	0.74%	0.34%	1.12%	2.06%	1.58%	9.95%	13.67%
CHLOROMETHYL METHYL ETHER	0.61%	2.82%	3.86%		2.91%	23.37%	34.14%
CHLOROPENTAFLUROETHANE	0.35%	0.10%	1.18%	2.45%	1.41%	9.64%	23.03%
CHLOROPRENE	0.48%	0.72%	3.00%		2.74%	20.87%	25.11%
CHLOROTRIFLUOROETHYLENE	0.41%	1.19%	1.88%		2.09%	13.94%	22.30%
CHLOROTRIFLUOROMETHANE	0.10%	0.28%	1.55%	1.77%	1.27%	8.52%	19.97%
CHRYSENE	0.58%	2.09%	4.35%	2.12%	5.06%	53.68%	51.57%
CINNAMIC ACID	2.41%	0.13%			2.38%	29.03%	44.77%
cis,trans-2,4-HEXADIENE	0.61%	1.00%	3.90%	2.39%	3.38%	27.10%	34.47%
cis-1,2-DICHLOROETHYLENE	2.06%	1.62%	7.40%	10.42%	2.51%	23.37%	29.69%
cis-1,2-DIMETHYLCYCLOHEXANE	1.27%	0.97%	5.48%	1.43%	2.98%	26.45%	24.28%
cis-1,2-DIMETHYLCYCLOPENTANE	0.24%	0.31%	1.55%	1.35%	2.00%	13.83%	22.88%
cis-1,3-DICHLOROPROPENE	0.91%	0.76%	2.67%		2.55%	20.39%	27.35%
cis-1,3-DIMETHYLCYCLOHEXANE	1.10%	0.69%	4.22%	1.27%	2.13%	19.04%	23.90%
cis-1,3-DIMETHYLCYCLOPENTANE	0.45%	0.45%	2.77%	2.09%	0.81%	6.67%	23.13%
cis-1,3-PENTADIENE	2.78%	0.88%	8.77%	5.68%	2.32%	25.10%	33.98%
cis-1,4-DIMETHYLCYCLOHEXANE	1.35%	0.93%	5.25%	1.81%	2.47%	22.65%	22.64%
cis-1,8-TERPIN	1.82%	2.94%	9.23%		1.94%	15.44%	18.51%
cis-1-PROPENYLBENZENE	0.50%	1.82%	2.72%	4.62%	2.98%	26.11%	35.99%
cis-2-BUTENE	0.10%	0.35%	2.19%	3.34%	1.86%	13.28%	22.52%
cis-2-DECENE	0.85%	0.49%	2.34%	4.33%	2.53%	24.16%	33.81%
cis-2-DODECENE	0.97%	0.49%	1.92%	5.15%	2.32%	24.07%	33.91%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
cis-2-HEPTENE	0.36%	0.68%	3.76%	1.70%	3.02%	22.76%	31.99%
cis-2-HEXENE	0.24%	0.66%	3.41%	1.51%	2.70%	20.58%	30.01%
cis-2-METHYLCYCLOHEXANOL	2.89%	1.02%	3.35%	3.47%	1.43%	6.47%	20.05%
cis-2-NONENE	0.27%	0.59%	3.61%		2.76%	24.71%	33.22%
cis-2-OCTENE	0.96%	0.66%	3.19%	3.04%	3.03%	23.71%	32.48%
cis-2-PENTENE	0.32%	1.02%	2.41%	2.00%	2.01%	14.94%	23.86%
cis-2-PHENYLBUTENE-2	0.67%	1.27%	3.48%		3.64%	31.18%	34.20%
cis-3-HEPTENE	0.49%	0.78%	3.87%	1.87%	2.62%	22.05%	26.33%
cis-3-HEXENE	0.23%	0.62%	2.40%	2.39%	2.26%	18.42%	26.78%
cis-3-METHYLCYCLOHEXANOL	1.97%	1.80%	2.92%	0.76%	0.28%	2.04%	22.20%
cis-3-OCTENE	0.62%	0.69%	3.16%	2.37%	2.95%	22.87%	32.08%
cis-4-METHYLCYCLOHEXANOL	0.66%	1.19%	3.38%	1.32%	0.14%	2.75%	21.62%
cis-4-OCTENE	0.49%	0.63%	5.11%	2.37%	2.91%	22.67%	31.84%
cis-CROTONALDEHYDE	0.29%	0.83%	2.11%	5.22%	2.94%	24.72%	30.16%
cis-CROTONIC ACID	0.77%	0.72%			3.04%	31.00%	41.30%
cis-CROTONITRILE	6.72%	3.03%	12.31%	5.46%	5.18%	53.51%	53.10%
cis-DECAHYDRONAPHTHALENE	0.43%	0.54%	5.51%	3.36%	2.41%	18.23%	26.95%
cis-STILBENE	0.49%	0.84%	2.01%		3.22%	26.24%	33.05%
CITRACONIC ACID	0.77%	1.58%	1.85%		3.57%	46.01%	59.37%
CROTYL GLYCOL ETHER	1.62%	0.43%			1.93%	21.54%	33.05%
CUMENE	0.22%	0.69%	2.41%	4.17%	2.36%	19.15%	25.57%
CYANOGEN	0.25%	0.05%	2.06%		2.33%	18.28%	23.98%
CYANOGEN CHLORIDE	1.20%	1.06%	7.25%	5.21%	4.56%	39.48%	27.45%
CYCLOBUTANE	0.82%	1.17%	1.43%	0.88%	1.75%	9.98%	21.89%
CYCLOHEPTANE	0.17%	0.48%	1.76%	1.82%	1.75%	12.56%	24.18%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
CYCLOHEPTENE	0.70%	0.68%	3.95%	3.75%	0.90%	9.57%	23.01%
CYCLOHEXANE	0.46%	0.19%	3.54%	1.45%	1.57%	11.55%	22.14%
CYCLOHEXANECARBOXALDEHYDE	0.64%	0.93%		1.47%	3.19%	24.47%	30.64%
CYCLOHEXANOL	5.84%	0.48%	8.74%	15.42%	0.74%	18.66%	31.35%
CYCLOHEXANONE	0.15%	1.26%	3.92%		4.30%	33.68%	45.48%
CYCLOHEXANONE OXIME	1.12%	1.72%	4.13%		0.79%	4.18%	14.50%
CYCLOHEXENE	0.40%	0.44%	1.33%	1.56%	1.82%	12.45%	22.69%
CYCLOHEXYL ACETATE	0.94%	0.38%	3.11%	0.80%	1.65%	16.15%	32.02%
CYCLOHEXYL FORMATE	0.47%	0.73%	2.06%	1.61%	2.49%	18.77%	32.25%
CYCLOHEXYL HYDROPEROXIDE	1.51%	1.20%	2.96%		0.09%	4.48%	26.67%
CYCLOHEXYL ISOCYANATE	0.84%	1.65%	3.25%		2.79%	27.45%	23.92%
CYCLOHEXYL MERCAPTAN	0.31%	0.61%	1.54%	2.62%	2.12%	14.69%	30.57%
CYCLOHEXYLAMINE	1.70%	0.21%	4.37%	2.69%	1.79%	9.03%	12.73%
CYCLOHEXYLBENZENE	2.27%	1.40%	4.26%		1.65%	18.79%	35.34%
CYCLOOCTANE	0.49%	0.61%	2.50%	5.02%	1.73%	13.97%	22.89%
CYCLOOCTENE	0.83%	0.28%	3.32%	7.85%	1.24%	12.18%	22.99%
CYCLOPENTADIENE	3.70%	1.19%	6.69%	4.88%	1.28%	8.55%	21.26%
CYCLOPENTANE	0.15%	1.11%	1.38%	1.66%	1.62%	11.14%	20.94%
CYCLOPENTANONE	0.99%	1.05%	4.08%	2.98%	3.81%	31.10%	45.84%
CYCLOPENTENE	0.22%	0.41%	1.81%	1.13%	1.49%	9.59%	19.48%
CYCLOPENTYLACETIC ACID	2.24%	0.14%		7.65%	1.54%	18.47%	32.21%
CYCLOPENTYLAMINE	0.86%	1.09%	3.81%		1.07%	10.51%	13.25%
CYCLOPROPANE	0.27%	0.33%	2.07%	3.77%	1.46%	8.06%	22.90%
CYCLOPROPANE CARBOXYLIC ACID	0.31%	0.35%		17.38%	1.06%	10.26%	25.08%
CYCLOPROPANECARBOXAMIDE	0.77%	2.04%	3.10%		4.77%	50.92%	49.30%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
CYCLOPROPYL CYANIDE	3.36%	2.65%		5.98%	6.48%	59.13%	58.96%
CYCLOPROPYLAMINE	1.32%	0.31%			2.35%	15.99%	29.07%
DECAFLUOROBUTANE	0.70%	0.27%	0.80%		1.30%	11.05%	21.94%
DECAMETHYLCYCLOPENTASILOXANE	2.08%	0.21%	3.00%		1.60%	21.46%	34.41%
DECAMETHYLTETRAILOXANE	1.18%	0.88%	3.82%		0.57%	8.47%	26.91%
DECANAL	2.17%	1.03%	1.46%		0.32%	7.04%	24.95%
DEHYDROABIETIC ACID	1.15%	0.56%	3.24%		0.87%	11.39%	33.81%
DEHYDROABIETYLAMINE	0.88%	0.33%	1.55%		2.02%	23.46%	37.93%
DEUTERIUM OXIDE	4.06%	1.72%	9.59%	11.88%	4.61%	44.86%	46.26%
DI-(2-CHLOROETHOXY)METHANE	0.21%	0.81%	2.27%		3.01%	28.13%	35.34%
DI(2-CHLOROETHYL)ETHER	0.55%	1.00%		6.11%	3.47%	30.83%	41.25%
DI-(2-ETHYLHEXYL) MALEATE	1.21%	1.01%	2.66%		2.88%	37.59%	50.78%
DI-2-ETHYLHEXYLAMINE	1.59%	0.67%	2.84%		0.73%	11.24%	34.37%
DIACETYL	1.46%	0.78%	3.05%		2.65%	25.12%	31.46%
DIALLYL MALEATE	1.13%	0.27%	1.95%		1.53%	18.85%	36.02%
DIALLYL PHTHALATE	1.16%	0.60%	2.12%		2.01%	23.42%	37.66%
DIALLYL SULFIDE	4.52%	0.71%			2.76%	28.85%	40.06%
DIALLYLAMINE	0.80%	2.59%	1.78%		1.36%	13.62%	18.40%
DIAMYL KETONE	1.26%	0.68%			2.24%	24.39%	32.43%
DIAMYLAMINE	0.58%	0.61%	1.38%		1.46%	15.52%	32.81%
DIBENZOFURAN	1.00%	1.69%	1.12%	1.67%	3.11%	20.79%	26.75%
DIBENZOTHIOPHENE	0.61%	0.22%	1.37%		1.98%	15.50%	25.79%
DIBENZYL ETHER	5.65%	0.86%	4.65%		0.12%	16.83%	32.68%
DIBORANE	0.18%	0.26%	1.73%	2.48%	0.81%	4.41%	14.48%
DIBROMODIFLUOROMETHANE	1.50%	1.70%		9.02%	3.03%	21.79%	30.72%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
DIBROMOMETHANE	0.44%	0.47%	1.04%	4.08%	0.91%	4.55%	5.91%
DIBUTYL MALEATE	1.18%	0.77%	2.32%		1.00%	13.82%	45.26%
DIBUTYL SEBACATE	1.93%	1.04%	5.15%	4.32%	0.59%	11.12%	53.57%
DIBUTYL TEREPHTHALATE	0.61%	0.71%	3.59%		1.51%	18.32%	47.02%
DICHLOROACETALDEHYDE	0.52%	0.87%	2.17%		2.97%	24.04%	30.02%
DICHLOROACETIC ACID	0.92%	1.53%	1.81%		2.31%	23.70%	38.77%
DICHLOROACETYL CHLORIDE	0.58%	0.18%	1.89%		1.69%	13.99%	24.27%
DICHLORODIETHYLSILANE	2.03%	0.36%	1.85%		0.87%	10.83%	18.42%
DICHLORODIFLUOROMETHANE	0.03%	0.33%	2.48%	3.97%	1.45%	9.35%	19.19%
DICHLOROFLUOROMETHANE	0.48%	0.39%	2.68%	2.55%	1.75%	12.93%	23.18%
DICHLOROMETHANE	0.95%	1.27%	5.32%	8.11%	3.01%	20.28%	25.66%
DICHLOROSILANE	0.83%	0.64%			1.24%	9.58%	14.80%
DICYANDIAMIDE	1.08%	0.24%	1.34%		1.34%	15.65%	31.56%
DICYCLOHEXYL SULFIDE	0.59%	0.76%	0.90%	6.78%	1.77%	15.53%	18.64%
DICYCLOPENTADIENE	0.72%	4.44%	5.47%	5.96%	3.15%	27.67%	34.33%
DIETHANOLAMINE	0.33%	1.99%	2.83%		2.67%	30.54%	36.99%
DIETHYL CARBONATE	4.68%	1.19%	4.93%		2.80%	18.33%	32.28%
DIETHYL DISULFIDE	1.67%	0.64%	1.83%	0.18%	2.25%	12.95%	28.43%
DIETHYL ETHER	0.27%	0.35%	3.21%	6.56%	2.25%	17.34%	26.91%
DIETHYL MALEATE	1.04%	0.20%			1.13%	10.81%	42.14%
DIETHYL MALONATE	1.04%	0.41%	5.41%		1.62%	19.79%	38.81%
DIETHYL PHTHALATE	0.85%	0.87%	2.19%		3.11%	30.05%	38.32%
DIETHYL SUCCINATE	1.84%	0.90%	3.34%	4.57%	2.74%	19.94%	28.00%
DIETHYL SULFIDE	0.77%	0.40%	3.07%	0.68%	1.81%	15.22%	22.62%
DIETHYLALUMINUM CHLORIDE	1.84%	3.69%	7.42%		6.11%	58.37%	35.51%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
DIETHYLAMINE	0.82%	0.32%	2.68%	1.67%	2.24%	19.49%	23.25%
DIETHYLENE GLYCOL	1.97%	1.02%			3.60%	34.05%	43.79%
DIETHYLENE GLYCOL DIETHYL ETHER	0.80%	0.27%	1.53%		1.47%	14.71%	30.77%
DIETHYLENE GLYCOL DIMETHYL ETHER	0.29%	0.89%	1.52%		2.13%	20.10%	39.62%
DIETHYLENE GLYCOL DI-n-BUTYL ETHER	2.64%	0.49%			1.77%	13.70%	33.35%
DIETHYLENE GLYCOL ETHYL ETHER ACETATE	2.08%	0.21%	3.82%		1.32%	17.59%	30.67%
DIETHYLENE GLYCOL MONOBUTYL ETHER ACETATE	1.18%	0.62%		4.06%	0.74%	13.06%	33.95%
DIETHYLENE GLYCOL MONOPROPYL ETHER	0.13%	0.33%	1.48%	6.87%	1.48%	13.80%	28.34%
DIETHYLENTRIAMINE	1.33%	0.67%	2.45%		1.48%	17.26%	30.18%
DIETHYLSULFITE	1.18%	0.44%	4.85%		0.82%	5.63%	22.98%
DIFLUOROMETHANE	1.88%	1.82%	5.46%	3.71%	4.40%	35.26%	36.84%
DIFLUOROMETHYL TRIFLUOROMETHYL ETHER	0.53%	1.42%	1.08%	1.91%	1.63%	12.82%	37.27%
DIGLYCOLIC ACID	0.92%	1.03%	1.45%		2.72%	37.86%	55.34%
DIHEXYL ADIPATE	1.05%	0.36%	3.52%	4.09%	0.80%	10.94%	53.37%
DIIODOMETHANE	2.38%	1.56%	8.96%	30.12%	4.95%	39.61%	39.15%
DIISOBUTYL ETHER	0.50%	0.66%	2.76%	1.10%	1.09%	9.95%	26.41%
DIISOBUTYL KETONE	0.71%	0.31%	1.60%		2.65%	17.12%	31.66%
DIISOBUTYL PHTHALATE	1.20%	0.96%	3.21%		0.69%	9.45%	33.16%
DIISOBUTYLAMINE	0.83%	0.83%			0.79%	9.07%	19.36%
DIISONONYL PHTHALATE	2.78%	0.48%	6.45%		0.47%	13.12%	42.49%
DIISOCTYL PHTHALATE	1.24%	0.73%	3.45%	0.72%	1.06%	14.96%	40.76%
DIISOPENTYLSULFIDE	0.40%	0.70%	3.17%		1.43%	13.93%	30.69%
DIISOPROPYL ETHER	0.97%	0.23%	5.71%	0.43%	1.18%	12.26%	24.66%
DIISOPROPYL KETONE	0.92%	0.43%	5.00%		1.44%	15.20%	27.07%
DIISOPROPYL SULFIDE	0.36%	0.24%	1.54%	3.57%	1.23%	7.95%	21.18%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
DIISOPROPYLAMINE	4.22%	0.74%	7.40%		1.87%	3.23%	8.38%
DIKETENE	1.17%	0.48%		2.87%	0.75%	9.15%	22.41%
DILACTIC ACID	1.35%	2.12%	7.38%	4.25%	1.10%	7.70%	20.56%
DIMERCAPTOETHYL ETHER	0.52%	1.19%	3.41%		3.70%	32.52%	43.06%
DIMETHYL CARBONATE	0.90%	0.77%	2.33%		3.85%	28.40%	34.46%
DIMETHYL DISULFIDE	0.42%	0.50%	2.10%	3.74%	1.44%	10.74%	26.19%
DIMETHYL ETHER	0.24%	0.53%	2.68%	1.61%	1.99%	11.89%	21.47%
DIMETHYL GLUTARATE	2.31%	0.88%			2.85%	32.16%	38.13%
DIMETHYL ISOPHTHALATE	0.16%	0.96%	1.26%		3.43%	34.86%	41.09%
DIMETHYL MALEATE	0.27%	0.88%	2.41%	2.15%	3.33%	33.01%	44.16%
DIMETHYL PEROXIDE	1.09%	0.22%	0.85%		1.15%	10.83%	22.20%
DIMETHYL PHTHALATE	0.54%	0.80%	1.22%		2.89%	29.38%	37.68%
DIMETHYL SILANE	1.93%	1.09%	2.71%		2.89%	13.89%	21.30%
DIMETHYL SUCCINATE	1.53%	0.52%			3.10%	21.98%	30.93%
DIMETHYL SULFIDE	0.56%	0.30%	2.30%	2.84%	2.36%	14.82%	25.43%
DIMETHYL SULFOXIDE	1.99%	2.60%	9.64%	1.17%	4.52%	46.56%	57.53%
DIMETHYL TEREPHTHALATE	0.77%	0.72%			3.78%	34.59%	47.57%
DIMETHYL-1,4-CYCLOHEXANEDICARBOXYLATE	0.88%	0.72%	1.41%		2.72%	27.54%	35.53%
DIMETHYL-2,6-NAPHTHALENEDICARBOXYLATE	0.40%	0.90%	1.51%		2.94%	31.88%	41.09%
DIMETHYLACETYLENE	0.23%	0.48%	3.20%	0.45%	2.26%	17.45%	21.85%
DIMETHYLALUMINUM CHLORIDE	2.89%	2.94%			5.88%	57.89%	48.10%
DIMETHYLAMINE	1.65%	0.69%	2.98%	11.13%	2.21%	16.93%	26.06%
DIMETHYLCHLOROSILANE	0.93%	0.59%	5.44%		2.14%	13.41%	20.86%
DIMETHYLDICHLOROSILANE	0.71%	0.63%	2.47%	5.02%	1.20%	11.41%	15.42%
DIMETHYLDIMETHOXSILANE	3.10%	0.31%			2.35%	27.90%	23.80%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
DIMETHYLETHANOLAMINE	1.22%	0.83%	2.19%		0.65%	8.13%	27.60%
DIMETHYLKETENE	1.55%	0.33%		20.33%	1.42%	6.60%	19.27%
DIMETHYLMALONATE	3.38%	1.57%			1.25%	1.59%	30.28%
DIMETHYLMERCURY	1.44%	0.19%			1.33%	5.18%	18.31%
DI-n-BUTYL DISULFIDE	0.62%	0.63%	2.13%		2.00%	18.95%	30.14%
DI-n-BUTYL ETHER	0.73%	0.36%	2.23%	0.48%	1.98%	18.26%	35.12%
DI-n-BUTYL PHTHALATE	1.57%	0.54%	2.47%		2.15%	27.29%	40.96%
DI-n-BUTYL SULFIDE	0.11%	0.59%			2.22%	18.90%	35.26%
DI-n-BUTYL SULFONE	0.86%	0.49%	1.52%		2.33%	25.72%	47.08%
DI-n-BUTYLAMINE	1.18%	0.31%	2.05%	2.57%	2.35%	14.73%	26.86%
DI-n-DECYL PHTHALATE	1.17%	0.89%	4.52%		1.13%	17.17%	50.89%
DI-n-HEPTYL PHTHALATE	1.61%	0.48%	4.12%		1.09%	16.53%	40.54%
DI-n-HEXYL ETHER	1.12%	0.49%	1.73%	1.87%	1.44%	17.06%	43.87%
DI-n-HEXYL PHTHALATE	1.48%	0.38%	3.26%		1.53%	20.90%	42.00%
DI-n-NONYL PHTHALATE	1.13%	0.53%	3.66%		1.50%	20.20%	48.49%
DI-n-OCTYL ETHER	1.13%	0.90%	2.63%	0.81%	1.01%	13.78%	49.53%
DI-n-OCTYL TEREPHTHALATE	1.20%	0.24%	3.57%	0.83%	1.25%	17.66%	41.86%
DI-n-OCTYLAMINE	0.58%	1.20%	1.94%		3.16%	38.05%	47.77%
DINONYL ETHER	1.16%	0.34%			0.90%	13.17%	53.83%
DINONYLPHENOL	0.57%	1.90%	1.59%		3.76%	52.98%	63.90%
DI-n-PENTYL ETHER	1.00%	0.35%	6.40%	1.85%	1.98%	17.98%	39.09%
DI-n-PROPYL DISULFIDE	0.95%	0.45%	3.01%	1.22%	1.57%	14.88%	33.35%
DI-n-PROPYL ETHER	0.50%	0.77%	1.69%	1.27%	2.11%	14.19%	27.13%
DI-n-PROPYL PHTHALATE	1.77%	0.62%	2.77%		2.37%	29.10%	40.15%
DI-n-PROPYL SULFIDE	0.39%	0.53%	1.76%	0.58%	2.61%	19.14%	32.79%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
DI-n-PROPYL SULFONE	0.93%	0.84%	2.97%		2.74%	29.88%	46.86%
DI-n-PROPYLAMINE	0.75%	0.31%	0.96%	1.55%	1.66%	11.26%	20.76%
DI-n-UNDECYL PHTHALATE	1.29%	0.73%			0.86%	14.47%	50.77%
DIPHENYL CARBONATE	0.76%	0.37%	1.24%		2.12%	22.63%	35.13%
DIPHENYL DISULFIDE	4.06%	3.62%			2.91%	15.16%	10.34%
DIPHENYL ETHER	1.48%	1.25%	3.05%		3.34%	24.14%	37.17%
DIPHENYLACETYLENE	0.59%	0.69%	2.55%		2.66%	23.12%	30.14%
DIPHENYLAMINE	0.89%	0.83%	2.42%		2.94%	25.91%	32.10%
DIPHENYLDICHLOROSILANE	2.13%	0.59%		7.39%	3.35%	31.96%	43.65%
DIPHENYLMETHANE	1.31%	0.93%	3.52%		2.98%	26.18%	31.35%
DIPROPYL MALEATE	0.60%	0.17%	1.62%		1.54%	17.52%	41.77%
DIPROPYLENE GLYCOL MONOMETHYL ETHER ACETATE	0.87%	0.31%	2.43%	3.87%	1.49%	12.79%	29.71%
DIPROPYLENE GLYCOL n-BUTYL ETHER	1.60%	1.19%			0.54%	2.74%	29.45%
DI-sec-BUTYL ETHER	0.57%	0.44%	2.12%	1.29%	1.88%	11.84%	23.96%
DISILANE	0.93%	2.58%	7.22%		2.45%	15.70%	4.66%
DI-t-BUTYL PEROXIDE	0.63%	0.81%	1.83%		0.47%	4.34%	20.33%
DI-tert-BUTYL DISULFIDE	0.71%	2.34%			0.71%	6.97%	16.81%
DI-tert-BUTYL ETHER	1.90%	0.28%	4.12%		2.26%	22.94%	34.74%
DI-tert-BUTYL SULFIDE	0.94%	0.15%	1.54%		1.77%	15.28%	28.69%
DIVINYL ETHER	0.47%	0.24%	1.02%		1.44%	8.96%	20.77%
DODECAMETHYLCYCLOHEXASILOXANE	1.72%	0.14%	2.67%		1.40%	18.49%	34.30%
DODECAMETHYLPENTASILOXANE	1.46%	0.41%	3.10%		1.14%	14.41%	31.64%
DODECANAL	1.26%	0.92%	4.24%		0.41%	6.36%	25.72%
DODECANEDIOIC ACID	1.58%	1.01%			1.26%	17.01%	51.43%
D-XYLOSE	0.44%	0.43%			1.14%	11.49%	32.18%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
EICOSAMETHYLNONASILOXANE	1.53%	0.96%	5.99%		0.66%	10.94%	39.70%
ERUCIC ACID	1.08%	1.00%	3.17%		1.67%	24.71%	41.84%
ETHANE	0.17%	0.29%	1.16%	5.75%	1.05%	5.23%	19.37%
ETHANESULFONYL CHLORIDE	1.39%	1.04%			3.24%	25.22%	31.17%
ETHANOL	1.18%	2.54%	5.14%	46.68%	1.88%	21.91%	38.17%
ETHYL ACETATE	0.65%	0.52%	2.40%	4.02%	2.92%	23.71%	30.70%
ETHYL ACETOACETATE	0.30%	0.33%			2.84%	25.70%	32.90%
ETHYL ACRYLATE	0.92%	0.36%	4.42%		2.29%	21.66%	28.94%
ETHYL BENZOATE	0.89%	0.85%	6.81%		2.19%	21.35%	24.40%
ETHYL CAPRATE	2.51%	0.48%			2.15%	26.85%	37.45%
ETHYL CAPRYLATE	0.76%	0.31%	1.47%		2.02%	20.96%	33.11%
ETHYL CHLORIDE	0.25%	0.57%	3.01%	5.44%	2.36%	16.55%	26.09%
ETHYL CHLOROFORMATE	1.64%	1.94%	5.59%	6.79%	1.18%	7.86%	14.22%
ETHYL CYANOACETATE	0.45%	1.20%			5.17%	54.10%	57.38%
ETHYL FLUORIDE	0.54%	0.74%	3.95%		3.12%	20.75%	30.11%
ETHYL FORMATE	0.33%	0.57%	3.91%	4.05%	2.82%	22.48%	29.81%
ETHYL HYDROPEROXIDE	2.65%	1.15%	1.85%		0.05%	6.95%	23.47%
ETHYL IODIDE	0.99%	1.26%	5.63%		3.68%	30.13%	32.49%
ETHYL ISOAMYL KETONE	2.73%	0.25%			1.66%	20.18%	29.83%
ETHYL ISOBUTYL ETHER	0.69%	0.56%	1.50%		1.15%	10.28%	22.59%
ETHYL ISOBUTYRATE	0.34%	0.59%	4.02%	0.29%	1.98%	17.30%	23.00%
ETHYL ISOPROPYL ETHER	0.47%	0.41%	1.68%	0.97%	0.97%	8.01%	20.80%
ETHYL ISOPROPYL KETONE	1.00%	1.35%	3.92%		1.83%	17.93%	28.27%
ETHYL ISOVALERATE	2.22%	0.34%	6.22%	0.66%	0.94%	15.47%	29.81%
ETHYL LACTATE	0.33%	0.12%			1.58%	13.94%	27.05%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
ETHYL LAURATE	2.77%	0.68%			2.34%	30.91%	41.28%
ETHYL LEVULINATE	0.25%	0.63%			2.73%	25.56%	35.19%
ETHYL LINOLEATE	0.63%	1.47%	2.44%		2.57%	32.14%	37.61%
ETHYL LINOLENATE	0.86%	1.74%	1.89%		2.55%	32.14%	35.20%
ETHYL MERCAPTAN	0.11%	0.49%	2.43%	5.83%	1.87%	13.23%	21.73%
ETHYL METHACRYLATE	0.51%	0.45%	3.59%		2.91%	24.91%	31.21%
ETHYL METHYL DISULFIDE	1.25%	0.48%			1.70%	9.43%	21.05%
ETHYL MYRISTATE	2.23%	0.98%			2.77%	35.46%	44.62%
ETHYL n-BUTYRATE	0.24%	0.70%	2.79%	7.19%	3.38%	27.20%	33.11%
ETHYL n-HEXYL ETHER	0.78%	0.41%	1.83%	1.40%	1.83%	17.44%	34.87%
ETHYL n-OCTYL SULFIDE	0.63%	0.44%	1.03%		1.32%	9.35%	15.33%
ETHYL n-PENTYL SULFIDE	0.69%	0.37%	1.58%		2.08%	19.02%	34.93%
ETHYL OLEATE	0.11%	0.92%			2.84%	34.16%	48.77%
ETHYL PHENYL ACETATE	0.53%	0.44%	1.61%		2.31%	22.08%	31.92%
ETHYL PHENYL CARBONATE	0.98%	0.39%	1.16%		2.19%	21.73%	31.46%
ETHYL PROPIONATE	0.55%	0.54%	4.30%	1.23%	2.80%	24.16%	30.46%
ETHYL PROPYL DISULFIDE	0.64%	1.03%			1.18%	7.75%	21.44%
ETHYL PROPYL ETHER	3.62%	0.99%		3.29%	2.24%	11.33%	21.35%
ETHYL PROPYL SULFIDE	0.45%	0.60%	1.17%		2.40%	16.33%	25.56%
ETHYL STEARATE	1.57%	1.61%	5.38%		3.38%	44.52%	53.31%
ETHYL t-BUTYL SULFIDE	0.52%	0.44%	1.89%	2.44%	1.58%	13.12%	26.37%
ETHYL TERT-BUTYL DISULFIDE	0.13%	0.37%	2.37%		1.66%	12.65%	23.61%
ETHYL tert-PENTYL ETHER	0.83%	0.23%	3.97%	2.70%	1.54%	15.63%	22.18%
ETHYL THIOLACETATE	0.55%	0.45%	2.62%		2.16%	17.70%	25.91%
ETHYL VANILLIN	1.50%	0.92%	3.78%		0.35%	7.73%	35.75%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
ETHYL VINYL ETHER	0.35%	1.00%	2.49%	8.84%	2.24%	15.77%	23.02%
ETHYL-3-ETHOXYPROPIONATE	0.87%	1.50%	2.38%	1.34%	2.30%	22.67%	41.27%
ETHYLACETYLENE	0.25%	0.28%	1.75%	2.75%	1.73%	13.29%	27.45%
ETHYLAL	1.54%	0.31%	3.62%	3.28%	2.00%	13.27%	26.87%
ETHYLAMINE	1.04%	0.77%	3.16%	7.43%	1.92%	17.54%	8.67%
ETHYLBENZENE	0.10%	0.63%	3.83%	0.53%	2.58%	19.52%	26.72%
ETHYLBENZENE HYDROPEROXIDE	1.03%	0.91%	2.89%	4.13%	0.53%	7.62%	29.55%
ETHYLCHLOROACETATE	1.23%	0.77%	4.23%		3.11%	29.07%	38.20%
ETHYLCYCLOHEXANE	1.21%	0.58%	4.31%	0.64%	2.36%	21.29%	29.15%
ETHYLCYCLOPENTANE	0.15%	0.74%	1.46%	1.72%	2.01%	14.78%	23.79%
ETHYLDIETHANOLAMINE	2.29%	1.25%	2.80%		0.85%	12.87%	29.11%
ETHYLENE	0.23%	0.37%	1.90%	4.15%	0.93%	4.84%	18.49%
ETHYLENE CARBONATE	5.36%	1.64%	5.69%		5.76%	46.04%	70.96%
ETHYLENE GLYCOL	1.91%	1.68%	2.13%		2.50%	27.29%	29.95%
ETHYLENE GLYCOL DIACETATE	1.45%	0.70%	2.23%		2.63%	28.18%	36.21%
ETHYLENE GLYCOL DIACRYLATE	0.78%	0.51%			2.41%	25.23%	36.53%
ETHYLENE GLYCOL DINITRATE	0.70%	0.25%	2.74%		1.36%	16.55%	23.94%
ETHYLENE GLYCOL MONOPROPYL ETHER	5.13%	1.58%		10.39%	3.40%	22.51%	34.58%
ETHYLENE OXIDE	0.23%	0.65%	3.99%	0.76%	3.19%	23.48%	28.90%
ETHYLENEDIAMINE	0.98%	0.27%	1.25%	5.00%	2.99%	20.95%	1.03%
ETHYLENEIMINE	3.37%	0.58%	10.28%	7.45%	3.77%	38.13%	25.59%
ETHYLIDENE DIACETATE	0.90%	0.09%	1.96%	4.14%	2.00%	19.74%	33.03%
ETHYLNORBORNENE	0.42%	1.00%	3.10%		3.29%	24.45%	29.54%
ETHYLTRIACETOXSILANE	2.09%	2.17%		2.86%	4.76%	53.67%	50.05%
ETHYLTRICHLOROSILANE	1.14%	1.26%	1.79%		1.18%	10.49%	15.64%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
ETHYNYLBENZENE	0.72%	1.42%	3.18%	7.87%	1.89%	15.28%	26.78%
EUGENOL	0.80%	0.44%	1.29%		2.61%	26.15%	37.49%
FLUORANTHENE	4.05%	2.43%	13.78%		5.73%	48.63%	46.72%
FLUORENE	0.49%	2.29%	6.01%	0.67%	5.38%	50.56%	45.63%
FLUORINE	0.11%	0.21%	1.01%	2.77%	0.33%	0.92%	16.04%
FLUOROBENZENE	0.28%	0.28%	2.29%		2.28%	16.58%	26.81%
FORMANILIDE	0.73%	1.25%	2.70%		3.29%	32.87%	38.92%
FUMARIC ACID	0.58%	0.12%	2.98%	2.57%	1.96%	24.59%	44.47%
FUMARONITRILE	0.50%	3.34%	7.30%	9.11%	8.01%	87.48%	70.09%
FURAN	0.73%	0.33%	3.10%	4.56%	1.59%	14.20%	13.30%
FURAN 2,5-DICARBOXYLIC ACID	0.38%	1.94%			5.14%	70.33%	73.47%
FURFURAL	0.60%	0.47%	3.79%	4.85%	1.96%	17.70%	30.22%
FURFURYL ALCOHOL	1.17%	2.23%		8.05%	0.53%	6.17%	24.49%
GALLIUM TRICHLORIDE	4.75%	2.94%			8.32%	81.73%	91.45%
gamma-AMINOPROPYLTRIETHOXYLANE	2.61%	0.92%		12.78%	0.67%	1.54%	15.19%
gamma-BUTYROLACTONE	0.80%	2.36%		4.70%	5.76%	52.55%	45.19%
gamma-TERPINENE	0.99%	1.20%	2.15%	0.65%	2.20%	20.23%	33.80%
gamma-VALEROLACTONE	2.25%	1.95%	4.16%		4.03%	27.48%	49.21%
GERMANIUM TETRACHLORIDE	1.15%	0.76%	2.68%	0.75%	2.00%	10.96%	22.95%
GERMANIUM TETRAFLUORIDE	0.31%	0.40%	4.09%		2.49%	18.30%	26.88%
GERMANIUM TETRAHYDRIDE	3.68%	1.07%			0.15%	8.49%	9.86%
GLUTARALDEHYDE	0.83%	1.94%	4.67%	2.75%	4.74%	49.45%	46.84%
GLUTARIC ACID	2.53%	0.33%	3.97%	6.12%	2.66%	35.10%	43.10%
GLUTARIC ANHYDRIDE	2.35%	1.31%	4.06%		3.17%	22.31%	45.61%
GLUTARONITRILE	3.89%	3.25%		5.03%	10.88%	110.12%	95.46%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
GLYCERYL TRIACETATE	1.01%	0.81%	2.90%		1.10%	13.66%	33.53%
GLYCOL ALDEHYDE	1.01%	3.35%	3.77%		5.52%	67.56%	52.19%
GLYCOLIC ACID	1.47%	1.21%	4.68%		0.02%	3.77%	31.95%
GUAIACOL	4.15%	0.20%	4.87%	4.37%	2.85%	8.34%	15.69%
HALOTHANE	1.55%	0.71%	5.77%	2.94%	2.54%	11.63%	18.47%
HEPTAFLUOROPROPYL METHYL ETHER	0.45%	0.48%	1.85%		2.36%	20.52%	29.35%
HEPTANAL	0.73%	0.84%	2.17%		2.68%	20.24%	25.29%
HEXACHLOROBENZENE	6.19%	1.70%			4.08%	54.65%	52.52%
HEXACHLOROCYCLOPENTADIENE	0.24%	0.83%	2.89%		2.93%	25.07%	30.59%
HEXACHLORODISILOXANE	2.09%	0.91%	2.55%		0.07%	5.01%	19.21%
HEXACHLOROETHANE	0.82%	1.65%	9.87%		4.92%	40.04%	39.98%
HEXACHLOROSILANE	1.75%	1.04%	2.85%		0.15%	4.49%	19.55%
HEXACOSAMETHYLDODECASILOXANE	1.21%	1.78%	6.41%		0.22%	0.42%	35.48%
HEXADECAMETHYLCYCLOOCTASILOXANE	0.82%	0.21%	3.04%		1.36%	16.46%	39.41%
HEXADECAMETHYLHEPTASILOXANE	2.61%	0.48%	4.10%		1.07%	18.77%	38.23%
HEXAETHYLBENZENE	1.11%	0.14%	2.46%	6.43%	1.25%	14.99%	29.48%
HEXAFLUORO-1,3-BUTADIENE	2.08%	0.25%	3.08%		1.20%	15.51%	26.86%
HEXAFLUROACETONE	1.29%	0.61%	0.59%	11.92%	1.51%	14.21%	6.04%
HEXAFLUROBENZENE	0.28%	0.46%	1.55%	2.11%	2.76%	23.09%	30.62%
HEXAFLUROETHANE	0.19%	0.19%	0.92%	1.90%	1.14%	8.14%	19.14%
HEXAMETHYLBENZENE	0.96%	0.20%	2.25%	3.31%	2.51%	24.51%	27.89%
HEXAMETHYLCYCLOTIRISILOXANE	2.06%	0.75%	1.78%		0.13%	9.42%	24.70%
HEXAMETHYLDISILAZANE	1.04%	0.29%	1.74%		2.27%	17.05%	28.10%
HEXAMETHYLDISILOXANE	0.94%	0.29%	3.49%	3.02%	1.10%	12.55%	22.61%
HEXAMETHYLENEDIAMINE	1.33%	0.29%	1.32%		1.13%	12.59%	19.64%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
HEXAMETHYLENEIMINE	1.30%	0.26%	2.54%		1.60%	9.83%	12.19%
HEXANAL	0.13%	0.80%	2.53%		2.59%	20.69%	25.87%
HEXANENITRILE	1.35%	1.36%	4.92%		4.34%	33.96%	36.14%
HMX	0.91%	2.62%	1.90%		5.02%	71.00%	75.67%
HYDRACRYLONITRILE	3.23%	0.79%		26.48%	6.60%	66.14%	51.62%
HYDRAZINE	0.90%	0.54%	3.67%	16.49%	2.03%	17.50%	22.06%
HYDRAZOBENZENE	0.70%	1.79%	2.60%		3.65%	40.04%	40.60%
HYDROGEN BROMIDE	0.86%	0.32%	2.39%	1.58%	0.30%	3.65%	17.69%
HYDROGEN CHLORIDE	2.82%	1.54%	4.57%	1.42%	2.14%	14.89%	33.67%
HYDROGEN CYANIDE	9.77%	6.70%			8.50%	92.74%	73.74%
HYDROGEN IODIDE	0.67%	0.47%	2.83%	6.98%	0.10%	0.29%	15.96%
HYDROGEN PEROXIDE	1.87%	0.97%	2.40%		2.46%	16.11%	20.02%
HYDROGEN SELENIDE	1.78%	0.32%	3.88%		0.06%	1.13%	6.45%
HYDROGEN SULFIDE	0.33%	0.29%	1.55%	7.08%	0.72%	4.97%	17.26%
HYDROXYACETONITRILE	1.00%	2.22%	4.15%	7.85%	4.74%	60.14%	59.14%
HYDROXYCAPROIC ACID	1.70%	1.82%	5.90%		0.64%	3.29%	29.36%
IBUPROFEN	1.14%	1.68%			2.37%	20.10%	6.51%
IMIDAZOLE	2.03%	1.58%	3.37%		0.70%	1.15%	16.19%
INDANE	0.44%	0.97%	11.19%	1.67%	2.30%	16.70%	21.35%
INDENE	3.14%	1.93%	3.18%	0.38%	3.26%	25.62%	35.44%
INDOLE	0.87%	1.07%	4.71%	1.28%	4.27%	39.89%	18.14%
IODINE	0.86%	1.06%	4.25%		0.52%	5.45%	25.68%
IODOBENZENE	0.29%	0.64%	2.56%	2.74%	2.29%	17.85%	26.00%
IRON PENTACARBONYL	3.61%	0.17%		2.97%	0.98%	15.19%	23.10%
ISOBUTANE	0.20%	0.50%	2.65%	0.93%	1.57%	9.84%	19.88%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
ISOBUTENE	0.38%	0.34%	2.70%	1.69%	1.95%	11.83%	21.15%
ISOBUTYL ACETATE	0.72%	0.66%	4.59%	5.33%	1.91%	20.37%	32.74%
ISOBUTYL ACRYLATE	0.31%	0.22%	1.99%		1.87%	16.39%	27.36%
ISOBUTYL CHLORIDE	0.35%	0.99%	2.93%	4.96%	2.35%	16.50%	25.07%
ISOBUTYL FORMATE	1.09%	0.79%	1.72%		0.43%	5.87%	11.86%
ISOBUTYL ISOBUTYRATE	1.78%	0.51%	2.27%		1.22%	14.05%	27.32%
ISOBUTYL MERCAPTAN	0.70%	0.67%	2.34%	2.44%	2.10%	12.44%	24.30%
ISOBUTYL METHACRYLATE	0.35%	0.39%	2.17%	1.31%	2.21%	19.67%	28.86%
ISOBUTYLAMINE	0.41%	0.84%	1.16%	2.99%	1.66%	10.72%	8.06%
ISOBUTYLBENZENE	0.47%	0.52%	2.41%	0.80%	1.24%	11.23%	23.57%
iso-BUTYLCYCLOHEXANE	0.77%	0.89%	2.18%		1.88%	16.65%	32.64%
ISOBUTYLENE GLYCOL	1.10%	1.27%	5.84%		0.32%	0.95%	20.59%
ISOBUTYL-tert-BUTYL ETHER	0.91%	0.52%	1.08%	1.38%	0.90%	8.80%	24.06%
ISOBUTYRIC ACID	1.05%	0.43%			4.61%	45.49%	55.20%
ISOBUTYRIC ANHYDRIDE	1.18%	1.03%			1.39%	9.76%	32.45%
ISOBUTYRONITRILE	1.86%	2.30%	6.23%	4.22%	4.87%	46.14%	49.80%
ISOPENTANE	0.11%	0.60%	2.21%	1.35%	1.82%	12.13%	23.37%
ISOPENTYL ACETATE	2.39%	0.73%	2.74%	4.16%	4.02%	22.11%	33.15%
ISOPENTYL BUTYRATE	0.84%	0.97%			2.26%	17.21%	27.77%
ISOPENTYL ISOVALERATE	1.88%	1.42%	2.14%	3.54%	2.19%	17.74%	33.74%
ISOPHORONE	1.65%	0.93%			3.36%	24.93%	31.13%
ISOPHTHALIC ACID	0.67%	1.71%	2.74%		4.08%	57.27%	66.64%
ISOPHTHALOYL CHLORIDE	1.12%	0.15%	1.98%		1.72%	19.68%	35.71%
ISOPIMARIC ACID	0.93%	0.11%	2.50%		1.56%	19.04%	36.00%
ISOPRENE	1.68%	0.55%	5.45%	4.79%	1.77%	17.49%	26.24%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
ISOPROPANOL	3.41%	2.06%	2.88%	21.71%	0.64%	16.12%	33.17%
ISOPROPYL ACETATE	1.25%	0.33%	4.81%	5.49%	2.13%	22.63%	33.38%
ISOPROPYL ACRYLATE	1.16%	0.26%		9.71%	1.74%	14.36%	24.70%
ISOPROPYL BUTYL ETHER	0.89%	0.28%	3.17%	1.10%	1.23%	11.84%	27.66%
ISOPROPYL CHLORIDE	0.87%	0.51%	0.94%	1.42%	1.23%	10.10%	20.86%
ISOPROPYL IODIDE	1.90%	0.42%	3.32%	3.99%	0.54%	1.81%	7.89%
ISOPROPYL ISOBUTYL ETHER	0.77%	0.25%	3.06%	1.18%	0.69%	6.97%	22.63%
ISOPROPYL MERCAPTAN	0.92%	0.37%	1.47%	3.42%	1.30%	5.62%	18.76%
ISOPROPYL PALMITATE	1.59%	1.21%	4.50%		3.07%	39.75%	49.86%
ISOPROPYLAMINE	1.54%	0.20%	4.05%	9.62%	1.35%	14.12%	30.34%
ISOPROPYLCYCLOHEXANE	0.06%	0.57%	1.81%		2.45%	18.51%	31.41%
ISOPROPYLCYCLOPENTANE	0.26%	0.55%	2.58%	3.35%	2.44%	17.16%	28.72%
ISOQUINOLINE	0.13%	0.28%	1.12%	0.44%	0.84%	6.17%	16.70%
ISOSORBIDE	1.22%	0.76%	3.00%		0.65%	8.95%	28.32%
ISOVALERIC ACID	1.35%	0.96%		7.63%	1.93%	22.13%	51.72%
ISOXAZOLE	1.14%	1.35%	4.36%		4.71%	32.49%	40.39%
ITACONIC ACID	0.79%	1.32%	1.73%		3.35%	42.96%	57.84%
KETENE	1.51%	0.24%	5.28%		1.12%	11.87%	22.57%
KRYPTON	0.37%	0.47%	1.58%		0.30%	1.63%	15.63%
LACTIC ACID	0.87%	2.19%	4.14%		0.56%	7.77%	25.05%
LACTONITRILE	1.07%	1.22%	3.73%		2.98%	36.52%	45.80%
L-ARABINOSE	0.43%	0.44%			1.14%	11.51%	32.18%
LEVOGLUCOSAN	1.16%	1.20%	4.69%		0.06%	3.12%	26.09%
LEVULINIC ACID	0.19%	1.57%	1.62%		3.40%	38.38%	48.34%
L-GLUTAMIC ACID	1.90%	2.14%	9.53%		1.10%	9.03%	24.94%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
LINOLEIC ACID	1.51%	1.92%	3.59%		0.88%	13.34%	53.87%
LINOLENIC ACID	1.22%	0.73%	3.75%		0.69%	11.01%	40.30%
L-MENTHOL	1.62%	1.79%	6.81%		1.01%	7.04%	26.25%
L-PHENYLALANINE	1.07%	0.30%	2.76%	1.49%	1.29%	15.43%	34.80%
LYSINE	1.59%	1.46%	5.83%		0.32%	0.01%	28.40%
MALEIC ACID	1.13%	0.28%	1.74%		1.77%	24.02%	44.55%
MALEIC ANHYDRIDE	4.57%	1.76%	8.12%		2.28%	6.20%	25.33%
MALONIC ACID	2.36%	0.17%			1.40%	19.76%	35.81%
MALTOL	1.51%	0.86%	2.65%		2.94%	31.15%	37.89%
m-CHLOROANILINE	0.17%	2.38%	9.93%		2.32%	20.49%	24.58%
m-CHLOROBENZOYL CHLORIDE	0.67%	0.95%	5.19%		3.07%	28.77%	34.30%
m-CHLORONITROBENZENE	2.00%	0.83%	5.03%	2.41%	3.69%	29.99%	19.60%
m-CHLOROPHENOL	3.05%	0.78%	7.29%		1.43%	6.53%	18.68%
m-CRESOL	2.04%	0.81%	3.45%	8.58%	2.18%	20.85%	37.50%
m-CYMENE	0.45%	0.56%	3.49%	3.29%	2.58%	23.43%	29.58%
m-DIBROMOBENZENE	1.22%	0.24%	1.37%	2.80%	1.63%	10.30%	21.67%
m-DICHLOROBENZENE	0.35%	1.45%	3.81%	1.32%	2.69%	21.59%	32.69%
m-DIETHYLBENZENE	0.85%	0.85%	2.84%	4.18%	2.55%	22.53%	30.74%
m-DIISOPROPYLBENZENE	2.65%	3.73%	4.74%		0.65%	13.93%	28.96%
m-DIVINYLBENZENE	0.46%	1.11%	5.34%		3.24%	29.54%	39.70%
MELAMINE	0.66%	2.10%			5.53%	59.09%	56.87%
MERCURY DICHLORIDE	0.33%	0.62%	3.02%		3.23%	24.25%	33.94%
MESITYL OXIDE	1.26%	1.03%	4.74%	1.61%	3.49%	32.23%	37.37%
MESITYLENE	0.36%	0.46%	2.87%	4.10%	2.75%	23.01%	30.45%
METHACROLEIN	0.42%	1.85%	4.71%		4.56%	35.30%	35.54%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
METHACRYLONITRILE	2.52%	3.10%	4.67%	8.85%	7.58%	52.61%	49.33%
METHANE	0.28%	0.35%	1.34%	6.28%	0.34%	1.12%	16.47%
METHANOL	1.94%	0.88%	10.50%	37.70%	4.47%	39.86%	50.17%
METHOXYACETIC ACID	1.43%	0.80%	2.01%		4.21%	42.10%	53.21%
METHOXYACETONE	0.86%	1.27%			3.62%	29.78%	33.88%
METHOXYDIHYDROPYRAN	0.68%	0.20%	1.36%		1.62%	14.23%	27.62%
METHYL ACETATE	0.36%	0.60%	2.60%	3.77%	3.18%	23.33%	29.63%
METHYL ACRYLATE	0.76%	0.42%	3.87%		3.31%	26.17%	29.46%
METHYL alpha-HYDROXYISOBUTYRATE	0.15%	0.42%	2.01%		2.36%	21.22%	31.70%
METHYL alpha-METHOXYISOBUTYRATE	0.51%	1.20%	2.46%		3.51%	31.55%	35.39%
METHYL BENZOATE	1.15%	1.65%	1.56%	4.07%	3.69%	25.49%	22.71%
METHYL CAPRYLATE	2.47%	0.51%	3.54%		1.40%	20.21%	32.48%
METHYL CHLORIDE	0.34%	0.92%	1.84%	1.26%	2.36%	15.10%	22.48%
METHYL CHLOROACETATE	0.68%	1.53%	2.21%	1.76%	3.21%	27.26%	36.86%
METHYL CHLOROFORMATE	0.79%	0.44%	1.35%		1.32%	12.13%	22.83%
METHYL CHLOROSILANE	3.80%	1.29%	2.98%	16.89%	2.05%	13.27%	19.42%
METHYL CYANOACETATE	0.35%	4.42%	4.25%		5.74%	58.16%	63.85%
METHYL DECANOATE	2.51%	0.64%	4.83%		2.33%	29.16%	37.30%
METHYL DICHLOROSILANE	2.13%	1.56%	2.46%	8.38%	2.53%	11.79%	17.26%
METHYL DIETHANOLAMINE	1.18%	0.86%	1.52%		1.68%	18.57%	30.41%
METHYL DODECANOATE	1.63%	0.83%	3.57%		2.67%	31.58%	40.70%
METHYL EICOSANOATE	2.01%	1.76%			3.71%	50.29%	56.85%
METHYL ERUCATE	0.93%	1.36%	2.23%		2.54%	35.04%	47.12%
METHYL ETHYL ETHER	1.40%	0.59%	4.00%	3.20%	1.22%	13.44%	24.78%
METHYL ETHYL KETONE	1.33%	1.33%	1.92%	3.12%	3.41%	26.95%	32.42%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
METHYL ETHYL SULFIDE	1.05%	0.78%	5.12%	3.17%	3.03%	25.09%	36.52%
METHYL FLUORIDE	0.68%	1.63%		1.94%	4.88%	32.25%	32.51%
METHYL FORMATE	0.33%	0.65%	3.37%	2.52%	3.00%	23.39%	30.84%
METHYL GLYOXAL	0.54%	1.08%	2.39%		3.00%	25.27%	28.85%
METHYL HYDROPEROXIDE	0.40%	0.82%	3.14%		0.70%	6.52%	22.10%
METHYL IODIDE	1.08%	1.05%	10.28%	10.30%	3.14%	16.06%	26.74%
METHYL ISOBUTYL ETHER	0.46%	0.49%	3.90%	1.08%	1.43%	11.42%	22.78%
METHYL ISOBUTYL KETONE	0.47%	0.65%	2.07%	2.60%	2.91%	22.37%	30.21%
METHYL ISOBUTYRATE	0.83%	0.46%	2.39%	2.00%	2.50%	21.32%	28.80%
METHYL ISOCYANATE	0.48%	2.80%	4.92%		4.32%	35.65%	22.18%
METHYL ISOPROPENYL KETONE	0.56%	1.35%	4.20%		3.66%	29.71%	33.53%
METHYL ISOPROPYL ETHER	0.43%	0.45%	2.72%	1.91%	1.73%	13.22%	23.98%
METHYL ISOPROPYL KETONE	0.54%	0.55%	1.09%	1.53%	2.89%	20.53%	30.06%
METHYL ISOPROPYL SULFIDE	0.45%	0.41%	1.49%		1.63%	12.34%	16.23%
METHYL LACTATE	0.15%	0.37%	2.21%		2.66%	24.34%	31.60%
METHYL LINOLENATE	0.23%	0.53%			1.43%	17.08%	40.74%
METHYL MERCAPTAN	1.13%	0.40%	2.12%	7.23%	2.44%	11.36%	24.24%
METHYL METHACRYLATE	1.80%	1.39%	6.11%		2.85%	26.68%	31.97%
METHYL MYRISTATE	3.21%	1.44%			2.38%	35.01%	45.58%
METHYL n-BUTYL ETHER	0.45%	0.59%	2.27%	2.31%	2.14%	16.85%	28.13%
METHYL n-BUTYL SULFIDE	0.14%	0.50%	2.09%	1.54%	2.50%	19.34%	31.56%
METHYL n-BUTYRATE	0.66%	0.38%	2.12%	5.44%	2.84%	23.48%	30.15%
METHYL NONAFLUORO-N-BUTYL ETHER	1.32%	0.61%		3.17%	2.74%	19.49%	28.24%
METHYL n-PENTYL ETHER	0.61%	0.48%	2.56%	1.67%	2.11%	17.89%	31.02%
METHYL n-PROPYL ETHER	0.99%	0.89%	2.24%	2.41%	2.62%	15.81%	25.82%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
METHYL n-PROPYL SULFIDE	0.16%	0.70%	1.88%	1.30%	2.14%	16.65%	28.48%
METHYL OLEATE	1.92%	0.60%	4.69%		2.26%	30.30%	44.69%
METHYL PALMITATE	3.37%	1.44%			2.57%	39.08%	48.74%
METHYL PALMITOLEATE	1.04%	0.35%	3.34%		1.16%	15.47%	52.51%
METHYL para-TOLUATE	3.40%	0.28%			1.61%	20.91%	29.71%
METHYL PENTYL SULFIDE	1.56%	0.45%	2.55%	1.96%	1.98%	19.54%	29.21%
METHYL PHENYL SULFIDE	1.12%	0.89%			1.94%	17.47%	19.82%
METHYL PROPIONATE	0.74%	0.50%	2.36%	1.87%	2.84%	23.19%	30.24%
METHYL RICINOLEATE	1.59%	0.62%	3.86%		2.19%	30.86%	49.87%
METHYL sec-BUTYL ETHER	0.60%	0.77%	4.34%	0.93%	1.62%	13.18%	23.02%
METHYL SILANE	1.35%	0.39%			0.88%	7.28%	1.40%
METHYL SILICATE	0.12%	0.26%	1.42%	1.96%	1.60%	13.32%	22.00%
METHYL STEARATE	3.54%	1.20%			2.73%	43.59%	52.45%
METHYL t-BUTYL SULFIDE	0.73%	0.24%	2.43%	2.37%	1.42%	11.99%	23.96%
METHYL tert-BUTYL ETHER	1.39%	0.34%	2.88%		1.92%	17.53%	27.44%
METHYL tert-PENTYL ETHER	0.57%	0.27%	2.25%	1.94%	2.52%	19.28%	26.12%
METHYL t-PENTYL SULFIDE	0.42%	0.79%	3.01%	3.91%	2.91%	22.32%	28.65%
METHYL TRICHLOROSILANE	1.21%	0.41%		5.44%	2.07%	13.74%	19.38%
METHYL VINYL DICHLOROSILANE	0.68%	0.57%	4.10%		3.44%	27.62%	25.41%
METHYL VINYL ETHER	0.93%	0.34%	3.60%		2.58%	19.26%	23.50%
METHYL-3-MERCAPTOPROPIONATE	0.84%	0.66%	2.32%		2.67%	24.27%	31.01%
METHYL-4-FORMYLBENZOATE	2.12%	0.74%			3.80%	36.20%	36.11%
METHYLACETYLENE	0.51%	0.41%	3.10%	2.66%	1.89%	13.54%	20.79%
METHYLAL	0.99%	0.34%	5.08%	11.57%	3.43%	29.85%	58.31%
METHYLAMINE	1.20%	0.45%	4.16%	1.44%	2.34%	21.60%	3.75%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
METHYLCYCLOHEXANE	0.35%	0.56%	2.47%	0.70%	1.88%	13.01%	23.47%
METHYLCYCLOPENTADIENE	0.62%	0.15%	1.93%		1.34%	10.48%	21.31%
METHYLCYCLOPENTADIENE DIMER	0.63%	0.63%	2.17%		2.65%	23.86%	30.98%
METHYLCYCLOPENTANE	0.59%	0.59%	1.39%	1.73%	1.53%	12.28%	22.11%
METHYLCYCLOPROPANE	0.20%	0.70%			1.54%	9.35%	24.63%
METHYLETHANOLAMINE	0.79%	0.24%	0.93%		1.95%	20.05%	32.21%
METHYLGERMANIUM TRICHLORIDE	1.56%	0.28%	2.68%	3.40%	1.62%	14.81%	24.30%
METHYLGLUTARONITRILE	0.58%	4.50%	4.84%		6.24%	70.23%	76.74%
METHYLNORBORNENE	0.42%	0.95%	3.65%		3.00%	22.00%	28.22%
m-ETHYLPHENOL	0.46%	0.26%	2.71%	16.81%	0.97%	7.97%	19.60%
m-ETHYLSTYRENE	0.69%	1.11%	2.44%		2.97%	26.50%	37.04%
m-ETHYLTOLUENE	0.56%	0.70%	4.75%		2.39%	21.57%	31.28%
METHYLTRICETOXYSILANE	0.35%	3.62%	4.84%	2.97%	7.09%	71.97%	59.76%
m-METHYLSTYRENE	0.58%	0.97%	3.92%	4.46%	3.39%	28.79%	35.98%
m-NITROANILINE	0.97%	0.23%	3.94%		2.10%	7.91%	25.87%
MONOCHLOROBENZENE	0.28%	0.38%	2.59%	2.02%	2.42%	17.66%	25.91%
MONOCHLOROSILANE	0.98%	0.18%	1.12%	1.17%	0.82%	6.76%	19.26%
MONOMETHYL TEREPHTHALATE	0.97%	0.99%			3.13%	39.04%	50.72%
MONOMETHYL UREA	4.80%	0.21%			1.20%	22.04%	34.66%
MONOOLEIN	1.00%	0.18%	3.20%		1.44%	19.87%	44.34%
MONOPALMITIN	1.27%	0.65%	4.45%		0.70%	11.12%	39.94%
MONO-TERT-BUTYLHYDROQUINONE	0.69%	2.05%			0.81%	8.49%	16.04%
MORPHOLINE	0.66%	0.18%	1.44%		2.00%	13.18%	23.84%
m-PHENYLENEDIAMINE	1.40%	1.04%	4.89%		2.95%	27.21%	16.94%
m-TERPHENYL	0.15%	0.12%	2.06%		2.30%	22.96%	36.30%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
m-tert-BUTYLPHENOL	1.95%	0.48%	2.42%		0.88%	12.36%	27.78%
m-TOLUALCOHOL	0.75%	2.27%	3.99%	2.21%	0.68%	3.65%	24.73%
m-TOLUALDEHYDE	0.92%	0.67%	3.68%		3.16%	29.97%	38.78%
m-TOLUIC ACID	3.04%	0.33%	2.91%		1.17%	18.26%	34.93%
m-TOLUIDINE	0.59%	0.59%	4.88%	6.07%	3.05%	23.73%	37.48%
m-XYLENE	0.47%	0.62%	2.96%	1.29%	2.57%	21.05%	28.43%
N-(2-HYDROXYETHYL)PIPERAZINE	2.31%	1.42%	3.73%		1.16%	1.16%	18.66%
N,N'-BIS(2-HYDROXYETHYL)ETHYLENEDIAMINE	1.31%	1.88%			0.72%	3.86%	28.87%
N,N'-DI(2-HYDROXYETHYL)PIPERAZINE	2.07%	1.74%	5.55%	3.89%	0.73%	2.04%	19.33%
N,N-DIETHYLANILINE	2.45%	0.34%	5.14%	1.88%	1.78%	23.48%	22.78%
N,N-DIETHYLHYDROXYLAMINE	1.39%	0.29%	3.18%		0.01%	3.73%	14.95%
N,N-DIETHYLMETHYLAMINE	0.14%	0.69%			1.50%	10.85%	22.33%
N,N-DIMETHYLACETAMIDE	0.78%	1.72%	7.14%		4.96%	47.78%	40.97%
N,N-DIMETHYLANILINE	1.01%	0.24%	7.07%		2.25%	22.74%	12.82%
N,N-DIMETHYLFORMAMIDE	2.60%	2.72%	7.69%	3.41%	8.56%	67.02%	55.47%
N,N-DIMETHYL-n-BUTYLAMINE	0.62%	0.42%	1.83%		1.89%	15.86%	21.74%
N,N'-DIPHENYL-p-PHENYLENEDIAMINE	0.62%	1.42%	1.13%		3.63%	40.12%	49.35%
N,N'-DI-tert-BUTYLETHYLENEDIAMINE	0.40%	1.73%	5.53%	10.00%	0.62%	4.57%	16.90%
N-AMINOETHYL ETHANOLAMINE	1.59%	1.42%	4.20%		0.08%	2.91%	32.24%
N-AMINOETHYL PIPERAZINE	0.23%	0.71%			1.53%	12.95%	25.33%
NAPHTHALENE	0.41%	0.67%	9.47%	3.61%	2.85%	20.81%	25.83%
n-BUTANE	0.10%	0.38%	2.04%	1.22%	1.81%	11.59%	21.72%
n-BUTYL ACETATE	0.22%	0.47%	1.93%	2.29%	2.48%	20.57%	32.67%
n-BUTYL ACRYLATE	1.48%	1.51%	2.25%		2.59%	19.75%	33.07%
n-BUTYL BENZOATE	0.50%	0.47%			2.15%	21.40%	39.59%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
n-BUTYL CHLORIDE	0.95%	0.91%	2.92%		3.35%	24.89%	31.24%
n-BUTYL ETHYL ETHER	0.37%	0.46%		4.85%	1.75%	15.32%	28.85%
n-BUTYL FORMATE	0.31%	0.36%	2.89%	2.11%	2.40%	21.34%	31.36%
n-BUTYL ISOCYANATE	0.62%	0.86%	3.92%		3.21%	28.56%	27.12%
n-BUTYL MERCAPTAN	0.85%	0.57%	3.10%	2.25%	2.95%	18.27%	29.64%
n-BUTYL METHACRYLATE	1.63%	0.32%	4.20%		1.95%	22.67%	35.61%
n-BUTYL n-BUTYRATE	0.21%	0.45%	1.54%	1.47%	2.31%	21.07%	36.06%
n-BUTYL PROPIONATE	1.23%	0.40%	3.15%	1.07%	1.95%	19.52%	33.15%
n-BUTYL STEARATE	0.83%	1.03%	3.18%	7.50%	0.73%	10.69%	55.09%
n-BUTYL VALERATE	0.64%	0.58%		0.95%	1.49%	17.05%	36.78%
n-BUTYLAMINE	0.91%	0.46%	1.53%	8.20%	1.77%	14.94%	13.22%
n-BUTYLBENZENE	0.06%	0.87%	1.72%	0.75%	2.48%	20.54%	27.45%
n-BUTYLCYCLOHEXANE	2.71%	0.62%	6.93%	4.49%	1.84%	22.71%	34.70%
n-BUTYLCYCLOPENTANE	0.56%	0.63%	5.27%	1.55%	2.67%	20.13%	31.00%
n-BUTYLHYDROPEROXIDE	1.70%	2.77%	6.97%		2.62%	19.95%	2.23%
n-BUTYRIC ACID	0.56%	0.57%			3.43%	33.28%	43.45%
n-CROTYL ACETATE	0.70%	0.39%	1.68%		2.16%	19.92%	29.17%
n-DECANE	0.49%	0.61%	1.90%	1.05%	2.59%	24.00%	31.50%
n-DECYL FORMATE	0.76%	0.16%		3.06%	1.59%	19.04%	34.27%
n-DECYL MERCAPTAN	0.82%	0.54%	0.82%	1.37%	3.24%	26.33%	45.13%
n-DECYLAMINE	1.35%	0.29%	2.84%	3.93%	2.33%	20.10%	34.00%
n-DECYLBENZENE	1.11%	0.95%	1.72%	0.99%	2.89%	24.00%	45.02%
n-DECYLCYCLOHEXANE	0.11%	0.73%	4.54%	1.88%	2.25%	23.00%	47.07%
n-DODECANE	0.42%	0.62%	1.99%	2.82%	2.54%	25.76%	32.71%
n-DODECANOIC ACID	2.88%	0.36%	4.78%	8.47%	1.05%	18.04%	39.11%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
n-DODECYLAMINE	2.06%	0.28%	4.63%	4.58%	2.79%	20.28%	39.60%
n-DODECYLBENZENE	0.74%	1.05%	1.12%	0.58%	2.07%	23.66%	50.13%
n-DOTRIACONTANE	0.53%	0.14%	1.57%	0.36%	1.53%	18.02%	41.68%
n-EICOSANE	0.49%	0.38%	1.22%	0.25%	1.96%	25.35%	36.93%
NEOABIETIC ACID	1.04%	0.32%	2.50%		1.22%	15.02%	35.03%
NEOHEXANOIC ACID	1.28%	1.47%	2.86%	3.27%	2.35%	25.24%	36.43%
NEON	1.01%	1.18%	6.34%		2.14%	15.09%	11.23%
NEOPENTANE	0.09%	0.15%	2.26%	3.33%	1.44%	9.76%	22.53%
N-ETHYL-2-METHYLALLYLAMINE	0.64%	0.78%	1.81%	3.87%	1.85%	16.11%	19.65%
N-ETHYLANILINE	1.14%	0.64%	5.16%		2.56%	25.13%	26.94%
N-ETHYLMORPHOLINE	0.56%	0.25%	1.08%	6.35%	1.57%	12.87%	23.81%
n-HENEICOSANE	0.55%	0.57%	1.60%	0.68%	2.35%	26.93%	37.77%
n-HEPTACOSANE	0.99%	0.17%	1.56%	0.63%	1.59%	21.06%	39.39%
n-HEPTADECANE	1.12%	0.56%	2.71%	0.73%	2.23%	27.90%	37.14%
n-HEPTADECANOIC ACID	1.22%	0.25%		13.16%	2.24%	25.85%	48.35%
n-HEPTADECYLBENZENE	0.86%	0.79%	1.82%	1.34%	1.87%	22.65%	57.66%
n-HEPTANE	0.36%	0.42%	2.35%	0.53%	2.40%	19.74%	27.66%
n-HEPTANOIC ACID	2.56%	0.47%	1.60%		0.88%	15.24%	32.37%
n-HEPTYL ACETATE	0.35%	0.49%	2.97%	1.30%	1.83%	18.52%	38.52%
n-HEPTYL FORMATE	1.20%	0.63%	2.55%	3.20%	2.71%	22.66%	38.71%
n-HEPTYL MERCAPTAN	0.76%	0.56%	2.09%	1.33%	3.28%	23.99%	38.78%
n-HEPTYLAMINE	1.17%	0.16%	4.57%	4.92%	2.47%	19.68%	25.32%
n-HEPTYLBENZENE	1.68%	1.17%	2.60%	1.74%	3.76%	26.48%	40.08%
n-HEXACOSANE	0.63%	0.28%	1.31%	1.12%	1.82%	23.12%	40.13%
n-HEXADECANE	1.10%	0.69%	3.36%	0.79%	2.41%	29.75%	37.62%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
n-HEXADECANOIC ACID	1.47%	0.13%		13.07%	1.73%	21.12%	43.86%
n-HEXADECYLBENZENE	1.30%	0.98%	2.34%	1.55%	1.42%	20.33%	56.59%
n-HEXANE	0.48%	0.37%	3.18%	0.98%	2.49%	17.87%	25.35%
n-HEXANOIC ACID	2.64%	1.31%			1.28%	20.55%	35.57%
n-HEXATRIACONTANE	2.18%	0.27%	0.00%	0.0113103	1.27%	11.54%	30.66%
n-HEXYL ACETATE	0.13%	0.44%	2.40%	1.74%	2.20%	19.69%	36.50%
n-HEXYL FORMATE	0.93%	0.49%	2.41%	4.10%	2.31%	22.24%	35.93%
n-HEXYL MERCAPTAN	0.46%	0.53%	2.32%	1.32%	3.07%	22.62%	36.07%
n-HEXYLAMINE	0.61%	0.33%	1.92%	5.62%	2.30%	18.71%	21.76%
n-HEXYLBENZENE	0.74%	0.74%	1.44%	1.48%	3.15%	24.76%	37.07%
NIACIN	0.66%	0.09%	1.13%		1.66%	16.77%	30.07%
NICKEL CARBONYL	2.82%	0.30%		2.33%	1.82%	8.18%	17.89%
NICOTINONITRILE	0.60%	1.29%	5.11%	6.97%	5.19%	48.71%	37.47%
NITRIC OXIDE	1.46%	2.09%	2.36%	31.96%	0.82%	11.49%	32.84%
NITROBENZENE	7.11%	2.38%	9.82%		3.33%	25.29%	29.77%
NITROETHANE	5.14%	2.45%	4.74%	2.42%	4.96%	36.90%	34.96%
NITROGEN	0.22%	0.30%	1.27%	4.18%	0.06%	0.52%	15.31%
NITROGEN TRIFLUORIDE	0.12%	0.27%	2.08%		1.03%	7.67%	22.43%
NITROMETHANE	4.08%	3.02%	5.09%	3.91%	6.17%	48.95%	49.32%
NITROSYL CHLORIDE	3.38%	1.38%	6.81%		0.40%	8.30%	3.66%
NITROUS OXIDE	1.51%	0.18%	2.52%	6.02%	1.04%	9.90%	21.58%
N-METHYL-2-PYRROLIDONE	0.63%	1.18%	1.66%		4.81%	37.05%	42.73%
N-METHYLACETAMIDE	0.75%	1.83%	4.94%		5.70%	53.78%	49.66%
N-METHYLANILINE	2.06%	0.93%	6.30%		0.55%	0.60%	0.24%
N-METHYLCYCLOHEXYLAMINE	0.55%	0.15%	1.02%		1.76%	15.09%	25.68%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
N-METHYLFORMAMIDE	1.68%	2.87%	7.46%		7.63%	78.23%	65.38%
N-METHYLPYRIDINE	1.48%	0.55%	1.41%		2.24%	13.99%	23.69%
N-METHYLPYRROLE	2.12%	2.96%	6.33%	5.43%	1.88%	19.89%	25.24%
N-METHYLPYRROLIDINE	0.47%	0.27%	1.82%		1.30%	9.61%	20.98%
N-NITROSODIETHANOLAMINE	1.06%	0.54%	3.75%		1.00%	13.77%	37.40%
N-NITROSODIMETHYLAMINE	1.32%	2.80%	6.38%	3.97%	6.24%	54.86%	45.77%
n-NONADECANE	1.08%	0.55%	2.88%	0.96%	2.22%	27.92%	37.79%
n-NONANE	0.26%	0.53%	1.74%	1.10%	2.43%	22.82%	30.60%
n-NONANOIC ACID	3.48%	0.24%	3.57%		0.64%	15.01%	34.16%
n-NONYL ACETATE	1.02%	0.57%	1.55%	1.07%	1.29%	15.39%	40.98%
n-NONYL FORMATE	0.73%	0.18%		2.82%	1.66%	19.03%	32.95%
n-NONYL MERCAPTAN	1.38%	0.67%	3.03%	2.64%	3.46%	25.35%	43.09%
n-NONYL n-UNDECYL PHTHALATE	0.46%	1.13%	2.20%		4.34%	54.79%	72.11%
n-NONYLAMINE	1.22%	0.34%	3.70%	4.06%	2.35%	19.52%	31.89%
n-OCTACOSANE	0.31%	0.17%	1.22%	1.04%	1.62%	20.72%	40.56%
n-OCTADECANE	1.40%	0.59%	3.60%	0.74%	2.29%	28.25%	36.99%
n-OCTADECYLBENZENE	0.80%	0.59%	1.79%	1.26%	1.95%	23.22%	59.41%
n-OCTANE	0.35%	0.60%	1.99%	0.54%	2.60%	22.07%	30.24%
n-OCTANOIC ACID	2.62%	0.95%	1.56%		0.90%	15.49%	32.39%
n-OCTYL ACETATE	0.45%	0.23%	3.33%	1.01%	1.65%	17.77%	40.08%
n-OCTYL FORMATE	2.76%	0.97%	2.17%	3.52%	3.46%	23.24%	40.26%
n-OCTYL MERCAPTAN	0.47%	0.54%	2.30%	1.90%	3.07%	25.12%	41.68%
n-OCTYLAMINE	0.90%	0.27%	3.35%	4.07%	2.25%	18.94%	28.54%
n-OCTYLBENZENE	1.09%	0.97%	1.93%	1.10%	3.29%	26.27%	42.28%
NONANAL	1.28%	0.14%	1.66%		1.44%	15.12%	25.41%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
NONYLPHENOL	0.83%	1.32%	4.79%		1.15%	13.03%	36.19%
n-PENTACOSANE	0.51%	0.37%	1.34%	0.59%	2.02%	23.94%	38.53%
n-PENTADECANE	1.29%	0.69%	3.48%	0.87%	2.47%	29.34%	36.82%
n-PENTADECANOIC ACID	1.36%	0.19%		11.27%	2.00%	22.50%	43.52%
n-PENTADECYLBENZENE	0.92%	1.05%	1.97%	1.18%	1.67%	21.55%	54.66%
n-PENTANE	0.11%	0.40%	2.38%	0.95%	2.11%	14.83%	23.41%
n-PENTANOIC ACID	1.21%	0.95%			2.19%	25.79%	39.43%
n-PENTASILANE	0.65%	0.90%	2.12%		0.42%	4.12%	18.23%
n-PENTYL ACETATE	0.40%	0.54%	2.90%	2.12%	2.86%	22.98%	35.80%
n-PENTYL FORMATE	3.48%	1.25%		3.96%	2.69%	17.22%	31.32%
n-PENTYL MERCAPTAN	0.60%	0.83%	2.25%	1.47%	2.79%	19.81%	33.04%
n-PENTYLAMINE	0.14%	0.31%	1.52%	5.58%	2.15%	17.40%	17.71%
n-PENTYLBENZENE	1.13%	0.71%		0.92%	3.21%	23.73%	31.57%
n-PENTYLCYCLOHEXANE	0.16%	0.42%	2.64%		2.27%	18.97%	28.96%
n-PROPYL ACETATE	0.49%	0.56%	3.71%	1.98%	2.83%	24.69%	31.43%
n-PROPYL ACRYLATE	0.80%	0.30%	1.91%		2.00%	18.47%	29.05%
n-PROPYL BENZOATE	1.59%	0.62%		2.37%	3.02%	23.35%	37.54%
n-PROPYL FORMATE	0.80%	0.51%	4.27%	5.48%	2.67%	22.92%	30.14%
n-PROPYL IODIDE	0.16%	0.87%	4.16%		3.77%	27.61%	30.02%
n-PROPYL ISOBUTYRATE	0.96%	0.23%	1.48%	3.20%	1.27%	13.04%	27.92%
n-PROPYL MERCAPTAN	0.92%	0.66%	2.84%	3.31%	2.57%	15.11%	26.46%
n-PROPYL METHACRYLATE	0.51%	1.07%	3.33%		2.85%	22.72%	33.29%
n-PROPYL n-BUTYRATE	1.11%	0.51%	5.12%	1.48%	2.27%	23.10%	36.86%
n-PROPYL PROPIONATE	0.44%	0.34%	3.05%	6.25%	2.20%	20.46%	32.39%
n-PROPYLAMINE	2.01%	0.27%	3.11%	7.22%	1.32%	17.07%	11.76%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
n-PROPYLBENZENE	0.06%	0.99%	2.11%	0.89%	2.42%	19.69%	25.65%
n-PROPYLCYCLOHEXANE	1.93%	0.64%	5.22%	1.39%	1.95%	20.72%	32.30%
n-PROPYLCYCLOPENTANE	0.08%	0.59%	1.70%	0.76%	2.29%	17.71%	27.79%
n-TETRACOSANE	0.92%	0.31%	1.05%	0.99%	1.80%	24.23%	39.49%
n-TETRADECANE	1.10%	0.74%	3.00%	0.76%	2.57%	29.33%	36.38%
n-TETRADECANOIC ACID	1.33%	0.15%		11.17%	2.01%	23.49%	44.88%
n-TETRADECYLAMINE	2.12%	0.23%		4.96%	2.52%	19.27%	43.50%
n-TETRADECYLBENZENE	0.75%	1.08%	1.57%	1.29%	1.84%	22.47%	53.76%
n-TETRASILANE	0.21%	1.06%	3.56%		0.25%	1.39%	16.43%
n-TRICOSANE	0.92%	0.37%	1.16%	0.99%	1.91%	25.20%	38.64%
n-TRIDECANE	0.81%	0.65%	2.57%	0.77%	2.52%	27.30%	34.81%
n-TRIDECANOIC ACID	2.02%	0.17%	6.01%	9.29%	1.55%	20.48%	40.99%
n-TRIDECYLBENZENE	0.53%	1.05%	1.45%	0.56%	2.09%	22.79%	51.26%
n-UNDECANE	0.47%	0.63%	2.39%	0.76%	2.60%	25.40%	32.58%
n-UNDECANOIC ACID	3.11%	0.36%		7.55%	1.00%	17.88%	37.68%
n-UNDECYLBENZENE	1.44%	1.06%	2.25%	1.12%	2.95%	23.01%	45.90%
o-ANISIDINE	1.05%	0.72%	2.03%		2.98%	23.23%	30.73%
o-CHLOROANILINE	1.45%	0.70%	1.71%		3.49%	21.90%	19.77%
o-CHLOROBENZOIC ACID	0.73%	1.44%			3.78%	41.39%	42.21%
o-CHLORONITROBENZENE	2.68%	1.72%		2.36%	3.24%	28.31%	22.02%
o-CHLOROPHENOL	4.46%	0.38%	8.11%		2.26%	9.33%	15.12%
o-CHLOROTOLUENE	0.22%	0.41%	2.93%		2.73%	21.22%	31.35%
o-CRESOL	0.31%	0.87%	1.78%	9.19%	1.09%	9.63%	36.84%
OCTADECAMETHYLOCTASILOXANE	2.02%	0.88%	4.72%		0.45%	10.41%	24.04%
OCTAFLUORO-2-BUTENE	0.55%	1.04%	3.99%	0.65%	3.84%	30.77%	34.37%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
OCTAFLUOROCYCLOBUTANE	0.72%	0.16%	1.12%	2.03%	1.19%	11.08%	19.31%
OCTAFLUOROPROPANE	0.81%	0.48%			0.83%	6.99%	19.34%
OCTAHYDRO-PENTALENE-1-CARBOXYLIC ACID	0.40%	1.23%		8.64%	3.53%	35.62%	42.80%
OCTAMETHYLCYCLOTETRAILOXANE	2.19%	0.18%	3.09%		1.18%	15.88%	25.41%
OCTAMETHYLTRISILOXANE	0.60%	0.23%	2.26%		1.31%	11.35%	23.43%
OCTANAL	0.99%	0.17%	1.52%		1.34%	13.37%	22.58%
o-CYMENE	0.86%	0.59%	5.48%		2.31%	22.60%	28.14%
o-DICHLOROBENZENE	1.98%	1.35%	6.83%	6.16%	2.69%	26.64%	36.77%
o-DIETHYLBENZENE	1.38%	0.85%	3.93%	2.27%	2.83%	26.14%	28.05%
o-ETHYLANILINE	0.99%	0.92%	3.06%		2.05%	20.43%	22.46%
o-ETHYLPHENOL	0.86%	0.60%	4.12%	6.95%	1.18%	7.53%	29.39%
o-ETHYLSTYRENE	0.56%	0.90%	3.43%		3.24%	28.50%	36.22%
o-ETHYLTOLUENE	0.43%	0.77%	2.46%	4.74%	2.43%	20.96%	28.23%
OLEIC ACID	2.41%	1.24%	3.51%		0.51%	10.76%	55.72%
o-METHYLSTYRENE	0.79%	0.74%	2.91%	4.67%	2.33%	21.56%	29.32%
o-NITROANISOLE	0.77%	0.91%	2.45%		2.86%	28.94%	36.59%
o-NITRODIPHENYLAMINE	1.15%	0.73%			0.66%	9.00%	29.43%
o-NITROTOLUENE	2.03%	1.92%	2.99%		4.09%	28.06%	19.07%
o-PHENYLENEDIAMINE	0.59%	0.49%	1.67%		2.30%	22.91%	32.65%
o-TERPHENYL	1.11%	0.18%	3.60%		0.49%	0.89%	8.67%
o-tert-BUTYLPHENOL	0.34%	0.67%	3.72%		0.93%	7.57%	23.99%
o-TOLUALDEHYDE	0.78%	1.30%			3.91%	32.86%	35.77%
o-TOLUIC ACID	0.95%	0.34%	1.05%		2.05%	22.33%	35.82%
o-TOLUIDINE	0.72%	0.74%	2.66%	6.15%	2.16%	14.75%	21.55%
OXAZOLE	1.20%	3.63%			3.20%	18.85%	2.51%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
OXYGEN	0.22%	0.32%	1.44%	6.26%	0.14%	0.19%	15.74%
o-XYLENE	0.29%	0.31%	2.27%	1.03%	2.59%	18.57%	25.46%
OZONE	2.71%	1.17%	5.67%	16.54%	3.08%	24.06%	45.92%
p.alpha-DIMETHYLBENZYL ALCOHOL	0.89%	0.52%	2.49%		1.09%	11.84%	27.55%
PALUSTRIC ACID	1.29%	1.16%	6.01%	25.28%	0.13%	3.18%	28.03%
p-AMINOAZOBENZENE	0.97%	0.15%	1.03%		1.45%	16.00%	30.55%
p-AMINODIPHENYL	0.75%	0.24%			1.42%	14.25%	27.68%
p-AMINODIPHENYLAMINE	1.24%	0.98%	2.41%		0.39%	6.47%	26.38%
PARALDEHYDE	1.01%	0.54%	1.85%	13.74%	0.34%	4.53%	25.61%
p-BROMOTOLUENE	1.03%	0.29%	3.43%		0.52%	6.79%	16.97%
p-CHLOROANILINE	0.32%	1.24%	2.29%		2.72%	24.05%	25.07%
p-CHLOROBENZOTRIFLUORIDE	0.58%	0.48%	3.47%		3.15%	27.34%	38.69%
p-CHLORONITROBENZENE	0.79%	0.19%	2.58%	2.33%	3.26%	30.83%	21.06%
p-CHLOROPHENOL	2.36%	0.78%	5.33%		2.02%	10.31%	18.30%
p-CHLOROTOLUENE	0.19%	0.49%	2.61%		2.58%	19.75%	29.95%
p-CRESOL	1.88%	1.24%	4.81%	7.90%	1.66%	6.51%	36.90%
p-CUMYLPHENOL	0.54%	0.29%	2.16%	3.99%	0.49%	6.47%	14.96%
p-CYMENE	0.27%	0.79%	1.95%	3.34%	2.97%	23.89%	29.85%
p-DICHLOROBENZENE	0.39%	1.17%	3.43%	4.41%	2.66%	21.70%	32.84%
p-DIETHYLBENZENE	0.16%	0.91%	1.71%	2.97%	2.89%	24.43%	30.89%
p-DIISOPROPYLBENZENE	2.28%	0.29%	4.72%		1.73%	20.40%	30.34%
p-DIISOPROPYLBENZENE HYDROPEROXIDE	1.24%	0.65%	2.67%	3.00%	0.80%	11.70%	34.76%
p-DIMETHYLAMINOBENZALDEHYDE	2.37%	2.46%	7.84%		5.91%	52.81%	59.47%
p-DIVINYLBENZENE	0.24%	1.31%	2.49%		3.69%	31.40%	34.81%
PENTACHLOROETHANE	1.19%	0.97%			3.48%	26.83%	35.72%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
PENTACHLOROFLUOROETHANE	0.89%	0.82%	5.66%		3.39%	26.72%	35.55%
PENTAETHYLBENZENE	0.26%	0.47%		7.77%	1.92%	18.66%	31.85%
PENTAETHYLENE GLYCOL DIMETHYL ETHER	1.31%	0.42%	4.22%		0.64%	10.93%	55.89%
PENTAETHYLENE GLYCOL MONOMETHYL ETHER	1.49%	0.32%	3.40%		1.17%	16.75%	39.62%
PENTAFLUORO(TRIFLUOROMETHYL)SULFUR	0.62%	0.83%	4.21%		0.48%	3.15%	8.10%
PENTAFLUOROETHANE	0.23%	0.19%	1.84%	4.36%	1.94%	15.21%	22.89%
PENTAFLUOROETHYL METHYL ETHER	0.34%	0.72%	2.04%		2.80%	23.14%	29.88%
PENTAFLUOROETHYL TRIFLUOROVINYL ETHER	1.15%	2.76%	6.52%		1.68%	10.75%	10.87%
PENTAFLUOROPHENOL	0.92%	0.53%			2.19%	15.80%	23.74%
PENTAMETHYLBENZENE	0.36%	0.98%	2.85%	7.86%	2.43%	22.55%	29.08%
PENTANAL	2.13%	0.50%	4.17%		1.49%	20.75%	30.37%
PERCHLORYL FLUORIDE	0.38%	0.42%	1.37%	4.45%	1.04%	6.52%	18.09%
PERFLUOROBUTANOIC ACID	1.84%	0.20%			1.65%	22.06%	38.23%
PERFLUOROMETHYLCYCLOPENTANE	0.99%	0.14%	0.91%		1.39%	13.37%	24.97%
PERFLUORO-n-DODECANE	0.42%	1.80%			4.84%	51.20%	50.57%
PERFLUORO-n-HEPTANE	0.79%	0.14%	1.50%		1.38%	17.81%	24.49%
PERFLUORO-n-HEXADECANE	2.73%	2.74%			6.35%	80.52%	69.24%
PERFLUORO-n-HEXANE	0.97%	0.25%	1.04%		1.37%	15.11%	22.81%
PERFLUORO-n-NONANE	0.58%	0.93%			3.03%	29.24%	36.13%
PERFLUORO-n-OCTANE	0.66%	0.44%	6.48%		2.24%	21.57%	31.08%
PERFLUORO-n-PENTANE	1.51%	0.36%	2.02%		1.07%	13.13%	24.29%
p-ETHYLPHENOL	2.10%	0.96%	2.25%	3.46%	0.03%	7.51%	23.76%
p-ETHYLSTYRENE	0.48%	1.43%	3.29%		3.11%	27.45%	38.91%
p-ETHYLTOLUENE	0.77%	1.42%	0.84%	3.74%	2.53%	17.99%	28.65%
PHENANTHRENE	0.94%	0.72%	3.72%	2.37%	5.96%	50.89%	49.91%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
PHENETOLE	0.63%	0.82%	1.21%		3.06%	24.05%	34.47%
PHENOL	1.26%	0.70%	3.75%	10.32%	1.32%	5.75%	37.07%
PHENOTHIAZINE	1.24%	1.57%	4.77%		0.51%	1.93%	18.18%
PHENYL ISOCYANATE	2.31%	1.72%	3.59%		3.54%	22.70%	20.47%
PHENYL MERCAPTAN	2.29%	0.94%	2.07%	3.17%	1.87%	16.96%	27.89%
PHENYLACETONITRILE	0.80%	1.13%	9.01%		4.63%	47.38%	49.96%
PHENYLHYDRAZINE	5.69%	1.94%			2.76%	19.91%	2.76%
PHENYLMETHYLDICHLOROSILANE	0.31%	1.66%	2.31%		2.06%	18.35%	30.97%
PHENYLTRICHLOROSILANE	0.18%	0.69%	2.48%		2.09%	17.76%	29.09%
PHOSGENE	0.48%	0.43%	0.91%	5.17%	1.17%	7.07%	16.97%
PHOSPHINE	0.81%	1.52%	2.57%	16.67%	0.04%	2.97%	21.79%
PHOSPHORUS PENTAFLUORIDE	1.08%	0.28%	1.79%		0.77%	6.73%	19.24%
PHOSPHORUS TRICHLORIDE	3.17%	0.86%	4.36%	1.90%	0.43%	1.23%	5.87%
PHOSPHORUS TRIFLUORIDE	0.96%	0.23%		9.50%	1.43%	7.14%	16.95%
PHTHALAN	0.29%	0.68%	2.13%		2.49%	20.66%	27.11%
PHTHALIC ACID	1.54%	1.18%	5.29%		0.01%	3.94%	32.38%
PHTHALIDE	3.48%	0.90%			2.84%	14.83%	20.53%
p-HYDROQUINONE	4.09%	0.52%			1.96%	27.48%	35.61%
p-HYDROXYBENZALDEHYDE	1.04%	0.41%	5.14%		2.66%	27.46%	29.85%
PIMARIC ACID	0.93%	0.10%	2.98%		1.58%	19.01%	36.00%
PIMELIC ACID	3.53%	2.22%			1.40%	23.22%	47.00%
PIPERAZINE	1.20%	3.19%	8.49%		2.82%	18.39%	3.14%
PIPERIDINE	1.03%	0.17%	2.93%	3.92%	1.17%	11.89%	14.94%
p-ISOPROPENYL PHENOL	1.56%	1.39%	4.13%		3.62%	38.42%	41.72%
p-MENTHANE HYDROPEROXIDE	1.64%	2.60%	6.52%		1.39%	10.30%	20.79%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
p-METHYLSTYRENE	0.63%	3.41%	3.86%	1.88%	2.61%	24.07%	27.27%
p-NITROANILINE	1.10%	0.41%	0.78%		1.13%	11.94%	31.43%
p-NITROTOLUENE	5.90%	2.54%			5.39%	54.05%	45.60%
p-PHENETIDINE	0.46%	1.97%	2.13%		2.31%	22.97%	31.24%
p-PHENYLENEDIAMINE	0.69%	0.65%	1.80%		2.58%	25.53%	34.35%
PROPADIENE	1.91%	0.97%	5.67%	3.22%	1.65%	15.63%	26.06%
PROPANAL	0.82%	1.30%	10.18%		3.33%	26.11%	35.80%
PROPANE	0.05%	0.49%	1.55%	2.28%	1.46%	8.73%	20.64%
PROPARGYL ALCOHOL	1.38%	1.71%			4.68%	37.87%	38.75%
PROPARGYL CHLORIDE	0.57%	0.53%	4.49%	12.24%	4.22%	28.93%	34.08%
PROPENYL CYCLOHEXENE	0.75%	0.37%	2.69%	3.88%	2.12%	18.57%	29.28%
PROPIONIC ACID	0.87%	0.45%			4.17%	43.25%	51.79%
PROPIONIC ANHYDRIDE	0.37%	1.01%	2.34%	1.75%	2.34%	18.92%	33.34%
PROPIONITRILE	3.65%	3.19%	5.33%		8.06%	66.92%	50.90%
PROPYL CHLORIDE	0.81%	0.56%	1.93%	8.76%	2.83%	19.24%	29.68%
PROPYLENE	0.66%	0.45%	1.74%	1.83%	1.16%	8.26%	18.82%
PROPYLENE GLYCOL 1-tert-BUTYL ETHER	0.71%	0.36%	1.40%		2.15%	20.70%	30.50%
PROPYLENE GLYCOL 2-tert-BUTYL ETHER	0.73%	0.37%	1.03%		2.17%	20.71%	30.48%
PROPYLENE GLYCOL alpha-METHYLBENZYL ETHER	0.35%	0.47%	1.60%	18.57%	2.35%	23.65%	35.10%
PROPYLENE GLYCOL ETHYL ETHER ACETATE	0.75%	0.43%	1.28%	30.09%	1.73%	17.06%	33.24%
PROPYLENE GLYCOL MONOALLYL ETHER	2.14%	0.23%	2.80%		1.57%	18.49%	29.79%
PROPYLENE GLYCOL MONOMETHYL ETHER	1.62%	0.56%	4.99%		1.83%	21.85%	37.57%
PROPYLENE GLYCOL MONOMETHYL ETHER ACETATE	1.03%	0.26%	3.27%	3.47%	1.58%	20.30%	30.81%
PROPYLENE GLYCOL n-BUTYL ETHER	1.75%	0.38%	2.20%		2.22%	23.90%	38.36%
PROPYLENE GLYCOL n-PROPYL ETHER	2.88%	0.40%			1.82%	22.66%	31.81%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
PROPYLENEIMINE	2.81%	0.77%			2.32%	23.84%	29.43%
p-TERPHENYL	0.75%	0.59%	3.62%	1.02%	0.15%	2.74%	15.45%
p-tert-AMYLPHENOL	0.59%	0.18%	1.12%		1.40%	14.39%	28.09%
p-tert-BUTYL ETHYLBENZENE	0.73%	0.61%	2.74%	0.84%	2.59%	24.13%	31.65%
p-tert-BUTYL CATECHOL	1.19%	1.15%	4.92%		0.74%	4.78%	11.64%
p-tert-BUTYLPHENOL	1.33%	0.25%	3.64%		1.34%	11.98%	23.54%
p-tert-BUTYLSTYRENE	1.10%	1.07%	2.18%	1.16%	3.48%	28.28%	33.39%
p-tert-OCTYLPHENOL	0.59%	0.21%	1.51%		1.70%	18.08%	32.09%
p-TOLUALDEHYDE	0.31%	0.92%	1.58%		3.21%	25.48%	31.38%
p-TOLUIC ACID	1.70%	0.98%	4.52%		3.13%	36.00%	43.46%
p-TOLUIDINE	3.52%	0.68%		0.67%	1.43%	23.11%	31.41%
p-XYLENE	0.26%	0.62%	1.65%	1.14%	2.92%	21.34%	27.61%
PYRAZINE	1.74%	1.44%	5.75%		3.89%	30.57%	15.34%
PYRAZOLE	0.46%	1.77%	5.91%		5.37%	44.16%	31.16%
PYRENE	1.56%	2.86%	3.69%	1.98%	6.90%	59.83%	50.59%
PYRIDAZINE	1.47%	2.91%		4.14%	7.29%	59.21%	42.60%
PYRIDINE	0.47%	1.18%	2.80%	2.47%	2.03%	16.26%	20.15%
PYRIMIDINE	0.27%	1.17%		12.16%	4.43%	32.85%	17.55%
PYRROLE	1.03%	0.23%	3.67%	2.45%	2.22%	20.63%	18.05%
PYRROLIDINE	1.15%	0.61%	1.72%		0.67%	8.01%	12.80%
QUATERPHENYL	1.29%	0.69%	1.82%		2.49%	30.21%	42.43%
QUINALDINE	2.02%	1.10%	6.97%		3.19%	35.39%	29.84%
QUINOLINE	0.85%	0.29%	2.43%	1.47%	1.43%	8.89%	20.22%
QUINONE	1.01%	1.34%	3.11%	10.19%	0.15%	2.07%	9.14%
RADON	3.10%	0.90%			0.55%	9.85%	21.03%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
RDX	1.79%	2.59%	8.99%	3.44%	1.49%	11.72%	19.76%
SACCHARIN	2.00%	6.15%	10.89%	5.45%	5.10%	35.27%	6.28%
SALICYLIC ACID	1.25%	1.82%	6.82%		0.71%	5.02%	21.29%
SALICYLIC ACID PHENYL ESTER	1.07%	0.53%	1.18%		2.36%	25.74%	36.64%
sec-BUTENYL ACETATE	1.43%	0.21%	1.80%	6.88%	1.56%	15.83%	26.27%
sec-BUTYL ACETATE	1.47%	0.32%	5.53%	1.01%	1.12%	13.71%	26.09%
sec-BUTYL ACRYLATE	1.51%	0.28%	1.49%		1.11%	14.27%	26.16%
sec-BUTYL CHLORIDE	1.31%	0.60%	4.07%	0.90%	2.16%	13.99%	23.32%
sec-BUTYL FORMATE	1.17%	0.65%	4.16%	3.90%	1.50%	15.74%	25.80%
sec-BUTYL MERCAPTAN	0.68%	0.60%	2.05%	1.89%	1.95%	11.07%	23.18%
sec-BUTYLAMINE	0.62%	0.56%	2.79%	1.46%	2.00%	16.14%	14.95%
sec-BUTYLBENZENE	1.24%	0.64%	2.53%	3.46%	2.31%	20.92%	25.62%
sec-BUTYLCYCLOHEXANE	0.74%	0.90%	2.82%		2.53%	21.90%	36.15%
sec-BUTYL-tert-BUTYL ETHER	0.65%	0.20%	0.82%	1.50%	1.25%	11.09%	24.31%
SILANE	2.33%	2.51%			0.14%	7.92%	16.38%
SITOSTEROL	0.55%	1.84%	1.73%		3.78%	51.86%	61.52%
STIGMASTEROL	0.57%	1.73%	1.48%		3.69%	49.95%	61.28%
STYRENE	0.44%	1.23%	4.23%	2.51%	3.02%	21.72%	30.40%
STYRENE GLYCOL	0.87%	0.40%	1.04%		2.15%	22.84%	34.40%
SUBERIC ACID	4.59%	0.39%			1.40%	25.84%	48.71%
SUCCINIC ANHYDRIDE	8.11%	3.23%	6.78%		4.57%	48.68%	49.77%
SUCCINIMIDE	1.06%	1.45%			4.95%	49.46%	46.98%
SUCROSE	1.29%	2.75%	4.92%		4.67%	43.59%	47.03%
SULFOLANE	0.59%	1.43%	3.86%		5.04%	42.09%	56.66%
SULFUR DIOXIDE	1.08%	0.67%	3.55%	4.38%	1.73%	16.61%	24.11%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
SULFUR HEXAFLUORIDE	0.61%	0.13%	1.04%		0.76%	7.62%	18.33%
SULFUR TRIOXIDE	9.11%	3.82%	9.32%		0.23%	17.26%	30.47%
SULFURYL CHLORIDE	2.32%	1.25%	7.82%		3.26%	30.75%	40.02%
SYRINGALDEHYDE	0.90%	0.77%			0.76%	6.29%	28.98%
SYRINGOL	0.63%	0.28%	2.23%		1.29%	13.76%	29.60%
t-BUTYL ACETOACETATE	0.72%	0.46%	2.24%		1.11%	11.60%	26.98%
t-BUTYL HYDROPEROXIDE	1.77%	1.34%	3.11%		0.25%	1.86%	21.55%
TEREPHTHALDEHYDE	0.68%	1.63%	3.48%	3.11%	4.21%	43.57%	45.71%
TEREPHTHALIC ACID	0.10%	1.56%			5.41%	70.63%	65.68%
TEREPHTHALOYL CHLORIDE	0.65%	1.07%	4.24%		0.23%	3.36%	16.36%
TERPINOLENE	1.25%	0.78%	3.87%	0.74%	2.36%	22.67%	32.97%
tert-BUTYL ACETATE	2.32%	0.66%	1.15%	6.00%	1.07%	13.04%	22.49%
tert-BUTYL CHLORIDE	0.46%	0.44%	1.67%	2.49%	1.20%	8.08%	20.10%
tert-BUTYL ETHYL ETHER	0.71%	0.34%	0.99%		1.65%	14.22%	22.13%
tert-BUTYL FORMATE	0.61%	1.44%	1.49%	5.43%	1.61%	13.25%	24.47%
tert-BUTYL MERCAPTAN	1.12%	0.34%	2.29%	4.38%	0.40%	3.48%	17.85%
tert-BUTYL METHACRYLATE	1.65%	0.28%	1.76%		1.14%	12.75%	24.30%
tert-BUTYLAMINE	1.02%	0.99%	3.39%	10.07%	1.07%	11.73%	19.20%
tert-BUTYLBENZENE	1.91%	1.20%	4.49%	0.75%	1.67%	18.66%	25.18%
tert-BUTYLCYCLOHEXANE	1.19%	1.24%	9.29%		1.98%	17.82%	33.20%
tert-BUTYLFORMAMIDE	0.63%	1.70%	3.86%		4.30%	40.28%	40.66%
tert-DODECYL MERCAPTAN	0.72%	0.33%	1.45%	2.30%	2.11%	21.60%	33.54%
tert-NONYL MERCAPTAN	1.00%	0.87%	4.02%	3.20%	2.96%	28.90%	34.57%
tert-OCTYL MERCAPTAN	0.56%	0.52%	3.06%	0.78%	2.30%	18.73%	26.83%
TETRACHLOROETHYLENE	1.28%	0.19%	2.33%	2.50%	1.60%	16.08%	54.31%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
TETRACHLOROSILANE	0.32%	0.15%	2.23%	4.51%	1.43%	12.83%	20.06%
TETRADECAMETHYLHEXASILOXANE	1.71%	0.35%	3.57%		1.29%	16.78%	34.11%
TETRADECANEDIOIC ACID	0.72%	1.44%			0.89%	11.47%	51.95%
TETRAETHYL LEAD	0.69%	2.79%	7.04%	0.19%	3.69%	30.60%	34.30%
TETRAETHYL SILANE	0.53%	0.50%	2.04%	5.99%	1.45%	13.04%	19.22%
TETRAETHYLENE GLYCOL	0.44%	1.06%	1.71%		2.10%	23.92%	50.83%
TETRAETHYLENE GLYCOL DIMETHYL ETHER	0.73%	0.55%			0.58%	10.27%	49.43%
TETRAETHYLENE GLYCOL MONOETHYL ETHER	1.48%	1.55%	4.93%		0.25%	0.33%	26.79%
TETRAETHYLENE GLYCOL MONOMETHYL ETHER	1.53%	1.93%	5.85%		0.67%	3.87%	25.36%
TETRAETHYLENEPENTAMINE	1.76%	1.83%	5.48%		0.40%	1.47%	33.31%
TETRAFLUROETHYLENE	0.39%	0.38%	2.37%	1.74%	1.80%	13.75%	25.20%
TETRAFLUROHYDRAZINE	6.47%	2.05%		8.95%	0.90%	5.91%	8.49%
TETRAHYDROFURAN	0.46%	0.37%	1.92%	2.37%	2.23%	14.82%	28.77%
TETRAHYDROFURFURYL ALCOHOL	5.12%	2.09%			3.33%	14.98%	31.05%
TETRAHYDROPYRAN	0.39%	0.66%	0.74%		1.23%	8.88%	26.49%
TETRAHYDROTHIOPHENE	0.76%	0.47%	3.34%	4.84%	2.60%	19.40%	36.32%
TETRAMETHYLETHYLENEDIAMINE	0.68%	0.20%	1.61%	1.31%	1.79%	15.86%	26.23%
TETRAMETHYLSILANE	0.71%	0.31%	2.76%	1.39%	1.31%	12.56%	24.26%
TETRANTROMETHANE	6.18%	1.48%			4.27%	40.11%	27.21%
TETRAPHENYLETHYLENE	0.50%	2.43%	4.01%		5.32%	62.19%	58.26%
TETRAPHENYLMETHANE	1.08%	2.18%	4.70%	1.50%	5.05%	59.39%	57.56%
TETRYL	1.75%	1.78%	6.32%		0.57%	3.27%	32.21%
THIACYCLOPROPANE	0.61%	1.00%	3.58%		2.98%	21.17%	33.89%
THIANDAN	0.77%	1.82%	3.99%		4.96%	38.93%	37.54%
THIOGLYCOLIC ACID	1.02%	1.17%			3.48%	34.30%	39.34%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
THIONYL CHLORIDE	2.94%	2.14%	8.48%		6.33%	57.53%	70.54%
THIOPHENE	0.62%	0.57%	2.60%	5.77%	1.90%	12.63%	28.85%
THIOUREA	0.85%	1.11%	2.31%		0.16%	0.57%	15.96%
THYMOL	1.00%	2.36%			0.44%	1.96%	30.24%
TIN(IV) CHLORIDE	0.59%	0.72%	2.35%	3.82%	2.13%	16.87%	24.83%
TITANIUM TETRACHLORIDE	3.72%	0.80%		12.91%	1.44%	4.85%	11.58%
TOLUENE	0.09%	0.55%	2.68%	1.42%	2.46%	18.03%	26.34%
trans,trans-2,4-HEXADIENE	0.39%	0.69%	3.81%	2.49%	3.27%	25.38%	33.72%
trans-1,2-DICHLOROETHYLENE	1.56%	0.97%	3.06%	4.44%	2.49%	10.66%	15.98%
trans-1,2-DIMETHYLCYCLOHEXANE	0.81%	0.60%	4.07%	1.12%	2.63%	21.95%	22.23%
trans-1,2-DIMETHYLCYCLOPENTANE	0.38%	0.44%	0.80%	4.66%	1.33%	8.39%	23.61%
trans-1,3,3,3-TETRAFLUOROPROPENE	1.08%	0.15%	1.56%	1.63%	1.92%	15.38%	23.19%
trans-1,3-DICHLOROPROPENE	1.65%	0.83%	3.95%	5.29%	2.51%	21.98%	28.54%
trans-1,3-DIMETHYLCYCLOHEXANE	1.39%	0.98%	5.38%	1.88%	2.48%	22.85%	22.61%
trans-1,3-DIMETHYLCYCLOPENTANE	0.37%	0.49%	1.33%	1.78%	1.26%	7.97%	23.58%
trans-1,3-HEXADIENE	0.32%	0.63%	1.70%		2.81%	21.35%	30.09%
trans-1,3-PENTADIENE	3.29%	0.94%	9.32%	7.48%	1.76%	22.11%	34.25%
trans-1,4-DIETHYLCYCLOHEXANE	0.96%	0.72%	1.68%		0.84%	8.65%	21.33%
trans-1,4-DIMETHYLCYCLOHEXANE	0.42%	0.66%	2.97%	0.73%	2.28%	18.17%	23.11%
trans-1,8-TERPIN	1.82%	2.56%	11.36%		1.57%	12.80%	19.85%
trans-1-PROPENYLBENZENE	0.66%	1.50%	3.32%	2.80%	3.10%	26.42%	35.78%
trans-2,2,4,6,6-PENTAMETHYL-3-HEPTENE	0.48%	1.31%	3.04%		3.78%	32.40%	34.94%
trans-2,n-HEXYL-DECAHYDRONAPHTHALENE	0.49%	2.09%	3.83%	8.81%	5.19%	49.83%	45.52%
trans-2-BUTENE	0.74%	0.36%	3.61%	2.40%	2.05%	12.34%	21.73%
trans-2-DECENE	0.84%	0.55%	2.28%	2.73%	2.56%	24.64%	33.38%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
trans-2-DODECENE	0.95%	0.68%	2.05%	4.12%	2.51%	25.93%	33.91%
trans-2-HEPTENE	0.19%	0.50%	2.50%	0.38%	2.63%	20.93%	31.38%
trans-2-HEXENE	0.30%	0.52%	3.00%	2.34%	2.39%	18.42%	29.27%
trans-2-METHYL-1,3-PENTADIENE	0.94%	0.99%	2.93%		2.95%	23.95%	29.41%
trans-2-METHYLCYCLOHEXANOL	1.22%	1.88%	2.65%	2.35%	0.75%	5.38%	20.64%
trans-2-NONENE	0.58%	0.48%	3.98%		2.47%	23.51%	33.00%
trans-2-OCTENE	0.41%	0.56%	2.82%	0.82%	2.95%	23.03%	32.44%
trans-2-PENTADECENE	0.65%	0.88%	1.50%		2.33%	25.24%	32.43%
trans-2-PENTENE	0.08%	0.43%	1.56%	2.64%	1.81%	12.85%	22.55%
trans-2-PHENYLBUTENE-2	0.71%	0.66%	2.47%		2.65%	22.71%	29.78%
trans-3,5-DIMETHOXYSTILBENE	0.72%	1.71%	1.45%		2.93%	30.90%	57.49%
trans-3-HEPTENE	0.33%	0.68%	2.67%	1.85%	2.65%	19.82%	29.34%
trans-3-HEXENE	0.21%	0.65%	2.56%	1.54%	2.00%	17.68%	26.78%
trans-3-METHYLCYCLOHEXANOL	1.11%	2.30%	2.66%	1.29%	0.39%	5.70%	22.59%
trans-3-OCTENE	0.39%	0.80%	2.73%	1.73%	3.01%	23.44%	28.46%
trans-4-METHYLCYCLOHEXANOL	1.29%	1.89%	3.30%	1.08%	0.04%	2.05%	21.62%
trans-4-OCTENE	0.62%	0.80%	2.31%	1.80%	3.06%	23.26%	28.23%
trans-CROTONIC ACID	1.74%	2.57%	2.99%		2.41%	27.10%	45.45%
trans-CROTONITRILE	1.99%	3.01%	6.89%		7.14%	59.51%	48.43%
trans-DECAHYDRONAPHTHALENE	0.43%	0.25%	1.13%	1.01%	1.79%	12.40%	23.96%
trans-STILBENE	2.19%	0.78%	5.73%		2.41%	30.05%	36.64%
TRIALLYLAMINE	0.41%	0.26%	0.81%	4.12%	1.87%	16.12%	28.01%
TRIAMYLAMINE	1.48%	1.15%	2.45%		0.77%	11.33%	36.56%
TRIBROMOMETHANE	1.64%	1.16%	2.49%	12.28%	0.66%	6.46%	10.75%
TRICAPRIN	0.20%	2.72%			5.14%	87.85%	89.51%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
TRICAPRYLIN	0.48%	2.53%	2.77%		5.08%	79.31%	79.84%
TRICHLOROACETALDEHYDE	0.70%	0.17%	1.85%		1.71%	14.59%	23.29%
TRICHLOROACETIC ACID	2.01%	0.17%	0.92%		0.96%	12.88%	28.29%
TRICHLOROACETYL CHLORIDE	0.71%	0.38%	1.82%		1.45%	6.83%	13.70%
TRICHLOROETHYLENE	0.77%	0.42%	4.31%	1.44%	1.50%	13.72%	25.90%
TRICHLOROFLUOROMETHANE	0.26%	0.33%	1.81%	1.47%	1.53%	9.71%	19.46%
TRICHLOROSILANE	0.48%	0.72%	1.76%	8.70%	0.86%	6.89%	18.79%
TRIDECAFLUOROHEPTANOIC ACID	3.40%	1.73%			0.71%	0.19%	27.65%
TRIDECANAL	0.23%	0.66%	4.95%		0.70%	6.76%	25.58%
TRIETHYL ALUMINUM	10.48%	11.26%	12.78%		7.26%	57.88%	8.49%
TRIETHYL ESTER PHOSPHOROUS ACID	2.17%	8.56%	9.48%		6.57%	40.22%	12.42%
TRIETHYL GALLIUM	0.15%	1.20%		27.53%	3.68%	33.83%	37.67%
TRIETHYL ORTHOFORMATE	0.33%	0.27%	3.61%		0.81%	7.71%	25.18%
TRIETHYLAMINE	0.34%	0.47%	2.57%	2.36%	1.66%	13.03%	25.10%
TRIETHYLENE GLYCOL BIS(2-ETHYLHEXANOATE)	0.99%	1.81%	3.52%		1.47%	19.12%	59.81%
TRIETHYLENE GLYCOL DIMETHYL ETHER	1.23%	2.18%	2.28%		0.67%	10.52%	42.53%
TRIETHYLENEDIAMINE	0.53%	0.55%	1.57%		0.80%	7.47%	21.54%
TRIETHYLENETETRAMINE	1.26%	1.26%	3.97%		0.09%	3.42%	30.24%
TRIFLUOROACETIC ACID	1.05%	1.78%		8.32%	8.17%	82.28%	104.85%
TRIFLUOROIODOMETHANE	0.33%	1.33%	1.32%		1.85%	11.59%	23.37%
TRIFLUOROMETHANE	0.31%	0.66%	5.03%	2.18%	3.23%	23.37%	30.35%
TRIFLUOROMETHYL TRIFLUOROVINYL ETHER	0.92%	2.16%	5.00%		1.14%	6.82%	11.93%
TRIISOBUTYL ALUMINUM	0.91%	1.01%			3.39%	26.52%	32.28%
TRIMETHYL BORATE	0.98%	2.01%			2.27%	15.69%	55.68%
TRIMETHYL SILANE	0.46%	0.69%	2.63%		1.75%	12.16%	20.68%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
TRIMETHYL SILANOL	4.35%	1.26%			0.91%	1.46%	17.51%
TRIMETHYLALUMINUM	3.55%	0.44%	14.96%		3.89%	41.31%	58.52%
TRIMETHYLAMINE	0.67%	0.46%	2.19%	0.98%	2.12%	13.12%	16.15%
TRIMETHYLCHLOROSILANE	0.10%	1.19%	1.53%	3.96%	1.73%	12.84%	17.79%
TRIMETHYLENE SULFIDE	0.72%	0.37%	4.78%	2.97%	3.20%	23.97%	30.60%
TRIMETHYLGALLIUM	4.65%	2.79%	10.47%	3.52%	0.84%	18.90%	65.81%
TRIMETHYLOLPROPANE	2.23%	2.21%			0.67%	13.12%	31.86%
TRI-n-BUTYL BORATE	0.49%	3.91%	2.91%		1.11%	8.60%	19.95%
TRI-n-BUTYL PHOSPHATE	0.23%	0.85%			1.83%	20.68%	40.69%
TRI-n-BUTYLAMINE	0.97%	1.14%	1.87%		1.41%	15.83%	34.91%
TRI-n-OCTYLAMINE	1.02%	0.89%			1.51%	17.33%	56.63%
TRIOXANE	0.67%	0.62%	1.89%	6.99%	2.56%	20.88%	28.40%
TRIPHENYLENE	0.26%	0.84%	1.88%		2.91%	28.86%	38.87%
TRIPHENYLETHYLENE	0.70%	1.03%	2.52%	1.00%	3.16%	32.65%	39.34%
TRIPHENYLMETHANE	1.18%	0.40%	2.71%	9.83%	2.61%	27.92%	44.71%
TRIPROPYLAMINE	1.85%	2.46%			0.51%	8.66%	24.60%
TRIPROPYLENE GLYCOL MONOETHYL ETHER	1.33%	2.68%		15.96%	1.25%	8.42%	29.41%
TRIPROPYLENE GLYCOL MONOMETHYL ETHER	1.15%	2.31%		0.47%	0.99%	7.06%	28.11%
TRIS(2-METHOXYETHOXY)VINYLSILANE	0.83%	2.41%	8.95%		0.87%	9.95%	29.63%
TRISILANE	1.12%	1.31%			0.00%	2.51%	13.57%
UNDECANAL	1.14%	0.85%	3.33%		0.54%	7.19%	25.65%
UNDECYL MERCAPTAN	1.15%	0.40%	2.62%	1.71%	3.25%	26.12%	47.01%
UNDECYLAMINE	2.77%	0.26%		4.87%	3.22%	22.76%	37.20%
VALERONITRILE	2.28%	1.59%	3.26%		5.29%	40.04%	38.15%
VANADIUM OXYTRICHLORIDE	1.75%	1.55%			4.59%	37.77%	62.52%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $c_{P,liq}^{sat}$	MAPE on V_c	MAPE on T_c	MAPE on P_c
VANADIUM TETRACHLORIDE	1.72%	1.89%			1.01%	7.90%	19.53%
VANILLIC ACID	1.19%	0.44%	3.85%		1.02%	13.36%	33.80%
VANILLIN	0.97%	0.70%	2.40%		0.69%	9.26%	29.40%
VINYL ACETATE	0.76%	0.54%	5.06%	10.07%	3.24%	28.50%	34.63%
VINYL CHLORIDE	2.31%	0.52%	6.36%		0.69%	9.10%	17.97%
VINYL FLUORIDE	2.48%	0.99%		2.28%	1.17%	8.98%	20.40%
VINYL FORMATE	2.28%	0.99%	5.28%		2.08%	21.30%	26.70%
VINYL PIVALATE	0.73%	0.40%	1.21%		1.18%	11.18%	23.49%
VINYL PROPIONATE	0.66%	0.47%	2.43%		2.21%	19.34%	27.31%
VINYLCETONITRILE	4.51%	2.85%	8.68%	5.23%	6.06%	60.46%	61.06%
VINYLCETYLENE	3.54%	0.85%	5.63%	4.58%	1.21%	17.76%	26.29%
VINYLCYCLOHEXANE	0.96%	0.59%	2.22%	7.06%	1.74%	14.92%	24.82%
VINYLETHYLENE CARBONATE	1.35%	0.89%	2.85%	3.48%	3.07%	30.68%	53.79%
VINYLNORBORNENE	0.52%	4.89%	4.18%		2.19%	18.16%	26.58%
VINYLTRICHLOROSILANE	0.37%	0.55%	3.98%		3.25%	25.43%	20.57%
VINYLTRIMETHOXSILANE	0.96%	0.55%		9.17%	2.02%	14.13%	30.19%
WATER	5.55%	2.72%	9.21%	18.12%	4.09%	40.74%	45.28%
XENON	0.41%	0.60%	1.95%		0.78%	3.27%	16.52%

Table S4. Compound-by-compound analysis of the performance of the I-PC-SAFT EoS for 1 800 compounds.

I-PC-SAFT EoS

Average MAPE (%) on:						
P^{sat}	v_{liq}^{sat}	$\Delta_{vap}H$	$C_{P,liq}^{sat}$	V_c	T_c	P_c
2.08	4.60	4.00	4.10	12.4	0	0
Global average deviation: 3.6%						

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c
(3,3,3-TRIFLUOROPROPYL)METHYLDICHLOROSILANE	1.40%	3.72%	3.72%		9.62%
(3-GLYCIDOXYPROPYL)METHYLDIETHOXYSILANE	2.25%	6.51%	4.98%		14.14%
(3-METHYLACRYLOXYPROPYL)TRICHLOROSILANE	2.48%	6.43%	4.54%		16.58%
[3-(2,3-EPOXYPROXY)PROPYL]TRIMETHOXYSILANE	2.56%	8.30%	5.00%	3.11%	18.84%
[3-(MERCAPTO)PROPYL]TRIETHOXYSILANE	0.25%	3.66%			12.33%
1-(4-ETHYLPHENYL)-2-(4-ETHYLPHENYL)ETHANE	1.62%	3.50%	5.22%		16.38%
1-(4-ETHYLPHENYL)-2-PHENYLETHANE	1.99%	4.15%	3.90%	4.60%	15.28%
1,1,1,2,2,3,4,5,5,5-DECAFLUOROPENTANE	4.77%	3.40%	3.64%		10.17%
1,1,1,2,2-PENTAFLUOROPROPANE	1.03%	3.70%	2.32%		7.16%
1,1,1,2,3,3,3-HEPTAFLUOROPROPANE	1.58%	3.63%	2.66%		13.39%
1,1,1,2,3,3-HEXAFLUOROPROPANE	1.18%	3.57%	2.95%		8.04%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
1,1,1,2-TETRACHLORODIFLUOROETHANE	1.66%	2.53%	4.34%		12.92%
1,1,1,2-TETRACHLOROETHANE	1.81%	3.66%	3.70%	7.61%	14.28%
1,1,1,2-TETRAFLUROETHANE	0.62%	3.65%	1.96%	5.04%	10.42%
1,1,1,3,3-HEXAFLUROPROPANE	1.92%	3.35%	4.31%		12.19%
1,1,1,3,3-PENTACHLOROPROPANE	2.87%	3.79%	4.85%		10.60%
1,1,1,3,3-PENTAFLUROBUTANE	6.55%	1.15%			10.87%
1,1,1,3,3-PENTAFLUROPROPANE	3.07%	3.46%	4.97%		8.89%
1,1,1-TRICHLOROETHANE	0.21%	2.23%	2.26%	2.67%	10.57%
1,1,1-TRICHLOROFLUROETHANE	0.98%	5.80%	2.66%		12.14%
1,1,1-TRICHLOROTRIFLUROETHANE	3.33%	2.42%	2.02%	1.73%	9.91%
1,1,1-TRIFLUROETHANE	0.31%	3.48%	2.84%	5.77%	11.49%
1,1,2,2,3-PENTAFLUROPROPANE	1.02%	3.26%	3.55%		7.87%
1,1,2,2-TETRACHLORODIFLUOROETHANE	0.71%	3.16%	2.83%		12.32%
1,1,2,2-TETRACHLOROETHANE	6.51%	4.44%			14.23%
1,1,2,2-TETRAFLUROETHANE	4.37%	2.70%	2.26%	0.25%	7.78%
1,1,2,2-TETRAPHENYLETHANE	2.33%	2.62%	5.69%	1.13%	12.18%
1,1,2-TRICHLOROETHANE	1.54%	2.92%	2.44%	7.46%	13.49%
1,1,2-TRICHLOROTRIFLUROETHANE	1.35%	2.22%	2.25%	2.88%	7.97%
1,1,2-TRIFLUROETHANE	2.55%	3.42%	2.54%	6.60%	9.81%
1,1,2-TRIMETHYLCYCLOPENTANE	1.12%	3.66%	3.76%		13.42%
1,1,2-TRIPHENYLETHANE	2.02%	3.93%	4.08%	1.91%	16.09%
1,1,3-TRIMETHYLCYCLOHEXANE	0.85%	2.07%	3.00%		8.90%
1,1,3-TRIMETHYLCYCLOPENTANE	3.45%	6.18%	3.28%		16.08%
1,1,5-TRIMETHYLINDAN	0.45%	4.81%	4.36%		11.94%
1,1-DIBROMOETHANE	11.19%	1.64%	11.51%	13.11%	0.13%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
1,1-DICHLORO-1-FLUOROETHANE	0.30%	2.32%	1.52%	3.06%	8.11%
1,1-DICHLOROETHANE	1.45%	2.34%	1.40%	1.37%	6.26%
1,1-DICHLOROETHYLENE	8.12%	3.02%	6.77%	11.04%	2.84%
1,1-DICHLOROPROPANE	1.03%	6.60%	2.02%	3.21%	8.32%
1,1-DICHLOROTETRAFLUROETHANE	0.09%	1.83%	2.37%	4.09%	6.64%
1,1-DIETHYLCYCLOHEXANE	1.94%	5.59%	3.08%	6.95%	10.72%
1,1-DIFLUOROETHANE	0.29%	4.55%	1.90%	8.83%	12.16%
1,1-DIFLUOROETHYLENE	3.29%	1.19%		2.87%	9.21%
1,1-DIMETHOXYETHANE	0.18%	3.99%	4.39%	5.20%	9.53%
1,1-DIMETHYLCYCLOHEXANE	1.95%	3.38%	2.63%	1.64%	6.79%
1,1-DIMETHYLCYCLOPENTANE	1.25%	1.85%	1.24%	1.94%	9.83%
1,1-DIPHENYLETHANE	1.46%	4.08%	2.44%		12.65%
1,2,3,4-TETRAHYDRONAPHTHALENE	0.29%	5.08%	1.51%	2.36%	15.40%
1,2,3,4-TETRAMETHYLBENZENE	1.66%	4.24%	3.42%	7.41%	10.78%
1,2,3,4-TETRAMETHYLCYCLOHEXANE	1.64%	5.33%	3.00%	2.69%	11.80%
1,2,3,5-TETRAETHYLBENZENE	2.68%	4.95%	5.10%	7.98%	13.04%
1,2,3,5-TETRAMETHYLBENZENE	0.43%	4.64%	3.49%	6.04%	11.43%
1,2,3,6-TETRAHYDROBENZALDEHYDE	1.21%	5.53%	3.85%	3.57%	12.61%
1,2,3,6-TETRAHYDROBENZYL ALCOHOL	1.65%	4.98%	4.00%		10.61%
1,2,3-TRICHLOROBENZENE	1.32%	0.26%	4.54%	6.10%	3.49%
1,2,3-TRICHLOROPROPANE	1.39%	4.78%	3.02%	4.55%	17.09%
1,2,3-TRIETHYLBENZENE	1.86%	5.77%	3.75%	6.49%	12.30%
1,2,3-TRIMETHYL-4-ETHYLBENZENE	1.51%	4.55%	4.12%		11.27%
1,2,3-TRIMETHYLBENZENE	0.70%	5.67%	3.38%	6.53%	10.12%
1,2,3-TRIMETHYLINDENE	2.00%	3.26%	3.72%	12.71%	14.25%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
1,2,4,5-TETRAISOPROPYLBENZENE	2.93%	3.24%	6.30%		15.13%
1,2,4,5-TETRAMETHYLBENZENE	1.36%	4.25%	3.26%	7.11%	12.36%
1,2,4-TRICHLOROBENZENE	1.80%	4.49%	1.95%	2.95%	15.37%
1,2,4-TRIETHYLBENZENE	0.29%	5.89%	2.91%	5.53%	11.78%
1,2,4-TRIMETHYL-3-ETHYLBENZENE	1.18%	4.34%			10.91%
1,2,4-TRIMETHYL-5-ETHYLBENZENE	0.67%	4.58%	4.68%		11.38%
1,2,4-TRIMETHYLBENZENE	0.39%	5.07%	3.03%	5.61%	10.27%
1,2-BENZENE DICARBOXYLIC ACID, HEPTYL, UNDECYL ESTER	2.39%	9.78%	5.56%		31.12%
1,2-BENZENEDICARBOXYLIC ACID, HEPTYL, NONYL ESTER	2.91%	7.80%	5.50%		26.28%
1,2-BENZENEDIOL	6.36%	0.91%	10.30%		9.50%
1,2-BUTADIENE	3.40%	3.02%	2.35%	4.13%	13.64%
1,2-BUTANEDIOL	4.40%	5.60%	4.65%		1.96%
1,2-DIBROMOETHANE	1.48%	2.68%	1.27%	1.54%	10.18%
1,2-DIBROMOPROPANE	0.62%	2.65%	3.20%		6.17%
1,2-DIBROMOTETRAFLUOROETHANE	0.89%	3.50%	2.46%		3.38%
1,2-DICHLORO-1,1,2-TRIFLUOROETHANE	0.43%	2.97%	1.79%	4.71%	10.90%
1,2-DICHLORO-4-NITROBENZENE	1.75%	5.29%	3.73%		10.79%
1,2-DICHLOROBUTANE	0.78%	6.87%	2.25%		11.29%
1,2-DICHLOROETHANE	2.91%	2.87%	4.75%	3.11%	14.96%
1,2-DICHLOROHEXAFLUOROCYCLOBUTANE	0.79%	3.09%	2.61%		11.24%
1,2-DICHLOROPROPANE	0.75%	4.56%	2.73%	2.59%	10.69%
1,2-DICHLOROTETRAFLUROETHANE	0.64%	2.62%	2.53%	4.29%	7.54%
1,2-DIETHOXYETHANE	0.74%	6.47%	2.23%	10.32%	12.58%
1,2-DIFLUOROBENZENE	0.45%	3.09%	3.44%		9.43%
1,2-DIFLUOROETHANE	0.66%	12.35%	3.56%	1.36%	22.49%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
1,2-DIMETHOXYETHANE	2.27%	4.67%	2.70%		22.13%
1,2-DIMETHOXYPROPANE	1.23%	3.01%	3.27%		9.19%
1,2-DIMETHYL-3-PROPYLBENZENE	0.54%	2.74%	4.54%		2.39%
1,2-DIPHENYLETHANE	1.04%	4.43%	4.84%		11.61%
1,2-EPOXY-2-METHYLPROPANE	0.47%	3.33%	2.89%	0.41%	13.05%
1,2-EPOXY-3-PHENOXYPROPANE	0.73%	4.27%	6.07%		19.99%
1,2-EPOXYBUTANE	1.71%	5.21%	2.57%	1.98%	10.06%
1,2-ETHANEDITHIOL	1.30%	4.18%	2.41%		40.48%
1,2-HEXADIENE	1.29%	5.63%	2.58%	0.66%	12.21%
1,2-PENTADIENE	6.20%	4.90%	6.68%	1.12%	13.88%
1,2-PROPANEDIAMINE	1.44%	0.67%	2.00%		12.77%
1,2-PROPYLENE GLYCOL	3.56%	8.68%	5.26%		5.85%
1,2-PROPYLENE OXIDE	1.25%	5.64%	3.08%	3.98%	22.51%
1,3,5,7-CYCLOOCTATETRAENE	0.34%	0.23%	3.73%	0.72%	11.13%
1,3,5-TRICHLOROBENZENE	1.65%	3.19%	2.73%	9.72%	7.11%
1,3,5-TRIETHYLBENZENE	1.20%	6.50%	2.98%	5.54%	15.22%
1,3,5-TRISOPROPYLBENZENE	2.42%	4.66%	5.29%		14.21%
1,3,5-TRI-tert-BUTYLBENZENE	3.70%	3.95%			12.24%
1,3-BENZENEDIOL	1.50%	1.11%	4.16%	3.81%	7.49%
1,3-BUTADIENE	0.90%	2.62%	2.18%	1.85%	9.37%
1,3-CYCLOHEXADIENE	1.00%	0.44%	2.30%	1.51%	6.64%
1,3-DIBROMOPROPANE	0.20%	3.41%	3.17%		7.20%
1,3-DICHLOROHEXAFLUOROPROPANE	1.15%	6.10%	2.76%		12.52%
1,3-DICHLOROPROPANE	0.79%	6.12%	3.08%	1.22%	15.98%
1,3-DIFLUOROBENZENE	0.93%	2.57%	3.82%		6.79%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
1,3-DIMETHYL UREA	2.17%	3.73%	5.00%		14.19%
1,3-DIMETHYL-2-IMIDAZOLIDINONE	0.59%	5.21%	4.25%		12.22%
1,3-DIMETHYL-5-NITROBENZENE	1.58%	7.90%	4.77%		20.26%
1,3-DIMETHYLADAMANTANE	0.19%	2.59%	3.61%	0.59%	3.13%
1,3-DIOXANE	1.22%	1.80%	2.50%	3.22%	16.78%
1,3-DIPHENYLTRIAZENE	1.85%	3.18%	4.14%		10.62%
1,3-DI-TERT-BUTYL GLYCERIN	1.58%	2.35%	4.25%		8.58%
1,3-PROPANEDIAMINE	2.37%	1.11%	3.88%		11.23%
1,3-PROPYLENE GLYCOL	3.60%	9.20%	5.62%		5.67%
1,3-PROPYLENE OXIDE	0.52%	4.67%	2.25%	2.72%	13.27%
1,4-BENZENEDICARBOXYLIC ACID, 2-HYDROXYETHYL METHYL ESTER	1.92%	2.98%	4.87%		10.78%
1,4-BIS(3-AMINOPROPYL)PIPERAZINE	1.04%	2.28%	5.68%	1.69%	4.06%
1,4-BUTANEDIISOCYANATE	0.72%	11.97%	5.01%	5.88%	23.59%
1,4-BUTANEDIOL	6.05%	7.23%	6.64%		5.28%
1,4-CYCLOHEXANEDICARBOXYLIC ACID	2.76%	1.41%	9.25%		11.31%
1,4-CYCLOHEXANEDIMETHANOL	4.62%	3.10%			9.58%
1,4-DIBROMOBENZENE	5.27%	1.64%			9.63%
1,4-DICHLOROBUTANE	2.03%	4.54%	2.83%	3.41%	20.07%
1,4-DICHLORO-cis-2-BUTENE	1.42%	3.86%	2.93%	0.75%	14.47%
1,4-DICHLORO-trans-2-BUTENE	1.48%	3.26%	3.20%	0.80%	14.55%
1,4-DICYANO-2-BUTENE	1.90%	30.78%	4.99%		36.20%
1,4-DIFLUOROBENZENE	1.22%	1.60%	4.13%		3.17%
1,4-DIOXANE	1.07%	2.40%	2.79%	9.69%	15.14%
1,4-DI-tert-BUTYLBENZENE	1.35%	1.83%	2.32%	0.49%	2.44%
1,4-HEXADIENE	0.44%	4.64%	2.46%	4.34%	10.59%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
1,4-PENTADIENE	9.12%	2.93%	11.40%	19.63%	6.28%
1,4-PENTANEDIOL	4.23%	4.62%	6.62%		11.53%
1,5,9-CYCLODODECATRIENE	1.73%	3.20%			8.47%
1,5-CYCLOOCTADIENE	1.20%	0.53%	2.10%	4.79%	12.18%
1,5-DICHLOROPENTANE	2.37%	5.08%	3.34%	4.78%	22.37%
1,5-HEXADIENE	0.81%	5.33%	2.38%		7.89%
1,5-NAPHTHALENE DIISOCYANATE	1.26%	2.91%	5.25%		11.25%
1,5-PENTANEDIAMINE	1.53%	1.26%			2.84%
1,6-DIMETHYLINDAN	0.49%	5.08%	4.55%		10.29%
1,6-HEXANEDIOL DIACRYLATE	0.30%	5.25%			14.16%
1,9-DECADIENE	1.28%	4.95%	4.24%		11.24%
1-AMINO-2-PROPANOL	1.95%	3.90%	8.92%		7.36%
1-BROMOBUTANE	3.71%	3.68%	6.08%		9.62%
1-BROMODECANE	2.03%	5.00%	4.63%		12.93%
1-BROMOHEPTANE	1.70%	2.94%			11.37%
1-BROMONAPHTHALENE	1.46%	4.65%	2.89%		15.48%
1-BROMOPROPANE	5.69%	5.01%	6.99%		7.53%
1-BUTANOL	7.02%	6.53%	7.61%	16.25%	10.03%
1-BUTENE	2.10%	4.03%	5.37%	2.94%	7.24%
1-CHLORO-1,1-DIFLUOROETHANE	0.31%	3.62%	1.06%	2.30%	9.52%
1-CHLORO-2,4-DINITROBENZENE	2.12%	5.78%	4.22%		9.93%
1-CHLORONAPHTHALENE	2.00%	4.97%	4.33%		23.07%
1-CHLOROPENTANE	0.73%	5.44%	3.44%		13.14%
1-cis-2-trans-3-TRIMETHYLCYCLOPENTANE	1.32%	5.73%	3.26%		14.45%
1-cis-2-trans-4-TRIMETHYLCYCLOPENTANE	0.75%	6.34%	3.41%		15.20%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
1-CYCLOHEXYLETHANONE	3.39%	4.26%	5.25%		10.34%
1-DECANOL	4.32%	5.10%		12.46%	7.37%
1-DECENE	0.66%	4.60%	4.57%	0.44%	11.99%
1-DECYNE	0.62%	3.85%	3.80%	6.11%	12.30%
1-DOCOSANOL	7.83%	3.52%			15.45%
1-DODECANOL	2.78%	5.10%		11.92%	7.38%
1-DODECENE	1.50%	4.91%	4.31%	2.65%	11.37%
1-EICOSANOL	3.87%	3.35%		7.78%	12.61%
1-EICOSENE	1.57%	3.93%	3.21%	0.82%	9.89%
1-ETHOXY-2-PROPANOL	4.72%	2.81%			9.29%
1-ETHYL-2-ISOPROPYLBENZENE	1.56%	4.81%	2.43%	1.98%	11.07%
1-ETHYLCYCLOHEXENE	1.31%	4.82%	3.65%		9.68%
1-ETHYL-DECALIN	1.39%	5.00%	4.04%		11.22%
1-ETHYLNAPHTHALENE	1.02%	5.41%	3.26%	1.94%	6.36%
1-ETHYLTETRALIN	1.42%	6.08%	4.09%		11.81%
1-HEPTADECANOL	1.84%	3.02%		8.75%	9.95%
1-HEPTADECENE	1.02%	4.33%	3.34%	0.95%	10.28%
1-HEPTANOL	6.28%	1.86%		10.89%	10.50%
1-HEPTENE	1.20%	4.49%	4.17%	0.66%	10.36%
1-HEPTYNE	1.14%	3.23%	4.97%	3.19%	6.87%
1-HEXADECANOL	1.97%	4.70%		9.63%	9.07%
1-HEXADECENE	0.77%	4.48%	3.13%	1.02%	10.55%
1-HEXANOL	6.49%	6.23%		10.95%	9.21%
1-HEXATRIACONTENE	3.85%	3.37%	5.61%		8.80%
1-HEXENE	2.12%	4.33%	3.46%	1.75%	9.48%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
1-HEXYNE	1.05%	4.50%	2.96%	2.48%	8.03%
1H-PERFLUORO-N-HEXANE	2.97%	3.72%	5.73%		9.49%
1-METHOXY-2-PROPANOL PROPANOATE	3.46%	5.14%	5.88%		12.03%
1-METHYL-1-ETHYLCYCLOPENTANE	2.23%	5.12%		0.98%	8.72%
1-METHYL-2-n-PROPYLBENZENE	1.73%	4.28%	4.62%	0.86%	11.02%
1-METHYL-3-(METHYLETHOXY)BENZENE	1.25%	3.23%	5.57%		13.50%
1-METHYL-3-HYDROXY-5-ISOPROPYL BENZENE	3.39%	1.84%	5.44%		7.57%
1-METHYL-3-HYDROXY-6-ISOPROPYL BENZENE	0.46%	1.44%	4.87%		7.45%
1-METHYL-3-n-PROPYLBENZENE	0.56%	3.66%	3.64%	0.82%	14.57%
1-METHYL-4-n-PROPYLBENZENE	0.69%	2.14%	3.78%	0.87%	15.60%
1-METHYL-4-VINYLCYCLOHEXENE	1.55%	4.71%	2.67%	6.20%	9.89%
1-METHYLCYCLOPENTENE	1.03%	3.61%	2.09%	2.70%	6.66%
1-METHYL-DECALIN	2.05%	4.59%	3.97%		10.35%
1-METHYLINDAN	0.75%	4.93%	4.06%		9.79%
1-METHYLINDENE	1.13%	4.18%	2.90%	0.54%	9.81%
1-METHYLNAPHTHALENE	2.69%	5.17%	2.45%	3.02%	8.81%
1-METHYLTETRALIN	1.60%	5.90%	3.81%		11.11%
1-METHYLVINYL ACETATE	1.96%	2.29%	4.03%		5.37%
1-n-BUTYLNAPHTHALENE	1.28%	5.02%	3.01%	2.59%	10.18%
1-n-DECYLNAPHTHALENE	2.17%	5.32%	4.94%		29.78%
1-n-HEXYL-1,2,3,4-TETRAHYDRONAPHTHALENE	2.06%	5.84%	3.79%	0.82%	22.00%
1-n-HEXYLNAPHTHALENE	1.93%	4.56%	3.20%	1.36%	14.17%
1-NITROBUTANE	6.09%	6.12%	6.01%		12.20%
1-NITROPROPANE	4.48%	6.18%	8.18%	5.47%	11.54%
1-n-NONYLNAPHTHALENE	1.74%	5.30%	4.84%		26.55%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
1-NONADECANOL	2.61%	3.61%			11.22%
1-NONADECENE	1.22%	4.07%	3.32%	0.96%	9.89%
1-NONANOL	4.62%	5.90%		15.12%	7.06%
1-NONENE	0.38%	4.50%	4.99%	0.98%	10.82%
1-NONYNE	1.34%	3.48%	3.06%	5.69%	10.27%
1-n-PENTYLNAPHTHALENE	1.36%	5.47%	3.57%	1.99%	12.07%
1-OCTADECANOL	1.94%	4.32%		9.22%	10.56%
1-OCTADECENE	1.06%	4.14%	3.26%	1.03%	10.18%
1-OCTANOL	6.19%	4.05%	11.02%	11.53%	8.42%
1-OCTENE	1.35%	4.35%	4.25%	1.31%	9.96%
1-OCTYNE	0.45%	3.78%	4.49%	3.68%	8.53%
1-PENTADECANOL	2.08%	5.07%		9.94%	7.75%
1-PENTADECENE	0.80%	4.50%	4.61%	0.93%	10.61%
1-PENTANOL	5.49%	6.31%	8.43%	10.56%	9.33%
1-PENTENE	0.17%	3.94%	3.82%	2.48%	8.88%
1-PENTENE-4-YNE	1.51%	3.03%	2.58%	0.50%	8.81%
1-PENTYNE	1.81%	2.71%	3.94%	1.94%	4.85%
1-PHENYLNAPHTHALENE	1.58%	5.18%	3.60%		12.92%
1-PROPANOL	5.82%	8.74%	4.70%	31.32%	10.63%
1-tert-BUTOXY-2-[2-(HYDROXY)PROPOXY]PROPANE	2.61%	2.93%	4.82%		13.83%
1-tert-BUTOXY-2-[2-(tert-BUTOXY)PROPOXY]PROPANE	1.68%	18.99%	4.76%		29.27%
1-tert-BUTYL GLYCERIN	2.56%	5.98%	4.68%		15.69%
1-TETRADECENE	1.99%	5.14%	4.66%	0.36%	12.20%
1-TRIACONTENE	3.65%	4.47%	5.45%		8.40%
1-TRIDECANOL	2.32%	4.79%		11.57%	7.44%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
1-TRIDECENE	1.50%	4.99%	4.43%	0.12%	11.74%
1-UNDECANOL	3.03%	4.27%		13.03%	7.57%
1-UNDECENE	1.06%	4.79%	4.58%	2.21%	11.05%
2-(2-ETHOXYETHOXY)ETHANOL	2.50%	5.30%	4.73%		11.89%
2-(2-HEXOXYETHOXY)ETHANOL	1.89%	1.38%		9.63%	8.45%
2-(2-METHOXYETHOXY)ETHANOL	2.27%	5.97%	4.45%		11.44%
2-(2-PENTOXYETHOXY)ETHANOL	5.42%	4.13%			10.96%
2-(5H)-FURANONE	0.97%	27.57%	4.43%		52.43%
2-(alpha-METHYLBENZYLOXY)-1-PROPANOL	1.78%	3.58%	5.02%	15.77%	16.41%
2-(DIFLUOROMETHOXY)-1,1,1-TRIFLUOROETHANE	1.40%	4.28%	2.85%		8.01%
2-(N-MORPHOLINO)-2'-HYDROXYDIETHYLETHER	1.52%	3.65%	4.80%	6.72%	11.31%
2,2,3,3-TETRAMETHYLBUTANE	0.62%	1.42%	3.01%	0.79%	6.04%
2,2,3,3-TETRAMETHYLHEXANE	1.36%	3.36%	4.29%	1.41%	8.58%
2,2,3,3-TETRAMETHYLPENTANE	0.69%	2.78%	2.88%	0.81%	13.40%
2,2,3,4-TETRAMETHYLPENTANE	0.63%	4.69%	2.94%	2.75%	13.18%
2,2,3-TRIMETHYLBUTANE	0.26%	2.73%	1.85%	0.87%	10.88%
2,2,3-TRIMETHYLPENTANE	0.55%	5.92%	1.80%	1.82%	14.45%
2,2,4,4,6,8,8-HEPTAMETHYLNONANE	0.76%	7.97%	3.49%	5.36%	19.09%
2,2,4,4-TETRAFLUOROPENTANE	1.20%	2.32%	3.91%		8.94%
2,2,4,4-TETRAMETHYL-1,3-CYCLOBUTANEDIOL	4.04%	2.89%	6.76%		12.17%
2,2,4,4-TETRAMETHYLPENTANE	0.63%	3.44%	2.65%	2.80%	11.67%
2,2,4-TRIMETHYL-1,3-PENTANEDIOL	6.37%	4.86%			17.04%
2,2,4-TRIMETHYLPENTANE	0.52%	4.25%	1.72%	4.39%	9.75%
2,2,5,5-TETRAMETHYLHEXANE	2.66%	2.95%	2.76%	1.51%	9.67%
2,2,5-TRIMETHYLHEXANE	1.65%	4.57%	3.51%	2.61%	13.19%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
2,2-DICHLORO-1,1,1-TRIFLUOROETHANE	0.65%	3.47%	1.60%	2.89%	8.55%
2,2-DICHLORO-1,1,2-TRIFLUOROETHANE	1.03%	3.18%	2.63%	4.82%	10.17%
2,2-DIMETHYL-1-PROPANOL	4.93%	0.95%	5.96%		6.28%
2,2-DIMETHYL-3-ETHYLPENTANE	1.24%	3.90%	2.73%	5.02%	9.38%
2,2-DIMETHYLBUTANE	0.49%	3.09%	2.30%	0.44%	8.70%
2,2-DIMETHYLHEPTANE	0.78%	4.91%	3.49%	1.78%	13.41%
2,2-DIMETHYLHEXANE	0.85%	4.95%	2.13%	0.64%	9.36%
2,2-DIMETHYLOCTANE	1.70%	4.74%	3.15%	0.95%	15.16%
2,2-DIMETHYLPENTANE	0.36%	4.73%	1.74%	0.66%	9.44%
2,2'-IMINOBIS-ACETONITRILE	2.01%	21.25%	5.11%		30.50%
2,3,3,3-TETRAFLUOROPROPENE	0.66%	3.93%	3.63%		9.83%
2,3,3,4-TETRAMETHYLPENTANE	0.56%	3.98%	3.03%	1.15%	10.63%
2,3,3-TRIMETHYL-1-BUTENE	1.04%	2.37%	2.07%	6.90%	10.31%
2,3,3-TRIMETHYLPENTANE	0.31%	4.55%	1.82%	1.24%	8.80%
2,3,4,5,2',3',4',5'-OCTAHYDRO-BIFURYL-(3,3')	0.57%	5.12%	4.28%		13.16%
2,3,4-TRIMETHYLPENTANE	0.61%	5.19%	2.02%	1.03%	9.04%
2,3,5-TRIMETHYLTHIOPHENE	0.69%	4.01%	3.75%		9.50%
2,3-BUTANEDIOL	3.67%	0.97%	12.98%		8.38%
2,3-DICHLOROBUTANE	0.51%	2.62%	1.60%		12.30%
2,3-DICHLOROPROPENE	4.22%	1.53%		0.56%	14.17%
2,3-DIHYDROFURAN	0.63%	4.04%	2.41%		13.32%
2,3-DIMETHYL-1,3-BUTADIENE	2.86%	3.89%	2.55%	0.43%	13.84%
2,3-DIMETHYL-1-BUTENE	0.96%	3.62%	1.99%	4.53%	10.86%
2,3-DIMETHYL-1-HEXENE	1.88%	4.19%	2.44%	5.34%	10.72%
2,3-DIMETHYL-2,3-DIPHENYLBUTANE	0.99%	6.00%	4.51%		18.82%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
2,3-DIMETHYL-2-BUTENE	3.82%	4.31%	3.19%	2.13%	13.33%
2,3-DIMETHYLBENZOTHIOPHENE	1.96%	4.56%	3.89%		17.33%
2,3-DIMETHYLBUTANE	0.15%	4.18%	1.23%	1.68%	7.66%
2,3-DIMETHYLDECANE	1.76%	6.00%	4.19%		11.86%
2,3-DIMETHYLDODECANE	1.69%	5.80%	4.43%		12.64%
2,3-DIMETHYLHEPTANE	1.23%	5.19%	3.79%	2.59%	10.21%
2,3-DIMETHYLHEXANE	0.78%	5.55%	2.68%	0.43%	9.78%
2,3-DIMETHYLNONANE	1.49%	6.35%	4.31%		11.43%
2,3-DIMETHYLOCTANE	0.83%	5.79%	4.11%		10.95%
2,3-DIMETHYLPENTANE	0.62%	6.20%	2.08%	2.05%	13.43%
2,3-DIMETHYLTHIOPHENE	1.06%	5.41%	3.26%		7.67%
2,3-DIMETHYLUDECANE	1.49%	5.90%	4.42%		12.22%
2,3-PENTADIENE	3.77%	4.85%	3.13%	1.78%	5.33%
2,3-XYLENOL	1.18%	1.12%	3.81%	3.58%	5.83%
2,4,4-TRIMETHYL-1-PENTENE	1.17%	4.03%	2.02%	1.11%	13.82%
2,4,4-TRIMETHYL-2-PENTENE	1.90%	4.60%	2.48%	2.40%	14.20%
2,4,4-TRIMETHYLHEXANE	0.62%	4.51%	3.54%	3.09%	11.75%
2,4,6-TRIMETHYLPYRIDINE	2.32%	6.68%	1.77%		9.81%
2,4-DIAMINOTOLUENE	2.86%	4.13%	3.31%		12.68%
2,4-DICHLOROBENZOTRIFLUORIDE	1.63%	4.60%	3.28%		19.72%
2,4-DICHLOROTOLUENE	1.73%	4.61%	2.29%		14.28%
2,4-DIMETHYL-1,3-DIOXOLANE-2-METHANOL	1.74%	4.28%	4.59%		12.15%
2,4-DIMETHYL-3-ETHYLPENTANE	0.55%	4.68%	3.28%		10.24%
2,4-DIMETHYLHEXANE	0.80%	4.27%	2.55%	0.13%	10.65%
2,4-DIMETHYLOCTANE	1.74%	3.05%	2.89%	3.28%	15.21%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
2,4-DIMETHYLPENTANE	0.67%	5.33%	1.84%	0.50%	9.59%
2,4-DINITROPHENOL	2.08%	3.56%	5.91%		15.03%
2,4-DIPHENYL-4-METHYLPENTENE-1	0.81%	5.01%	4.00%		13.94%
2,4-TOLUENE DIISOCYANATE	1.52%	3.90%			4.58%
2,4-XYLENOL	0.53%	3.76%	3.63%	2.47%	0.62%
2,5-DIHYDROFURAN	3.31%	4.94%	2.98%	0.83%	14.78%
2,5-DIMETHYL-1,5-HEXADIENE	1.72%	4.36%	2.12%	0.58%	10.45%
2,5-DIMETHYL-2,4-HEXADIENE	3.65%	4.37%	6.87%	0.59%	18.93%
2,5-DIMETHYLFURAN	2.37%	2.92%	3.76%		8.49%
2,5-DIMETHYLHEXANE	0.60%	4.61%	2.25%	0.74%	9.68%
2,5-DIMETHYLOCTANE	0.65%	4.78%	3.30%	3.48%	14.68%
2,5-DIMETHYLTETRAHYDROFURAN	0.17%	3.10%	3.77%		11.38%
2,5-DIMETHYLTHIOPHENE	1.26%	2.50%			7.86%
2,5-XYLENOL	1.40%	1.79%	5.83%	6.83%	5.45%
2,6,8-TRIMETHYL-4-NONANONE	1.70%	5.61%	4.71%		15.56%
2,6-DIETHYLNAPHTHALENE	2.08%	4.31%	3.91%	1.37%	13.97%
2,6-DIMETHYL-4-HEPTANOL	2.22%	2.48%	4.96%		6.87%
2,6-DIMETHYLHEPTANE	2.46%	5.42%	2.23%	1.06%	15.03%
2,6-DIMETHYLNAPHTHALENE	1.58%	2.31%	2.99%	3.16%	11.97%
2,6-DIMETHYLOCTANE	1.71%	3.08%	3.03%	2.25%	15.89%
2,6-DIMETHYLPYRIDINE	2.42%	4.49%	2.34%	1.77%	5.45%
2,6-DINITROPHENOL	3.61%	4.32%	6.60%		13.65%
2,6-DI-tert-BUTYL-p-CRESOL	0.69%	4.45%			7.55%
2,6-NAPHTHALENEDICARBOXYLIC ACID	3.15%	1.67%	8.18%		13.52%
2,6-TOLUENE DIISOCYANATE	5.09%	4.77%	4.71%		13.49%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
2,6-XYLENOL	1.43%	1.47%	3.71%	3.32%	6.62%
2,7-DIMETHYLBENZOTHIOPHENE	0.94%	3.55%	4.10%		10.59%
2,7-DIMETHYLNAPHTHALENE	1.28%	1.26%	2.63%	4.54%	4.00%
2,7-DIMETHYLOCTANE	1.80%	4.59%	2.61%	1.90%	16.49%
2-ACETOACETOXY ETHYL METHACRYLATE	2.62%	6.02%	5.85%		17.62%
2-AMINO-2-METHYL-1-PROPANOL	4.56%	3.37%	7.24%		15.71%
2-AMINODIPHENYL	1.86%	1.12%	4.17%		6.14%
2-AMINOETHOXYETHANOL	1.95%	0.23%	4.17%	9.65%	6.04%
2-BROMOBUTANE	1.19%	3.64%	2.02%	1.25%	2.31%
2-BROMOPROPANE	3.65%	6.90%	5.05%	1.57%	0.04%
2-BUTANOL	6.43%	6.39%	9.15%		11.29%
2-BUTOXIME	3.01%	6.34%	5.42%	4.06%	9.76%
2-BUTOXYETHANOL	1.51%	5.68%	4.04%	9.47%	7.51%
2-BUTYL-2-ETHYL-1,3-PROPANEDIOL	3.90%	4.49%			13.30%
2-BUTYLBENZOTHIOPHENE	1.61%	2.39%	5.07%		9.50%
2-BUTYL-NONAN-1-OL	2.79%	2.64%	5.18%		11.30%
2-BUTYNE-1,4-DIOL	1.77%	1.57%	5.07%		7.01%
2-CHLORO-1,1,1,2-TETRAFLUOROETHANE	0.55%	6.66%	10.08%	4.56%	8.19%
2-CHLORO-1,1,1-TRIFLUOROETHANE	0.71%	4.15%	2.81%	1.75%	10.93%
2-CHLORO-1,1-DIFLUOROETHYLENE	3.06%	3.50%	2.38%	2.90%	10.52%
2-CHLORO-1,3-PROPANEDIOL	1.78%	2.34%	5.71%		8.03%
2-CHLOROETHANOL	2.35%	8.78%			7.04%
2-CHLOROPROPENE	0.66%	0.63%	1.59%	1.16%	8.45%
2-CYCLOHEXENE-1-ONE	0.93%	5.54%	3.77%		11.66%
2-CYCLOHEXENYL CYCLOHEXANONE	1.86%	4.33%	4.05%		10.47%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
2-ETHOXY-1-PROPANOL	0.83%	3.67%	4.96%		6.85%
2-ETHOXYETHYL ACETATE	1.28%	2.90%	3.27%		1.44%
2-ETHYL BUTYRIC ACID	2.11%	3.26%	3.64%		16.02%
2-ETHYL HEXANOIC ACID	2.79%	7.16%	5.17%		6.94%
2-ETHYL-1-BUTANOL	5.50%	3.22%			9.86%
2-ETHYL-1-BUTENE	2.55%	3.74%	2.15%	2.81%	9.64%
2-ETHYL-1-HEXANOL	5.36%	4.91%			11.18%
2-ETHYL-1-HEXENE	1.58%	4.37%	3.55%		12.14%
2-ETHYL-1-PENTENE	1.63%	3.88%	2.52%	9.60%	11.29%
2-ETHYL-2-HEXENAL	0.55%	7.80%	3.60%	2.62%	20.42%
2-ETHYLBENZOTHIOPHENE	1.49%	3.83%	3.76%	2.47%	13.42%
2-ETHYLHEXANAL	1.81%	3.60%	3.89%		13.42%
2-ETHYLHEXYL ACRYLATE	1.49%	5.19%		9.94%	11.62%
2-ETHYLHEXYL BENZOATE	1.83%	6.35%	4.79%		12.87%
2-ETHYL-m-XYLENE	0.36%	3.54%	2.23%	0.91%	9.57%
2-ETHYLNAPHTHALENE	1.44%	5.93%	4.18%	1.97%	9.58%
2-ETHYL-p-XYLENE	1.77%	4.74%	4.04%	0.79%	12.44%
2-ETHYL-TETRAHYDROTHIOPHENE	3.23%	4.09%	4.55%		9.80%
2-ETHYLTHIOPHENE	0.58%	2.68%	3.31%		7.97%
2-FORMYL BENZOIC ACID	2.95%	5.52%	4.45%	8.30%	21.06%
2-HEPTANOL	7.71%	4.95%			7.26%
2-HEPTANONE	0.58%	4.29%	4.42%		11.06%
2-HEXANOL	9.62%	4.90%	10.14%		8.54%
2-HEXANONE	0.61%	5.30%	4.01%		10.77%
2-HEXYNE	3.31%	2.41%	4.20%		12.56%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
2-HYDROXYPROPYL METHACRYLATE	2.35%	4.42%	3.98%	3.55%	11.22%
2-MERCAPTOBENZOTHAZOLE	0.94%	2.13%	3.93%		10.13%
2-METHOXY PROPANOL-1	0.51%	5.35%	4.94%		12.69%
2-METHOXYETHANOL	0.21%	7.15%	5.12%		0.74%
2-METHYL BENZOTHIOPHENE	0.96%	3.75%	4.42%	1.83%	13.18%
2-METHYL OCTANAL	2.14%	4.13%	4.44%		11.09%
2-METHYL THIAINDAN	0.87%	4.54%	3.28%		10.56%
2-METHYL-, 3-HYDROXY-2,2,4-TRIMETHYLPENTYL PROPANOATE	0.75%	5.90%			13.98%
2-METHYL-1,3-PROPANEDIOL	2.61%	2.27%	3.24%	4.82%	7.37%
2-METHYL-1-BUTANOL	5.24%	6.61%	8.63%		5.35%
2-METHYL-1-BUTENE	1.82%	4.82%	1.39%	2.83%	10.88%
2-METHYL-1-BUTENE-3-YNE	1.20%	1.59%	1.32%	0.48%	13.08%
2-METHYL-1-HEPTANOL	1.96%	2.24%	4.42%		8.55%
2-METHYL-1-HEPTENE	0.69%	4.52%	3.75%	2.92%	14.22%
2-METHYL-1-HEXANOL	2.43%	4.48%	3.91%	8.89%	7.75%
2-METHYL-1-HEXENE	1.59%	4.48%	1.91%	0.64%	12.61%
2-METHYL-1-NONENE	1.53%	4.76%	3.32%	1.61%	19.26%
2-METHYL-1-OCTENE	1.32%	5.82%	3.98%	2.93%	15.11%
2-METHYL-1-PENTANOL	6.22%	5.64%			8.91%
2-METHYL-1-PENTENE	1.24%	4.78%	2.05%	1.01%	11.27%
2-METHYL-1-PROPANOL	8.11%	8.06%	8.11%	8.11%	9.11%
2-METHYL-2-AMINOBUTANE	1.20%	0.74%	3.18%		2.38%
2-METHYL-2-BUTANOL	9.49%	3.55%	8.49%	17.53%	7.81%
2-METHYL-2-BUTENE	1.39%	7.16%	3.62%	5.83%	11.11%
2-METHYL-2-PENTENAL	1.55%	3.83%	3.12%	3.10%	21.13%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
2-METHYL-2-PENTENE	3.40%	4.87%	2.76%	4.27%	7.11%
2-METHYL-2-PROPANOL	7.85%	2.48%	5.75%	13.03%	9.43%
2-METHYL-3-ETHYLPENTANE	0.63%	6.56%	1.68%	2.94%	13.91%
2-METHYLBENZOFURAN	0.85%	4.13%	2.92%		10.48%
2-METHYLBUTYRALDEHYDE	0.42%	3.54%	5.13%	0.33%	9.55%
2-METHYLBUTYRIC ACID	1.99%	5.28%	3.71%		11.50%
2-METHYLDECANE	2.23%	4.75%	3.83%		11.48%
2-METHYL-DODECAN-1-OL	2.90%	2.76%	5.28%		11.55%
2-METHYLDODECANE	1.22%	4.94%	4.70%		12.45%
2-METHYLHEPTANAL	3.76%	3.88%	6.11%		10.78%
2-METHYLHEPTANE	0.91%	5.68%	2.22%	0.93%	9.08%
2-METHYLHEXANAL	1.74%	4.40%	3.20%	0.99%	11.10%
2-METHYLHEXANE	0.72%	5.09%	3.02%	0.27%	10.40%
2-METHYLHEXANOIC ACID	2.51%	4.09%	4.93%		11.07%
2-METHYLINDENE	1.35%	4.41%	2.66%	0.49%	10.58%
2-METHYLNAPHTHALENE	4.49%	4.39%	2.16%	4.39%	10.14%
2-METHYLNONANE	0.77%	4.87%	3.60%	0.71%	16.15%
2-METHYLOCTANE	0.95%	4.58%	4.08%	3.17%	10.83%
2-METHYLOCTANOIC ACID	2.14%	4.16%	4.85%		11.49%
2-METHYLPENTANE	0.46%	4.51%	1.99%	0.52%	8.28%
2-METHYLPROPANAL	1.33%	3.86%	4.25%		10.73%
2-METHYLPYRIDINE	0.39%	3.27%	1.86%	1.01%	2.49%
2-METHYLTETRAHYDROFURAN	0.61%	8.32%	4.30%		24.69%
2-METHYLTHIACYCLOPENTANE	1.31%	4.65%	3.54%		9.85%
2-METHYLTHIOPHENE	0.52%	1.31%	2.31%	1.67%	12.08%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
2-METHYLTRIDECANE	1.23%	5.23%	4.86%		12.96%
2-METHYLUNDECANE	1.56%	5.01%	4.33%		11.88%
2-NITROPROPANE	5.53%	5.62%	8.62%	4.14%	8.35%
2-NONANOL	4.15%	2.89%			5.53%
2-NONANONE	0.38%	3.70%	4.94%		10.14%
2-NORBORNENE	0.85%	1.54%	2.55%	0.47%	9.12%
2-n-PROPYLTHIOPHENE	0.42%	3.01%	3.93%		8.53%
2-OCTANOL	5.69%	5.65%			5.27%
2-OCTANONE	0.53%	3.38%	4.82%		10.85%
2-PENTANETHIOL	1.79%	3.05%	2.91%		4.77%
2-PENTANOL	9.20%	6.09%			9.49%
2-PENTANONE	0.52%	4.65%	3.75%		11.92%
2-PENTOXYETHANOL	1.82%	3.89%	4.00%	6.71%	10.11%
2-PENTYNE	2.67%	2.48%	5.16%	1.12%	12.37%
2-PHENYL-1-PROPANOL	2.18%	2.42%	3.11%	14.18%	6.93%
2-PHENYL-2-PROPANOL	1.22%	2.88%	7.52%		3.64%
2-PHENYLBUTENE-1	2.33%	4.52%	2.54%		15.03%
2-PHENYLETHANOL	3.78%	5.96%	12.44%		6.00%
2-PROPYLBENZOTHIOPHENE	1.58%	2.13%	4.31%		8.39%
2-PYRROLIDONE	0.62%	4.55%	5.95%	11.98%	13.60%
3-(METHYLMERCAPTO)PROPANAL	1.79%	4.63%	3.28%	3.85%	18.91%
3-(N,N-DIMETHYLAMINO) PROPYLAMINE	0.38%	3.63%	4.96%		8.91%
3-(TRIETHOXSILYL)PROPIONITRILE	0.44%	6.64%	4.90%	5.50%	16.11%
3,3,3-TRIFLUOROPROPENE	3.33%	3.35%			15.60%
3,3,5-TRIMETHYLHEPTANE	0.35%	4.67%	1.20%	1.84%	9.60%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
3,3-DIETHYLPENTANE	0.91%	4.04%	3.64%	0.71%	16.51%
3,3-DIMETHYL-1-BUTENE	2.21%	1.92%	2.98%	4.52%	10.10%
3,3-DIMETHYL-1-BUTYNE	0.81%	1.20%	1.94%		7.29%
3,3-DIMETHYL-2-BUTANONE	0.99%	2.60%	4.43%	3.07%	5.44%
3,3-DIMETHYLHEXANE	0.49%	7.70%	1.82%	0.75%	14.41%
3,3-DIMETHYLPENTANE	0.36%	2.56%	1.91%	1.21%	8.16%
3,4-DICHLORO-1-BUTENE	2.81%	4.21%			10.16%
3,4-DICHLOROANILINE	1.37%	4.71%	3.76%		9.64%
3,4-DICHLOROPHENYL ISOCYANATE	4.33%	4.85%			11.99%
3,4-DIMETHYLHEXANE	0.66%	5.45%	2.69%	0.33%	9.03%
3,4-DIMETHYLTHIOPHENE	1.11%	3.71%	3.15%		8.84%
3,4-XYLENOL	1.09%	2.42%	4.18%	2.79%	5.56%
3,5-DIISOPROPYLTOLUENE	1.48%	5.09%	4.07%		11.70%
3,5-DIMETHYLBENZOFURAN	0.22%	5.08%	5.26%		11.70%
3,5-DIMETHYLBENZOTHIOPHENE	1.94%	4.64%			10.56%
3,5-XYLENOL	3.07%	4.51%	6.34%	4.98%	4.76%
3-AMINO-1-PROPANOL	2.49%	3.37%	4.30%		11.93%
3-BUTEN-2-ONE	1.24%	4.77%	3.89%		17.60%
3-CHLORO- <i>o</i> -XYLENE	1.55%	4.22%	4.02%		11.12%
3-CHLOROPROPENE	2.07%	3.89%		0.73%	12.29%
3-CHLOROPROPYLDIMETHYLCHLOROSILANE	0.72%	5.75%	5.07%		11.40%
3-CHLOROPROPYLTRIMETHOXSILANE	0.22%	7.02%		7.74%	13.77%
3-ETHYL-1-HEPTANOL	2.16%	2.92%	4.85%	10.78%	10.40%
3-ETHYL-1-HEXENE	0.89%	4.84%	3.85%	3.64%	12.04%
3-ETHYL-1-PENTENE	1.19%	3.25%	2.53%	3.54%	8.13%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
3-ETHYL-2,5-DIMETHYLTHIOPHENE	1.38%	6.39%	3.50%		11.99%
3-ETHYLBENZOTHIOPHENE	0.72%	4.41%	4.47%		10.19%
3-ETHYLDODECANE	1.60%	4.94%	4.37%		12.05%
3-ETHYLHEPTANE	0.68%	5.94%	3.49%	6.34%	11.08%
3-ETHYLHEXANE	0.84%	6.38%	2.98%	0.37%	13.32%
3-ETHYL-o-XYLENE	3.03%	5.01%	3.11%	0.96%	8.49%
3-ETHYLPENTANE	0.79%	3.90%	2.87%	1.79%	8.80%
3-HEPTANOL	3.31%	3.77%			8.78%
3-HEPTANONE	2.32%	5.28%	4.14%	0.53%	11.88%
3-HEXANONE	0.87%	4.72%	2.65%	0.86%	9.53%
3-HEXYNE	5.35%	4.26%			11.41%
3-HYDROXY-2-METHYL PROPIONALDEHYDE	2.24%	3.92%	4.03%	5.56%	11.42%
3-HYDROXYBUTYROLACTONE	1.13%	4.79%	5.64%		18.03%
3-MERCAPTOPROPIONIC ACID	1.80%	1.24%	5.21%	2.39%	22.61%
3-METHOXY-3-BUTEN-2-ONE	0.63%	4.09%			10.24%
3-METHOXYISOPROPYLAMINE	1.60%	0.79%	3.30%		0.78%
3-METHOXYPROPIONITRILE	1.58%	16.12%	5.73%		24.95%
3-METHYL SULFOLANE	1.57%	4.75%	3.30%		26.04%
3-METHYL-1,2-BUTADIENE	4.32%	2.58%	3.77%	5.98%	6.24%
3-METHYL-1,4-PENTADIENE	0.76%	3.58%	3.56%	5.01%	8.56%
3-METHYL-1-BUTANOL	7.23%	7.69%	8.86%		6.05%
3-METHYL-1-BUTENE	0.13%	3.39%	1.21%	8.19%	4.08%
3-METHYL-1-BUTYNE	6.53%	0.53%	8.49%	1.70%	2.54%
3-METHYL-1-HEXENE	1.18%	4.43%	2.56%	0.65%	9.55%
3-METHYL-1-PENTANOL	0.94%	6.50%	10.08%		7.07%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
3-METHYL-1-PENTENE	1.72%	3.82%	2.97%	1.28%	8.16%
3-METHYL-2-BUTANOL	9.25%	4.94%	10.11%		5.27%
3-METHYL-2-PENTANONE	0.63%	5.23%	3.01%	3.61%	10.67%
3-METHYL-3-ETHYLPENTANE	0.11%	4.10%	1.76%	0.91%	9.57%
3-METHYL-3-PENTANOL	2.99%	3.17%			4.09%
3-METHYLBUTYRALDEHYDE	0.95%	2.49%	3.72%		8.22%
3-METHYL-cis-2-PENTENE	2.30%	4.69%	1.57%	2.01%	10.07%
3-METHYLCYCLOPENTANONE	2.78%	5.20%	4.41%		11.67%
3-METHYLCYCLOPENTENE	0.94%	3.24%	1.64%	2.44%	4.85%
3-METHYLDECANE	0.72%	5.47%	5.21%		11.57%
3-METHYLDODECANE	0.64%	5.69%			12.52%
3-METHYLHEPTANE	0.66%	6.77%	2.12%	1.13%	13.12%
3-METHYLHEXANAL	1.24%	5.40%	5.38%	2.58%	15.27%
3-METHYLHEXANE	0.92%	6.65%	2.07%	0.63%	12.72%
3-METHYLNONANE	1.52%	5.80%	2.90%	1.43%	14.42%
3-METHYLOCTANE	0.72%	5.34%	3.17%	1.16%	13.05%
3-METHYLPENTANE	0.55%	5.65%	1.68%	0.50%	6.67%
3-METHYLPYRIDINE	0.08%	3.75%	2.26%	1.48%	3.33%
3-METHYLTHIOPHENE	0.59%	2.43%	1.96%	1.84%	11.60%
3-METHYL-trans-2-PENTENE	2.51%	6.26%	3.76%	6.88%	12.07%
3-METHYLTRIDECANE	1.31%	5.52%	4.82%		13.10%
3-METHYLUDECANE	0.53%	5.36%			12.05%
3-NITROBENZOTRIFLUORIDE	0.79%	4.85%	4.13%		18.67%
3-NONANONE	3.17%	4.30%	0.0527227	0.00%	10.08%
3-OCTANONE	1.57%	5.12%	3.66%		9.16%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
3-PENTANOL	11.17%	5.73%			9.04%
3-PENTANONE	1.75%	3.41%	7.02%	0.74%	5.52%
3-PHENYL-1-PROPANOL	2.03%	2.96%		19.66%	9.19%
4-((2-HYDROXYETHOXY)CARBONYL) BENZOIC ACID	2.33%	2.32%	6.09%		11.41%
4-(2-METHOXYETHYL)MORPHOLINE	3.00%	5.09%	5.16%		12.02%
4,4'-DIISOPROPYLBIPHENYL	1.68%	4.30%	4.77%		14.74%
4,4'-DINITRODIPHENYLAMINE	2.29%	2.74%	5.46%		13.15%
4,4'-DINITROTRIPHENYLAMINE	2.70%	3.17%	5.39%		13.90%
4,6-DIMETHYLDIBENZOTHIOPHENE	1.58%	3.95%	4.76%		17.23%
4-[2-(2-AMINOETHOXY)ETHYL]MORPHOLINE	1.91%	2.09%	4.34%	3.21%	8.33%
4-CHLORO-3-NITROBENZOTRIFLUORIDE	0.94%	5.17%	4.66%		16.47%
4-CHLORO-o-XYLENE	1.47%	5.68%	3.82%		16.39%
4-ETHYL-m-XYLENE	0.97%	4.83%	4.29%	0.81%	12.79%
4-ETHYL-o-XYLENE	1.24%	5.34%	2.08%	0.82%	11.06%
4-HEPTANONE	0.74%	3.82%	2.69%	1.29%	11.71%
4-HYDROXYACETOPHENONE	4.42%	4.04%			13.64%
4-HYDROXYBUTYRALDEHYDE	2.25%	4.79%	5.34%	2.49%	13.97%
4-HYDROXYMETHYL BENZOIC ACID	3.66%	0.51%	6.80%		7.51%
4-HYDROXYSTYRENE	1.75%	2.02%	3.38%	3.48%	7.88%
4-ISOBUTYLSTYRENE	1.41%	4.44%	3.50%	1.19%	14.53%
4-METHOXYPHENYLACETIC ACID	2.19%	0.67%	4.14%		6.48%
4-METHYL DIBENZOTHIOPHENE	1.53%	4.56%			11.23%
4-METHYL-1-HEPTENE	0.89%	5.25%	4.00%		12.46%
4-METHYL-1-HEXENE	1.35%	4.16%	2.72%	1.56%	8.17%
4-METHYL-1-OCTANOL	0.41%	3.19%			11.67%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
4-METHYL-1-PENTENE	0.96%	3.93%	1.62%	3.36%	9.61%
4-METHYL-2-PENTANOL	3.88%	4.16%	3.11%		5.68%
4-METHYL-cis-2-PENTENE	1.37%	3.77%	2.68%	4.75%	9.46%
4-METHYL-CYCLOHEXANE-METHANOL	4.04%	2.03%	6.05%		17.68%
4-METHYLCYCLOPENTENE	0.69%	2.20%	2.55%	2.48%	5.49%
4-METHYLGUAIACOL	1.20%	2.27%	4.38%		6.00%
4-METHYLHEPTANE	0.87%	6.35%	2.21%	1.24%	10.43%
4-METHYLNONANE	0.92%	4.65%	4.71%	1.45%	14.68%
4-METHYLOCTANE	0.64%	5.68%	3.26%	0.78%	13.87%
4-METHYLPHENANTHRENE	2.96%	5.03%	4.21%		18.38%
4-METHYLPYRIDINE	0.16%	3.08%	2.05%	1.44%	1.85%
4-METHYL-trans-2-PENTENE	1.34%	3.97%	2.43%	3.30%	9.79%
4-NONANONE	2.05%	2.92%	3.93%		10.38%
4-OCTANONE	3.67%	3.94%	5.40%		9.46%
5-(HYDROXYMETHYL) FURFURAL	2.22%	4.29%	4.77%		11.99%
5-ETHYLIDENE-2-NORBORNENE	1.17%	3.79%	1.95%		9.41%
5-ETHYL-m-XYLENE	0.66%	6.05%	2.36%	0.88%	15.25%
5-HEXEN-2-ONE	0.35%	6.14%			17.01%
5-METHYL FURFURAL	0.53%	4.53%	4.83%		10.27%
5-METHYL-1-HEXANOL	2.60%	0.28%	4.28%		11.86%
5-METHYL-1-HEXENE	1.49%	4.83%	2.61%	5.63%	11.44%
5-METHYL-2-HEXANONE	0.42%	5.04%	3.69%		11.73%
5-METHYLINDAN	0.95%	4.54%			9.91%
5-METHYLNONANE	1.24%	5.18%	4.24%	1.61%	14.31%
5-NONANONE	0.67%	5.33%	4.85%	1.13%	13.07%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
5-o-TOLYL-2-PENTENE	1.50%	4.91%	4.06%		13.98%
6-AMINOHEXANAMIDE	1.92%	4.30%	4.48%	4.85%	12.29%
6-AMINOHEXANOL	3.57%	1.24%	5.33%		8.27%
6-HYDROXYHEXANOIC ACID	2.09%	1.74%			10.02%
6-METHYL-1-HEPTENE	0.92%	5.38%	2.91%	3.96%	12.88%
6-METHYL-1-OCTANOL	0.74%	3.12%			11.60%
7-METHYL-1-OCTENE	1.63%	5.62%	3.10%	2.90%	11.61%
8-HYDROXYQUINOLINE	1.78%	1.85%	3.20%		4.71%
8-METHYL-1-NONANOL	7.09%	4.72%			11.41%
8-METHYL-1-NONENE	1.69%	4.28%	3.42%	1.87%	15.69%
8-METHYLQUINOLINE	1.56%	3.30%	3.79%	2.91%	2.61%
ACENAPHTHALENE	2.31%	2.97%	3.74%	3.34%	9.43%
ACENAPHTHENE	3.31%	7.96%	6.57%	3.87%	8.39%
ACETAL	3.00%	1.78%	7.95%	5.17%	5.14%
ACETALDEHYDE	0.81%	5.25%	10.31%		26.33%
ACETALDOL	1.98%	8.23%			8.80%
ACETALDOXIME	0.38%	1.86%	5.06%		1.98%
ACETAMIDE	3.38%	20.26%	5.30%	2.81%	23.81%
ACETAMINOPHEN	2.44%	0.27%	4.25%	2.44%	4.04%
ACETANILIDE	1.95%	3.43%	3.94%		17.62%
ACETIC ACID	4.11%	14.14%		6.30%	33.08%
ACETIC ANHYDRIDE	0.74%	4.48%	4.90%	2.10%	14.83%
ACETOACETANILIDE	2.09%	5.02%	4.33%		15.20%
ACETOACETIC ACID	2.62%	4.33%	5.55%		13.51%
ACETOIN	2.28%	4.07%	5.24%		12.62%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
ACETONE	0.28%	4.14%	4.20%	8.91%	17.81%
ACETONE CYANOHYDRIN	2.47%	4.40%	4.07%		12.96%
ACETONITRILE	4.14%	39.66%	9.82%		35.08%
ACETOPHENONE	0.46%	3.70%	2.84%		8.33%
ACETOVANILLONE	2.37%	2.30%	4.58%		10.14%
ACETOXYACETIC ACID	1.92%	17.11%	5.77%		28.41%
ACETYL CHLORIDE	6.47%	5.44%	6.89%	7.74%	9.24%
ACETYLENE	0.40%	1.48%	3.01%	3.04%	10.26%
ACETYLSALICYLIC ACID	2.58%	3.29%	5.39%	3.17%	13.48%
ACRIDINE	0.70%	4.77%	4.19%	0.36%	7.70%
ACROLEIN	4.96%	5.59%	7.92%	6.61%	19.18%
ACROLEIN CYANOHYDRIN	2.20%	6.40%			14.42%
ACRYLIC ACID	2.11%	4.24%		7.26%	20.06%
ACRYLONITRILE	0.91%	13.96%			24.51%
ACRYLOXY PROPIONIC ACID	0.57%	5.32%			14.42%
ADAMANTANE	0.22%	6.51%		0.64%	15.87%
ADIPIC ACID	3.77%	3.33%			16.69%
ADIPONITRILE	1.27%	32.90%			54.21%
AGATHADIOL	3.01%	1.51%	5.99%		10.30%
AIR	2.50%	1.01%	4.50%	5.60%	1.96%
ALLYL ACETATE	1.54%	5.93%	8.32%		11.11%
ALLYL ACRYLATE	2.89%	4.73%	4.56%		10.75%
ALLYL ALCOHOL	1.72%	7.97%	3.96%	6.15%	8.63%
ALLYL ETHER	2.41%	4.93%	3.75%		10.87%
ALLYL GLYCIDYL ETHER	1.02%	4.40%	3.99%		10.70%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
ALLYL METHACRYLATE	1.88%	4.78%	5.44%		12.40%
ALLYLAMINE	1.36%	6.79%	2.76%		6.36%
ALLYLIDENE DIACETATE	2.53%	4.52%	4.72%		11.42%
ALLYL-TERT-BUTYLPEROXIDE	0.89%	2.71%	3.84%		7.97%
alpha-EPICHLOROHYDRIN	2.57%	3.98%	4.31%		25.31%
alpha-HYDROXYISOBUTYRAMIDE	1.33%	2.46%	4.75%		9.57%
alpha-HYDROXYISOBUTYRIC ACID	2.26%	1.30%	5.39%		8.67%
alpha-METHYLBENZYL ALCOHOL	4.22%	4.46%	6.15%		10.99%
alpha-METHYLBENZYL ALCOHOL FORMATE	1.67%	4.93%	2.53%		12.27%
alpha-METHYLSTYRENE	1.74%	3.28%	2.62%	1.19%	15.42%
alpha-PHELLANDRENE	3.11%	2.16%	2.70%	0.48%	13.72%
alpha-PINENE	4.17%	5.78%			21.05%
alpha-TERPINENE	1.31%	6.15%	2.20%	0.46%	12.29%
alpha-TERPINEOL	0.83%	2.36%	5.64%		9.17%
alpha-TOCOPHEROL	2.70%	6.20%	5.38%		15.03%
AMINOACETONITRILE	1.82%	4.49%	3.61%	5.73%	17.92%
AMINOCAPRONITRILE	1.55%	3.76%	4.36%	1.85%	17.62%
AMMONIA	1.17%	3.13%	2.46%	15.19%	15.44%
AMMONIUM CHLORIDE	0.27%	8.33%			46.48%
AMMONIUM SULFIDE	2.34%	54.38%			47.92%
ANETHOLE	1.45%	4.64%	3.57%		18.95%
ANILINE	1.30%	2.44%	1.79%	6.84%	4.59%
ANISOLE	0.87%	3.73%	2.21%		8.38%
ANTHRACENE	3.24%	8.53%	8.02%	1.57%	24.96%
ANTHRAQUINONE	5.30%	3.74%	7.88%		11.54%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
ANTIMONY TRICHLORIDE	1.13%	18.97%			42.57%
ARGON	0.62%	0.66%	2.30%	5.11%	9.76%
ARSENIC (III) CHLORIDE	0.25%	3.65%	3.92%	0.84%	10.41%
ARSINE	1.08%	0.56%	3.68%	12.70%	50.31%
AZELAIC ACID	6.29%	5.29%			21.11%
BENZALDEHYDE	0.94%	4.54%	1.72%	3.15%	9.77%
BENZAMIDE	1.85%	3.24%	4.93%		11.03%
BENZENE	0.75%	2.06%	1.89%	2.41%	9.76%
BENZENE-1,2,4-TRICARBOXYLIC ACID TRIMETHYL ESTER	1.76%	5.38%			13.54%
BENZIDINE	2.03%	3.25%	4.08%		11.23%
BENZO[b]FLUORANTHENE	0.36%	24.16%			32.28%
BENZOIC ACID	8.41%	3.34%	7.48%	13.56%	13.13%
BENZONITRILE	0.97%	4.30%	3.73%		23.30%
BENZOPHENONE	1.35%	3.28%	2.50%		4.58%
BENZOTHIOPHENE	2.21%	1.57%	3.95%		5.46%
BENZOTRICHLORIDE	1.00%	4.59%	2.51%		15.98%
BENZOTRIFLUORIDE	1.57%	4.78%	4.23%	0.56%	14.95%
BENZOYL CHLORIDE	1.20%	3.24%	5.24%		11.49%
BENZYL ACETATE	1.02%	3.01%	3.57%		15.90%
BENZYL ALCOHOL	7.46%	5.81%			0.20%
BENZYL CHLORIDE	2.45%	4.99%	2.53%	10.75%	14.35%
BENZYL DICHLORIDE	0.96%	3.61%	6.38%		16.96%
BENZYL ETHYL ETHER	1.89%	5.70%	4.19%		12.62%
BENZYL FORMATE	1.51%	3.81%	2.99%	3.26%	15.15%
BENZYL MERCAPTAN	0.78%	2.86%	3.80%	0.69%	15.08%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
BENZYLAMINE	0.62%	4.06%	2.92%		1.41%
beta-PHELLANDRENE	2.27%	3.10%	2.48%	0.39%	13.69%
beta-PINENE	1.39%	5.02%	3.47%		10.95%
beta-TERPINEOL	2.16%	1.90%	4.65%		8.26%
BICYCLO[2.2.1]HEPTANE	0.46%	1.73%	3.70%		10.53%
BICYCLO[2.2.2]OCTANE	0.82%	3.73%		3.17%	5.20%
BICYCLOHEXYL	1.32%	4.78%	4.79%		11.93%
BIPHENYL	0.82%	4.30%	3.77%	1.14%	8.54%
BIS-(2-AMINOETHYL)ETHER	5.06%	0.27%			3.80%
BIS(alpha-METHYLBENZYL) ETHER	3.60%	4.99%			14.36%
BIS(CHLOROMETHYL)ETHER	1.33%	4.30%	2.84%		15.06%
BIS(CYANOETHYL)ETHER	0.57%	21.43%	4.02%		64.65%
BIS(DIFLUOROMETHYL)ETHER	1.39%	4.30%	2.75%		7.26%
BIS(TRIFLUOROMETHYL)SULFIDE	1.44%	2.01%			7.62%
BIS[3-(TRIMETHOXSILYL)PROPYL]DISULFIDE	2.47%	3.81%	5.76%		16.28%
BORON TRIBROMIDE	3.67%	2.34%			7.82%
BORON TRICHLORIDE	2.03%	6.65%	4.36%		84.39%
BORON TRIFLUORIDE	1.72%	4.13%	6.28%	1.76%	0.82%
BROMINE	2.40%	0.95%	2.72%	2.41%	11.39%
BROMOBENZENE	1.16%	3.93%	2.84%	1.50%	10.04%
BROMOCHLORODIFLUOROMETHANE	0.55%	3.13%	2.91%	5.41%	1.01%
BROMOCHLOROMETHANE	1.13%	2.00%	1.78%		3.72%
BROMODIFLUOROMETHANE	1.32%	4.86%	7.85%		17.31%
BROMOETHANE	2.81%	2.16%	4.26%		9.83%
BROMOMETHANE	1.09%	2.25%	3.11%	1.53%	8.89%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
BROMOTRICHLOROMETHANE	0.42%	1.80%	1.72%	1.14%	7.87%
BROMOTRIFLUOROETHYLENE	0.67%	0.50%	2.44%	1.09%	1.11%
BROMOTRIFLUOROMETHANE	0.31%	2.49%	2.90%	11.04%	6.83%
BUTANAL	0.19%	4.81%	4.19%		12.34%
BUTYL VINYL ETHER	0.96%	4.18%	2.93%		12.97%
BUTYRONITRILE	2.31%	7.64%	7.14%		20.07%
CAMPHENE	1.38%	4.03%	2.78%		8.92%
CAMPHOR	0.53%	2.12%	4.31%		10.78%
CARBAMYL CHLORIDE	1.21%	0.29%	2.56%		1.92%
CARBON DIOXIDE	0.66%	0.96%	1.63%	8.63%	7.77%
CARBON DISULFIDE	0.62%	1.90%	2.48%	3.06%	9.74%
CARBON MONOXIDE	0.54%	0.30%	1.51%	11.57%	6.16%
CARBON TETRACHLORIDE	0.40%	2.17%	1.85%	4.60%	8.98%
CARBON TETRAFLUORIDE	0.33%	1.69%	2.01%	3.15%	7.12%
CARBONYL FLUORIDE	3.52%	0.29%	4.84%	18.03%	3.00%
CARBONYL SULFIDE	1.39%	1.59%	2.83%	9.46%	13.26%
CHLORINE	2.31%	0.96%	2.93%	8.18%	11.28%
CHLORINE TRIFLUORIDE	5.28%	36.12%	4.76%	4.36%	36.41%
CHLOROACETALDEHYDE	1.26%	7.57%	4.76%		19.24%
CHLOROACETIC ACID	1.81%	5.49%	5.01%		22.97%
CHLOROACETYL CHLORIDE	1.94%	3.76%			9.67%
CHLOROCYCLOHEXANE	0.31%	3.74%	3.23%		9.74%
CHLORODIFLUOROMETHANE	0.30%	3.50%	2.16%	1.65%	8.93%
CHLOROFLUOROMETHANE	2.88%	3.76%	5.85%	3.52%	14.99%
CHLOROFORM	0.93%	1.98%	2.59%	1.01%	1.78%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
CHLOROMETHYL METHYL ETHER	1.30%	1.11%	2.30%		16.02%
CHLOROPENTAFLUOROETHANE	0.55%	1.86%	2.14%	1.60%	10.00%
CHLOROPRENE	1.39%	4.91%	1.81%		8.19%
CHLOROTRIFLUOROETHYLENE	0.44%	1.83%	2.82%		8.35%
CHLOROTRIFLUOROMETHANE	0.30%	2.25%	1.19%	2.52%	8.25%
CHRYSENE	1.74%	14.49%	5.54%	0.85%	24.67%
CINNAMIC ACID	3.47%	4.53%			17.94%
cis,trans-2,4-HEXADIENE	1.31%	5.25%	2.52%	0.68%	13.90%
cis-1,2-DICHLOROETHYLENE	4.77%	2.64%	4.51%	11.39%	12.56%
cis-1,2-DIMETHYLCYCLOHEXANE	3.00%	4.57%	3.07%	0.89%	5.60%
cis-1,2-DIMETHYLCYCLOPENTANE	0.16%	2.92%	1.89%	1.00%	8.26%
cis-1,3-DICHLOROPROPENE	1.80%	3.59%	3.14%		10.19%
cis-1,3-DIMETHYLCYCLOHEXANE	2.55%	3.54%	2.62%	1.30%	7.60%
cis-1,3-DIMETHYLCYCLOPENTANE	0.78%	1.88%	2.80%	2.14%	11.22%
cis-1,3-PENTADIENE	6.55%	4.80%	7.37%	7.79%	15.20%
cis-1,4-DIMETHYLCYCLOHEXANE	3.13%	4.15%	2.97%	1.66%	5.46%
cis-1,8-TERPIN	3.05%	0.51%	6.06%		6.78%
cis-1-PROPENYLBENZENE	1.44%	3.58%	2.76%	5.66%	15.70%
cis-2-BUTENE	0.44%	3.46%	1.43%	1.10%	8.43%
cis-2-DECENE	1.71%	5.45%	3.46%	3.68%	12.74%
cis-2-DODECENE	1.95%	5.15%	3.85%	4.64%	12.02%
cis-2-HEPTENE	0.16%	5.84%	5.59%	0.96%	12.72%
cis-2-HEXENE	0.64%	5.53%	3.80%	2.57%	11.93%
cis-2-METHYLCYCLOHEXANOL	3.89%	3.06%	3.48%	1.53%	5.06%
cis-2-NONENE	1.13%	5.50%	5.04%		12.52%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
cis-2-OCTENE	0.75%	5.62%	4.16%	1.48%	12.58%
cis-2-PENTENE	0.68%	2.53%	3.60%	1.53%	9.27%
cis-2-PHENYLBUTENE-2	1.30%	5.22%	3.12%		12.16%
cis-3-HEPTENE	1.52%	5.57%	2.70%	0.87%	8.29%
cis-3-HEXENE	1.20%	4.71%	1.68%	1.21%	9.94%
cis-3-METHYLCYCLOHEXANOL	3.24%	2.83%	3.22%	1.45%	7.48%
cis-3-OCTENE	0.42%	6.48%	4.25%	0.75%	12.39%
cis-4-METHYLCYCLOHEXANOL	1.16%	2.29%	3.87%	1.46%	7.17%
cis-4-OCTENE	0.33%	6.34%	6.51%	0.78%	12.21%
cis-CROTONALDEHYDE	1.44%	5.49%	3.13%	4.47%	10.68%
cis-CROTONIC ACID	1.89%	4.50%			16.51%
cis-CROTONITRILE	2.96%	13.61%	3.98%	8.54%	27.82%
cis-DECAHYDRONAPHTHALENE	0.53%	3.98%	1.88%	2.17%	10.25%
cis-STILBENE	0.77%	5.15%	3.07%		11.83%
CITRACONIC ACID	2.49%	7.64%	4.83%		27.03%
CROTYL GLYCOL ETHER	2.87%	5.00%			12.11%
CUMENE	0.80%	4.47%	2.15%	4.66%	8.50%
CYANOGEN	0.77%	2.52%	3.98%		7.39%
CYANOGEN CHLORIDE	1.01%	6.20%	4.05%	11.09%	6.68%
CYCLOBUTANE	1.11%	4.35%	3.26%	4.74%	8.64%
CYCLOHEPTANE	0.34%	2.03%	1.90%	2.78%	10.11%
CYCLOHEPTENE	2.12%	1.04%	2.21%	3.73%	10.33%
CYCLOHEXANE	0.85%	1.90%	0.76%	0.67%	8.74%
CYCLOHEXANECARBOXALDEHYDE	0.45%	4.05%		1.85%	10.98%
CYCLOHEXANOL	9.58%	3.73%	10.05%	18.15%	12.36%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
CYCLOHEXANONE	0.42%	4.61%	2.39%		21.89%
CYCLOHEXANONE OXIME	1.68%	1.19%	3.18%		6.14%
CYCLOHEXENE	0.30%	2.97%	2.03%	0.60%	8.94%
CYCLOHEXYL ACETATE	1.99%	4.56%	3.20%	0.63%	14.15%
CYCLOHEXYL FORMATE	0.30%	3.76%	2.66%	0.62%	14.36%
CYCLOHEXYL HYDROPEROXIDE	2.46%	2.92%	3.69%		9.77%
CYCLOHEXYL ISOCYANATE	1.71%	4.29%	3.32%		3.70%
CYCLOHEXYL MERCAPTAN	0.24%	3.32%	1.93%	1.23%	14.90%
CYCLOHEXYLAMINE	2.77%	2.08%	3.67%	1.99%	0.65%
CYCLOHEXYLBENZENE	3.81%	1.97%	4.21%		17.01%
CYCLOOCTANE	1.23%	2.01%	2.17%	4.55%	8.40%
CYCLOOCTENE	2.25%	3.22%	2.65%	7.79%	8.65%
CYCLOPENTADIENE	4.22%	2.89%	9.38%	3.33%	8.43%
CYCLOPENTANE	0.41%	4.64%	2.62%	0.51%	7.31%
CYCLOPENTANONE	0.71%	5.48%	2.47%	4.08%	22.24%
CYCLOPENTENE	0.21%	2.65%	2.91%	3.70%	7.21%
CYCLOPENTYLACETIC ACID	3.08%	4.09%		7.62%	11.59%
CYCLOPENTYLAMINE	1.98%	4.35%	3.24%		0.03%
CYCLOPROPANE	0.51%	1.67%	1.51%	2.96%	11.68%
CYCLOPROPANE CARBOXYLIC ACID	0.75%	2.69%		18.08%	8.65%
CYCLOPROPANECARBOXAMIDE	1.95%	12.31%	5.88%		23.11%
CYCLOPROPYL CYANIDE	1.51%	16.34%		10.83%	32.95%
CYCLOPROPYLAMINE	1.64%	3.17%			12.53%
DECAFLUOROBUTANE	1.02%	3.04%	3.33%		7.64%
DECAMETHYLCYCLOPENTASILOXANE	4.30%	4.79%	4.46%		12.45%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
DECAMETHYLTETRAILOXANE	2.39%	3.50%	4.87%		9.89%
DECANAL	3.27%	2.86%	3.23%		10.10%
DEHYDROABIETIC ACID	2.10%	2.50%	5.32%		11.84%
DEHYDROABIETYLAMINE	2.19%	5.12%	4.28%		13.63%
DEUTERIUM OXIDE	1.55%	12.27%	2.94%	17.94%	22.19%
DI-(2-CHLOROETHOXY)METHANE	0.93%	5.62%	4.73%		12.65%
DI(2-CHLOROETHYL)ETHER	1.47%	5.83%		4.66%	17.84%
DI-(2-ETHYLHEXYL) MALEATE	3.58%	4.70%	5.78%		20.01%
DI-2-ETHYLHEXYLAMINE	3.18%	3.38%	4.26%		12.18%
DIACETYL	2.81%	3.45%	5.19%		11.22%
DIALLYL MALEATE	2.36%	5.09%	4.13%		12.76%
DIALLYL PHTHALATE	2.36%	6.70%	4.78%		13.38%
DIALLYL SULFIDE	8.46%	5.51%			20.41%
DIALLYLAMINE	1.52%	1.15%	2.86%		4.44%
DIAMYL KETONE	2.37%	4.15%			10.48%
DIAMYLAMINE	1.36%	4.66%	3.98%		12.37%
DIBENZOFURAN	1.98%	2.12%	4.72%	0.27%	9.20%
DIBENZOTHIOPHENE	0.53%	3.22%	3.68%		9.44%
DIBENZYL ETHER	10.64%	4.74%	1.27%		11.77%
DIBORANE	0.30%	0.77%	1.47%	0.49%	5.47%
DIBROMODIFLUOROMETHANE	2.03%	8.10%		7.02%	12.71%
DIBROMOMETHANE	1.10%	0.51%	2.07%	2.12%	3.02%
DIBUTYL MALEATE	2.59%	5.18%	4.27%		20.44%
DIBUTYL SEBACATE	4.11%	4.40%	6.08%	4.23%	24.82%
DIBUTYL TEREPHTHALATE	1.60%	5.61%	5.75%		19.49%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
DICHLOROACETALDEHYDE	0.87%	4.10%	3.21%		10.69%
DICHLOROACETIC ACID	1.94%	2.78%	3.66%		16.84%
DICHLOROACETYL CHLORIDE	1.25%	3.05%	2.39%		9.09%
DICHLORODIETHYLSILANE	3.31%	2.87%	4.85%		4.86%
DICHLORODIFLUOROMETHANE	0.04%	2.44%	1.97%	5.41%	7.17%
DICHLOROFLUOROMETHANE	0.87%	3.14%	2.36%	2.46%	9.19%
DICHLOROMETHANE	1.06%	3.15%	1.95%	3.67%	9.20%
DICHLOROSILANE	1.39%	1.31%			3.57%
DICYANDIAMIDE	2.10%	2.46%	5.27%		11.26%
DICYCLOHEXYL SULFIDE	1.11%	2.58%	3.72%	7.15%	3.41%
DICYCLOPENTADIENE	2.02%	1.29%	2.06%	5.08%	15.02%
DIETHANOLAMINE	0.78%	7.48%	6.04%		8.88%
DIETHYL CARBONATE	6.27%	4.29%	7.43%		13.08%
DIETHYL DISULFIDE	3.01%	3.95%	4.82%	3.09%	12.96%
DIETHYL ETHER	0.73%	4.20%	2.89%	5.57%	10.35%
DIETHYL MALEATE	1.19%	2.68%			22.70%
DIETHYL MALONATE	2.77%	4.26%	5.23%		16.98%
DIETHYL PHTHALATE	1.07%	5.98%	6.01%		13.62%
DIETHYL SUCCINATE	3.25%	3.49%	2.65%	2.88%	7.70%
DIETHYL SULFIDE	1.38%	4.28%	2.33%	1.88%	7.19%
DIETHYLALUMINUM CHLORIDE	3.52%	12.32%	5.30%		13.45%
DIETHYLAMINE	1.95%	3.47%	3.16%	1.27%	6.32%
DIETHYLENE GLYCOL	2.50%	6.64%			18.08%
DIETHYLENE GLYCOL DIETHYL ETHER	1.14%	3.96%	3.65%		11.15%
DIETHYLENE GLYCOL DIMETHYL ETHER	0.59%	3.57%	2.88%		18.46%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c
DIETHYLENE GLYCOL DI-n-BUTYL ETHER	3.32%	4.38%			11.81%
DIETHYLENE GLYCOL ETHYL ETHER ACETATE	3.82%	4.33%	6.34%		11.10%
DIETHYLENE GLYCOL MONOBUTYL ETHER ACETATE	3.22%	4.13%		4.07%	11.97%
DIETHYLENE GLYCOL MONOPROPYL ETHER	0.36%	3.34%	2.07%	7.31%	10.34%
DIETHYLENTRIAMINE	3.16%	3.14%	3.98%		12.19%
DIETHYLSULFITE	1.11%	2.20%	6.02%		9.69%
DIFLUOROMETHANE	1.00%	3.63%	4.07%	10.07%	14.74%
DIFLUOROMETHYL TRIFLUOROMETHYL ETHER	0.90%	5.67%	3.32%	2.90%	20.08%
DIGLYCOLIC ACID	2.75%	4.36%	5.74%		21.71%
DIHEXYL ADIPATE	2.32%	3.19%	4.57%	3.97%	25.74%
DIIODOMETHANE	2.94%	4.12%	5.57%	27.01%	17.65%
DIISOBUTYL ETHER	1.07%	3.62%	3.29%	0.81%	11.42%
DIISOBUTYL KETONE	2.28%	4.68%	4.55%		13.10%
DIISOBUTYL PHTHALATE	2.17%	4.21%	4.34%		11.65%
DIISOBUTYLAMINE	1.69%	3.52%			4.92%
DIISONONYL PHTHALATE	6.70%	3.42%	7.16%		16.16%
DIISOCTYL PHTHALATE	3.05%	5.37%	4.86%	0.81%	13.83%
DIISOPENTYLSULFIDE	0.96%	4.83%	5.21%		12.03%
DIISOPROPYL ETHER	2.11%	3.11%	3.86%	0.26%	9.75%
DIISOPROPYL KETONE	2.24%	4.26%	4.07%		10.19%
DIISOPROPYL SULFIDE	0.59%	2.18%	3.39%	2.96%	8.70%
DIISOPROPYLAMINE	8.04%	1.71%	8.19%		1.41%
DIKETENE	2.16%	2.50%		2.86%	8.59%
DILACTIC ACID	2.17%	0.98%	4.78%	3.35%	7.88%
DIMERCAPTOETHYL ETHER	1.08%	6.15%	3.45%		19.19%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
DIMETHYL CARBONATE	1.20%	4.27%	4.91%		12.84%
DIMETHYL DISULFIDE	0.87%	2.08%	1.79%	2.79%	12.90%
DIMETHYL ETHER	0.59%	2.49%	2.88%	2.21%	8.23%
DIMETHYL GLUTARATE	3.90%	4.91%			14.35%
DIMETHYL ISOPHTHALATE	1.03%	3.82%	5.28%		15.66%
DIMETHYL MALEATE	1.31%	4.77%	3.96%	0.99%	18.96%
DIMETHYL PEROXIDE	2.11%	2.75%	3.43%		8.39%
DIMETHYL PHTHALATE	1.50%	5.81%	4.61%		13.43%
DIMETHYL SILANE	2.83%	2.53%	1.81%		8.20%
DIMETHYL SUCCINATE	3.08%	4.05%			10.14%
DIMETHYL SULFIDE	0.88%	4.14%	2.36%	0.62%	10.28%
DIMETHYL SULFOXIDE	5.91%	7.47%	3.86%	0.69%	32.08%
DIMETHYL TEREPHTHALATE	0.40%	3.58%			21.60%
DIMETHYL-1,4-CYCLOHEXANEDICARBOXYLATE	1.89%	5.30%	4.60%		12.61%
DIMETHYL-2,6-NAPHTHALENEDICARBOXYLATE	1.63%	3.29%	4.74%		15.22%
DIMETHYLACETYLENE	1.01%	2.53%	1.95%	1.97%	6.19%
DIMETHYLALUMINUM CHLORIDE	7.04%	15.05%			24.75%
DIMETHYLAMINE	2.32%	4.81%	4.19%	10.05%	9.26%
DIMETHYLCHLOROSILANE	0.92%	4.45%	7.90%		6.33%
DIMETHYLDICHLOROSILANE	1.93%	1.57%	1.17%	4.88%	2.69%
DIMETHYLDIMETHOXYSilANE	6.42%	6.01%			4.09%
DIMETHYLETHANOLAMINE	1.75%	3.22%	3.82%		10.07%
DIMETHYLKETENE	2.30%	2.36%		25.32%	7.49%
DIMETHYLMALONATE	6.23%	3.38%			13.96%
DIMETHYLMERCURY	2.59%	1.87%			7.71%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
DI-n-BUTYL DISULFIDE	1.34%	5.71%	4.65%		10.91%
DI-n-BUTYL ETHER	1.42%	4.97%	3.09%	0.85%	15.93%
DI-n-BUTYL PHTHALATE	3.43%	6.67%	5.75%		14.49%
DI-n-BUTYL SULFIDE	0.46%	5.79%			15.55%
DI-n-BUTYL SULFONE	1.95%	4.86%	4.05%		21.17%
DI-n-BUTYLAMINE	2.60%	4.12%	3.16%	0.93%	9.71%
DI-n-DECYL PHTHALATE	3.66%	6.44%	5.89%		18.18%
DI-n-HEPTYL PHTHALATE	4.01%	5.21%	5.56%		13.58%
DI-n-HEXYL ETHER	2.27%	5.01%	3.83%	1.63%	20.74%
DI-n-HEXYL PHTHALATE	3.47%	6.00%	5.44%		14.69%
DI-n-NONYL PHTHALATE	3.03%	6.35%	5.42%		17.42%
DI-n-OCTYL ETHER	2.60%	4.67%	4.41%	0.65%	23.50%
DI-n-OCTYL TEREPHTHALATE	2.95%	4.55%	5.32%	0.93%	14.00%
DI-n-OCTYLAMINE	2.08%	3.98%	5.22%		19.12%
DINONYL ETHER	2.88%	3.34%			26.59%
DINONYLPHENOL	2.85%	11.55%	4.97%		27.78%
DI-n-PENTYL ETHER	0.93%	5.01%	8.48%	1.00%	18.01%
DI-n-PROPYL DISULFIDE	1.68%	3.88%	3.50%	1.68%	15.90%
DI-n-PROPYL ETHER	0.85%	5.08%	4.16%	0.97%	10.95%
DI-n-PROPYL PHTHALATE	3.51%	6.53%	6.16%		14.32%
DI-n-PROPYL SULFIDE	0.58%	5.33%	3.64%	1.31%	14.32%
DI-n-PROPYL SULFONE	2.52%	5.18%	3.15%		21.00%
DI-n-PROPYLAMINE	1.03%	3.22%	2.91%	1.86%	6.11%
DI-n-UNDECYL PHTHALATE	4.19%	5.10%			17.53%
DIPHENYL CARBONATE	1.70%	4.13%	4.86%		12.56%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
DIPHENYL DISULFIDE	5.91%	0.74%			5.09%
DIPHENYL ETHER	1.86%	3.76%	6.74%		16.59%
DIPHENYLACETYLENE	1.31%	4.11%	3.01%		10.76%
DIPHENYLAMINE	0.62%	4.59%	4.51%		10.64%
DIPHENYLDICHLOROSILANE	2.59%	6.08%		6.77%	19.62%
DIPHENYLMETHANE	1.71%	4.58%	5.22%		10.82%
DIPROPYL MALEATE	1.48%	4.32%	4.40%		18.16%
DIPROPYLENE GLYCOL MONOMETHYL ETHER ACETATE	0.71%	3.61%	4.29%	4.36%	10.74%
DIPROPYLENE GLYCOL n-BUTYL ETHER	2.54%	2.91%			9.91%
DI-sec-BUTYL ETHER	1.38%	3.75%	3.28%	1.11%	8.85%
DISILANE	1.23%	0.71%	2.47%		5.36%
DI-t-BUTYL PEROXIDE	0.78%	2.11%	3.24%		8.42%
DI-tert-BUTYL DISULFIDE	0.94%	1.89%			9.90%
DI-tert-BUTYL ETHER	3.71%	5.19%	4.19%		14.86%
DI-tert-BUTYL SULFIDE	1.67%	3.47%	3.69%		12.39%
DIVINYL ETHER	0.74%	2.60%	2.61%		7.96%
DODECAMETHYLCYCLOHEXASILOXANE	3.72%	4.01%	5.06%		12.41%
DODECAMETHYLPENTASILOXANE	2.89%	3.32%	5.11%		11.69%
DODECANAL	2.03%	2.52%	5.39%		9.51%
DODECANEDIOIC ACID	2.99%	4.64%			22.38%
D-XYLOSE	0.55%	3.02%			11.44%
EICOSAMETHYLNONASILOXANE	4.66%	4.54%	6.19%		14.84%
ERUCIC ACID	3.63%	4.20%	5.49%		10.33%
ETHANE	0.85%	1.26%	1.87%	7.92%	10.06%
ETHANESULFONYL CHLORIDE	1.27%	5.48%			11.11%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
ETHANOL	2.73%	9.84%	6.37%	48.34%	14.06%
ETHYL ACETATE	1.07%	5.01%	2.89%	5.35%	11.10%
ETHYL ACETOACETATE	0.42%	5.99%			10.81%
ETHYL ACRYLATE	2.34%	5.54%	3.09%		9.81%
ETHYL BENZOATE	1.80%	3.88%	6.94%		5.93%
ETHYL CAPRATE	4.19%	5.50%			13.37%
ETHYL CAPRYLATE	1.62%	4.83%	4.45%		11.85%
ETHYL CHLORIDE	0.61%	3.77%	3.06%	3.09%	10.64%
ETHYL CHLOROFORMATE	2.34%	0.74%	3.71%	6.01%	2.76%
ETHYL CYANOACETATE	2.03%	11.15%			29.91%
ETHYL FLUORIDE	0.68%	4.25%	4.59%		12.49%
ETHYL FORMATE	1.15%	4.40%	1.71%	2.14%	11.20%
ETHYL HYDROPEROXIDE	4.57%	3.53%	5.24%		8.93%
ETHYL IODIDE	2.95%	5.77%	2.58%		12.11%
ETHYL ISOAMYL KETONE	4.38%	4.26%			10.73%
ETHYL ISOBUTYL ETHER	1.29%	3.49%	3.34%		8.46%
ETHYL ISOBUTYRATE	0.82%	3.50%	5.14%	1.32%	6.33%
ETHYL ISOPROPYL ETHER	0.86%	1.82%	2.58%	0.65%	8.46%
ETHYL ISOPROPYL KETONE	2.21%	2.04%	2.66%		11.24%
ETHYL ISOVALERATE	4.95%	3.99%	4.39%	1.42%	12.45%
ETHYL LACTATE	0.36%	3.23%			9.23%
ETHYL LAURATE	4.88%	4.81%			15.23%
ETHYL LEVULINATE	0.39%	5.21%			12.50%
ETHYL LINOLEATE	2.20%	5.37%	5.49%		9.47%
ETHYL LINOLENATE	2.59%	4.55%	5.05%		7.69%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
ETHYL MERCAPTAN	0.60%	3.97%	1.20%	3.29%	7.79%
ETHYL METHACRYLATE	1.51%	6.30%	1.81%		10.83%
ETHYL METHYL DISULFIDE	1.74%	3.28%			7.99%
ETHYL MYRISTATE	4.43%	3.97%			17.23%
ETHYL n-BUTYRATE	0.27%	6.35%	4.36%	5.35%	11.93%
ETHYL n-HEXYL ETHER	1.47%	5.02%	3.33%	0.87%	15.49%
ETHYL n-OCTYL SULFIDE	0.98%	1.80%	1.72%		1.60%
ETHYL n-PENTYL SULFIDE	1.44%	4.52%	3.84%		15.69%
ETHYL OLEATE	1.17%	4.88%			18.37%
ETHYL PHENYL ACETATE	1.29%	4.89%	4.33%		11.42%
ETHYL PHENYL CARBONATE	1.93%	4.64%	4.36%		11.29%
ETHYL PROPIONATE	1.22%	4.97%	1.79%	0.43%	10.58%
ETHYL PROPYL DISULFIDE	0.65%	3.80%			8.15%
ETHYL PROPYL ETHER	5.48%	3.17%		1.21%	7.22%
ETHYL PROPYL SULFIDE	0.70%	4.56%	3.98%		9.36%
ETHYL STEARATE	4.34%	5.82%	7.20%		22.57%
ETHYL t-BUTYL SULFIDE	1.28%	3.94%	2.28%	2.04%	11.20%
ETHYL TERT-BUTYL DISULFIDE	0.24%	3.67%	4.51%		8.73%
ETHYL tert-PENTYL ETHER	2.40%	3.82%	2.75%	3.39%	6.38%
ETHYL THIOLACETATE	1.22%	3.87%	2.79%		9.30%
ETHYL VANILLIN	2.93%	2.67%	4.91%		12.32%
ETHYL VINYL ETHER	0.55%	2.50%	2.21%	7.05%	8.06%
ETHYL-3-ETHOXYPROPIONATE	1.76%	3.05%	3.25%	0.72%	19.95%
ETHYLACETYLENE	0.89%	3.21%	1.47%	1.65%	12.54%
ETHYLAL	1.63%	3.66%	6.37%	1.29%	10.91%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
ETHYLAMINE	2.49%	2.55%	2.72%	7.08%	5.43%
ETHYLBENZENE	0.41%	4.68%	0.47%	2.00%	9.48%
ETHYLBENZENE HYDROPEROXIDE	1.83%	3.24%	4.06%	4.08%	10.62%
ETHYLCHLOROACETATE	2.46%	5.23%	2.86%		15.55%
ETHYLCYCLOHEXANE	2.83%	5.55%	2.83%	1.00%	11.05%
ETHYLCYCLOPENTANE	0.38%	5.06%	1.77%	0.76%	8.39%
ETHYLDIETHANOLAMINE	3.63%	5.45%	5.77%		9.76%
ETHYLENE	0.54%	0.76%	1.18%	3.58%	9.75%
ETHYLENE CARBONATE	6.61%	7.45%	10.47%		42.24%
ETHYLENE GLYCOL	3.75%	8.12%	5.64%		7.56%
ETHYLENE GLYCOL DIACETATE	2.72%	5.45%	5.47%		12.89%
ETHYLENE GLYCOL DIACRYLATE	1.54%	5.25%			13.01%
ETHYLENE GLYCOL DINITRATE	1.82%	3.52%	4.75%		3.56%
ETHYLENE GLYCOL MONOPROPYL ETHER	6.58%	7.64%		8.54%	13.09%
ETHYLENE OXIDE	0.73%	4.96%	1.38%	4.91%	10.56%
ETHYLENEDIAMINE	1.90%	4.46%	5.25%	1.95%	15.80%
ETHYLENEIMINE	7.48%	4.68%	6.21%	8.63%	5.68%
ETHYLIDENE DIACETATE	1.77%	3.93%	3.64%	3.95%	12.90%
ETHYLNORBORNENE	0.60%	4.92%	2.76%		10.69%
ETHYLTRIACETOXSILANE	3.87%	12.49%		1.22%	23.93%
ETHYLTRICHLOROSILANE	1.72%	0.47%	2.64%		3.62%
ETHYNYLBENZENE	1.57%	1.39%	1.78%	7.03%	11.98%
EUGENOL	1.77%	5.71%	4.51%		14.55%
FLUORANTHENE	4.97%	7.39%	7.68%		20.83%
FLUORENE	1.90%	10.75%	3.57%	1.07%	21.42%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
FLUORINE	0.80%	0.41%	1.70%	0.88%	9.75%
FLUOROBENZENE	0.62%	3.37%	2.42%		10.75%
FORMANILIDE	1.78%	4.03%	3.77%		14.79%
FUMARIC ACID	2.66%	2.10%	8.43%	0.65%	15.44%
FUMARONITRILE	1.79%	37.54%	6.02%	3.78%	40.42%
FURAN	2.39%	2.73%	2.08%	4.47%	0.03%
FURAN 2,5-DICARBOXYLIC ACID	2.35%	30.74%			36.96%
FURFURAL	1.38%	3.59%	3.01%	6.06%	12.75%
FURFURYL ALCOHOL	1.77%	4.72%		8.55%	7.42%
GALLIUM TRICHLORIDE	3.74%	33.76%			59.14%
gamma-AMINOPROPYLTRIETHOXSILANE	4.12%	1.27%		12.03%	0.12%
gamma-BUTYROLACTONE	1.83%	8.92%		8.70%	21.33%
gamma-TERPINENE	1.88%	3.01%	2.90%	0.52%	15.22%
gamma-VALEROLACTONE	2.92%	3.93%	7.76%		26.45%
GERMANIUM TETRACHLORIDE	1.76%	1.62%	4.34%	1.56%	9.80%
GERMANIUM TETRAFLUORIDE	1.34%	1.40%	4.08%		10.07%
GERMANIUM TETRAHYDRIDE	9.42%	0.51%			5.61%
GLUTARALDEHYDE	2.08%	7.43%	3.88%	1.23%	21.40%
GLUTARIC ACID	4.49%	4.23%	7.28%	5.71%	16.12%
GLUTARIC ANHYDRIDE	3.01%	3.27%	8.07%		23.80%
GLUTARONITRILE	4.58%	41.80%		12.82%	60.77%
GLYCERYL TRIACETATE	1.91%	4.39%	4.94%		11.10%
GLYCOL ALDEHYDE	2.61%	22.41%	7.62%		23.31%
GLYCOLIC ACID	2.65%	1.81%	5.46%		10.81%
GUAIACOL	8.70%	2.48%	3.85%	1.49%	2.47%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
HALOTHANE	3.44%	2.48%	1.88%	0.24%	5.43%
HEPTAFLUOROPROPYL METHYL ETHER	1.07%	4.47%	3.88%		10.75%
HEPTANAL	0.61%	3.61%	5.69%		7.68%
HEXACHLOROBENZENE	8.90%	19.09%			26.46%
HEXACHLOROCYCLOPENTADIENE	0.97%	4.55%	3.25%		10.60%
HEXACHLORODISILOXANE	3.35%	2.17%	5.05%		7.46%
HEXACHLOROETHANE	1.80%	7.95%	3.63%		17.56%
HEXACHLOROSILANE	2.69%	2.18%	4.89%		7.35%
HEXACOSAMETHYLDODECASILOXANE	4.18%	2.75%	5.65%		11.54%
HEXADECAMETHYLCYCLOCTASILOXANE	2.37%	3.71%	5.26%		15.31%
HEXADECAMETHYLHEPTASILOXANE	6.73%	5.62%	3.85%		13.27%
HEXAETHYLBENZENE	2.10%	2.40%	5.13%	6.70%	9.11%
HEXAFLUORO-1,3-BUTADIENE	4.24%	3.87%	3.47%		10.23%
HEXAFLUROACETONE	2.03%	3.98%	4.10%	11.71%	7.60%
HEXAFLUROBENZENE	0.75%	3.25%	4.20%	0.76%	10.97%
HEXAFLUROETHANE	0.34%	1.42%	3.56%	2.23%	7.06%
HEXAMETHYLBENZENE	1.91%	3.78%	5.02%	3.91%	7.22%
HEXAMETHYLCYCLOTRISILOXANE	4.57%	2.24%	4.04%		9.14%
HEXAMETHYLDISILAZANE	1.20%	2.60%	4.55%		10.11%
HEXAMETHYLDISILOXANE	2.32%	3.18%	4.13%	3.10%	7.26%
HEXAMETHYLENEDIAMINE	2.32%	2.06%	4.90%		4.48%
HEXAMETHYLENEIMINE	1.67%	2.26%	4.06%		0.13%
HEXANAL	0.43%	3.79%	3.89%		8.19%
HEXANENITRILE	1.34%	5.59%	9.36%		13.32%
HMX	2.97%	26.64%	7.19%		36.84%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
HYDRACRYLONITRILE	3.22%	15.68%		28.98%	22.53%
HYDRAZINE	1.61%	3.03%	2.27%	24.98%	32.33%
HYDRAZOBENZENE	1.91%	3.90%	4.27%		14.96%
HYDROGEN BROMIDE	1.82%	0.79%	1.60%	0.23%	9.66%
HYDROGEN CHLORIDE	2.81%	1.31%	3.07%	6.81%	18.32%
HYDROGEN CYANIDE	5.76%	50.91%			44.86%
HYDROGEN IODIDE	1.08%	0.35%	2.80%	9.23%	10.24%
HYDROGEN PEROXIDE	2.42%	2.51%	5.15%		4.93%
HYDROGEN SELENIDE	2.38%	0.35%	3.92%		0.58%
HYDROGEN SULFIDE	0.49%	0.59%	1.37%	9.59%	8.37%
HYDROXYACETONITRILE	3.16%	14.32%	4.61%	7.29%	28.53%
HYDROXYCAPROIC ACID	2.88%	1.54%	4.99%		10.06%
IBUPROFEN	1.84%	2.71%			0.43%
IMIDAZOLE	3.73%	1.69%	4.33%		6.45%
INDANE	0.30%	2.81%	6.48%	3.24%	6.06%
INDENE	2.77%	3.49%	4.24%	1.86%	14.86%
INDOLE	2.47%	4.49%	3.56%	2.82%	1.36%
IODINE	1.88%	0.33%	3.67%		20.66%
IODOBENZENE	1.10%	3.52%	1.59%	2.10%	9.79%
IRON PENTACARBONYL	5.94%	2.51%		4.87%	7.51%
ISOBUTANE	0.23%	3.44%	1.25%	2.65%	7.33%
ISOBUTENE	0.70%	3.10%	0.98%	2.44%	7.83%
ISOBUTYL ACETATE	2.63%	6.15%	3.51%	4.86%	12.88%
ISOBUTYL ACRYLATE	0.84%	3.92%	3.51%		9.94%
ISOBUTYL CHLORIDE	0.48%	6.16%	2.71%	2.98%	8.76%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
ISOBUTYL FORMATE	1.79%	2.66%	2.33%		0.22%
ISOBUTYL ISOBUTYRATE	2.97%	2.73%	5.51%		11.21%
ISOBUTYL MERCAPTAN	1.08%	3.69%	1.62%	0.25%	10.13%
ISOBUTYL METHACRYLATE	1.16%	4.17%	2.51%	0.60%	10.46%
ISOBUTYLAMINE	0.70%	4.05%	3.32%	1.60%	4.64%
ISOBUTYLBENZENE	1.01%	1.95%	3.59%	0.65%	9.32%
iso-BUTYLCYCLOHEXANE	1.47%	3.05%	3.39%		15.60%
ISOBUTYLENE GLYCOL	1.68%	1.71%	5.37%		5.21%
ISOBUTYL-tert-BUTYL ETHER	1.52%	1.30%	3.04%	1.34%	10.91%
ISOBUTYRIC ACID	1.44%	6.73%			27.53%
ISOBUTYRIC ANHYDRIDE	1.49%	0.88%			16.33%
ISOBUTYRONITRILE	1.27%	6.72%	3.10%	4.89%	25.30%
ISOPENTANE	0.10%	4.15%	1.36%	0.35%	9.29%
ISOPENTYL ACETATE	5.58%	5.03%	3.55%	0.93%	13.54%
ISOPENTYL BUTYRATE	1.21%	6.17%			8.73%
ISOPENTYL ISOVALERATE	1.51%	6.85%	2.55%	2.36%	13.33%
ISOPHORONE	1.48%	4.56%			11.16%
ISOPHTHALIC ACID	2.77%	19.69%	7.03%		30.86%
ISOPHTHALOYL CHLORIDE	2.36%	4.12%	3.14%		13.99%
ISOPIMARIC ACID	2.29%	3.06%	6.24%		12.74%
ISOPRENE	4.12%	3.90%	4.21%	5.73%	10.73%
ISOPROPANOL	6.53%	6.88%	4.91%	20.50%	11.45%
ISOPROPYL ACETATE	3.38%	4.70%	2.28%	5.06%	13.49%
ISOPROPYL ACRYLATE	1.65%	3.76%		10.97%	8.76%
ISOPROPYL BUTYL ETHER	1.60%	2.80%	2.98%	0.91%	12.27%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
ISOPROPYL CHLORIDE	1.78%	3.30%	2.40%	1.42%	7.95%
ISOPROPYL IODIDE	4.09%	0.78%	5.84%	5.44%	1.33%
ISOPROPYL ISOBUTYL ETHER	1.34%	1.69%	2.99%	1.21%	9.91%
ISOPROPYL MERCAPTAN	1.66%	1.78%	1.70%	1.42%	8.06%
ISOPROPYL PALMITATE	4.07%	4.30%	7.01%		20.19%
ISOPROPYLAMINE	3.21%	3.40%	3.93%	10.31%	14.36%
ISOPROPYLCYCLOHEXANE	0.25%	4.47%	1.80%		13.75%
ISOPROPYLCYCLOPENTANE	0.43%	5.32%	3.35%	2.99%	11.74%
ISOQUINOLINE	0.11%	1.10%	2.43%	0.60%	5.57%
ISOSORBIDE	2.11%	3.09%	4.72%		10.38%
ISOVALERIC ACID	2.55%	6.57%		8.32%	25.56%
ISOXAZOLE	1.35%	5.29%	2.42%		17.82%
ITACONIC ACID	2.47%	7.66%	5.86%		25.83%
KETENE	4.09%	2.43%	2.98%		9.93%
KRYPTON	0.38%	0.49%	1.62%		10.08%
LACTIC ACID	1.52%	4.90%	5.43%		3.65%
LACTONITRILE	2.98%	6.40%	4.84%		17.89%
L-ARABINOSE	0.56%	3.02%			11.44%
LEVOGLUCOSAN	1.92%	2.00%	5.37%		9.54%
LEVULINIC ACID	1.71%	6.65%	4.35%		20.33%
L-GLUTAMIC ACID	2.62%	0.81%	6.50%		8.56%
LINOLEIC ACID	3.43%	6.46%	4.82%		23.03%
LINOLENIC ACID	3.04%	3.99%	4.74%		13.35%
L-MENTHOL	1.58%	3.94%	8.57%		8.56%
L-PHENYLALANINE	1.87%	2.03%	6.54%	1.17%	12.21%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
LYSINE	2.65%	1.41%	5.51%		10.06%
MALEIC ACID	2.60%	3.75%	5.55%		15.49%
MALEIC ANHYDRIDE	7.74%	0.91%	12.55%		12.96%
MALONIC ACID	4.00%	3.57%			12.74%
MALTOL	2.99%	2.82%	6.42%		14.11%
m-CHLOROANILINE	0.86%	1.03%	5.26%		7.59%
m-CHLOROBENZOYL CHLORIDE	1.54%	5.05%	4.22%		12.14%
m-CHLORONITROBENZENE	1.73%	5.22%	7.41%	2.47%	0.60%
m-CHLOROPHENOL	4.13%	0.67%	10.17%		6.38%
m-CRESOL	2.72%	5.85%	5.62%	8.39%	16.56%
m-CYMENE	1.68%	5.26%	2.95%	4.08%	10.12%
m-DIBROMOBENZENE	1.44%	2.90%	3.12%	4.51%	8.28%
m-DICHLOROBENZENE	1.17%	2.87%	2.56%	2.62%	14.49%
m-DIETHYLBENZENE	1.67%	4.78%	2.87%	4.64%	11.75%
m-DIISOPROPYLBENZENE	5.34%	3.51%	5.15%		14.86%
m-DIVINYLBENZENE	1.79%	5.87%	3.13%		17.09%
MELAMINE	0.43%	19.72%			27.97%
MERCURY DICHLORIDE	0.17%	3.02%	3.83%		14.11%
MESITYL OXIDE	2.88%	4.81%	2.98%	0.66%	14.96%
MESITYLENE	0.61%	5.01%	3.35%	6.00%	10.91%
METHACROLEIN	0.92%	3.79%	2.73%		13.80%
METHACRYLONITRILE	3.85%	10.46%	8.29%	0.61%	25.10%
METHANE	0.75%	0.37%	1.92%	7.39%	11.14%
METHANOL	1.75%	6.49%	10.51%	48.50%	23.89%
METHOXYACETIC ACID	0.47%	5.51%	4.83%		25.79%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
METHOXYACETONE	1.04%	4.85%			12.11%
METHOXYDIHYDROPYRAN	1.40%	3.36%	2.84%		11.44%
METHYL ACETATE	0.70%	5.06%	3.02%	1.02%	10.59%
METHYL ACRYLATE	0.89%	6.70%	3.31%		9.07%
METHYL alpha-HYDROXYISOBUTYRATE	0.43%	4.10%	5.11%		11.44%
METHYL alpha-METHOXYISOBUTYRATE	1.31%	4.81%	4.09%		12.78%
METHYL BENZOATE	2.16%	3.59%	4.26%	1.68%	4.17%
METHYL CAPRYLATE	4.89%	3.80%	3.86%		12.54%
METHYL CHLORIDE	0.31%	2.13%	2.51%	3.27%	8.43%
METHYL CHLOROACETATE	1.00%	3.74%	3.58%	3.04%	15.23%
METHYL CHLOROFORMATE	1.56%	3.58%	2.77%		7.73%
METHYL CHLOROSILANE	4.50%	4.09%	5.38%	14.38%	4.92%
METHYL CYANOACETATE	1.12%	13.36%	3.85%		35.42%
METHYL DECANOATE	4.66%	5.43%	5.75%		13.41%
METHYL DICHLOROSILANE	3.70%	5.74%	6.66%	5.66%	3.23%
METHYL DIETHANOLAMINE	2.24%	6.02%	4.41%		9.63%
METHYL DODECANOATE	3.27%	4.61%	5.82%		15.12%
METHYL EICOSANOATE	5.37%	9.62%			25.35%
METHYL ERUCATE	3.47%	4.12%	5.34%		15.04%
METHYL ETHYL ETHER	3.60%	3.89%	1.41%	1.93%	9.83%
METHYL ETHYL KETONE	0.77%	4.84%	3.36%	4.96%	11.94%
METHYL ETHYL SULFIDE	2.45%	5.16%	2.99%	1.97%	16.59%
METHYL FLUORIDE	1.32%	4.27%		14.00%	11.54%
METHYL FORMATE	1.17%	4.71%	1.78%	2.26%	11.95%
METHYL GLYOXAL	1.31%	2.74%	4.74%		9.25%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_c
METHYL HYDROPEROXIDE	0.83%	2.95%	4.32%		8.39%
METHYL IODIDE	3.26%	2.71%	6.51%	1.09%	11.76%
METHYL ISOBUTYL ETHER	0.93%	3.48%	2.86%	0.63%	8.49%
METHYL ISOBUTYL KETONE	0.59%	4.85%	4.03%	2.86%	11.32%
METHYL ISOBUTYRATE	1.37%	4.70%	2.90%	0.95%	10.20%
METHYL ISOCYANATE	1.30%	1.86%	3.61%		2.36%
METHYL ISOPROPENYL KETONE	1.35%	4.70%	2.65%		12.32%
METHYL ISOPROPYL ETHER	0.85%	3.64%	2.55%	2.72%	9.37%
METHYL ISOPROPYL KETONE	0.71%	4.76%	3.09%	5.10%	11.87%
METHYL ISOPROPYL SULFIDE	0.93%	3.63%	2.65%		2.81%
METHYL LACTATE	0.78%	6.36%	5.01%		10.20%
METHYL LINOLENATE	0.80%	5.47%			14.04%
METHYL MERCAPTAN	2.80%	3.05%	3.80%	1.10%	11.06%
METHYL METHACRYLATE	3.38%	3.65%	5.19%		11.97%
METHYL MYRISTATE	6.45%	3.26%			18.75%
METHYL n-BUTYL ETHER	0.85%	5.24%	2.69%	1.27%	11.13%
METHYL n-BUTYL SULFIDE	0.46%	4.95%	2.09%	0.37%	13.50%
METHYL n-BUTYRATE	1.01%	5.96%	3.26%	4.22%	10.39%
METHYL NONAFLUORO-N-BUTYL ETHER	1.45%	4.86%		0.68%	10.15%
METHYL n-PENTYL ETHER	1.27%	4.00%	2.71%	0.92%	13.49%
METHYL n-PROPYL ETHER	1.55%	3.21%	2.44%	0.06%	10.44%
METHYL n-PROPYL SULFIDE	0.79%	3.57%	1.70%	0.27%	12.29%
METHYL OLEATE	4.39%	5.93%	7.57%		15.82%
METHYL PALMITATE	7.22%	4.11%			20.41%
METHYL PALMITOLEATE	2.46%	4.16%	5.19%		24.66%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
METHYL para-TOLUATE	5.61%	3.76%			10.76%
METHYL PENTYL SULFIDE	2.76%	5.07%	4.05%	1.85%	10.94%
METHYL PHENYL SULFIDE	2.17%	2.70%			4.30%
METHYL PROPIONATE	1.09%	5.08%	3.16%	0.41%	10.94%
METHYL RICINOLEATE	4.38%	5.66%	6.63%		17.90%
METHYL sec-BUTYL ETHER	1.18%	4.54%	2.98%	0.35%	7.91%
METHYL SILANE	1.86%	1.48%			1.88%
METHYL SILICATE	0.39%	2.22%	4.35%	2.22%	6.57%
METHYL STEARATE	8.28%	6.46%			22.38%
METHYL t-BUTYL SULFIDE	1.62%	2.95%	2.41%	2.17%	9.98%
METHYL tert-BUTYL ETHER	2.79%	4.03%	3.22%		10.90%
METHYL tert-PENTYL ETHER	0.87%	4.58%	2.48%	4.34%	8.84%
METHYL t-PENTYL SULFIDE	0.72%	4.71%	2.62%	2.69%	10.41%
METHYL TRICHLOROSILANE	1.33%	2.84%		2.78%	5.29%
METHYL VINYL DICHLOROSILANE	1.23%	6.50%	2.15%		5.66%
METHYL VINYL ETHER	1.53%	5.12%	2.01%		6.74%
METHYL-3-MERCAPTOPROPIONATE	1.81%	4.77%	3.76%		11.02%
METHYL-4-FORMYLBENZOATE	1.64%	5.39%			11.88%
METHYLACETYLENE	0.92%	2.42%	1.09%	0.93%	6.84%
METHYLAL	2.43%	6.53%	3.66%	10.02%	32.71%
METHYLAMINE	3.14%	3.93%	2.29%	1.42%	11.01%
METHYLCYCLOHEXANE	0.40%	3.47%	2.03%	1.88%	9.27%
METHYLCYCLOPENTADIENE	1.16%	2.49%	1.60%		8.16%
METHYLCYCLOPENTADIENE DIMER	1.38%	5.12%	3.82%		10.96%
METHYLCYCLOPENTANE	1.38%	3.97%	1.59%	0.88%	8.12%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
METHYLCYCLOPROPANE	0.26%	3.85%			11.98%
METHYLETHANOLAMINE	1.72%	3.94%	3.89%		11.63%
METHYLGERMANIUM TRICHLORIDE	2.83%	3.12%	3.68%	3.26%	9.32%
METHYLGLUTARONITRILE	1.84%	19.74%	4.27%		44.94%
METHYLNORBORNENE	0.81%	4.26%	2.52%		10.61%
m-ETHYLPHENOL	0.64%	2.36%	4.50%	16.64%	5.59%
m-ETHYLSTYRENE	1.52%	5.68%	4.20%		15.70%
m-ETHYLTOLUENE	1.69%	5.02%	3.59%		12.36%
METHYLTRIACTOXSILANE	0.97%	24.44%	5.34%	2.33%	32.30%
m-METHYLSTYRENE	1.34%	6.28%	3.11%	5.36%	14.26%
m-NITROANILINE	1.31%	2.27%	1.49%		9.58%
MONOCHLOROBENZENE	0.56%	3.91%	2.45%	2.22%	9.59%
MONOCHLOROSILANE	1.75%	1.65%	2.44%	0.79%	8.73%
MONOMETHYL TEREPHTHALATE	2.53%	6.67%			20.78%
MONOMETHYL UREA	7.74%	4.18%			12.50%
MONOOLEIN	2.84%	4.92%	5.30%		15.24%
MONOPALMITIN	3.06%	3.30%	5.55%		13.44%
MONO-TERT-BUTYLHYDROQUINONE	0.75%	1.00%			6.61%
MORPHOLINE	1.06%	2.75%	3.85%		8.87%
m-PHENYLENEDIAMINE	1.90%	4.38%	7.40%		2.47%
m-TERPHENYL	0.89%	5.18%	4.69%		13.41%
m-tert-BUTYLPHENOL	3.22%	3.16%	5.79%		10.18%
m-TOLUALCOHOL	1.51%	2.55%	3.24%	2.52%	11.18%
m-TOLUALDEHYDE	2.12%	5.92%	3.15%		15.53%
m-TOLUIC ACID	4.80%	3.39%	7.64%		13.02%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
m-TOLUIDINE	0.83%	5.16%	3.68%	4.10%	16.56%
m-XYLENE	1.12%	4.09%	2.60%	2.64%	10.35%
N-(2-HYDROXYETHYL)PIPERAZINE	5.23%	1.37%	3.45%		8.45%
N,N'-BIS(2-HYDROXYETHYL)ETHYLENEDIAMINE	2.63%	1.54%			9.74%
N,N'-DI(2-HYDROXYETHYL)PIPERAZINE	3.09%	1.56%	5.53%	3.30%	7.60%
N,N-DIETHYLANILINE	5.20%	5.52%	4.08%	2.14%	3.58%
N,N-DIETHYLHYDROXYLAMINE	2.32%	0.98%	3.70%		0.80%
N,N-DIETHYLMETHYLAMINE	0.22%	3.89%			8.39%
N,N-DIMETHYLACETAMIDE	3.04%	7.59%	2.69%		17.78%
N,N-DIMETHYLANILINE	2.52%	5.01%	3.96%		4.32%
N,N-DIMETHYLFORMAMIDE	1.37%	16.20%	3.91%	4.41%	30.16%
N,N-DIMETHYL-n-BUTYLAMINE	1.16%	3.02%	2.66%		6.16%
N,N'-DIPHENYL-p-PHENYLENEDIAMINE	0.26%	4.13%	4.77%		19.90%
N,N'-DI-tert-BUTYLETHYLENEDIAMINE	0.63%	1.23%	4.16%	9.97%	6.86%
N-AMINOETHYL ETHANOLAMINE	2.81%	2.89%	4.37%		11.20%
N-AMINOETHYL PIPERAZINE	0.38%	4.35%			8.50%
NAPHTHALENE	0.53%	3.46%	3.70%	2.68%	8.31%
n-BUTANE	0.24%	2.82%	1.81%	4.11%	8.45%
n-BUTYL ACETATE	0.30%	4.51%	3.17%	1.04%	13.38%
n-BUTYL ACRYLATE	1.30%	2.52%	2.50%		14.43%
n-BUTYL BENZOATE	1.24%	4.57%			17.72%
n-BUTYL CHLORIDE	1.44%	5.52%	3.48%		11.99%
n-BUTYL ETHYL ETHER	1.07%	4.53%		4.06%	11.93%
n-BUTYL FORMATE	1.29%	5.59%	2.21%	0.98%	12.05%
n-BUTYL ISOCYANATE	1.48%	8.04%	2.82%		5.93%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
n-BUTYL MERCAPTAN	1.38%	5.12%	1.60%	0.81%	12.50%
n-BUTYL METHACRYLATE	3.75%	5.91%	2.57%		14.55%
n-BUTYL n-BUTYRATE	0.85%	5.96%	3.00%	0.65%	15.44%
n-BUTYL PROPIONATE	2.27%	5.45%	3.10%	1.26%	13.50%
n-BUTYL STEARATE	2.14%	0.90%	4.59%	7.37%	28.90%
n-BUTYL VALERATE	2.12%	5.35%		1.27%	16.10%
n-BUTYLAMINE	1.52%	3.92%	3.07%	7.69%	1.29%
n-BUTYLBENZENE	0.53%	4.36%	2.36%	2.04%	9.44%
n-BUTYLCYCLOHEXANE	5.67%	4.70%	6.16%	4.83%	15.24%
n-BUTYLCYCLOPENTANE	0.88%	5.54%	1.97%	0.55%	12.48%
n-BUTYLHYDROPEROXIDE	2.47%	1.49%	2.85%		3.25%
n-BUTYRIC ACID	0.41%	5.65%			17.25%
n-CROTYL ACETATE	1.52%	4.52%	3.79%		10.46%
n-DECANE	1.19%	4.51%	3.05%	0.30%	10.83%
n-DECYL FORMATE	2.08%	4.53%		3.19%	12.20%
n-DECYL MERCAPTAN	1.34%	7.22%	4.24%	0.93%	20.36%
n-DECYLAMINE	1.17%	4.75%	5.67%	2.86%	12.32%
n-DECYLBENZENE	1.76%	4.58%	4.14%	0.48%	20.77%
n-DECYLCYCLOHEXANE	0.83%	4.41%	7.76%	2.43%	22.60%
n-DODECANE	1.46%	4.79%	4.22%	2.22%	10.52%
n-DODECANOIC ACID	5.23%	4.15%	7.47%	8.38%	14.00%
n-DODECYLAMINE	3.89%	4.92%	8.21%	3.16%	16.09%
n-DODECYLBENZENE	1.96%	4.06%	3.23%	0.85%	24.17%
n-DOTRIACONTANE	1.56%	4.24%	3.53%	0.74%	9.91%
n-EICOSANE	2.48%	5.09%	3.68%	0.26%	10.23%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
NEOABIETIC ACID	2.07%	2.69%	5.43%		12.39%
NEOHEXANOIC ACID	2.67%	7.84%	3.49%	2.92%	12.88%
NEON	0.58%	0.49%	1.01%		2.26%
NEOPENTANE	0.17%	1.34%	1.52%	2.24%	9.86%
N-ETHYL-2-METHYLALLYLAMINE	1.31%	2.36%	2.75%	3.42%	4.31%
N-ETHYLANILINE	2.51%	5.87%	5.47%		7.04%
N-ETHYLMORPHOLINE	1.03%	3.43%	3.34%	6.11%	8.89%
n-HENEICOSANE	1.45%	5.18%	3.32%	0.70%	10.31%
n-HEPTACOSANE	2.85%	4.57%	3.33%	0.89%	9.59%
n-HEPTADECANE	3.11%	5.32%	4.67%	0.66%	11.35%
n-HEPTADECANOIC ACID	2.24%	5.23%		12.43%	18.03%
n-HEPTADECYLBENZENE	2.11%	4.29%	4.38%	1.46%	28.07%
n-HEPTANE	0.96%	4.57%	2.19%	2.62%	9.85%
n-HEPTANOIC ACID	4.43%	4.02%	1.95%		10.94%
n-HEPTYL ACETATE	1.22%	3.80%	4.71%	0.77%	17.63%
n-HEPTYL FORMATE	0.88%	4.57%	2.47%	2.45%	17.22%
n-HEPTYL MERCAPTAN	1.19%	5.19%	2.78%	1.03%	17.69%
n-HEPTYLAMINE	0.90%	4.43%	3.46%	3.46%	6.77%
n-HEPTYLBENZENE	3.07%	5.16%	4.76%	0.57%	17.67%
n-HEXACOSANE	2.15%	4.81%	3.34%	0.85%	10.42%
n-HEXADECANE	3.21%	5.04%	4.93%	0.68%	12.05%
n-HEXADECANOIC ACID	2.66%	4.41%		12.51%	16.09%
n-HEXADECYLBENZENE	3.50%	3.29%	4.41%	1.57%	28.22%
n-HEXANE	0.35%	4.23%	1.55%	2.42%	8.75%
n-HEXANOIC ACID	5.03%	6.38%			11.74%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
n-HEXATRIACONTANE	7.93%	3.53%	0.00%	0.012461	8.26%
n-HEXYL ACETATE	0.48%	4.82%	4.60%	0.83%	16.03%
n-HEXYL FORMATE	1.83%	6.16%	3.26%	3.37%	14.70%
n-HEXYL MERCAPTAN	0.67%	5.62%	2.94%	0.81%	16.06%
n-HEXYLAMINE	0.56%	4.51%	4.19%	4.33%	4.24%
n-HEXYLBENZENE	1.12%	5.62%	3.54%	2.08%	15.62%
NIACIN	1.53%	1.86%	5.74%		10.81%
NICKEL CARBONYL	3.79%	2.01%		5.24%	4.90%
NICOTINONITRILE	1.86%	9.31%	3.86%	9.90%	14.51%
NITRIC OXIDE	2.94%	3.73%	5.78%	31.60%	14.71%
NITROBENZENE	7.78%	4.63%	6.32%		8.81%
NITROETHANE	6.29%	4.30%	8.60%	8.84%	12.67%
NITROGEN	0.56%	0.43%	1.54%	4.03%	10.14%
NITROGEN TRIFLUORIDE	0.80%	1.95%	0.26%		11.48%
NITROMETHANE	4.71%	9.31%	8.34%	12.86%	24.85%
NITROSYL CHLORIDE	4.65%	0.54%	6.18%		7.57%
NITROUS OXIDE	2.16%	1.15%	2.49%	7.22%	9.56%
N-METHYL-2-PYRROLIDONE	0.86%	4.65%	6.77%		19.19%
N-METHYLACETAMIDE	1.65%	11.80%	4.34%		24.57%
N-METHYLANILINE	3.27%	1.48%	8.12%		8.16%
N-METHYLCYCLOHEXYLAMINE	1.05%	3.10%	3.11%		9.46%
N-METHYLFORMAMIDE	1.69%	27.76%	3.88%		37.85%
N-METHYLPYRROLIDINE	2.15%	2.96%	3.80%		8.89%
N-METHYLPYRROLE	4.59%	0.65%	4.44%	6.74%	9.82%
N-METHYLPYRROLIDINE	0.84%	2.73%	2.00%		8.23%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
N-NITROSODIETHANOLAMINE	2.12%	4.48%	5.31%		12.89%
N-NITROSODIMETHYLAMINE	2.73%	11.86%	4.56%	0.39%	22.25%
n-NONADECANE	2.96%	5.34%	5.44%	0.49%	10.97%
n-NONANE	1.45%	4.58%	3.05%	0.32%	10.77%
n-NONANOIC ACID	5.91%	3.06%	5.82%		12.42%
n-NONYL ACETATE	2.08%	2.74%	3.09%	0.83%	19.55%
n-NONYL FORMATE	1.96%	4.52%		2.94%	11.82%
n-NONYL MERCAPTAN	2.29%	5.18%	5.38%	1.34%	20.18%
n-NONYL n-UNDECYL PHTHALATE	2.34%	10.50%	5.36%		37.46%
n-NONYLAMINE	1.05%	3.85%	6.41%	2.86%	11.55%
n-OCTACOSANE	1.22%	4.56%	3.35%	0.99%	10.22%
n-OCTADECANE	3.10%	5.33%	4.16%	0.60%	10.74%
n-OCTADECYLBENZENE	1.92%	4.64%	4.32%	1.41%	28.75%
n-OCTANE	0.93%	4.24%	2.54%	0.70%	11.11%
n-OCTANOIC ACID	4.51%	4.66%	3.14%		10.52%
n-OCTYL ACETATE	1.31%	4.09%	5.06%	0.61%	18.33%
n-OCTYL FORMATE	4.15%	4.32%	4.55%	2.56%	18.35%
n-OCTYL MERCAPTAN	0.61%	5.66%	2.89%	0.87%	19.45%
n-OCTYLAMINE	0.65%	3.70%	5.69%	2.88%	9.29%
n-OCTYLBENZENE	1.65%	5.25%	4.23%	0.78%	18.95%
NONANAL	2.21%	3.22%	4.84%		8.43%
NONYLPHENOL	1.43%	5.33%	6.64%		13.29%
n-PENTACOSANE	1.68%	4.87%	3.39%	0.99%	9.66%
n-PENTADECANE	3.03%	5.30%	4.26%	0.71%	11.73%
n-PENTADECANOIC ACID	2.12%	5.15%		10.68%	15.84%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
n-PENTADECYL BENZENE	2.63%	3.49%	4.58%	1.23%	26.92%
n-PENTANE	0.07%	3.98%	1.24%	2.87%	8.33%
n-PENTANOIC ACID	2.71%	7.52%			13.90%
n-PENTASILANE	1.07%	2.48%	3.09%		7.24%
n-PENTYL ACETATE	0.59%	5.12%	4.52%	0.76%	15.22%
n-PENTYL FORMATE	5.22%	3.12%		1.89%	13.02%
n-PENTYL MERCAPTAN	0.89%	3.85%	2.23%	0.95%	14.98%
n-PENTYLAMINE	0.41%	4.41%	3.59%	4.43%	1.51%
n-PENTYLBENZENE	1.65%	5.96%		2.06%	11.44%
n-PENTYLCYCLOHEXANE	0.28%	4.62%	5.36%		10.51%
n-PROPYL ACETATE	1.27%	5.66%	2.40%	1.13%	11.21%
n-PROPYL ACRYLATE	1.57%	4.15%	3.05%		10.85%
n-PROPYL BENZOATE	1.64%	5.47%		1.52%	16.14%
n-PROPYL FORMATE	1.80%	5.08%	3.72%	4.32%	11.13%
n-PROPYL IODIDE	0.50%	6.20%	3.91%		10.14%
n-PROPYL ISOBUTYRATE	1.76%	3.38%	3.07%	3.00%	11.25%
n-PROPYL MERCAPTAN	1.39%	3.43%	1.76%	0.11%	11.29%
n-PROPYL METHACRYLATE	0.51%	4.19%	4.64%		13.86%
n-PROPYL n-BUTYRATE	2.61%	5.59%	4.06%	0.97%	15.91%
n-PROPYL PROPIONATE	1.28%	4.73%	4.04%	5.31%	12.93%
n-PROPYLAMINE	5.11%	3.97%	3.41%	8.59%	3.03%
n-PROPYLBENZENE	0.68%	3.88%	2.13%	1.71%	8.57%
n-PROPYLCYCLOHEXANE	4.18%	4.54%	4.07%	1.33%	14.03%
n-PROPYLCYCLOPENTANE	0.42%	5.43%	1.75%	2.53%	10.61%
n-TETRACOSANE	2.80%	4.99%	3.16%	0.82%	10.58%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
n-TETRADECANE	2.73%	5.28%	4.95%	0.75%	11.79%
n-TETRADECANOIC ACID	2.19%	4.83%		10.52%	16.70%
n-TETRADECYLAMINE	4.02%	4.82%		3.84%	18.38%
n-TETRADECYLBENZENE	2.24%	3.69%	4.43%	1.35%	26.50%
n-TETRASILANE	0.15%	2.11%	3.98%		6.79%
n-TRICOSANE	2.81%	5.08%	3.36%	0.87%	10.24%
n-TRIDECANE	2.14%	5.09%	4.33%	0.75%	11.37%
n-TRIDECANOIC ACID	3.42%	4.79%	8.80%	8.99%	14.82%
n-TRIDECYLBENZENE	1.23%	3.86%	4.59%	0.61%	24.87%
n-UNDECANE	1.43%	4.83%	4.12%	0.15%	10.96%
n-UNDECANOIC ACID	5.43%	4.22%		7.50%	13.41%
n-UNDECYLBENZENE	2.89%	4.13%	4.20%	0.48%	21.43%
o-ANISIDINE	1.58%	4.43%	5.41%		10.96%
o-CHLOROANILINE	3.15%	4.46%	5.97%		2.38%
o-CHLOROBENZOIC ACID	1.99%	5.95%			16.36%
o-CHLORONITROBENZENE	2.23%	4.06%		2.16%	1.90%
o-CHLOROPHENOL	6.18%	2.37%	9.28%		2.34%
o-CHLOROTOLUENE	0.75%	4.68%	2.03%		12.78%
o-CRESOL	0.74%	3.33%	3.85%	8.90%	20.60%
OCTADECAMETHYLOCTASILOXANE	5.52%	1.05%	5.40%		3.72%
OCTAFLUORO-2-BUTENE	1.21%	7.28%	2.81%	4.45%	12.61%
OCTAFLUOROCYCLOBUTANE	1.41%	1.63%	3.06%	1.68%	5.46%
OCTAFLUOROPROPANE	1.17%	2.46%			7.11%
OCTAHYDRO-PENTALENE-1-CARBOXYLIC ACID	0.42%	4.02%		10.36%	16.53%
OCTAMETHYLCYCLOTETRAILOXANE	3.70%	2.88%	6.42%		7.04%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
OCTAMETHYLTRISILOXANE	0.71%	2.92%	4.38%		7.63%
OCTANAL	1.78%	2.87%	3.94%		6.91%
o-CYMENE	2.52%	5.12%	2.71%		9.20%
o-DICHLOROBENZENE	4.73%	3.83%	4.05%	6.33%	16.46%
o-DIETHYLBENZENE	2.57%	4.80%	3.79%	2.42%	8.30%
o-ETHYLANILINE	2.11%	3.63%	3.14%		4.67%
o-ETHYLPHENOL	1.23%	0.98%	5.28%	6.13%	15.40%
o-ETHYLSTYRENE	1.33%	6.16%	3.59%		14.24%
o-ETHYLTOLUENE	1.46%	4.40%	2.18%	5.41%	10.22%
OLEIC ACID	4.94%	4.44%	4.35%		25.75%
o-METHYLSTYRENE	2.20%	4.39%	2.31%	5.02%	10.86%
o-NITROANISOLE	1.79%	5.42%	3.63%		13.05%
o-NITRODIPHENYLAMINE	2.06%	3.02%			10.75%
o-NITROTOLUENE	3.49%	3.74%	7.83%		0.21%
o-PHENYLENEDIAMINE	1.69%	3.63%	3.80%		11.61%
o-TERPHENYL	2.65%	0.24%	2.49%		0.68%
o-tert-BUTYLPHENOL	0.31%	2.91%	5.15%		9.02%
o-TOLUALDEHYDE	0.65%	5.26%			13.02%
o-TOLUIC ACID	1.94%	3.55%	4.74%		13.17%
o-TOLUIDINE	1.09%	2.58%	1.81%	4.52%	6.42%
OXAZOLE	1.43%	0.36%			3.30%
OXYGEN	0.42%	0.51%	1.53%	6.12%	10.58%
o-XYLENE	0.44%	4.04%	2.32%	2.99%	8.55%
OZONE	1.64%	7.24%	5.41%	12.09%	23.82%
p.alpha-DIMETHYLBENZYL ALCOHOL	1.64%	3.79%	4.53%		10.09%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
PALUSTRIC ACID	2.05%	1.76%	6.37%	25.17%	9.91%
p-AMINOAZOBENZENE	1.83%	3.33%	4.00%		10.95%
p-AMINODIPHENYL	1.46%	3.69%			10.09%
p-AMINODIPHENYLAMINE	2.14%	2.91%	3.66%		9.78%
PARALDEHYDE	1.53%	1.38%	3.60%	14.02%	12.97%
p-BROMOTOLUENE	1.87%	0.92%	2.70%		5.42%
p-CHLOROANILINE	1.13%	3.04%	3.37%		6.13%
p-CHLOROBENZOTRIFLUORIDE	1.40%	5.40%	2.89%		16.57%
p-CHLORONITROBENZENE	1.67%	4.97%	4.33%	2.39%	0.43%
p-CHLOROPHENOL	3.66%	1.39%	8.83%		4.72%
p-CHLOROTOLUENE	0.31%	3.62%	2.57%		12.11%
p-CRESOL	3.63%	3.59%	5.96%	6.19%	21.54%
p-CUMYLPHENOL	1.31%	1.78%	3.20%	3.98%	0.25%
p-CYMENE	0.59%	5.03%	3.18%	5.04%	10.48%
p-DICHLOROBENZENE	1.26%	2.55%	2.55%	3.69%	14.27%
p-DIETHYLBENZENE	0.56%	4.54%	3.05%	3.39%	11.04%
p-DIISOPROPYLBENZENE	4.16%	4.26%	3.88%		11.40%
p-DIISOPROPYLBENZENE HYDROPEROXIDE	2.50%	3.86%	4.31%	2.98%	12.13%
p-DIMETHYLAMINO BENZALDEHYDE	1.86%	9.89%	9.46%		31.94%
p-DIVINYLBENZENE	0.86%	4.25%	4.17%		12.53%
PENTACHLOROETHANE	0.58%	5.19%			14.94%
PENTACHLOROFLUOROETHANE	1.22%	2.78%	3.95%		14.72%
PENTAETHYLBENZENE	0.53%	5.46%		8.34%	10.86%
PENTAETHYLENE GLYCOL DIMETHYL ETHER	3.07%	2.24%	5.26%		27.25%
PENTAETHYLENE GLYCOL MONOMETHYL ETHER	3.16%	4.58%	5.43%		13.70%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
PENTAFLURO(TRIFLUOROMETHYL)SULFUR	0.85%	0.36%	3.06%		1.44%
PENTAFLUROETHANE	0.75%	2.57%	2.52%	8.03%	7.48%
PENTAFLUROETHYL METHYL ETHER	0.88%	4.34%	3.82%		10.77%
PENTAFLUROETHYL TRIFLUOROVINYL ETHER	1.51%	1.20%	3.47%		5.21%
PENTAFLUROPHENOL	1.63%	2.28%			6.92%
PENTAMETHYLBENZENE	1.22%	3.47%	3.79%	8.66%	9.65%
PENTANAL	5.56%	5.51%	4.55%		11.47%
PERCHLORYL FLUORIDE	0.48%	1.08%	1.41%	5.80%	7.54%
PERFLUROBUTANOIC ACID	3.55%	3.86%			13.54%
PERFLUROMETHYLCYCLOPENTANE	1.68%	2.47%	4.72%		9.18%
PERFLURO-n-DODECANE	1.56%	14.37%			23.66%
PERFLURO-n-HEPTANE	3.04%	3.51%	4.23%		5.95%
PERFLURO-n-HEXADECANE	1.67%	38.28%			38.69%
PERFLURO-n-HEXANE	2.21%	2.90%	4.29%		6.08%
PERFLURO-n-NONANE	1.39%	4.08%			12.84%
PERFLURO-n-OCTANE	1.43%	3.31%	8.25%		10.99%
PERFLURO-n-PENTANE	2.99%	3.65%	4.04%		8.48%
p-ETHYLPHENOL	4.55%	2.59%	2.98%	4.64%	8.82%
p-ETHYLSTYRENE	1.29%	4.50%	3.57%		17.15%
p-ETHYLTOLUENE	0.95%	2.39%	3.21%	4.78%	11.94%
PHENANTHRENE	1.01%	9.22%	5.10%	5.05%	24.51%
PHENETOLE	0.77%	4.46%	3.63%		14.10%
PHENOL	2.42%	2.44%	4.93%	9.04%	22.83%
PHENOTHIAZINE	1.84%	1.51%	4.53%		7.24%
PHENYL ISOCYANATE	3.09%	2.88%	7.86%		3.36%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
PHENYL MERCAPTAN	3.27%	2.38%	3.61%	3.56%	11.77%
PHENYLACETONITRILE	2.62%	7.01%	5.17%		24.54%
PHENYLHYDRAZINE	7.02%	3.28%			12.69%
PHENYLMETHYLDICHLOROSILANE	1.10%	1.82%	2.39%		13.63%
PHENYLTRICHLOROSILANE	0.79%	3.36%	3.24%		11.73%
PHOSGENE	0.70%	2.58%	1.80%	2.77%	5.68%
PHOSPHINE	3.35%	2.55%	3.77%	12.90%	18.15%
PHOSPHORUS PENTAFLUORIDE	1.34%	1.12%	3.07%		8.32%
PHOSPHORUS TRICHLORIDE	5.70%	0.84%	6.60%	5.53%	1.05%
PHOSPHORUS TRIFLUORIDE	1.63%	1.44%		5.76%	5.83%
PHTHALAN	0.87%	3.65%	3.85%		9.10%
PHTHALIC ACID	2.79%	1.78%	5.96%		11.18%
PHTHALIDE	5.27%	2.31%			4.87%
p-HYDROQUINONE	6.98%	3.67%			12.57%
p-HYDROXYBENZALDEHYDE	1.96%	5.93%	5.33%		6.90%
PIMARIC ACID	2.18%	2.51%	7.16%		12.74%
PIMELIC ACID	5.63%	1.30%			20.79%
PIPERAZINE	1.31%	0.24%	2.34%		3.25%
PIPERIDINE	2.72%	2.09%	1.59%	3.65%	1.98%
p-ISOPROPENYL PHENOL	3.08%	3.90%	5.80%		17.29%
p-MENTHANE HYDROPEROXIDE	2.33%	1.13%	3.99%		8.72%
p-METHYLSTYRENE	2.15%	0.35%	2.33%	2.00%	9.80%
p-NITROANILINE	1.82%	2.77%	1.44%		11.36%
p-NITROTOLUENE	2.95%	15.02%			21.26%
p-PHENETIDINE	1.49%	2.21%	4.52%		11.26%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
p-PHENYLENEDIAMINE	1.70%	3.52%	4.56%		12.23%
PROPADIENE	4.32%	1.90%	3.76%	5.00%	12.39%
PROPANAL	0.20%	4.76%	4.70%		15.36%
PROPANE	0.24%	2.39%	1.56%	5.48%	9.04%
PROPARGYL ALCOHOL	1.31%	3.83%			15.34%
PROPARGYL CHLORIDE	0.78%	7.31%	2.17%	8.26%	13.25%
PROPENYL CYCLOHEXENE	1.66%	4.77%	2.68%	3.77%	11.55%
PROPIONIC ACID	1.97%	5.96%			25.09%
PROPIONIC ANHYDRIDE	0.65%	3.02%	5.15%	3.34%	13.90%
PROPIONITRILE	4.11%	18.79%	8.51%		26.15%
PROPYL CHLORIDE	1.19%	4.66%	3.04%	5.50%	12.57%
PROPYLENE	1.11%	2.02%	1.88%	1.80%	7.79%
PROPYLENE GLYCOL 1-tert-BUTYL ETHER	1.59%	4.31%	4.06%		10.96%
PROPYLENE GLYCOL 2-tert-BUTYL ETHER	1.54%	3.90%	4.23%		10.94%
PROPYLENE GLYCOL alpha-METHYLBENZYL ETHER	1.10%	4.53%	4.86%	18.17%	12.54%
PROPYLENE GLYCOL ETHYL ETHER ACETATE	1.46%	4.88%	3.46%	30.76%	13.70%
PROPYLENE GLYCOL MONOALLYL ETHER	3.58%	4.52%	5.48%		10.81%
PROPYLENE GLYCOL MONOMETHYL ETHER	4.04%	6.35%	4.16%		16.35%
PROPYLENE GLYCOL MONOMETHYL ETHER ACETATE	3.71%	4.77%	2.69%	3.33%	11.07%
PROPYLENE GLYCOL n-BUTYL ETHER	3.03%	6.49%	4.07%		16.04%
PROPYLENE GLYCOL n-PROPYL ETHER	4.76%	5.35%			11.32%
PROPYLENEIMINE	5.44%	3.93%			10.74%
p-TERPHENYL	1.14%	1.07%	4.48%	1.11%	2.57%
p-tert-AMYLPHENOL	1.43%	2.88%	3.72%		10.18%
p-tert-BUTYL ETHYLBENZENE	1.71%	5.01%	2.53%	0.62%	11.34%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
p-tert-BUTYLCAATECHOL	1.52%	0.40%	3.93%		0.80%
p-tert-BUTYLPHENOL	1.53%	2.48%	6.74%		7.60%
p-tert-BUTYLSTYRENE	0.83%	5.55%	3.38%	0.88%	11.87%
p-tert-OCTYLPHENOL	1.55%	3.25%	4.19%		11.70%
p-TOLUALDEHYDE	0.35%	4.63%	4.14%		11.27%
p-TOLUIC ACID	3.27%	3.98%	7.01%		17.74%
p-TOLUIDINE	7.82%	3.28%		1.71%	11.81%
p-XYLENE	0.29%	3.67%	3.67%	3.55%	9.56%
PYRAZINE	2.56%	3.25%	3.31%		2.96%
PYRAZOLE	1.34%	6.36%	3.06%		9.94%
PYRENE	2.06%	15.01%	6.36%	4.22%	24.77%
PYRIDAZINE	1.89%	14.20%		1.79%	19.98%
PYRIDINE	1.37%	1.97%	1.93%	1.25%	5.53%
PYRIMIDINE	0.77%	3.82%		8.46%	1.14%
PYRROLE	2.83%	4.76%	2.79%	2.71%	1.30%
PYRROLIDINE	2.64%	2.66%	2.36%		1.05%
QUATERPHENYL	2.81%	5.46%	5.52%		15.29%
QUINALDINE	5.14%	4.01%	3.43%		8.50%
QUINOLINE	1.15%	2.29%	4.62%	2.96%	7.39%
QUINONE	1.43%	1.86%	3.39%	10.88%	1.44%
RADON	7.44%	0.24%			12.63%
RDX	2.48%	0.78%	5.88%	2.33%	7.26%
SACCHARIN	2.00%	0.75%	3.10%	2.48%	1.54%
SALICYLIC ACID	1.44%	1.15%	5.56%		8.13%
SALICYLIC ACID PHENYL ESTER	2.18%	5.01%	4.98%		13.06%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
sec-BUTENYL ACETATE	2.53%	3.85%	3.97%	6.75%	9.49%
sec-BUTYL ACETATE	3.18%	3.27%	3.75%	0.92%	10.14%
sec-BUTYL ACRYLATE	3.37%	3.72%	3.71%		9.40%
sec-BUTYL CHLORIDE	1.57%	4.44%	4.02%	3.41%	8.25%
sec-BUTYL FORMATE	2.83%	4.96%	2.63%	3.74%	9.18%
sec-BUTYL MERCAPTAN	1.24%	3.32%	1.98%	0.29%	9.66%
sec-BUTYLAMINE	1.35%	4.84%	2.67%	0.60%	0.06%
sec-BUTYLBENZENE	2.45%	4.63%	6.40%	3.62%	8.11%
sec-BUTYLCYCLOHEXANE	1.49%	5.05%	3.61%		16.62%
sec-BUTYL-tert-BUTYL ETHER	1.23%	2.25%	3.27%	1.59%	10.03%
SILANE	7.88%	5.10%			14.72%
SITOSTEROL	2.91%	11.56%	5.11%		26.94%
STIGMASTEROL	2.63%	10.80%	5.91%		26.62%
STYRENE	0.53%	3.29%	2.05%	1.24%	12.29%
STYRENE GLYCOL	1.89%	4.17%	4.76%		12.30%
SUBERIC ACID	7.33%	4.86%			19.67%
SUCCINIC ANHYDRIDE	5.57%	13.03%	10.07%		23.87%
SUCCINIMIDE	2.46%	10.12%			21.97%
SUCROSE	1.29%	9.28%	3.71%		22.83%
SULFOLANE	0.36%	4.64%	3.28%		30.77%
SULFUR DIOXIDE	3.25%	2.23%	1.96%	4.92%	8.52%
SULFUR HEXAFLUORIDE	1.83%	0.80%	2.39%		6.79%
SULFUR TRIOXIDE	12.28%	2.72%	11.23%		12.59%
SULFURYL CHLORIDE	5.33%	4.53%	3.88%		18.11%
SYRINGALDEHYDE	0.81%	2.35%			10.38%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
SYRINGOL	1.35%	3.27%	4.69%		10.68%
t-BUTYL ACETOACETATE	1.38%	3.52%	4.26%		9.86%
t-BUTYL HYDROPEROXIDE	2.88%	1.87%	3.87%		7.67%
TEREPHTHALDEHYDE	1.80%	7.31%	5.12%	1.42%	20.04%
TEREPHTHALIC ACID	2.77%	35.09%			31.77%
TEREPHTHALOYL CHLORIDE	1.06%	2.08%	4.85%		2.59%
TERPINOLENE	2.52%	4.31%	2.56%	0.60%	13.39%
tert-BUTYL ACETATE	3.76%	3.78%	5.43%	6.53%	7.21%
tert-BUTYL CHLORIDE	0.70%	1.01%	4.21%	1.78%	8.53%
tert-BUTYL ETHYL ETHER	1.38%	3.08%	3.44%		7.14%
tert-BUTYL FORMATE	1.12%	0.53%	2.64%	4.85%	10.18%
tert-BUTYL MERCAPTAN	1.59%	0.24%	2.90%	4.78%	8.44%
tert-BUTYL METHACRYLATE	2.72%	3.28%	4.49%		8.73%
tert-BUTYLAMINE	2.80%	3.81%	1.82%	10.29%	5.15%
tert-BUTYLBENZENE	4.15%	2.41%	4.70%	1.67%	8.91%
tert-BUTYLCYCLOHEXANE	2.10%	2.24%	5.43%		16.09%
tert-BUTYLFORMAMIDE	1.57%	3.94%	3.70%		16.98%
tert-DODECYL MERCAPTAN	1.50%	4.69%	3.70%	2.17%	12.06%
tert-NONYL MERCAPTAN	2.20%	5.58%	3.15%	2.52%	12.26%
tert-OCTYL MERCAPTAN	1.18%	4.24%	2.56%	0.28%	9.80%
TETRACHLOROETHYLENE	3.57%	3.47%	2.94%	2.07%	35.12%
TETRACHLOROSILANE	1.78%	2.69%	1.66%	4.18%	6.22%
TETRADECAMETHYLHEXASILOXANE	3.77%	4.75%	5.23%		12.01%
TETRADECANEDIOIC ACID	1.80%	4.26%			22.81%
TETRAETHYL LEAD	0.91%	9.56%	3.21%	2.31%	11.47%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
TETRAETHYL SILANE	1.10%	4.00%	2.74%	4.80%	4.25%
TETRAETHYLENE GLYCOL	1.09%	7.82%	4.60%		21.22%
TETRAETHYLENE GLYCOL DIMETHYL ETHER	2.10%	1.74%			24.83%
TETRAETHYLENE GLYCOL MONOETHYL ETHER	2.38%	2.28%	4.80%		9.67%
TETRAETHYLENE GLYCOL MONOMETHYL ETHER	2.42%	1.78%	4.89%		9.11%
TETRAETHYLENEPENTAMINE	3.14%	2.47%	4.87%		10.97%
TETRAFLUROETHYLENE	0.99%	2.25%	2.09%	0.68%	10.56%
TETRAFLUROHYDRAZINE	7.28%	2.37%		5.53%	2.42%
TETRAHYDROFURAN	0.67%	3.99%	2.28%	1.07%	13.20%
TETRAHYDROFURFURYL ALCOHOL	8.32%	7.79%			11.19%
TETRAHYDROPYRAN	0.75%	3.13%	2.72%		13.29%
TETRAHYDROTHIOPHENE	1.43%	5.78%	1.73%	2.58%	18.03%
TETRAMETHYLETHYLENEDIAMINE	1.30%	3.55%	2.88%	0.79%	9.60%
TETRAMETHYLSILANE	2.24%	2.29%	1.39%	1.48%	10.20%
TETRANITROMETHANE	7.07%	6.68%			3.69%
TETRAPHENYLETHYLENE	2.03%	19.27%	5.33%		28.72%
TETRAPHENYLMETHANE	2.08%	19.89%	6.23%	1.03%	28.74%
TETRYL	3.14%	1.50%	5.23%		10.47%
THIACYCLOPROPANE	0.26%	4.26%	1.48%		16.12%
THIAINDAN	0.77%	3.74%	3.82%		15.07%
THIOGLYCOLIC ACID	1.79%	4.62%			15.01%
THIONYL CHLORIDE	7.46%	11.94%	5.78%		45.09%
THIOPHENE	0.71%	2.13%	1.94%	3.80%	14.55%
THIOUREA	1.61%	1.32%	2.95%		6.42%
THYMOL	1.07%	3.78%			14.55%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
TIN(IV) CHLORIDE	1.16%	2.71%	3.49%	2.64%	9.05%
TITANIUM TETRACHLORIDE	6.04%	1.42%		21.07%	1.28%
TOLUENE	0.42%	4.26%	1.85%	1.32%	9.84%
trans,trans-2,4-HEXADIENE	0.72%	4.45%	3.16%	0.69%	13.59%
trans-1,2-DICHLOROETHYLENE	4.10%	1.45%	2.46%	1.49%	3.79%
trans-1,2-DIMETHYLCYCLOHEXANE	2.02%	4.92%	2.29%	1.55%	5.07%
trans-1,2-DIMETHYLCYCLOPENTANE	0.57%	2.07%	1.80%	5.22%	11.09%
trans-1,3,3,3-TETRAFLUOROPROPENE	1.46%	2.63%	5.11%	0.71%	7.54%
trans-1,3-DICHLOROPROPENE	3.16%	3.25%	4.44%	5.24%	10.66%
trans-1,3-DIMETHYLCYCLOHEXANE	3.17%	4.14%	3.12%	1.78%	5.38%
trans-1,3-DIMETHYLCYCLOPENTANE	0.50%	2.64%	1.93%	2.16%	11.04%
trans-1,3-HEXADIENE	0.56%	3.98%	3.47%		11.88%
trans-1,3-PENTADIENE	7.85%	2.90%	7.81%	11.10%	17.06%
trans-1,4-DIETHYLCYCLOHEXANE	1.70%	3.35%	3.37%		7.64%
trans-1,4-DIMETHYLCYCLOHEXANE	1.21%	3.09%	2.08%	0.72%	7.09%
trans-1,8-TERPIN	2.76%	0.63%	7.15%		7.21%
trans-1-PROPENYLBENZENE	1.41%	3.88%	2.82%	3.35%	15.15%
trans-2,2,4,4,6,6-PENTAMETHYL-3-HEPTENE	1.15%	5.08%	3.82%		12.75%
trans-2,n-HEXYL-DECAHYDRONAPHTHALENE	1.40%	7.25%	4.43%	7.37%	20.89%
trans-2-BUTENE	1.21%	2.61%	1.99%	5.94%	8.05%
trans-2-DECENE	1.71%	5.13%	3.50%	2.10%	12.22%
trans-2-DODECENE	1.94%	5.04%	3.91%	3.58%	11.55%
trans-2-HEPTENE	0.64%	5.30%	4.25%	1.43%	12.70%
trans-2-HEXENE	0.75%	5.10%	3.50%	3.85%	11.94%
trans-2-METHYL-1,3-PENTADIENE	1.80%	3.82%	3.67%		10.71%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
trans-2-METHYLCYCLOHEXANOL	1.04%	3.96%	3.09%	1.49%	5.36%
trans-2-NONENE	1.81%	5.42%	4.75%		12.59%
trans-2-OCTENE	0.22%	5.32%	5.72%	0.72%	12.77%
trans-2-PENTADECENE	1.68%	4.51%	4.87%		9.45%
trans-2-PENTENE	0.20%	3.68%	1.61%	4.25%	8.31%
trans-2-PHENYLBUTENE-2	1.36%	4.33%	3.15%		10.73%
trans-3,5-DIMETHOXYSTILBENE	0.48%	4.57%	5.46%		27.75%
trans-3-HEPTENE	0.38%	5.56%	3.55%	0.84%	11.36%
trans-3-HEXENE	1.69%	3.54%	1.74%	1.59%	10.31%
trans-3-METHYLCYCLOHEXANOL	1.82%	4.50%	3.97%	1.40%	6.48%
trans-3-OCTENE	0.58%	5.37%	3.08%	0.29%	9.57%
trans-4-METHYLCYCLOHEXANOL	1.93%	3.11%	3.96%	1.48%	7.02%
trans-4-OCTENE	0.87%	4.95%	2.88%	0.34%	9.49%
trans-CROTONIC ACID	3.00%	1.12%	5.94%		21.26%
trans-CROTONITRILE	1.76%	13.65%	6.93%		23.80%
trans-DECAHYDRONAPHTHALENE	0.37%	3.05%	2.80%	0.90%	9.53%
trans-STILBENE	4.91%	3.71%	3.41%		13.37%
TRIALLYLAMINE	0.53%	4.19%	3.45%	3.77%	10.22%
TRIAMYLAMINE	2.91%	4.32%	4.01%		14.58%
TRIBROMOMETHANE	2.59%	0.64%	3.12%	13.59%	1.43%
TRICAPRIN	2.98%	33.66%			43.08%
TRICAPRYLIN	2.58%	27.76%	6.60%		38.71%
TRICHLOROACETALDEHYDE	1.43%	3.51%	2.56%		7.79%
TRICHLOROACETIC ACID	3.34%	2.35%	3.98%		10.93%
TRICHLOROACETYL CHLORIDE	1.97%	1.43%	4.14%		2.79%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
TRICHLOROETHYLENE	2.32%	2.75%	1.80%	1.77%	11.31%
TRICHLOROFUOROMETHANE	0.30%	2.16%	0.77%	0.94%	7.25%
TRICHLOROSILANE	1.08%	2.92%	3.63%	8.31%	7.25%
TRIDECAFLUOROHEPTANOIC ACID	5.61%	1.81%			9.83%
TRIDECANAL	0.42%	2.35%	6.11%		8.71%
TRIETHYL ALUMINUM	3.86%	6.31%	5.09%		23.43%
TRIETHYL ESTER PHOSPHOROUS ACID	0.85%	1.74%	2.77%		0.42%
TRIETHYL GALLIUM	0.77%	4.99%		26.05%	14.16%
TRIETHYL ORTHOFORMATE	0.70%	2.28%	4.86%		10.38%
TRIETHYLAMINE	0.75%	3.99%	3.04%	2.36%	9.99%
TRIETHYLENE GLYCOL BIS(2-ETHYLHEXANOATE)	2.66%	8.56%	5.43%		27.90%
TRIETHYLENE GLYCOL DIMETHYL ETHER	2.45%	1.31%	3.85%		22.47%
TRIETHYLENEDIAMINE	0.99%	1.36%	4.13%		8.11%
TRIETHYLENETETRAMINE	2.02%	2.62%	4.46%		10.55%
TRIFLUOROACETIC ACID	0.53%	32.54%		1.61%	69.53%
TRIFLUOROIODOMETHANE	0.42%	0.52%	2.77%		10.48%
TRIFLUOROMETHANE	0.35%	4.47%	2.56%	7.65%	11.51%
TRIFLUOROMETHYL TRIFLUOROVINYL ETHER	1.24%	1.40%	3.11%		5.44%
TRIISOBUTYL ALUMINUM	0.78%	4.50%			11.48%
TRIMETHYL BORATE	1.03%	5.94%			34.36%
TRIMETHYL SILANE	0.74%	2.09%	1.61%		7.74%
TRIMETHYL SILANOL	6.48%	1.23%			4.25%
TRIMETHYLALUMINUM	8.30%	5.29%	8.60%		33.26%
TRIMETHYLAMINE	0.96%	2.78%	3.32%	2.31%	2.93%
TRIMETHYLCHLOROSILANE	0.30%	1.03%	1.78%	4.07%	4.49%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
TRIMETHYLENE SULFIDE	1.59%	6.20%	2.22%	0.43%	11.74%
TRIMETHYLGALLIUM	10.11%	6.21%	9.23%	0.50%	42.70%
TRIMETHYLOLPROPANE	6.58%	0.47%			9.37%
TRI-n-BUTYL BORATE	0.60%	4.99%	1.58%		10.49%
TRI-n-BUTYL PHOSPHATE	1.01%	4.52%			15.62%
TRI-n-BUTYLAMINE	1.90%	6.03%	3.92%		13.54%
TRI-n-OCTYLAMINE	2.10%	3.11%			28.70%
TRIOXANE	1.20%	2.56%	4.31%	5.52%	10.20%
TRIPHENYLENE	0.47%	4.36%	5.81%		13.84%
TRIPHENYLETHYLENE	1.73%	4.63%	3.80%	1.13%	14.64%
TRIPHENYLMETHANE	2.43%	5.32%	3.94%	9.42%	19.65%
TRIPROPYLAMINE	3.06%	6.29%			6.56%
TRIPROPYLENE GLYCOL MONOETHYL ETHER	3.15%	1.75%		16.79%	11.26%
TRIPROPYLENE GLYCOL MONOMETHYL ETHER	2.27%	1.66%		0.69%	10.24%
TRIS(2-METHOXYETHOXY)VINYLSILANE	1.53%	6.30%	10.02%		10.68%
TRISILANE	1.86%	1.68%			5.84%
UNDECANAL	1.85%	2.67%	4.72%		9.67%
UNDECYL MERCAPTAN	1.95%	6.74%	3.24%	0.57%	21.56%
UNDECYLAMINE	4.43%	5.42%		3.15%	14.08%
VALERONITRILE	3.16%	4.90%	8.73%		15.17%
VANADIUM OXYTRICHLORIDE	1.79%	4.38%			37.56%
VANADIUM TETRACHLORIDE	2.05%	0.92%			14.69%
VANILLIC ACID	2.12%	2.34%	6.86%		11.96%
VANILLIN	1.86%	2.79%	4.32%		10.74%
VINYL ACETATE	1.89%	6.25%	2.57%	8.34%	12.89%

Name	MAPE on P^{sat}	MAPE on ρ_{liq}^{sat}	MAPE on $\Delta_{vap}H$	MAPE on $C_{P,liq}^{sat}$	MAPE on V_C
VINYL CHLORIDE	4.35%	2.66%	6.70%		7.06%
VINYL FLUORIDE	3.68%	3.72%		1.78%	8.30%
VINYL FORMATE	4.45%	3.26%	2.85%		9.07%
VINYL PIVALATE	1.45%	3.33%	2.78%		8.71%
VINYL PROPIONATE	1.42%	4.07%	2.86%		9.53%
VINYLACETONITRILE	1.30%	16.40%	6.47%	6.34%	34.47%
VINYLACETYLENE	8.35%	1.94%	6.57%	1.42%	11.82%
VINYLCYCLOHEXANE	1.76%	4.58%	3.02%	6.49%	9.20%
VINYLETHYLENE CARBONATE	2.75%	7.58%	4.19%	3.83%	27.71%
VINYLNORBORNENE	1.26%	4.17%	2.55%		12.80%
VINYLTRICHLOROSILANE	0.92%	6.04%	2.68%		2.27%
VINYLTRIMETHOXYSILANE	1.61%	4.58%		11.10%	12.35%
WATER	2.34%	7.89%	3.81%	24.45%	21.49%
XENON	2.00%	0.38%	1.59%		10.25%

Appendix A8 – Numerical values of the experimental data included in the benchmark database with the corresponding references and experimental data visualization.

A light MS Excel file including only numerical values of the experimental data and corresponding references is provided free of charge in the following link:

https://pubs.acs.org/doi/suppl/10.1021/acs.iecr.0c01734/suppl_file/ie0c01734_si_001.xls

Additionally, nine large-size MS Excel files for each of the Binary Association Codes (BAC), including numerical values of the experimental data, corresponding reference and data visualization are provided free of charge in the following links:

- BAC₁
https://pubs.acs.org/doi/suppl/10.1021/acs.iecr.0c01734/suppl_file/ie0c01734_si_002.xlsx2.
- BAC₂
https://pubs.acs.org/doi/suppl/10.1021/acs.iecr.0c01734/suppl_file/ie0c01734_si_003.xlsx
- BAC₃
https://pubs.acs.org/doi/suppl/10.1021/acs.iecr.0c01734/suppl_file/ie0c01734_si_004.xlsx4.ie0c01734_si_005.xlsx
- (BAC₄)
https://pubs.acs.org/doi/suppl/10.1021/acs.iecr.0c01734/suppl_file/ie0c01734_si_005.xlsx
- BAC₅
https://pubs.acs.org/doi/suppl/10.1021/acs.iecr.0c01734/suppl_file/ie0c01734_si_006.xlsx
- BAC₆
https://pubs.acs.org/doi/suppl/10.1021/acs.iecr.0c01734/suppl_file/ie0c01734_si_007.xlsx
- BAC₇
https://pubs.acs.org/doi/suppl/10.1021/acs.iecr.0c01734/suppl_file/ie0c01734_si_008.xlsx
- BAC₈
https://pubs.acs.org/doi/suppl/10.1021/acs.iecr.0c01734/suppl_file/ie0c01734_si_009.xlsx
- BAC₉

https://pubs.acs.org/doi/suppl/10.1021/acs.iecr.0c01734/suppl_file/ie0c01734_si_010.xlsx

Appendix A9 – 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 free of charge on Table S1 of the file found in the following link:

https://pubs.acs.org/doi/suppl/10.1021/acs.iecr.0c01734/suppl_file/ie0c01734_si_011.pdf

Appendix A10 – System-by-system analysis of the {PR EoS + classical mixing rules with a I-dependent k_{ij} } performances to correlate the data included in the proposed database.

Provided free of charge in Table S2 of the file found in the following link:

https://pubs.acs.org/doi/suppl/10.1021/acs.iecr.0c01734/suppl_file/ie0c01734_si_011.pdf

Bibliography

- (1) European Federation of Chemical Engineers. Thermodynamics and Transport Properties Working Party.
- (2) 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* (22), 11131–11141. <https://doi.org/10.1021/ie101231b>.
- (3) Kontogeorgis, G. M.; Dohrn, R.; Economou, I. G.; de Hemptinne, J.-C.; ten Kate, A.; Kuitunen, S.; Mooijer, M.; Žilnik, L. F.; Vesovic, V. Industrial Requirements for Thermodynamic and Transport Properties: 2020. *Ind. Eng. Chem. Res.* **2021**, *60* (13), 4987–5013. <https://doi.org/10.1021/acs.iecr.0c05356>.
- (4) Chapman, W. G. Theory and Simulation of Associating Liquid Mixtures, Cornell University, 1988.
- (5) Chapman, W. G.; Jackson, G.; Gubbins, K. E. Phase Equilibria of Associating Fluids: Chain Molecules with Multiple Bonding Sites. *Molecular Physics* **1988**, *65* (5), 1057–1079. <https://doi.org/10.1080/00268978800101601>.
- (6) Chapman, W. G.; Gubbins, K. E.; Jackson, G.; Radosz, M. New Reference Equation of State for Associating Liquids. *Ind. Eng. Chem. Res.* **1990**, *29* (8), 1709–1721. <https://doi.org/10.1021/ie00104a021>.
- (7) Chapman, W. G.; Gubbins, K. E.; Jackson, G.; Radosz, M. SAFT: Equation-of-State Solution Model for Associating Fluids. *Fluid Phase Equilibria* **1989**, *52*, 31–38. [https://doi.org/10.1016/0378-3812\(89\)80308-5](https://doi.org/10.1016/0378-3812(89)80308-5).
- (8) 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. *The Journal of Chemical Physics* **1997**, *106* (10), 4168–4186. <https://doi.org/10.1063/1.473101>.
- (9) FELIPE J. BLAS and LOURDES F. VEGA. Thermodynamic Behaviour of Homonuclear and Heteronuclear Lennard-Jones Chains with Association Sites from Simulation and Theory. *Molecular Physics* **1997**, *92* (1), 135–150. <https://doi.org/10.1080/002689797170707>.
- (10) Nguyen-Huynh, D.; Passarello, J.-P.; Tobaly, P.; de Hemptinne, J.-C. Modeling Phase Equilibria of Asymmetric Mixtures Using a Group-Contribution SAFT (GC-SAFT) with a k_{ij} Correlation Method Based on London's Theory. 1. Application to CO₂ + n -Alkane, Methane + n -Alkane, and Ethane + n -Alkane Systems. *Ind. Eng. Chem. Res.* **2008**, *47* (22), 8847–8858. <https://doi.org/10.1021/ie071643r>.
- (11) Nguyen-Huynh, D.; Tran, T. K. S.; Tamouza, S.; Passarello, J.-P.; Tobaly, P.; de Hemptinne, J.-C. Modeling Phase Equilibria of Asymmetric Mixtures Using a Group-Contribution SAFT (GC-SAFT) with a k_{ij} Correlation Method Based on London's Theory. 2. Application to Binary Mixtures Containing Aromatic Hydrocarbons, n -Alkanes, CO₂, N₂, and H₂S. *Ind. Eng. Chem. Res.* **2008**, *47* (22), 8859–8868. <https://doi.org/10.1021/ie071644j>.
- (12) 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* (4), 1244–1260. <https://doi.org/10.1021/ie0003887>.
- (13) Gross, J.; Sadowski, G. Application of the Perturbed-Chain SAFT Equation of State to Associating Systems. *Ind. Eng. Chem. Res.* **2002**, *41* (22), 5510–5515. <https://doi.org/10.1021/ie010954d>.
- (14) Lafitte, T.; Apostolakou, A.; Avendaño, C.; Galindo, A.; Adjiman, C. S.; Müller, E. A.; Jackson, G. Accurate Statistical Associating Fluid Theory for Chain Molecules Formed from Mie Segments. *The Journal of Chemical Physics* **2013**, *139* (15), 154504. <https://doi.org/10.1063/1.4819786>.

- (15) Riedemann, A.; Walker, P.; Yew, P.; Putalapattu, R.; Ahaslam62; Ames, A.; Sakse; TJP-Karpowski. *Ypaul21/Clapeyron.Jl: V0.3.1*; Zenodo, 2022. <https://doi.org/10.5281/ZENODO.5968475>.
- (16) Baird, Z. *PC-SAFT*; 2021.
- (17) Polishuk, I. Standardized Critical Point-Based Numerical Solution of Statistical Association Fluid Theory Parameters: The Perturbed Chain-Statistical Association Fluid Theory Equation of State Revisited. *Ind. Eng. Chem. Res.* **2014**, *53* (36), 14127–14141. <https://doi.org/10.1021/ie502633e>.
- (18) Moine, E.; Piña-Martinez, A.; Jaubert, J.-N.; Sirjean, B.; Privat, R. *I*-PC-SAFT: An Industrialized 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* (45), 20815–20827. <https://doi.org/10.1021/acs.iecr.9b04660>.
- (19) Voutsas, E.; Louli, V.; Boukouvalas, C.; Magoulas, K.; Tassios, D. Thermodynamic Property Calculations with the Universal Mixing Rule for EoS/GE Models: Results with the Peng–Robinson EoS and a UNIFAC Model. *Fluid Phase Equilibria* **2006**, *241* (1–2), 216–228. <https://doi.org/10.1016/j.fluid.2005.12.028>.
- (20) 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* (19), 6238–6246. <https://doi.org/10.1021/ie049580p>.
- (21) Jaubert, J.-N.; Le Guennec, Y.; Piña-Martinez, A.; Ramirez-Velez, N.; Lasala, S.; Schmid, B.; Nikolaidis, I. K.; Economou, I. G.; Privat, R. Benchmark Database Containing Binary-System-High-Quality-Certified Data for Cross-Comparing Thermodynamic Models and Assessing Their Accuracy. *Ind. Eng. Chem. Res.* **2020**, *59* (33), 14981–15027. <https://doi.org/10.1021/acs.iecr.0c01734>.
- (22) Poling, B. E.; Prausnitz, J. M.; O’Connell, J. P. *The Properties of Gases and Liquids*, 5th ed.; McGraw-Hill: New York, 2001.
- (23) Connecticut Academy of Arts and Sciences. *Transactions of the Connecticut Academy of Arts and Sciences*; Published by the Academy,; New Haven :, 1874; Vol. v.3 (1874-1878).
- (24) Jaubert, J.-N., Privat Romain. *Thermodynamic Models for Chemical Engineering: Design, Develop, Analyse and Optimize*; 2021.
- (25) Elliott, J. R.; Lira, C. T. *Introductory Chemical Engineering Thermodynamics*, 2nd ed.; Prentice Hall: Upper Saddle River, NJ, 2012.
- (26) Kontogeorgis, G. M.; Folas, G. K. *Thermodynamic Models for Industrial Applications: From Classical and Advanced Mixing Rules to Association Theories*; Wiley: Chichester, U.K, 2010.
- (27) Span, R.; Wagner, W. A New Equation of State for Carbon Dioxide Covering the Fluid Region from the Triple-Point Temperature to 1100 K at Pressures up to 800 MPa. *Journal of Physical and Chemical Reference Data* **1996**, *25* (6), 1509–1596. <https://doi.org/10.1063/1.555991>.
- (28) *The GERG-2004 Wide-Range Equation of State for Natural Gases and Other Mixtures*, Als Ms. gedr.; Kunz, O., European Gas Research Group, Eds.; Fortschritt-Berichte VDI Reihe 6, Energietechnik; VDI-Verl: Düsseldorf, 2007.
- (29) Kunz, O.; Wagner, W. The GERG-2008 Wide-Range Equation of State for Natural Gases and Other Mixtures: An Expansion of GERG-2004. *J. Chem. Eng. Data* **2012**, *57* (11), 3032–3091. <https://doi.org/10.1021/je300655b>.
- (30) Waals, J. D. van der; Rowlinson, J. S. *On the Continuity of the Gaseous and Liquid States*; Studies in statistical mechanics; North-Holland ; Sole distributors for the U.S.A.

and Canada, Elsevier Science Pub. Co: Amsterdam ; New York : New York, N.Y., U.S.A, 1988.

- (31) Piña-Martinez, A.; Privat, R.; Lasala, S.; Soave, G.; Jaubert, J.-N. Search for the Optimal Expression of the Volumetric Dependence of the Attractive Contribution in Cubic Equations of State. *Fluid Phase Equilibria* **2020**, *522*, 112750. <https://doi.org/10.1016/j.fluid.2020.112750>.
- (32) 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 Equilibria* **2016**, *429*, 301–312. <https://doi.org/10.1016/j.fluid.2016.09.003>.
- (33) Soave, G. Equilibrium Constants from a Modified Redlich-Kwong Equation of State. *Chemical Engineering Science* **1972**, *27* (6), 1197–1203. [https://doi.org/10.1016/0009-2509\(72\)80096-4](https://doi.org/10.1016/0009-2509(72)80096-4).
- (34) Peng, D.-Y.; Robinson, D. B. A New Two-Constant Equation of State. *Ind. Eng. Chem. Fund.* **1976**, *15* (1), 59–64. <https://doi.org/10.1021/i160057a011>.
- (35) Le Guennec, Y.; Lasala, S.; Privat, R.; Jaubert, J.-N. A Consistency Test for α -Functions of Cubic Equations of State. *Fluid Phase Equilibria* **2016**, *427*, 513–538. <https://doi.org/10.1016/j.fluid.2016.07.026>.
- (36) Trebble, M. A.; Bishnoi, P. R. Development of a New Four-Parameter Cubic Equation of State. *Fluid Phase Equilibria* **1987**, *35* (1–3), 1–18. [https://doi.org/10.1016/0378-3812\(87\)80001-8](https://doi.org/10.1016/0378-3812(87)80001-8).
- (37) Melhem, G. A.; Saini, R.; Goodwin, B. M. A Modified Peng-Robinson Equation of State. *Fluid Phase Equilibria* **1989**, *47* (2–3), 189–237. [https://doi.org/10.1016/0378-3812\(89\)80176-1](https://doi.org/10.1016/0378-3812(89)80176-1).
- (38) Twu, C. H. A Modified Redlich-Kwong Equation of State for Highly Polar, Supercritical Systems.; 1988; pp 148–169.
- (39) Twu, C. H.; Bluck, D.; Cunningham, J. R.; Coon, J. E. A Cubic Equation of State with a New Alpha Function and a New Mixing Rule. *Fluid Phase Equilibria* **1991**, *69*, 33–50. [https://doi.org/10.1016/0378-3812\(91\)90024-2](https://doi.org/10.1016/0378-3812(91)90024-2).
- (40) Privat, R.; Visconte, M.; Zazoua-Khames, A.; Jaubert, J.-N.; Gani, R. Analysis and Prediction of the Alpha-Function Parameters Used in Cubic Equations of State. *Chemical Engineering Science* **2015**, *126*, 584–603. <https://doi.org/10.1016/j.ces.2014.12.040>.
- (41) Jaubert, J.-N.; Privat, R.; Le Guennec, Y.; Coniglio, L. Note on the Properties Altered by Application of a Pénélox–Type Volume Translation to an Equation of State. *Fluid Phase Equilibria* **2016**, *419*, 88–95. <https://doi.org/10.1016/j.fluid.2016.03.012>.
- (42) Pénélox, A.; Rauzy, E.; Fréze, R. A Consistent Correction for Redlich-Kwong-Soave Volumes. *Fluid Phase Equilibria* **1982**, *8* (1), 7–23. [https://doi.org/10.1016/0378-3812\(82\)80002-2](https://doi.org/10.1016/0378-3812(82)80002-2).
- (43) Pina-Martinez, A.; Privat, R.; Jaubert, J.-N. Use of 300,000 Experimental Data over 1800 Pure Fluids to Assess the Performance of 4 Cubic EoS: SRK, PR, Tc-RK, Tc-PR. *AIChE J.* <https://doi.org/under review>.
- (44) *REFPROP*; National Institute of Standards and Technology: United States of America.
- (45) Huang, S. H.; Radosz, M. Equation of State for Small, Large, Polydisperse, and Associating Molecules. *Ind. Eng. Chem. Res.* **1990**, *29* (11), 2284–2294. <https://doi.org/10.1021/ie00107a014>.
- (46) Huang, S. H.; Radosz, M. Equation of State for Small, Large, Polydisperse, and Associating Molecules: Extension to Fluid Mixtures. *Ind. Eng. Chem. Res.* **1991**, *30* (8), 1994–2005. <https://doi.org/10.1021/ie00056a050>.

- (47) Wertheim, M. S. Fluids with Highly Directional Attractive Forces. I. Statistical Thermodynamics. *J Stat Phys* **1984**, 35 (1–2), 19–34. <https://doi.org/10.1007/BF01017362>.
- (48) Wertheim, M. S. Fluids with Highly Directional Attractive Forces. II. Thermodynamic Perturbation Theory and Integral Equations. *J Stat Phys* **1984**, 35 (1–2), 35–47. <https://doi.org/10.1007/BF01017363>.
- (49) Wertheim, M. S. Fluids with Highly Directional Attractive Forces. III. Multiple Attraction Sites. *J Stat Phys* **1986**, 42 (3–4), 459–476. <https://doi.org/10.1007/BF01127721>.
- (50) Carnahan, N. F.; Starling, K. E. Equation of State for Nonattracting Rigid Spheres. *The Journal of Chemical Physics* **1969**, 51 (2), 635–636. <https://doi.org/10.1063/1.1672048>.
- (51) Carnahan, N. F.; Starling, K. E. Thermodynamic Properties of a Rigid-Sphere Fluid. *The Journal of Chemical Physics* **1970**, 53 (2), 600–603. <https://doi.org/10.1063/1.1674033>.
- (52) Boublik, T. Hard-Sphere Equation of State. *The Journal of Chemical Physics* **1970**, 53 (1), 471–472. <https://doi.org/10.1063/1.1673824>.
- (53) Mansoori, G. A.; Carnahan, N. F.; Starling, K. E.; Leland, T. W. Equilibrium Thermodynamic Properties of the Mixture of Hard Spheres. *The Journal of Chemical Physics* **1971**, 54 (4), 1523–1525. <https://doi.org/10.1063/1.1675048>.
- (54) Chen, S. S.; Kreglewski, A. Applications of the Augmented van Der Waals Theory of Fluids.: I. Pure Fluids. *Berichte der Bunsengesellschaft für physikalische Chemie* **1977**, 81 (10), 1048–1052. <https://doi.org/10.1002/bbpc.19770811037>.
- (55) Lafitte, T.; Bessieres, D.; Piñeiro, M. M.; Daridon, J.-L. Simultaneous Estimation of Phase Behavior and Second-Derivative Properties Using the Statistical Associating Fluid Theory with Variable Range Approach. *The Journal of Chemical Physics* **2006**, 124 (2), 024509. <https://doi.org/10.1063/1.2140276>.
- (56) Barker, J. A.; Henderson, D. Perturbation Theory and Equation of State for Fluids. II. A Successful Theory of Liquids. *The Journal of Chemical Physics* **1967**, 47 (11), 4714–4721. <https://doi.org/10.1063/1.1701689>.
- (57) Johnson, J. K.; Zollweg, J. A.; Gubbins, K. E. The Lennard-Jones Equation of State Revisited. *Molecular Physics* **1993**, 78 (3), 591–618. <https://doi.org/10.1080/00268979300100411>.
- (58) von Solms, N.; Michelsen, M. L.; Kontogeorgis, G. M. Computational and Physical Performance of a Modified PC-SAFT Equation of State for Highly Asymmetric and Associating Mixtures. *Ind. Eng. Chem. Res.* **2003**, 42 (5), 1098–1105. <https://doi.org/10.1021/ie020753p>.
- (59) Jog, P. K.; Chapman, W. G. Application of Wertheim’s Thermodynamic Perturbation Theory to Dipolar Hard Sphere Chains. *Molecular Physics* **1999**, 97 (3), 307–319. <https://doi.org/10.1080/00268979909482832>.
- (60) Tumakaka, F.; Gross, J.; Sadowski, G. Thermodynamic Modeling of Complex Systems Using PC-SAFT. *Fluid Phase Equilibria* **2005**, 228–229, 89–98. <https://doi.org/10.1016/j.fluid.2004.09.037>.
- (61) Ji, X.; Held, C.; Sadowski, G. Modeling Imidazolium-Based Ionic Liquids with EPC-SAFT. *Fluid Phase Equilibria* **2012**, 335, 64–73. <https://doi.org/10.1016/j.fluid.2012.05.029>.
- (62) Cameretti, L. F.; Sadowski, G.; Mollerup, J. M. Modeling of Aqueous Electrolyte Solutions with Perturbed-Chain Statistical Associated Fluid Theory. *Ind. Eng. Chem. Res.* **2005**, 44 (9), 3355–3362. <https://doi.org/10.1021/ie0488142>.
- (63) Gani, R. Group Contribution-Based Property Estimation Methods: Advances and Perspectives. *Current Opinion in Chemical Engineering* **2019**, 23, 184–196. <https://doi.org/10.1016/j.coche.2019.04.007>.

- (64) Tamouza, S.; Passarello, J.-P.; Tobaly, P.; de Hemptinne, J.-C. Group Contribution Method with SAFT EOS Applied to Vapor Liquid Equilibria of Various Hydrocarbon Series. *Fluid Phase Equilibria* **2004**, *222–223*, 67–76. <https://doi.org/10.1016/j.fluid.2004.06.038>.
- (65) Tamouza, S.; Passarello, J.-P.; Tobaly, P.; de Hemptinne, J.-C. Application to Binary Mixtures of a Group Contribution SAFT EOS (GC-SAFT). *Fluid Phase Equilibria* **2005**, *228–229*, 409–419. <https://doi.org/10.1016/j.fluid.2004.10.003>.
- (66) *PRO/II Process Engineering*; AVEVA.
- (67) *ProSimPlus*; ProSim.
- (68) Nguyen, T.-B.; de Hemptinne, J.-C.; Creton, B.; Kontogeorgis, G. M. GC-PPC-SAFT Equation of State for VLE and LLE of Hydrocarbons and Oxygenated Compounds. Sensitivity Analysis. *Ind. Eng. Chem. Res.* **2013**, *52* (21), 7014–7029. <https://doi.org/10.1021/ie3028069>.
- (69) Lafitte, T.; Piñeiro, M. M.; Daridon, J.-L.; Bessières, D. A Comprehensive Description of Chemical Association Effects on Second Derivative Properties of Alcohols through a SAFT-VR Approach. *J. Phys. Chem. B* **2007**, *111* (13), 3447–3461. <https://doi.org/10.1021/jp0682208>.
- (70) Postnikov, E. B.; Goncharov, A. L.; Cohen, N.; Polishuk, I. Estimating the Liquid Properties of 1-Alkanols from C5 to C12 by FT-EoS and CP-PC-SAFT: Simplicity versus Complexity. *The Journal of Supercritical Fluids* **2015**, *104*, 193–203. <https://doi.org/10.1016/j.supflu.2015.06.007>.
- (71) Dufal, S.; Lafitte, T.; Galindo, A.; Jackson, G.; Haslam, A. J. Developing Intermolecular-potential Models for Use with the SAFT - VR M Ie Equation of State. *AIChE J.* **2015**, *61* (9), 2891–2912. <https://doi.org/10.1002/aic.14808>.
- (72) Liang, X.; Maribo-Mogensen, B.; Thomsen, K.; Yan, W.; Kontogeorgis, G. M. Approach to Improve Speed of Sound Calculation within PC-SAFT Framework. *Ind. Eng. Chem. Res.* **2012**, *51* (45), 14903–14914. <https://doi.org/10.1021/ie3018127>.
- (73) Liang, X.; Thomsen, K.; Yan, W.; Kontogeorgis, G. M. Prediction of the Vapor–Liquid Equilibria and Speed of Sound in Binary Systems of 1-Alkanols and n-Alkanes with the Simplified PC-SAFT Equation of State. *Fluid Phase Equilibria* **2013**, *360*, 222–232. <https://doi.org/10.1016/j.fluid.2013.09.037>.
- (74) Pakraves, A.; Zarei, F.; Zarei, H. PpT Parameterization of SAFT Equation of State: Developing a New Parameterization Method for Equations of State. *Fluid Phase Equilibria* **2021**, *538*, 113024. <https://doi.org/10.1016/j.fluid.2021.113024>.
- (75) McCabe, C.; Kiselev, S. B. Application of Crossover Theory to the SAFT-VR Equation of State: SAFT-VRX for Pure Fluids. *Ind. Eng. Chem. Res.* **2004**, *43* (11), 2839–2851. <https://doi.org/10.1021/ie034288n>.
- (76) Eriksen, D. K.; Lazarou, G.; Galindo, A.; Jackson, G.; Adjiman, C. S.; Haslam, A. J. Development of Intermolecular Potential Models for Electrolyte Solutions Using an Electrolyte SAFT-VR Mie Equation of State. *Molecular Physics* **2016**, *114* (18), 2724–2749. <https://doi.org/10.1080/00268976.2016.1236221>.
- (77) Müller, E. A.; Mejía, A. Extension of the SAFT-VR Mie EoS To Model Homonuclear Rings and Its Parametrization Based on the Principle of Corresponding States. *Langmuir* **2017**, *33* (42), 11518–11529. <https://doi.org/10.1021/acs.langmuir.7b00976>.
- (78) Crippwell, J. T.; Schwarz, C. E.; Burger, A. J. SAFT-VR-Mie with an Incorporated Polar Term for Accurate Holistic Prediction of the Thermodynamic Properties of Polar Components. *Fluid Phase Equilibria* **2018**, *455*, 24–42. <https://doi.org/10.1016/j.fluid.2017.09.027>.
- (79) Lymperiadis, A.; Adjiman, C. S.; Galindo, A.; Jackson, G. A Group Contribution Method for Associating Chain Molecules Based on the Statistical Associating Fluid Theory

- (SAFT- γ). *The Journal of Chemical Physics* **2007**, *127* (23), 234903. <https://doi.org/10.1063/1.2813894>.
- (80) Perdomo-Hurtado, L.; Valadez-Pérez, N. E.; Millan-Malo, B.; Castañeda-Priego, R. Generalized Equation of State for Fluids: From Molecular Liquids to Colloidal Dispersions. *J. Chem. Phys.* **2021**, *154* (8), 084902. <https://doi.org/10.1063/5.0037630>.
- (81) Alkhatib, I. I. I.; Pereira, L. M. C.; Torne, J.; Vega, L. F. Polar Soft-SAFT: Theory and Comparison with Molecular Simulations and Experimental Data of Pure Polar Fluids. *Phys. Chem. Chem. Phys.* **2020**, *22* (23), 13171–13191. <https://doi.org/10.1039/D0CP00846J>.
- (82) Llovel, F.; Pàmies, J. C.; Vega, L. F. Thermodynamic Properties of Lennard-Jones Chain Molecules: Renormalization-Group Corrections to a Modified Statistical Associating Fluid Theory. *The Journal of Chemical Physics* **2004**, *121* (21), 10715–10724. <https://doi.org/10.1063/1.1809112>.
- (83) Dias, A. M. A.; Llovel, F.; Coutinho, J. A. P.; Marrucho, I. M.; Vega, L. F. Thermodynamic Characterization of Pure Perfluoroalkanes, Including Interfacial and Second Order Derivative Properties, Using the Crossover Soft-SAFT EoS. *Fluid Phase Equilibria* **2009**, *286* (2), 134–143. <https://doi.org/10.1016/j.fluid.2009.08.018>.
- (84) Pàmies, J. C.; Vega, L. F. Vapor–Liquid Equilibria and Critical Behavior of Heavy n -Alkanes Using Transferable Parameters from the Soft-SAFT Equation of State. *Ind. Eng. Chem. Res.* **2001**, *40* (11), 2532–2543. <https://doi.org/10.1021/ie000944x>.
- (85) Castro-Marcano, F.; Colina, C. M.; Olivera-Fuentes, C. Parametrization of Molecular-Based Equations of State: The PC-SAFT, Soft-SAFT, PHSC and PSCT Models. *Pol. J. Chem* **2006**, *80*, 37–49.
- (86) Oliveira, M. B.; Llovel, F.; Coutinho, J. A. P.; Vega, L. F. New Procedure for Enhancing the Transferability of Statistical Associating Fluid Theory (SAFT) Molecular Parameters: The Role of Derivative Properties. *Ind. Eng. Chem. Res.* **2016**, *55* (37), 10011–10024. <https://doi.org/10.1021/acs.iecr.6b02205>.
- (87) Ferrando, N.; de Hemptinne, J.-C.; Mougin, P.; Passarello, J.-P. Prediction of the PC-SAFT Associating Parameters by Molecular Simulation. *J. Phys. Chem. B* **2012**, *116* (1), 367–377. <https://doi.org/10.1021/jp209313a>.
- (88) Fuenzalida, M.; Cuevas-Valenzuela, J.; Pérez-Correa, J. R. Improved Estimation of PC-SAFT Equation of State Parameters Using a Multi-Objective Variable-Weight Cost Function. *Fluid Phase Equilibria* **2016**, *427*, 308–319. <https://doi.org/10.1016/j.fluid.2016.07.001>.
- (89) Jaber, M.; Babe, W.; Sauer, E.; Gross, J.; Lugo, R.; de Hemptinne, J. C. An Improved Group Contribution Method for PC-SAFT Applied to Branched Alkanes: Data Analysis and Parameterization. *Fluid Phase Equilibria* **2018**, *473*, 183–191. <https://doi.org/10.1016/j.fluid.2018.06.014>.
- (90) Matsukawa, H.; Kitahara, M.; Otake, K. Estimation of Pure Component Parameters of PC-SAFT EoS by an Artificial Neural Network Based on a Group Contribution Method. *Fluid Phase Equilibria* **2021**, *548*, 113179. <https://doi.org/10.1016/j.fluid.2021.113179>.
- (91) Anoune, I.; Mimoune, Z.; Madani, H.; Merzougui, A. New Modified PC-SAFT Pure Component Parameters for Accurate VLE and Critical Phenomena Description. *Fluid Phase Equilibria* **2021**, *532*, 112916. <https://doi.org/10.1016/j.fluid.2020.112916>.
- (92) Polishuk, I. About the Numerical Pitfalls Characteristic for SAFT EOS Models. *Fluid Phase Equilibria* **2010**, *298* (1), 67–74. <https://doi.org/10.1016/j.fluid.2010.07.003>.
- (93) Privat, R.; Gani, R.; Jaubert, J.-N. Are Safe Results Obtained When the PC-SAFT Equation of State Is Applied to Ordinary Pure Chemicals? *Fluid Phase Equilibria* **2010**, *295* (1), 76–92. <https://doi.org/10.1016/j.fluid.2010.03.041>.

- (94) Privat, R.; Moine, E.; Sirjean, B.; Gani, R.; Jaubert, J.-N. Application of the Corresponding-State Law to the Parametrization of Statistical Associating Fluid Theory (SAFT)-Type Models: Generation and Use of “Generalized Charts.” *Ind. Eng. Chem. Res.* **2019**, *58* (21), 9127–9139. <https://doi.org/10.1021/acs.iecr.8b06083>.
- (95) Ramírez-Vélez, N.; Piña-Martinez, A.; Jaubert, J.-N.; Privat, R. Parameterization of SAFT Models: Analysis of Different Parameter Estimation Strategies and Application to the Development of a Comprehensive Database of PC-SAFT Molecular Parameters. *J. Chem. Eng. Data* **2020**, *65* (12), 5920–5932. <https://doi.org/10.1021/acs.jced.0c00792>.
- (96) Pina-Martinez, A.; Le Guennec, Y.; Privat, R.; Jaubert, J.-N.; Mathias, P. M. Analysis of the Combinations of Property Data That Are Suitable for a Safe Estimation of Consistent Two α -Function Parameters: Updated Parameter Values for the Translated-Consistent T_c -PR and T_c -RK Cubic Equations of State. *J. Chem. Eng. Data* **2018**, *63* (10), 3980–3988. <https://doi.org/10.1021/acs.jced.8b00640>.
- (97) 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 Equilibria* **2017**, *445*, 45–53. <https://doi.org/10.1016/j.fluid.2017.04.015>.
- (98) McCabe, C.; Jackson, G. SAFT-VR Modelling of the Phase Equilibrium of Long-Chain n-Alkanes. *Phys. Chem. Chem. Phys.* **1999**, *1* (9), 2057–2064. <https://doi.org/10.1039/a808085b>.
- (99) Blas, F. J.; Galindo, A. Study of the High Pressure Phase Behaviour of CO₂+n-Alkane Mixtures Using the SAFT-VR Approach with Transferable Parameters. *Fluid Phase Equilibria* **2002**, *194–197*, 501–509. [https://doi.org/10.1016/S0378-3812\(01\)00651-3](https://doi.org/10.1016/S0378-3812(01)00651-3).
- (100) Forte, E.; Llovel, F.; Trusler, J. P. M.; Galindo, A. Application of the Statistical Associating Fluid Theory for Potentials of Variable Range (SAFT-VR) Coupled with Renormalisation-Group (RG) Theory to Model the Phase Equilibria and Second-Derivative Properties of Pure Fluids. *Fluid Phase Equilibria* **2013**, *337*, 274–287. <https://doi.org/10.1016/j.fluid.2012.09.022>.
- (101) Dias, A. M. A.; Pàmies, J. C.; Coutinho, J. A. P.; Marrucho, I. M.; Vega, L. F. SAFT Modeling of the Solubility of Gases in Perfluoroalkanes. *J. Phys. Chem. B* **2004**, *108* (4), 1450–1457. <https://doi.org/10.1021/jp036225o>.
- (102) Andreu, J. S.; Vega, L. F. Capturing the Solubility Behavior of CO₂ in Ionic Liquids by a Simple Model. *J. Phys. Chem. C* **2007**, *111* (43), 16028–16034. <https://doi.org/10.1021/jp074353x>.
- (103) de Villiers, A. J.; Schwarz, C. E.; Burger, A. J.; Kontogeorgis, G. M. Evaluation of the PC-SAFT, SAFT and CPA Equations of State in Predicting Derivative Properties of Selected Non-Polar and Hydrogen-Bonding Compounds. *Fluid Phase Equilibria* **2013**, *338*, 1–15. <https://doi.org/10.1016/j.fluid.2012.09.035>.
- (104) Soltani Panah, H. Modeling Binary Vapor–Liquid Equilibrium Data Containing Perfluorocarbons Using the Peng–Robinson and the PC-SAFT Equations of State. *International Journal of Refrigeration* **2018**, *85*, 13–26. <https://doi.org/10.1016/j.ijrefrig.2017.09.008>.
- (105) Britannica, T. E. Chemical Association. *Encyclopedia Britannica*; 2016.
- (106) Grinberg, N.; Grushka, E. *Advances in Chromatography. Volume 54*; 2018.
- (107) Dufal, S.; Lafitte, T.; Haslam, A. J.; Galindo, A.; Clark, G. N. I.; Vega, C.; Jackson, G. The A in SAFT: Developing the Contribution of Association to the Helmholtz Free Energy within a Wertheim TPT1 Treatment of Generic Mie Fluids. *Molecular Physics* **2015**, *113* (9–10), 948–984. <https://doi.org/10.1080/00268976.2015.1029027>.

- (108) 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* (11), 4310–4318. <https://doi.org/10.1021/ie9600203>.
- (109) Arunan, E.; Desiraju, G. R.; Klein, R. A.; Sadlej, J.; Scheiner, S.; Alkorta, I.; Clary, D. C.; Crabtree, R. H.; Dannenberg, J. J.; Hobza, P.; Kjaergaard, H. G.; Legon, A. C.; Mennucci, B.; Nesbitt, D. J. Definition of the Hydrogen Bond (IUPAC Recommendations 2011). *Pure and Applied Chemistry* **2011**, *83* (8), 1637–1641. <https://doi.org/10.1351/PAC-REC-10-01-02>.
- (110) Gilli, P.; Pretto, L.; Bertolasi, V.; Gilli, G. Predicting Hydrogen-Bond Strengths from Acid–Base Molecular Properties. The pK_a Slide Rule: Toward the Solution of a Long-Lasting Problem. *Acc. Chem. Res.* **2009**, *42* (1), 33–44. <https://doi.org/10.1021/ar800001k>.
- (111) Silverstein, K. A. T.; Haymet, A. D. J.; Dill, K. A. The Strength of Hydrogen Bonds in Liquid Water and Around Nonpolar Solutes. *J. Am. Chem. Soc.* **2000**, *122* (33), 8037–8041. <https://doi.org/10.1021/ja000459t>.
- (112) Chaplin, M. Water’s Hydrogen Bond Strength. *arXiv:0706.1355 [cond-mat, physics:physics]* **2007**.
- (113) Arunan, E.; Desiraju, G. R.; Klein, R. A.; Sadlej, J.; Scheiner, S.; Alkorta, I.; Clary, D. C.; Crabtree, R. H.; Dannenberg, J. J.; Hobza, P.; Kjaergaard, H. G.; Legon, A. C.; Mennucci, B.; Nesbitt, D. J. Defining the Hydrogen Bond: An Account (IUPAC Technical Report). *Pure and Applied Chemistry* **2011**, *83* (8), 1619–1636. <https://doi.org/10.1351/PAC-REP-10-01-01>.
- (114) Eckert, F.; Klamt, A. Fast Solvent Screening via Quantum Chemistry: COSMO-RS Approach. *AIChE J.* **2002**, *48* (2), 369–385. <https://doi.org/10.1002/aic.690480220>.
- (115) *COSMOtherm*; COSMOlogic GmbH 1 Co.: Leverkusen, Germany, 2015.
- (116) Zaitseva, K. V.; Varfolomeev, M. A.; Solomonov, B. N. Thermodynamic Functions of Hydrogen Bonding of Amines in Methanol Derived from Solution Calorimetry Data and Headspace Analysis. *Thermochimica Acta* **2012**, *535*, 8–16. <https://doi.org/10.1016/j.tca.2012.02.005>.
- (117) Belford. Hydrogen Bonds <https://chem.libretexts.org/@go/page/42086> (accessed 2021 - 11 -23).
- (118) Klamt, A. Conductor-like Screening Model for Real Solvents: A New Approach to the Quantitative Calculation of Solvation Phenomena. *J. Phys. Chem.* **1995**, *99* (7), 2224–2235. <https://doi.org/10.1021/j100007a062>.
- (119) Klamt, A.; Eckert, F. COSMO-RS: A Novel and Efficient Method for the a Priori Prediction of Thermophysical Data of Liquids. *Fluid Phase Equilibria* **2000**, *172* (1), 43–72. [https://doi.org/10.1016/S0378-3812\(00\)00357-5](https://doi.org/10.1016/S0378-3812(00)00357-5).
- (120) Klamt, A.; Jonas, V.; Bürger, T.; Lohrenz, J. C. W. Refinement and Parametrization of COSMO-RS. *J. Phys. Chem. A* **1998**, *102* (26), 5074–5085. <https://doi.org/10.1021/jp980017s>.
- (121) Khan, I.; Kurnia, K. A.; Mutelet, F.; Pinho, S. P.; Coutinho, J. A. P. Probing the Interactions between Ionic Liquids and Water: Experimental and Quantum Chemical Approach. *J. Phys. Chem. B* **2014**, *118* (7), 1848–1860. <https://doi.org/10.1021/jp4113552>.
- (122) Klamt, A.; Eckert, F.; Arlt, W. COSMO-RS: An Alternative to Simulation for Calculating Thermodynamic Properties of Liquid Mixtures. *Annu. Rev. Chem. Biomol. Eng.* **2010**, *1* (1), 101–122. <https://doi.org/10.1146/annurev-chembioeng-073009-100903>.

- (123) Klamt, A.; Reinisch, J.; Eckert, F.; Hellweg, A.; Diedenhofen, M. Polarization Charge Densities Provide a Predictive Quantification of Hydrogen Bond Energies. *Phys. Chem. Chem. Phys.* **2012**, *14* (2), 955–963. <https://doi.org/10.1039/C1CP22640A>.
- (124) Klamt, A.; Reinisch, J.; Eckert, F.; Graton, J.; Le Questel, J.-Y. Interpretation of Experimental Hydrogen-Bond Enthalpies and Entropies from COSMO Polarisation Charge Densities. *Phys. Chem. Chem. Phys.* **2013**, *15* (19), 7147. <https://doi.org/10.1039/c3cp44611e>.
- (125) Abranches, D. O.; Silva, L. P.; Martins, M. A. R.; Pinho, S. P.; Coutinho, J. A. P. Understanding the Formation of Deep Eutectic Solvents: Betaine as a Universal Hydrogen Bond Acceptor. *ChemSusChem* **2020**, *13* (18), 4916–4921. <https://doi.org/10.1002/cssc.202001331>.
- (126) Abranches, D. O.; Benfica, J.; Soares, B. P.; Leal-Duaso, A.; Sintra, T. E.; Pires, E.; Pinho, S. P.; Shimizu, S.; Coutinho, J. A. P. Unveiling the Mechanism of Hydrotropy: Evidence for Water-Mediated Aggregation of Hydrotropes around the Solute. *Chem. Commun.* **2020**, *56* (52), 7143–7146. <https://doi.org/10.1039/D0CC03217D>.
- (127) Piña-Martinez, A.; Privat, R.; Jaubert, J. Use of 300,000 Pseudo-experimental Data over 1800 Pure Fluids to Assess the Performance of Four Cubic Equations of State: SRK, PR, TC -RK, and TC -PR. *AIChE Journal* **2022**, *68* (2). <https://doi.org/10.1002/aic.17518>.
- (128) 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 and Fuels* **2013**, *27* (11), 7150–7178. <https://doi.org/10.1021/ef401605c>.
- (129) Nikolaidis, I. K.; Privat, R.; Jaubert, J.-N.; Economou, I. G. Assessment of the Perturbed Chain-Statistical Associating Fluid Theory Equation of State against a Benchmark Database of High-Quality Binary-System Data. *Ind. Eng. Chem. Res.* **2021**, *60* (24), 8935–8946. <https://doi.org/10.1021/acs.iecr.1c01234>.
- (130) Piña-Martinez, A.; Privat, R.; Nikolaidis, I. K.; Economou, I. G.; Jaubert, J.-N. What Is the Optimal Activity Coefficient Model To Be Combined with the *Translated – Consistent* Peng–Robinson Equation of State through Advanced Mixing Rules? Cross-Comparison and Grading of the Wilson, UNIQUAC, and NRTL a^E Models against a Benchmark Database Involving 200 Binary Systems. *Ind. Eng. Chem. Res.* **2021**, *60* (47), 17228–17247. <https://doi.org/10.1021/acs.iecr.1c03003>.
- (131) Agarwal, R.; Li, Y.-K.; Santollani, O.; Satyro, M. A.; Vieler, A. Uncovering the Realities of Simulation. Part II. *Chemical Engineering Progress* **2001**, *97* (6), 64–72.
- (132) DIPPR's Project 801 Database <https://www.aiche.org/dippr>.
- (133) 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 Equilibria* **2016**, *427*, 414–420. <https://doi.org/10.1016/j.fluid.2016.07.035>.
- (134) Wertheim, M. S. Fluids with Highly Directional Attractive Forces. IV. Equilibrium Polymerization. *J Stat Phys* **1986**, *42* (3–4), 477–492. <https://doi.org/10.1007/BF01127722>.
- (135) Joslin, C. G.; Gray, C. G.; Chapman, W. G.; Gubbins, K. E. Theory and Simulation of Associating Liquid Mixtures. II. *Molecular Physics* **1987**, *62* (4), 843–860. <https://doi.org/10.1080/00268978700102621>.
- (136) Zmpitas, W.; Gross, J. Detailed Pedagogical Review and Analysis of Wertheim's Thermodynamic Perturbation Theory. *Fluid Phase Equilibria* **2016**, *428*, 121–152. <https://doi.org/10.1016/j.fluid.2016.07.033>.

- (137) de Villiers, A. J.; Schwarz, C. E.; Burger, A. J. New Association Scheme for 1-Alcohols in Alcohol/Water Mixtures with SPC-SAFT: The 2C Association Scheme. *Ind. Eng. Chem. Res.* **2011**, *50* (14), 8711–8725. <https://doi.org/10.1021/ie200521k>.
- (138) Kruger, F.; Kontogeorgis, G. M.; von Solms, N. New Association Schemes for Mono-Ethylene Glycol: Cubic-Plus-Association Parameterization and Uncertainty Analysis. *Fluid Phase Equilibria* **2018**, *458*, 211–233. <https://doi.org/10.1016/j.fluid.2017.11.026>.
- (139) Abolala, M.; Pourdehjad, Z.; Peyvandi, K. Extension of 2C Association Scheme to Polyols Phase Equilibria. *Ind. Eng. Chem. Res.* **2017**, *56* (48), 14369–14383. <https://doi.org/10.1021/acs.iecr.7b03453>.
- (140) Janecek, J.; Paricaud, P. Influence of Cyclic Dimer Formation on the Phase Behavior of Carboxylic Acids. *J. Phys. Chem. B* **2012**, *116* (27), 7874–7882. <https://doi.org/10.1021/jp303051j>.
- (141) Tan, S. P.; Piri, M. Modeling the Solubility of Nitrogen Dioxide in Water Using Perturbed-Chain Statistical Associating Fluid Theory. *Ind. Eng. Chem. Res.* **2013**, *52* (45), 16032–16043. <https://doi.org/10.1021/ie402417p>.
- (142) Dietz, C. H. J. T.; van Osch, D. J. G. P.; Kroon, M. C.; Sadowski, G.; van Sint Annaland, M.; Gallucci, F.; Zubeir, L. F.; Held, C. PC-SAFT Modeling of CO₂ Solubilities in Hydrophobic Deep Eutectic Solvents. *Fluid Phase Equilibria* **2017**, *448*, 94–98. <https://doi.org/10.1016/j.fluid.2017.03.028>.
- (143) Cripwell, J. T.; Kruger, F. J.; Burger, A. J. Accounting for Cross Association in Non-Self-Associating Species Using a Physically Consistent SAFT-VR Mie Approach. *Fluid Phase Equilibria* **2019**, *483*, 1–13. <https://doi.org/10.1016/j.fluid.2018.11.003>.
- (144) Suresh, S. J.; Elliott, J. R. Multiphase Equilibrium Analysis via a Generalized Equation of State for Associating Mixtures. *Ind. Eng. Chem. Res.* **1992**, *31* (12), 2783–2794. <https://doi.org/10.1021/ie00012a025>.
- (145) von Solms, N.; Michelsen, M. L.; Passos, C. P.; Derawi, S. O.; Kontogeorgis, G. M. Investigating Models for Associating Fluids Using Spectroscopy. *Ind. Eng. Chem. Res.* **2006**, *45* (15), 5368–5374. <https://doi.org/10.1021/ie051341u>.
- (146) Luck, W. A. P. A Model of Hydrogen-Bonded Liquids. *Angew. Chem. Int. Ed. Engl.* **1980**, *19* (1), 28–41. <https://doi.org/10.1002/anie.198000281>.
- (147) 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* (14), 4855–4868. <https://doi.org/10.1021/ie051305v>.
- (148) Clark, G. N. I.; Haslam, A. J.; Galindo, A.; Jackson, G. Developing Optimal Wertheim-like Models of Water for Use in Statistical Associating Fluid Theory (SAFT) and Related Approaches. *Molecular Physics* **2006**, *104* (22–24), 3561–3581. <https://doi.org/10.1080/00268970601081475>.
- (149) Mac Dowell, N.; Llovel, F.; Adjiman, C. S.; Jackson, G.; Galindo, A. Modeling the Fluid Phase Behavior of Carbon Dioxide in Aqueous Solutions of Monoethanolamine Using Transferable Parameters with the SAFT-VR Approach. *Ind. Eng. Chem. Res.* **2010**, *49* (4), 1883–1899. <https://doi.org/10.1021/ie901014t>.
- (150) Haarmann, N.; Enders, S.; Sadowski, G. Heterosegmental Modeling of Long-Chain Molecules and Related Mixtures Using PC-SAFT: 2. Associating Compounds. *Ind. Eng. Chem. Res.* **2019**, *58* (11), 4625–4643. <https://doi.org/10.1021/acs.iecr.9b00157>.
- (151) Fouad, W. A.; Wang, L.; Haghmoradi, A.; Asthagiri, D.; Chapman, W. G. Understanding the Thermodynamics of Hydrogen Bonding in Alcohol-Containing Mixtures: Cross-Association. *J. Phys. Chem. B* **2016**, *120* (13), 3388–3402. <https://doi.org/10.1021/acs.jpcc.5b12375>.

- (152) Tybjerg, P. C. V.; Kontogeorgis, G. M.; Michelsen, M. L.; Stenby, E. H. Phase Equilibria Modeling of Methanol-Containing Systems with the CPA and SPC-SAFT Equations of State. *Fluid Phase Equilibria* **2010**, *288* (1–2), 128–138. <https://doi.org/10.1016/j.fluid.2009.10.021>.
- (153) Yarrison, M.; Chapman, W. G. A Systematic Study of Methanol+n-Alkane Vapor–Liquid and Liquid–Liquid Equilibria Using the CK-SAFT and PC-SAFT Equations of State. *Fluid Phase Equilibria* **2004**, *226*, 195–205. <https://doi.org/10.1016/j.fluid.2004.09.024>.
- (154) Llovel, 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* (3), 1350–1362. <https://doi.org/10.1021/jp0551465>.
- (155) Pamies, J. Bulk and Interfacial Properties of Chain Fluids: A Molecular Modelling Approach, Universitat Rovira i virgili, Tarragona, Spain, 2003.
- (156) Kontogeorgis, G. M.; Tsvintzelis, I.; von Solms, N.; Grenner, A.; Bøgh, D.; Frost, M.; Knage-Rasmussen, A.; Economou, I. G. Use of Monomer Fraction Data in the Parametrization of Association Theories. *Fluid Phase Equilibria* **2010**, *296* (2), 219–229. <https://doi.org/10.1016/j.fluid.2010.05.028>.
- (157) Ribeiro, R. T. C. S.; Alberton, A. L.; Paredes, M. L. L.; Kontogeorgis, G. M.; Liang, X. Extensive Study of the Capabilities and Limitations of the CPA and SPC-SAFT Equations of State in Modeling a Wide Range of Acetic Acid Properties. *Ind. Eng. Chem. Res.* **2018**, *57* (16), 5690–5704. <https://doi.org/10.1021/acs.iecr.8b00148>.
- (158) Grenner, A.; Schmelzer, J.; von Solms, N.; Kontogeorgis, G. M. Comparison of Two Association Models (Elliott–Suresh–Donohue and Simplified PC-SAFT) for Complex Phase Equilibria of Hydrocarbon–Water and Amine-Containing Mixtures. *Ind. Eng. Chem. Res.* **2006**, *45* (24), 8170–8179. <https://doi.org/10.1021/ie0605332>.
- (159) Vega, L. F.; Llovel, F.; Blas, F. J. Capturing the Solubility Minima of n -Alkanes in Water by Soft-SAFT. *J. Phys. Chem. B* **2009**, *113* (21), 7621–7630. <https://doi.org/10.1021/jp9018876>.
- (160) Grenner, A.; Kontogeorgis, G. M.; von Solms, N.; Michelsen, M. L. Modeling Phase Equilibria of Alkanols with the Simplified PC-SAFT Equation of State and Generalized Pure Compound Parameters. *Fluid Phase Equilibria* **2007**, *258* (1), 83–94. <https://doi.org/10.1016/j.fluid.2007.05.009>.
- (161) Belkadi, A.; Hadj-Kali, M. K.; Llovel, F.; Gerbaud, V.; Vega, L. F. Soft-SAFT Modeling of Vapor–Liquid Equilibria of Nitriles and Their Mixtures. *Fluid Phase Equilibria* **2010**, *289* (2), 191–200. <https://doi.org/10.1016/j.fluid.2009.12.012>.
- (162) Yushu, C.; Afef, A.; Fabrice, M.; Roland, S.; Jeday, M. R. Thermodynamic Modeling of Mixtures Containing Carboxylic Acids Using the PC-SAFT Equation of State. *Ind. Eng. Chem. Res.* **2012**, *51* (42), 13846–13852. <https://doi.org/10.1021/ie301930q>.
- (163) Ramirez-Velez, N.; Privat, R.; Pina-Martinez, A.; Jaubert, J.-N. Assessing the Performance of Non-Associating SAFT-Type EoS to Reproduce , , and Data of 1 800 Pure Fluids. *AIChE J.*
- (164) *ASPEN Plus*; AspenTech.
- (165) Britt, H. I.; Luecke, R. H. The Estimation of Parameters in Nonlinear, Implicit Models. *Technometrics* **1973**, *15* (2), 233–247. <https://doi.org/10.1080/00401706.1973.10489037>.
- (166) Van Rossum, G.; Drake, F. L. *Python 3*; CreateSpace: Scotts Valley, California, 2009.
- (167) Caswell, T. A.; Droettboom, M.; Lee, A.; De Andrade, E. S.; Hoffmann, T.; Hunter, J.; Klymak, J.; Firing, E.; Stansby, D.; Varoquaux, N.; Nielsen, J. H.; Root, B.; May, R.; Elson, P.; Seppänen, J. K.; Dale, D.; Jae-Joon Lee; McDougall, D.; Straw, A.; Hobson, P.; Hannah; Gohlke, C.; Vincent, A. F.; Yu, T. S.; Ma, E.; Silvester, S.; Moad, C.;

- Kniazhev, N.; Ernest, E.; Ivanov, P. *Matplotlib/Matplotlib: REL: V3.5.1*; Zenodo, 2021. <https://doi.org/10.5281/ZENODO.592536>.
- (168) Kontogeorgis, G. M.; Liang, X.; Arya, A.; Tsvintzelis, I. Equations of State in Three Centuries. Are We Closer to Arriving to a Single Model for All Applications? *Chemical Engineering Science: X* **2020**, *7*, 100060. <https://doi.org/10.1016/j.cesx.2020.100060>.
- (169) Chen, C.-C.; Mathias, P. M. Applied Thermodynamics for Process Modeling. *AIChE J.* **2002**, *48* (2), 194–200. <https://doi.org/10.1002/aic.690480202>.
- (170) Danner, R. P.; Gess, M. A. A Data Base Standard for the Evaluation of Vapor-Liquid-Equilibrium Models. *Fluid Phase Equilibria* **1990**, *56*, 285–301. [https://doi.org/10.1016/0378-3812\(90\)85109-N](https://doi.org/10.1016/0378-3812(90)85109-N).
- (171) Privat, R.; Jaubert, J.-N. Classification of Global Fluid-Phase Equilibrium Behaviors in Binary Systems. *Chemical Engineering Research and Design* **2013**, *91* (10), 1807–1839. <https://doi.org/10.1016/j.cherd.2013.06.026>.
- (172) Konynenburg, P. H. V.; Scott, R. L. Critical Lines and Phase Equilibria in Binary Van Der Waals Mixtures. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* **1980**, *298* (1442), 495–540. <https://doi.org/10.1098/rsta.1980.0266>.
- (173) 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 Grandes Gammes de Températures et de Pressions, Institut National Polytechnique de Lorraine, Nancy, 2011.
- (174) 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. *Journal of Chemical Thermodynamics* **2000**, *32* (3), 401–411. <https://doi.org/10.1006/jcht.1999.0613>.
- (175) Llovel, 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* (23), 11427–11437. <https://doi.org/10.1021/jp0608022>.
- (176) Llovel, F.; Peters, C. J.; Vega, L. F. Second-Order Thermodynamic Derivative Properties of Selected Mixtures by the Soft-SAFT Equation of State. *Fluid Phase Equilibria* **2006**, *248* (2), 115–122. <https://doi.org/10.1016/j.fluid.2006.07.018>.
- (177) Llovel, 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. *The Journal of Supercritical Fluids* **2007**, *41* (2), 204–216. <https://doi.org/10.1016/j.supflu.2006.10.001>.
- (178) 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. *Journal of Molecular Liquids* **2020**, *300*, 112294. <https://doi.org/10.1016/j.molliq.2019.112294>.
- (179) 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. *Journal of Molecular Liquids* **2019**, *291*, 111321. <https://doi.org/10.1016/j.molliq.2019.111321>.
- (180) Polishuk, I.; Privat, R.; Jaubert, J.-N. Novel Methodology for Analysis and Evaluation of SAFT-Type Equations of State. *Industrial and Engineering Chemistry Research* **2013**, *52* (38), 13875–13885. <https://doi.org/10.1021/ie4020155>.
- (181) 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. *Journal of Molecular Liquids* **2019**, *279*, 492–502. <https://doi.org/10.1016/j.molliq.2019.01.151>.

- (182) Polishuk, I.; Garrido, J. M. Comparison of SAFT-VR-Mie and CP-PC-SAFT in Predicting Phase Behavior of Associating Systems II. Ammonia – Hydrocarbons. *Journal of Molecular Liquids* **2018**, *269*, 657–665. <https://doi.org/10.1016/j.molliq.2018.08.098>.
- (183) 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. *Journal of Molecular Liquids* **2018**, *265*, 639–653. <https://doi.org/10.1016/j.molliq.2018.05.112>.
- (184) Atkins, P. W.; De Paula, J. *Atkins' Physical Chemistry*; Oxford University Press: Oxford, 2011.
- (185) Privat, R.; Jaubert, J.-N. Discussion around the Paradigm of Ideal Mixtures with Emphasis on the Definition of the Property Changes on Mixing. *Chemical Engineering Science* **2012**, *82*, 319–333. <https://doi.org/10.1016/j.ces.2012.07.030>.
- (186) Van Ness, H. C.; Byer, S. M.; Gibbs, R. E. Vapor-Liquid Equilibrium: Part I. An Appraisal of Data Reduction Methods. *AIChE Journal* **1973**, *19* (2), 238–244. <https://doi.org/10.1002/aic.690190206>.
- (187) Redlich, O.; Kister, A. T. Algebraic Representation of Thermodynamic Properties and the Classification of Solutions. *Industrial & Engineering Chemistry* **1948**, *40* (2), 345–348. <https://doi.org/10.1021/ie50458a036>.
- (188) Kojima, K.; Man Moon, H.; Ochi, K. Thermodynamic Consistency Test of Vapor-Liquid Equilibrium Data. *Fluid Phase Equilibria* **1990**, *56*, 269–284. [https://doi.org/10.1016/0378-3812\(90\)85108-M](https://doi.org/10.1016/0378-3812(90)85108-M).
- (189) Wisniak, J.; Ortega, J.; Fernández, L. A Fresh Look at the Thermodynamic Consistency of Vapour-Liquid Equilibria Data. *The Journal of Chemical Thermodynamics* **2017**, *105*, 385–395. <https://doi.org/10.1016/j.jct.2016.10.038>.
- (190) Poon, D. P. L.; Lu, B. C.-Y. Phase Equilibria for Systems Containing Nitrogen, Methane, and Propane. In *Advances in Cryogenic Engineering*; 1995; pp 292–299.
- (191) Wichterle, I.; Kobayashi, R. Vapor-Liquid Equilibrium of Methane-Propane System at Low Temperatures and High Pressures. *Journal of Chemical & Engineering Data* **1972**, *17* (1), 4–9. <https://doi.org/10.1021/je60052a019>.
- (192) Price, A. R.; Kobayashi, R. Low Temperature Vapor-Liquid Equilibrium in Light Hydrocarbon Mixtures: Methane-Ethane-Propane System. *Journal of Chemical & Engineering Data* **1959**, *4* (1), 40–52. <https://doi.org/10.1021/je60001a007>.
- (193) Wichterle, I.; Kobayashi, R. Vapor-Liquid Equilibrium of Methane-Ethane-Propane System at Low Temperatures and High Pressures. *Journal of Chemical & Engineering Data* **1972**, *17* (1), 13–18. <https://doi.org/10.1021/je60052a017>.
- (194) Webster, L. A.; Kidnay, A. J. Vapor-Liquid Equilibria for the Methane-Propane-Carbon Dioxide Systems at 230 K and 270 K. *Journal of Chemical & Engineering Data* **2001**, *46* (3), 759–764. <https://doi.org/10.1021/je000307d>.
- (195) Akers, W. W.; Burns, J. F.; Fairchild, W. R. Low-Temperature Phase Equilibria: Methane-Propane System. *Industrial & Engineering Chemistry* **1954**, *46* (12), 2531–2534. <https://doi.org/10.1021/ie50540a038>.
- (196) Reamer, H. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane-Propane System. *Industrial & Engineering Chemistry* **1950**, *42* (3), 534–539. <https://doi.org/10.1021/ie50483a037>.
- (197) Watanabe, K.; Kuroki, M.; Ogura, M.; Saito, I. Vapour-Liquid-Equilibrium of LNG. *TEION KOGAKU (Journal of Cryogenics and Superconductivity Society of Japan)* **1969**, *4* (6), 292–301. <https://doi.org/10.2221/jcsj.4.292>.

- (198) Miller, R. C.; Staveley, L. A. K. Excess Enthalpies for Some Binary Liquid Mixtures of Low-Molecular-Weight Alkanes. In *Advances in Cryogenic Engineering*; 1960; pp 493–500.
- (199) Cutler, A. J. B.; Morrison, J. A. Excess Thermodynamic Functions for Liquid Mixtures of Methane + Propane. *Transactions of the Faraday Society* **1965**, *61*, 429. <https://doi.org/10.1039/tf9656100429>.
- (200) Hutchings, D. J.; Lewis, E. J.; Wormald, C. J. Excess Enthalpies of Mixtures of Methane + Each of the N-Alkanes from Ethane to n-Octane. *The Journal of Chemical Thermodynamics* **1978**, *10* (6), 559–566. [https://doi.org/10.1016/0021-9614\(78\)90044-7](https://doi.org/10.1016/0021-9614(78)90044-7).
- (201) Roof, J. G.; Baron, J. D. Critical Loci of Binary Mixtures of Propane with Methane, Carbon Dioxide, and Nitrogen. *Journal of Chemical & Engineering Data* **1967**, *12* (3), 292–293. <https://doi.org/10.1021/je60034a003>.
- (202) Sage, B. H.; Lacey, W. N.; Schaafsma, J. G. Phase Equilibria in Hydrocarbon Systems II. Methane-Propane System. *Industrial & Engineering Chemistry* **1934**, *26* (2), 214–217. <https://doi.org/10.1021/ie50290a020>.
- (203) Lin, Y.-N.; Chen, R. J. J.; Chappellear, P. S.; Kobayashi, R. Vapor-Liquid Equilibrium of the Methane-n-Hexane System at Low Temperature. *Journal of Chemical & Engineering Data* **1977**, *22* (4), 402–408. <https://doi.org/10.1021/je60075a007>.
- (204) 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. *Journal of Chemical & Engineering Data* **2011**, *56* (12), 4301–4309. <https://doi.org/10.1021/je200101x>.
- (205) Stepanova, G. S.; Vybornova, Y. I. Phase Equilibriums of Methane-Hexane System. *Tr. Vses. Nauchno Issled. Inst. Prir. Gazov.* **1962**, 203–208.
- (206) Shim, J.; Kohn, J. P. Multiphase and Volumetric Equilibria of Methane-n-Hexane Binary System at Temperatures Between -110° and 150° C. *Journal of Chemical & Engineering Data* **1962**, *7* (1), 3–8. <https://doi.org/10.1021/je60012a002>.
- (207) Poston, R. S.; McKetta, J. J. Vapor-Liquid Equilibrium in the Methane-n-Hexane System. *Journal of Chemical & Engineering Data* **1966**, *11* (3), 362–363. <https://doi.org/10.1021/je60030a021>.
- (208) 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 Journal* **1974**, *20* (2), 347–353. <https://doi.org/10.1002/aic.690200221>.
- (209) Marteau, Ph.; Obriot, J.; Barreau, A.; Ruffier-Meray, V.; Behar, E. Experimental Determination of the Phase Behavior of Binary Mixtures: Methane-Hexane and Methane-Benzene. *Fluid Phase Equilibria* **1997**, *129* (1–2), 285–305. [https://doi.org/10.1016/S0378-3812\(96\)03125-1](https://doi.org/10.1016/S0378-3812(96)03125-1).
- (210) Elliott, D. G.; Lin, Y. N.; Chu, T. C.; Chappellear, P. S.; Kobayashi, R. K-Values for the Methane - n-Butane, Methane - n-Pentane, and Methane - n-Hexane Systems. *GPA Research Report* **1976**, 1–19.
- (211) 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 Journal* **1966**, *12* (6), 1212–1216. <https://doi.org/10.1002/aic.690120629>.
- (212) Reamer, H. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Methane- n-Heptane System. *Industrial & Engineering Chemistry Chemical & Engineering Data Series* **1956**, *1* (1), 29–42. <https://doi.org/10.1021/i460001a007>.

- (213) Oscarson, J. L.; Coxam, J. Y.; Gillespie, S. E.; Izatt, R. M. Excess Enthalpies of Mixing Methane with Methanol, n-Heptane, Toluene and Methylcyclohexane at 255.4 and 310.9 K and 13.8 MPa. *Fluid Phase Equilibria* **1996**, *114* (1–2), 161–174. [https://doi.org/10.1016/0378-3812\(95\)02813-7](https://doi.org/10.1016/0378-3812(95)02813-7).
- (214) Chen, R. J. J.; Chappellear, P. S.; Kobayashi, R. Vapor Phase Data for the Binary Systems of Methane with N-Butane, n-Pentane, n-Hexane, and n-Heptane. *GPA Research Report* **1976**, 1–14.
- (215) Stryjek, R.; Chappellear, P. S.; Kobayashi, R. Low-Temperature Vapor-Liquid Equilibria of Nitrogen-Ethane System. *Journal of Chemical & Engineering Data* **1974**, *19* (4), 340–343. <https://doi.org/10.1021/je60063a024>.
- (216) Grausø, L.; Fredenslund, A.; Mollerup, J. Vapour-Liquid Equilibrium Data for the Systems C₂H₆ + N₂, C₂H₄ + N₂, C₃H₈ + N₂, and C₃H₆ + N₂. *Fluid Phase Equilibria* **1977**, *1* (1), 13–26. [https://doi.org/10.1016/0378-3812\(77\)80022-8](https://doi.org/10.1016/0378-3812(77)80022-8).
- (217) Brown, T. S.; Sloan, E. D.; Kidnay, A. J. Vapor-Liquid Equilibria in the Nitrogen + Carbon Dioxide + Ethane System. *Fluid Phase Equilibria* **1989**, *51*, 299–313. [https://doi.org/10.1016/0378-3812\(89\)80372-3](https://doi.org/10.1016/0378-3812(89)80372-3).
- (218) Zeck, S.; Knapp, H. Vapor—Liquid and Vapor—Liquid—Liquid Phase Equilibria for Binary and Ternary Systems for Nitrogen, Ethane and Methanol: Experiment and Data Reduction. *Fluid Phase Equilibria* **1986**, *25* (3), 303–322. [https://doi.org/10.1016/0378-3812\(86\)80006-1](https://doi.org/10.1016/0378-3812(86)80006-1).
- (219) Gupta, M. K.; Gardner, G. C.; Hegarty, M. J.; Kidnay, A. J. Liquid-Vapor Equilibria for the N₂ + CH₄ + C₂H₆ System from 260 to 280 K. *Journal of Chemical & Engineering Data* **1980**, *25* (4), 313–318. <https://doi.org/10.1021/je60087a016>.
- (220) Ellington, R. T.; Eakin, B. E.; Parent, J. D.; Gami, D. C.; Bloomer, O. T. Vapor-Liquid Phase Equilibria in the Binary Systems of CH₄, C₂H₆, and N₂. *Thermodynamic and Transport Properties of Gases, Liquids, and Solids, Papers Presented at the Symposium on Thermal Properties* **1959**, *1*, 180–194.
- (221) Guedes, H. J. R.; Zollweg, J. A.; Filipe, E. J. M.; Martins, L. F. G.; Calado, J. C. G. Thermodynamics of Liquid (Nitrogen + Ethane). *The Journal of Chemical Thermodynamics* **2002**, *34* (5), 669–678. <https://doi.org/10.1006/jcht.2001.0936>.
- (222) Yu, P.; Elshayal, I. M.; Lu, B. C.-Y. Liquid-Liquid-Vapor Equilibria in the Nitrogen-Methane-Ethane System. *The Canadian Journal of Chemical Engineering* **1969**, *47* (5), 495–498. <https://doi.org/10.1002/cjce.5450470516>.
- (223) Koonce, K. T.; Kobayashi, Riki. A Method for Determining the Solubility of Gases in Relatively Nonvolatile Liquids: Solubility of Methane in n-Decane. *Journal of Chemical & Engineering Data* **1964**, *9* (4), 490–494. <https://doi.org/10.1021/je60023a004>.
- (224) Lentz, H.; Nuennerich, P. Die Bestimmung Der Zusammensetzung Koexistierender Phasen Binärer Mischungen Aus Nodenlinien Und Volumen. *Chem. Ing. Tech.* **2001**, *73*, 1162–1164. [https://doi.org/10.1002/1522-2640\(200109\)73:9<1162::AID-CITE1162>3.0.CO;2-4](https://doi.org/10.1002/1522-2640(200109)73:9<1162::AID-CITE1162>3.0.CO;2-4).
- (225) Reamer, H. H.; Olds, R. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. *Industrial & Engineering Chemistry* **1942**, *34* (12), 1526–1531. <https://doi.org/10.1021/ie50396a025>.
- (226) Lavender, H. M.; Sage, B. H.; Lacey, W. N. Gas-Liquid Equilibrium Constants, Methane-Decane System. *Oil Gas J.* **1940**, *39*, 48–49.
- (227) 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. *Journal of Chemical & Engineering Data* **1979**, *24* (2), 146–149. <https://doi.org/10.1021/je60081a004>.

- (228) Wiese, H. C.; Reamer, H. H.; Sage, B. H. Phase Equilibriums in Hydrocarbon Systems. Phase Behavior in the Methane-Propane-n-Decane System. *Journal of Chemical & Engineering Data* **1970**, *15* (1), 75–82. <https://doi.org/10.1021/je60044a018>.
- (229) Kay, W. B. Liquid-Vapor Phase Equilibrium Relations in the Ethane-n-Heptane System. *Industrial & Engineering Chemistry* **1938**, *30* (4), 459–465. <https://doi.org/10.1021/ie50340a023>.
- (230) Cota, H. M.; Thodos, G. Critical Temperatures and Critical Pressures of Hydrocarbon Mixtures. Methane Ethane-n-Butane System. *Journal of Chemical & Engineering Data* **1962**, *7* (1), 62–65. <https://doi.org/10.1021/je60012a018>.
- (231) Mehra, V. S.; Thodos, G. Vapor-Liquid Equilibrium in the Ethane-n-Heptane System. *Journal of Chemical & Engineering Data* **1965**, *10* (3), 211–214. <https://doi.org/10.1021/je60026a001>.
- (232) Ekiner, O.; Thodos, G. Critical Temperatures and Pressures of the Ethane-n-Heptane System. *The Canadian Journal of Chemical Engineering* **1965**, *43* (4), 205–208. <https://doi.org/10.1002/cjce.5450430411>.
- (233) Mehra, V. S.; Thodos, George. Vapor-Liquid Equilibrium Constants for the Ethane-Butane-n-Heptane System at 300° and 350°F. *Journal of Chemical & Engineering Data* **1968**, *13* (2), 155–160. <https://doi.org/10.1021/je60037a004>.
- (234) Singh, H.; Lucien, F. P.; Foster, N. R. Critical Properties for Binary Mixtures of Ethane Containing Low Concentrations of N-Alkane. *Journal of Chemical & Engineering Data* **2000**, *45* (1), 131–135. <https://doi.org/10.1021/je990220w>.
- (235) Kurata, F.; Swift, G. W. Experimental Measurements of Vapor-Liquid Equilibrium Data for the Ethane - Carbon Dioxide and Nitrogen - n-Pentane Binary Systems. *GPA Research Report* **1971**, 1–10.
- (236) Kalra, H.; Robinson, D. B.; Besserer, G. J. The Equilibrium Phase Properties of the Nitrogen-n-Pentane System. *Journal of Chemical & Engineering Data* **1977**, *22* (2), 215–218. <https://doi.org/10.1021/je60073a023>.
- (237) 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 Equilibria* **2006**, *250* (1–2), 37–48. <https://doi.org/10.1016/j.fluid.2006.09.018>.
- (238) Azarnoosh, A.; McKetta, J. J. Nitrogen-n-Decane System in the Two-Phase Region. *Journal of Chemical & Engineering Data* **1963**, *8* (4), 494–496. <https://doi.org/10.1021/je60019a005>.
- (239) 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. *Journal of Chemical & Engineering Data* **2009**, *54* (5), 1560–1568. <https://doi.org/10.1021/je800881t>.
- (240) Flöter, E.; de Loos, Th. W.; de Swaan Arons, J. High Pressure Solid-Fluid and Vapour-Liquid Equilibria in the System (Methane + Tetracosane). *Fluid Phase Equilibria* **1997**, *127* (1–2), 129–146. [https://doi.org/10.1016/S0378-3812\(96\)03157-3](https://doi.org/10.1016/S0378-3812(96)03157-3).
- (241) Huang, C.-P.; Jan, D.-S.; Tsai, F.-N. Modeling of Methane Solubility in Heavy N-Paraffins. *JOURNAL OF CHEMICAL ENGINEERING OF JAPAN* **1992**, *25* (2), 182–186. <https://doi.org/10.1252/jcej.25.182>.
- (242) 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 Equilibria* **1996**, *124* (1–2), 177–207. [https://doi.org/10.1016/S0378-3812\(96\)03101-9](https://doi.org/10.1016/S0378-3812(96)03101-9).
- (243) Suleiman, D.; Eckert, C. A. Phase Equilibria of Alkanes in Natural Gas Systems. 1. Alkanes in Methane. *Journal of Chemical & Engineering Data* **1995**, *40* (1), 2–11. <https://doi.org/10.1021/je00017a001>.

- (244) Schwarz, C. E.; Nieuwoudt, I.; Knoetze, J. H. Phase Equilibria of Long Chain N-Alkanes in Supercritical Ethane: Review, Measurements and Prediction. *The Journal of Supercritical Fluids* **2008**, *46* (3), 226–232. <https://doi.org/10.1016/j.supflu.2008.05.007>.
- (245) Tsai, F. N.; Huang, S. H.; Lin, H. M.; Chao, K. C. Solubility of Methane, Ethane, and Carbon Dioxide in n-Hexatriacontane. *Journal of Chemical & Engineering Data* **1987**, *32* (4), 467–469. <https://doi.org/10.1021/jc00050a025>.
- (246) 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. *Journal of Chemical & Engineering Data* **1989**, *34* (2), 187–191. <https://doi.org/10.1021/jc00056a012>.
- (247) Martin, M.; Youings, J. Vapour Pressures and Excess Gibbs Free Energies of Cyclohexane + N-Hexane, + n-Heptane and + n-Octane at 298. 15 K. *Australian Journal of Chemistry* **1980**, *33* (10), 2133. <https://doi.org/10.1071/CH9802133>.
- (248) Benson, G. C.; Benson, G. C.; Anand, S. C.; Kiyohara, O. Thermodynamic Properties of Some Cycloalkane-Cycloalkanol Systems at 298. 15.Deg.K. II. *Journal of Chemical & Engineering Data* **1974**, *19* (3), 258–261. <https://doi.org/10.1021/jc00062a027>.
- (249) 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.* **1963**, *37* (8), 938–943.
- (250) Ridgway, K.; Butler, P. A. Physical Properties of the Ternary System Benzene-Cyclohexane-Hexane. *Journal of Chemical & Engineering Data* **1967**, *12* (4), 509–515. <https://doi.org/10.1021/jc00035a012>.
- (251) Myers, H. S. [Vapor-Liquid] Equilibrium for Naphthenes and Paraffins. *Pet. Refiner* **1957**, *36* (3), 175–178.
- (252) Siddiqi, M. A.; Lucas, K. An Isothermal High-Pressure Flow Calorimeter the Excess Enthalpy of (Cyclohexane + n-Hexane) at Different Pressures at 288.15, 298.15, and 313.15 K. *The Journal of Chemical Thermodynamics* **1982**, *14* (12), 1183–1190. [https://doi.org/10.1016/0021-9614\(82\)90042-8](https://doi.org/10.1016/0021-9614(82)90042-8).
- (253) Ewing, M. B.; Marsh, K. N. The Enthalpy of Mixing of N-Hexane + Cyclohexane at 288.15 and 318.15 K. *The Journal of Chemical Thermodynamics* **1970**, *2* (2), 295–296. [https://doi.org/10.1016/0021-9614\(70\)90094-7](https://doi.org/10.1016/0021-9614(70)90094-7).
- (254) Christensen, J. J.; Izatt, R. M.; Eatough, D. J.; Hansen, L. D. The Effect of Pressure on the Excess Enthalpies of Cyclohexane + N-Hexane at 298.15 K. *The Journal of Chemical Thermodynamics* **1978**, *10* (1), 25–34. [https://doi.org/10.1016/0021-9614\(78\)90145-3](https://doi.org/10.1016/0021-9614(78)90145-3).
- (255) Heintz, A.; Lichtenthaler, R. N. An Isothermal Flow Calorimeter for Pressures to 600 Bar. *Berichte der Bunsengesellschaft für physikalische Chemie* **1979**, *83* (8), 853–856. <https://doi.org/10.1002/bbpc.19790830816>.
- (256) Gmehling, J.; Meents, B. Excess Enthalpy. Cyclohexane-Hexane System. *Int. Data Ser. Sel. Data Mixtures Ser. A* **1992**, No. 3, 144.
- (257) 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* (3), 181–190.
- (258) Saito, A.; Tanaka, R. Excess Volumes and Heat Capacities of Binary Mixtures Formed from Cyclohexane, Hexane, and Heptane at 298.15 K. *The Journal of Chemical Thermodynamics* **1988**, *20* (7), 859–865. [https://doi.org/10.1016/0021-9614\(88\)90075-4](https://doi.org/10.1016/0021-9614(88)90075-4).
- (259) Hissong, D. W.; Kay, W. B. Critical Properties of Hydrocarbons. II. Correlational Studies. *Proc. Am. Pet. Inst. Refin. Dep.* **1968**, *48*, 397–463.

- (260) Kassmann, K.-D.; Knapp, H. Vapor-Liquid Equilibria for Binary and Ternary Mixtures of Benzene, Toluene and n-Butyraldehyde. *Berichte der Bunsengesellschaft für physikalische Chemie* **1986**, *90* (5), 452–458. <https://doi.org/10.1002/bbpc.19860900514>.
- (261) Saito, S. Separation of Hydrocarbons. 2. Vapor-Liquid Equilibriums of Normal Paraffin-Aromatic Systems. *Asahi Garasu Kogyo Gijutsu Shoreikai Kenkyu Hokoku* **1969**, *15*, 397–407.
- (262) Jin, Z.; Hu, A.; Liu, K.; Zhangli, Jin. VLE of Binary and Ternary Systems for BTX Mixtures. *Chemical Engineering (China)* **1991**, *19* (6), 56–60.
- (263) Schubert, H. Phasengleichgewichtsmessungen. II. Vorausberechnung von Gleichgewichtsdaten Dampfförmig-Flüssig Idealer Binärer Systeme Und Prüfung Derselben Mittels Einer Neuen Gleichgewichtsapparatur. *Journal für Praktische Chemie* **1958**, *6* (2), 129–138. <https://doi.org/10.1002/prac.19580060209>.
- (264) Baud, E. Thermal Analysis of Binary Mixtures. *Bull. Soc. Chim. Fr.* **1915**, *17*, 329–345.
- (265) 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. *The Journal of Chemical Thermodynamics* **1975**, *7* (5), 435–442. [https://doi.org/10.1016/0021-9614\(75\)90273-6](https://doi.org/10.1016/0021-9614(75)90273-6).
- (266) Murakami, S.; Lam, V. T.; Benson, G. C. The Thermodynamic Properties of Binary Aromatic Systems II. Excess Enthalpies and Volumes of Benzene + Toluene and Toluene + Isomeric Xylene Mixtures at 25 °C. *The Journal of Chemical Thermodynamics* **1969**, *1* (4), 397–407. [https://doi.org/10.1016/0021-9614\(69\)90070-6](https://doi.org/10.1016/0021-9614(69)90070-6).
- (267) Diaz Pena, M.; Menduina, C. Semicontinuous Calorimeter for Measuring Heats of Mixing. *An. Quim.* **1973**, *69*, 857–868.
- (268) Fortier, J. L.; Benson, G. C. Heat Capacities of Some Binary Aromatic Hydrocarbon Mixtures Containing Benzene or Toluene. *Journal of Chemical & Engineering Data* **1979**, *24* (1), 34–37. <https://doi.org/10.1021/je60080a015>.
- (269) Kay, W. B.; Hissong, D. The Critical Properties of Hydrocarbons. I. Simple Mixtures. *Proc. Am. Pet. Inst. Refin. Dep.* **1967**, *47*, 653–722.
- (270) Vaughan, W. E.; Collins, F. C. P-V-T-x Relations of the System Propane-Isopentane. *Industrial & Engineering Chemistry* **1942**, *34* (7), 885–890. <https://doi.org/10.1021/ie50391a027>.
- (271) Zhang, X.; Zheng, Y.; Zhao, W. Measurement and Correlation of Vapor Liquid Equilibrium Data for Benzene Cyclohexane Methyl Cyclohexane DMF Systems. *Natural Gas Chemical Industry* **1997**, *22* (5), 52–55.
- (272) 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. *The Journal of Chemical Thermodynamics* **1975**, *7* (4), 369–376. [https://doi.org/10.1016/0021-9614\(75\)90175-5](https://doi.org/10.1016/0021-9614(75)90175-5).
- (273) Ott, J. B.; Marsh, K. N.; Stokes, R. H. Excess Enthalpies, Excess Gibbs Free Energies, and Excess Volumes for (Cyclohexane + n-Hexane), and Excess Gibbs Free Energies and Excess Volumes for (Cyclohexane + Methylcyclohexane) at 298.15 and 308.15 K. *The Journal of Chemical Thermodynamics* **1980**, *12* (12), 1139–1148. [https://doi.org/10.1016/S0021-9614\(80\)80006-1](https://doi.org/10.1016/S0021-9614(80)80006-1).
- (274) Tamura, K. Excess Heat Capacities of the Mixtures Containing Methylcyclohexane at 298.15 K. *Fluid Phase Equilibria* **2001**, *182* (1–2), 303–312. [https://doi.org/10.1016/S0378-3812\(01\)00407-1](https://doi.org/10.1016/S0378-3812(01)00407-1).
- (275) Djordjevich, L.; Budenholzer, R. A. Vapor-Liquid Equilibrium Data for Ethane-Propane System at Low Temperatures. *Journal of Chemical & Engineering Data* **1970**, *15* (1), 10–12. <https://doi.org/10.1021/je60044a020>.

- (276) Hirata, M.; Suda, S.; Hakuta, T.; Nagahama, K. Light Hydrocarbon Vapor-Liquid Equilibria. *Mem. Fac. Technol. Tokyo Metropol. Univ.* **1969**, *19*, 103–122.
- (277) 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* (1), 35–36.
- (278) Blanc, C. J.; Setier, J. C. B. Vapor-Liquid Equilibria for the Ethane-Propane System at Low Temperature. *Journal of Chemical & Engineering Data* **1988**, *33* (2), 111–115. <https://doi.org/10.1021/je00052a015>.
- (279) Clark, A. Q.; Stead, K. (Vapour + Liquid) Phase Equilibria of Binary, Ternary, and Quaternary Mixtures of CH₄, C₂H₆, C₃H₈, C₄H₁₀, and CO₂. *The Journal of Chemical Thermodynamics* **1988**, *20* (4), 413–427. [https://doi.org/10.1016/0021-9614\(88\)90178-4](https://doi.org/10.1016/0021-9614(88)90178-4).
- (280) Kahre, L. C. Liquid Density of Light Hydrocarbon Mixtures. *Journal of Chemical & Engineering Data* **1973**, *18* (3), 267–270. <https://doi.org/10.1021/je60058a030>.
- (281) Pöll, H.; Huemer, H.; Moser, F. Eine Apparatur Zur Bestimmung von Dampf-Flüssigkeits-Gleichgewichten Unter Erhöhtem Druck. *Monatshefte für Chemie* **1980**, *111* (5), 1159–1164. <https://doi.org/10.1007/BF00909673>.
- (282) Miksovsky, J.; Wichterle, I. Liquid-Vapor Equilibrium. LXX. Vapor -Liquid Equilibriums in the Ethane-Propane System at High Pressures. *Collect. Czech. Chem. Commun.* **1975**, *40* (2), 365–370. <https://doi.org/10.1135/cccc19750365>.
- (283) Matschke, D. E.; Thodos, G. Vapor-Liquid Equilibriums for the Ethane-Propane System. *J. Chem. Eng. Data* **1962**, *7* (2), 232–234. <https://doi.org/10.1021/je60013a022>.
- (284) Ott, J. B.; Brown, P. R.; Moore, J. D.; Lewellen, A. C. Excess Molar Enthalpies and Excess Molar Volumes for (Propane + Ethane) over the Temperature Range from 273.15 K to 373.15 K and the Pressure Range from 5 MPa to 15 MPa. *The Journal of Chemical Thermodynamics* **1997**, *29* (2), 149–178. <https://doi.org/10.1006/jcht.1996.0144>.
- (285) Horstmann, S.; Fischer, K.; Gmehling, J. Experimental Determination of Critical Data of Mixtures and Their Relevance for the Development of Thermodynamic Models. *Chemical Engineering Science* **2001**, *56* (24), 6905–6913. [https://doi.org/10.1016/S0009-2509\(01\)00332-3](https://doi.org/10.1016/S0009-2509(01)00332-3).
- (286) 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 Equilibria* **1999**, *165* (2), 157–168. [https://doi.org/10.1016/S0378-3812\(99\)00275-7](https://doi.org/10.1016/S0378-3812(99)00275-7).
- (287) Uchytel, 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 Equilibria* **1983**, *15* (2), 209–217. [https://doi.org/10.1016/0378-3812\(83\)80153-8](https://doi.org/10.1016/0378-3812(83)80153-8).
- (288) Kahre, L. C. Low-Temperature K Data for Methane-Butane. *Journal of Chemical & Engineering Data* **1974**, *19* (1), 67–71. <https://doi.org/10.1021/je60060a014>.
- (289) Elliot, D. G.; Chen, R. J. J.; Chappellear, P. S.; Kobayashi, R. Vapor-Liquid Equilibrium of Methane-Butane System at Low Temperatures and High Pressures. *Journal of Chemical & Engineering Data* **1974**, *19* (1), 71–77. <https://doi.org/10.1021/je60060a015>.
- (290) Wiese, H. C.; Jacobs, J.; Sage, B. H. Phase Equilibriums in the Hydrocarbon Systems. Phase Behavior in the Methane-Propane-n-Butane System. *Journal of Chemical & Engineering Data* **1970**, *15* (1), 82–91. <https://doi.org/10.1021/je60044a021>.
- (291) Sage, R. H.; Hicks, B. L.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. *Industrial & Engineering Chemistry* **1940**, *32* (8), 1085–1092. <https://doi.org/10.1021/ie50368a014>.

- (292) Rigas, T. J.; Mason, D. F.; Thodos, G. Vapor-Liquid Equilibria. Microsampling Technique Applied to a New Variable-Volume Cell. *Industrial & Engineering Chemistry* **1958**, *50* (9), 1297–1300. <https://doi.org/10.1021/ie50585a039>.
- (293) Sprow, F. B.; Prausnitz, J. M. Vapor-Liquid Equilibria for Five Cryogenic Mixtures. *AIChE Journal* **1966**, *12* (4), 780–784. <https://doi.org/10.1002/aic.690120427>.
- (294) Calado, J. C. G.; Staveley, L. A. K. Excess Gibbs Energy of Argon-Methane Liquid Mixtures at 115.77°K. *The Journal of Chemical Physics* **1972**, *56* (9), 4718–4719. <https://doi.org/10.1063/1.1677927>.
- (295) Shatskaya, L. V.; Zhirnova, N. A. Liquid-Vapor Phase Equilibria in Two-Component Systems at Low Temperatures. I. Argon-Methane System. *Russ. J. Phys. Chem.* **1976**, *50* (2), 298–298.
- (296) Kehlen, H.; Schneider, F.-U.; Haufe, S.; Barnitzke, W. Auswertung von Taudruckmessungen Binärer Systeme Im Mitteldruckbereich. *Zeitschrift für Physikalische Chemie* **1983**, *264O* (1). <https://doi.org/10.1515/zpch-1983-26497>.
- (297) Christiansen, L. J.; Fredenslund, Aa. Vapour-Liquid Equilibria of the CH₄-Ar-CO System. *Cryogenics* **1974**, *14* (1), 10–14. [https://doi.org/10.1016/0011-2275\(74\)90037-X](https://doi.org/10.1016/0011-2275(74)90037-X).
- (298) Christiansen, L. J.; Fredenslund, Aa.; Mollerup, J. Vapour-Liquid Equilibrium of the CH₄-Ar, CH₄-CO, and Ar-CO Systems at Elevated Pressures. *Cryogenics* **1973**, *13* (7), 405–413. [https://doi.org/10.1016/0011-2275\(73\)90076-3](https://doi.org/10.1016/0011-2275(73)90076-3).
- (299) Lewis, K. L.; Saville, G.; Staveley, L. A. K. Excess Enthalpies of Liquid Oxygen + Argon, Oxygen + Nitrogen, and Argon + Methane. *The Journal of Chemical Thermodynamics* **1975**, *7* (4), 389–400. [https://doi.org/10.1016/0021-9614\(75\)90178-0](https://doi.org/10.1016/0021-9614(75)90178-0).
- (300) Mosedale, S. E.; Wormald, C. J. The Enthalpy of Mixing of Argon + Methane at 123, 130, 140, and 145 K, at Pressures up to 9.12 MPa. *The Journal of Chemical Thermodynamics* **1977**, *9* (5), 483–490. [https://doi.org/10.1016/0021-9614\(77\)90149-5](https://doi.org/10.1016/0021-9614(77)90149-5).
- (301) Lewis, K. L.; Mosedale, S. E.; Wormald, C. J. The Enthalpies of Mixing of Methane + Argon, Methane + Nitrogen, and Methane + Hydrogen in the Gaseous and Two-Phase Regions. *The Journal of Chemical Thermodynamics* **1977**, *9* (2), 121–131. [https://doi.org/10.1016/0021-9614\(77\)90077-5](https://doi.org/10.1016/0021-9614(77)90077-5).
- (302) 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. *The Journal of Chemical Thermodynamics* **1977**, *9* (1), 27–42. [https://doi.org/10.1016/0021-9614\(77\)90194-X](https://doi.org/10.1016/0021-9614(77)90194-X).
- (303) Paul, H. I.; Krug, J.; Knapp, H. Measurements of VLE, vE and HE for Binary Mixtures of n-Alkanes with Chloro-Alkylbenzenes. *Fluid Phase Equilibria* **1988**, *39* (3), 307–324. [https://doi.org/10.1016/0378-3812\(88\)85010-6](https://doi.org/10.1016/0378-3812(88)85010-6).
- (304) Bayles, J. W.; Letcher, T. M. Thermodynamics of Some Binary Liquid Mixtures Containing Aliphatic Amines. *Journal of Chemical & Engineering Data* **1971**, *16* (3), 266–271. <https://doi.org/10.1021/je60050a026>.
- (305) 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 Equilibria* **2006**, *240* (1), 109–113. <https://doi.org/10.1016/j.fluid.2005.11.020>.
- (306) 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* (4), 47–49.
- (307) 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* (4), 384–388.

- (308) 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* (2), 367–373. <https://doi.org/10.1051/jcp/1973700367>.
- (309) Bendiab, H.; Roux-Desgranges, G.; Roux, A. H.; Grolier, J.-P. E.; Patterson, D. Excess Heat Capacities of Ternary Systems Containing Chlorobenzene or Chloronaphthalene. *Journal of Solution Chemistry* **1994**, *23* (2), 307–323. <https://doi.org/10.1007/BF00973552>.
- (310) Díaz Peña, M.; Compostizo, A.; Crespo Colín, A.; Escudero, I. Activity Coefficients and Excess Gibbs Free Energies at 348.15 K in Cyclohexane+chlorobenzene, +fluorobenzene, and +thiophene. *The Journal of Chemical Thermodynamics* **1980**, *12* (11), 1051–1055. [https://doi.org/10.1016/0021-9614\(80\)90160-3](https://doi.org/10.1016/0021-9614(80)90160-3).
- (311) 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. *Journal of Chemical & Engineering Data* **2001**, *46* (2), 256–260. <https://doi.org/10.1021/je0000591>.
- (312) Tanaka, R.; Murakami, S.; Fujishiro, R. Excess Enthalpies of Mixing of a Polar Liquid + a Non-Polar Liquid at 298.15 K. *The Journal of Chemical Thermodynamics* **1974**, *6* (3), 209–218. [https://doi.org/10.1016/0021-9614\(74\)90172-4](https://doi.org/10.1016/0021-9614(74)90172-4).
- (313) 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. *Bulletin of the Chemical Society of Japan* **1961**, *34* (9), 1278–1285. <https://doi.org/10.1246/bcsj.34.1278>.
- (314) Anantaraman, A. V.; Bhattacharyya, S. N.; Palit, S. R. Weak Dipolar Interaction in Solutions. Systems: Cyclohexane+chlorobenzene and Carbon Tetrachloride+chlorobenzene. *Transactions of the Faraday Society* **1961**, *57*, 40. <https://doi.org/10.1039/tf9615700040>.
- (315) 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. *Journal of Chemical & Engineering Data* **1990**, *35* (3), 266–271. <https://doi.org/10.1021/je00061a012>.
- (316) Azpiazu, Y.; Royo, F.; Gutiérrez Losa, C. Vapour Pressures of (Tetrachloromethane + α,ω -Dichloroalkane). *The Journal of Chemical Thermodynamics* **1984**, *16* (6), 561–565. [https://doi.org/10.1016/0021-9614\(84\)90007-7](https://doi.org/10.1016/0021-9614(84)90007-7).
- (317) Sagnes, Michele.; Sanchez, Victor. Vapor-Liquid Equilibria for Fourteen Systems Consisting of Chlorinated Hydrocarbons and Alcohols. *Journal of Chemical & Engineering Data* **1971**, *16* (3), 351–354. <https://doi.org/10.1021/je60050a038>.
- (318) Baños, I.; Valero, J.; Gracia, M.; Losa, C. G. Conformational Equilibrium and Calorimetric Behaviour of Systems Containing 1,2-Dichloroethane. *Berichte der Bunsengesellschaft für physikalische Chemie* **1983**, *87* (10), 866–871. <https://doi.org/10.1002/bbpc.19830871007>.
- (319) Marongiu, B. Excess Enthalpies of Alpha, Omega-Dichloroalkane (C1 - C6) + Tetrachloromethane. *Int. Data Ser. Sel. Data Mixtures Ser. A* **1988**, No. 1, 1–6.
- (320) Wilhelm, E.; Faradjzadeh, A.; Grolier, J.-P. E. Molar Excess Heat Capacities and Excess Volumes of 1,2-Dichloroethane + Cyclooctane, + Mesitylene, and + Tetrachloromethane. *The Journal of Chemical Thermodynamics* **1979**, *11* (10), 979–984. [https://doi.org/10.1016/0021-9614\(79\)90047-8](https://doi.org/10.1016/0021-9614(79)90047-8).
- (321) Ellis, S. R. M.; Contractor, R. M. Vapor-Liquid Equilibria at Reduced Pressure. *Chem. Eng. London* **1964**, *15* (1), 10–13.

- (322) Rollet, A. P.; Toledano, P.; Elkaim, G.; Sonez, M. Ebulliometry of Volatile Solutes. II. *Publ. Sci. Univ. Alger Ser. B* **1956**, *2*, 403–425.
- (323) Tschamler, H. Über Binäre Flüssige Mischungen VI: Mischungswärmen, Molwärmen, Volumeffekte Und Zustands-Diagramme von 1,2-Dichloräthan Mit Benzol Und n-Alkylbenzolen. *Monatshefte für Chemie* **1948**, *79* (6), 499–507. <https://doi.org/10.1007/BF00898687>.
- (324) 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* (3), 111–120.
- (325) 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. *Berichte der Bunsengesellschaft für physikalische Chemie* **1977**, *81* (10), 925–930. <https://doi.org/10.1002/bbpc.19770811009>.
- (326) Parrish, W. R.; Hiza, M. J. Liquid-Vapor Equilibria in the Nitrogen-Methane System between 95 and 120 K. In *Advances in Cryogenic Engineering*; 1995; pp 300–308.
- (327) 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. *Journal of Chemical & Engineering Data* **2012**, *57* (5), 1621–1626. <https://doi.org/10.1021/je201299u>.
- (328) Stryjek, R.; Chappellear, P. S.; Kobayashi, R. Low-Temperature Vapor-Liquid Equilibria of Nitrogen-Methane System. *Journal of Chemical & Engineering Data* **1974**, *19* (4), 334–339. <https://doi.org/10.1021/je60063a023>.
- (329) Cines, M. R.; Roach, J. T.; Hogan, R. J.; Roland, C. H. Nitrogen-Methane Vapor-Liquid Equilibria. *Chem. Eng. Progr. Symp. Ser.* **1953**, *49* (6), 1–10.
- (330) Bloomer, O. T.; Parent, J. D. Liquid-Vapor Phase Behavior of the Methane-Nitrogen System. *Chem. Eng. Progr. Symp. Ser.* **1953**, *49* (6), 11–24.
- (331) 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* (9), 531–540. [https://doi.org/10.1016/0011-2275\(75\)90149-6](https://doi.org/10.1016/0011-2275(75)90149-6).
- (332) Brandt, L. W.; Stroud, Lowell. Phase Equilibria in Natural Gas Systems. Apparatus with Windowed Cell for 800 P.S.I.G. and Temperatures to –320° F. *Industrial & Engineering Chemistry* **1958**, *50* (5), 849–852. <https://doi.org/10.1021/ie50581a046>.
- (333) McClure, D. W.; Lewis, K. L.; Miller, R. C.; Staveley, L. A. K. Excess Enthalpies and Gibbs Free Energies for Nitrogen + Methane at Temperatures below the Critical Point of Nitrogen. *The Journal of Chemical Thermodynamics* **1976**, *8* (8), 785–792. [https://doi.org/10.1016/0021-9614\(76\)90057-4](https://doi.org/10.1016/0021-9614(76)90057-4).
- (334) Klein, R. R.; Bennett, C. O.; Dodge, B. F. Experimental Heats of Mixing for Gaseous Nitrogen and Methane. *AIChE Journal* **1971**, *17* (4), 958–965. <https://doi.org/10.1002/aic.690170432>.
- (335) Gomes de Azevedo, E. J. S.; Calado, J. C. G. Thermodynamics of Liquid Methane+ethane. *Fluid Phase Equilibria* **1989**, *49*, 21–34. [https://doi.org/10.1016/0378-3812\(89\)80003-2](https://doi.org/10.1016/0378-3812(89)80003-2).
- (336) Miller, R. C.; Kidnay, A. J.; Hiza, M. J. Liquid + Vapor Equilibria in Methane + Ethene and in Methane + Ethane from 150.00 to 190.00 K. *The Journal of Chemical Thermodynamics* **1977**, *9* (2), 167–178. [https://doi.org/10.1016/0021-9614\(77\)90082-9](https://doi.org/10.1016/0021-9614(77)90082-9).
- (337) Wichterle, I.; Kobayashi, R. Vapor-Liquid Equilibrium of Methane-Ethane System at Low Temperatures and High Pressures. *Journal of Chemical & Engineering Data* **1972**, *17* (1), 9–12. <https://doi.org/10.1021/je60052a022>.
- (338) 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 Temperatures from 207 to 270 K. *Journal of Chemical & Engineering Data* **1995**, *40* (4), 726–731. <https://doi.org/10.1021/je00020a002>.
- (339) 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. *Journal of Chemical & Engineering Data* **1976**, *21* (1), 81–84. <https://doi.org/10.1021/je60068a030>.
- (340) Werner, G.; Schubert, H. Das Phasengleichgewicht Flüssig-Flüssig Des Systems Benzol/n-Heptan/Acetonitril Sowie Die Phasengleichgewichte Dampförmig-Flüssig Der Entsprechenden Binären Systeme Bei 20,0 °C. *Journal für Praktische Chemie* **1966**, *31* (5–6), 225–239. <https://doi.org/10.1002/prac.19660310501>.
- (341) 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. *The Journal of Chemical Thermodynamics* **1970**, *2* (6), 805–811. [https://doi.org/10.1016/0021-9614\(70\)90023-6](https://doi.org/10.1016/0021-9614(70)90023-6).
- (342) Sun, Y.; Yen, W. H. Vapor Pressures and Excess Gibbs Free Energies of Benzene-Cyclohexane, Benzene-n-Heptane and Cyclohexane-n-Heptane. *Gaodeng Xuexiao Huaxue Xuebao* **1986**, *7* (1), 54–58.
- (343) Messow, U.; Schuetze, D.; Pfestorf, R.; Kuchenbecker, D.; Suehnel, K. Thermodynamische Untersuchungen an Lösungsmittel/n-Paraffin-Systemen. *Z. Phys. Chem. Leipzig* **1977**, *258* (1), 24–32.
- (344) Palmer, D. A.; Smith, B. D. Thermodynamic Excess Property Measurements for Acetonitrile-Benzene-n-Heptane System at 45°C. *Journal of Chemical & Engineering Data* **1972**, *17* (1), 71–76. <https://doi.org/10.1021/je60052a037>.
- (345) 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* (4), 292–296.
- (346) Hanson, D. O.; Van Winkle, M. Alteration of the Relative Volatility of Hexane-1-Hexene by Oxygenated and Chlorinated Solvents. *Journal of Chemical & Engineering Data* **1967**, *12* (3), 319–325. <https://doi.org/10.1021/je60034a009>.
- (347) Brown, I. Liquid-Vapour Equilibria. III. The Systems Benzene- n-Heptane, n-Hexane-Chlorobenzene, and Cyclohexane-Nitrobenzene. *Australian Journal of Chemistry* **1952**, *5* (3), 530. <https://doi.org/10.1071/CH9520530>.
- (348) Brown, I.; Ewald, A. Liquid-Vapour Equilibria II. The System Benzene-Heptane. *Australian Journal of Chemistry* **1951**, *4* (2), 198. <https://doi.org/10.1071/CH9510198>.
- (349) Nielsen, R. L.; Weber, J. H. Vapor-Liquid Equilibria at Subatmospheric Pressures. Binary and Ternary Systems Containing Ethyl Alcohol, Benzene, and n-Heptane. *Journal of Chemical & Engineering Data* **1959**, *4* (2), 145–151. <https://doi.org/10.1021/je60002a011>.
- (350) Sieg, L. Flüssigkeit-Dampf-Gleichgewichte in Binären Systemen von Kohlenwasserstoffen Verschiedenen Typs: Flüssigkeit-Dampf-Gleichgewichte in Binären Systemen von Kohlenwasserstoffen Verschiedenen Typs. *Chemie Ingenieur Technik* **1950**, *22* (15), 322–326. <https://doi.org/10.1002/cite.330221503>.
- (351) Michishita, T.; Arai, Y.; Saito, S. Vapor-Liquid Equilibriums of Hydrocarbons at Atmospheric Pressure. *Kagaku Kogaku* **1971**, *35* (1), 111–0. <https://doi.org/10.1252/kakoronbunshu1953.35.111>.
- (352) Wang, Q.; Chen, G.; Han, S. Study on the Vapor-Liquid Equilibria under Pressure for Binary Systems. *Ranliao Huaxue Xuebao* **1990**, *18* (2), 185–192.
- (353) Vilcu, R.; Stanciu, F. Excess Thermodynamic Functions from Calorimetric Data. *Rev. Roum. Chim.* **1966**, *11* (2), 175–182.

- (354) Hammerl, I.; Raetzsch, M. T. Enthalpies of Mixing of Normal Paraffins with Aromatics. *Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg* **1973**, *15* (3), 175–178.
- (355) Tanaka, R. Excess Heat Capacities for Mixture of Benzene with N-Heptane at 293.15, 298.15, and 303.15 K. *Journal of Chemical & Engineering Data* **1987**, *32* (2), 176–177. <https://doi.org/10.1021/je00048a014>.
- (356) 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* (2), 95–96.
- (357) 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. *Chemical Engineering Science* **1978**, *33* (2), 189–197. [https://doi.org/10.1016/0009-2509\(78\)85053-2](https://doi.org/10.1016/0009-2509(78)85053-2).
- (358) Mentzer, R. A.; Greenkorn, R. A.; Chao, K. C. Bubble Pressures and Vapor-Liquid Equilibria for Four Binary Hydrocarbon Mixtures. *The Journal of Chemical Thermodynamics* **1982**, *14* (9), 817–830. [https://doi.org/10.1016/0021-9614\(82\)90155-0](https://doi.org/10.1016/0021-9614(82)90155-0).
- (359) Kurihara, K.; Uchiyama, M.; Kojima, K. Isothermal Vapor–Liquid Equilibria for Benzene + Cyclohexane + 1-Propanol and for Three Constituent Binary Systems. *Journal of Chemical & Engineering Data* **1997**, *42* (1), 149–154. <https://doi.org/10.1021/je9602475>.
- (360) Boublík, T. An Estimate of Limiting Values of Relative Volatility with Help of the Theorem of Corresponding States. II. Binary Systems of Tetrachloromethane, Benzene, and Cyclohexane. *Collection of Czechoslovak Chemical Communications* **1963**, *28* (7), 1771–1779. <https://doi.org/10.1135/cccc19631771>.
- (361) Scatchard, George.; Wood, S. E.; Mochel, J. M. Vapor–Liquid Equilibrium. III. Benzene–Cyclohexane Mixtures. *The Journal of Physical Chemistry* **1939**, *43* (1), 119–130. <https://doi.org/10.1021/j150388a009>.
- (362) 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. *Journal of Chemical & Engineering Data* **2011**, *56* (5), 2386–2392. <https://doi.org/10.1021/je101304x>.
- (363) Wiśniewska, B.; Gregorowicz, J.; Malanowski, S. Development of a Vapour-Liquid Equilibrium Apparatus to Work at Pressures up to 3 MPa. *Fluid Phase Equilibria* **1993**, *86*, 173–186. [https://doi.org/10.1016/0378-3812\(93\)87174-Y](https://doi.org/10.1016/0378-3812(93)87174-Y).
- (364) Lafuente, C.; Pardo, J.; Santate, J.; Royo, F.; Urieta, J. Use of a Fischer-Labodest Apparatus to Study the Liquid-Vapor Equilibrium of the Benzene-Cyclohexane System at Different Pressures. *Rev. Acad. Cienc. Exact. Fis. Quim. Nat. Zaragoza* **1992**, *47*, 183–190.
- (365) Rao, V. N. K.; Swami, D. R.; Rao, M. N. Vapor-Liquid Equilibria of Benzene–n-Hexane and Benzene-Cyclohexane Systems. *AIChE Journal* **1957**, *3* (2), 191–197. <https://doi.org/10.1002/aic.690030213>.
- (366) Elliott, K.; Wormald, C. J. A Precision Differential Flow Calorimeter the Excess Enthalpy of Benzene + Cyclohexane between 280.15 K and 393.15 K. *The Journal of Chemical Thermodynamics* **1976**, *8* (9), 881–893. [https://doi.org/10.1016/0021-9614\(76\)90166-X](https://doi.org/10.1016/0021-9614(76)90166-X).
- (367) Yan, W.-D.; Lin, R.-S.; Yen, W.-H. Excess Enthalpies of Seven Binary Liquid Systems. *Thermochimica Acta* **1990**, *169*, 171–184. [https://doi.org/10.1016/0040-6031\(90\)80143-M](https://doi.org/10.1016/0040-6031(90)80143-M).
- (368) Didaoui-Nemouchi, S.; Ait-Kaci, A.; Rogalski, M. Enthalpies of Mixing of Binary and Ternary Mixtures Containing Diisopropylether, Benzene and Cyclohexane at 303.15 K. *Journal of Thermal Analysis and Calorimetry* **2005**, *79* (1), 85–88. <https://doi.org/10.1007/s10973-004-0566-5>.

- (369) van Ness, H. C.; Abbott, M. M. Excess Enthalpy. Benzene-Cyclohexane System. *Int. Data Ser. Sel. Data Mixtures Ser. A* **1974**, 1974 (3), 160–161.
- (370) Lohmann, J.; Bölts, R.; Gmehling, J. Excess Enthalpy Data for Seven Binary Systems at Temperatures between 50 and 140 °C. *Journal of Chemical & Engineering Data* **2001**, 46 (2), 208–211. <https://doi.org/10.1021/jc000297g>.
- (371) 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. *The Journal of Chemical Thermodynamics* **1982**, 14 (3), 259–268. [https://doi.org/10.1016/0021-9614\(82\)90016-7](https://doi.org/10.1016/0021-9614(82)90016-7).
- (372) Páramo, R.; Zouine, M.; Casanova, C. New Batch Cells Adapted To Measure Saturated Heat Capacities of Liquids. *Journal of Chemical & Engineering Data* **2002**, 47 (3), 441–448. <https://doi.org/10.1021/jc0155103>.
- (373) 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. *Thermochimica Acta* **1977**, 21 (2), 297–300. [https://doi.org/10.1016/0040-6031\(77\)85030-2](https://doi.org/10.1016/0040-6031(77)85030-2).
- (374) Grolier, J.-P. E.; Wilhelm, E.; Hamed, M. H. Molar Heat Capacity and Isothermal Compressibility of Binary Liquid Mixtures: Carbon Tetrachloride + Benzene, Carbon Tetrachloride + Cyclohexane and Benzene + Cyclohexane. *Berichte der Bunsengesellschaft für physikalische Chemie* **1978**, 82 (12), 1282–1290. <https://doi.org/10.1002/bbpc.19780821204>.
- (375) Calado, J. C. G.; Soares, V. A. M. Thermodynamics of Liquid Ethylene + Xenon at 161.38 K. *The Journal of Chemical Thermodynamics* **1977**, 9 (9), 911–913. [https://doi.org/10.1016/0021-9614\(77\)90176-8](https://doi.org/10.1016/0021-9614(77)90176-8).
- (376) Nunes da Ponte, M.; Chokappa, D.; Calado, J. C. G.; Zollweg, J.; Streett, W. B. Vapor-Liquid Equilibrium in the Xenon + Ethene System. *J. Phys. Chem.* **1986**, 90 (6), 1147–1152. <https://doi.org/10.1021/j100278a037>.
- (377) Lainez, A.; Rebelo, L. P. N.; Calado, J. C. G.; Streett, W. B.; Zollweg, J. A. Excess Enthalpies of Liquid (Ethene + Xenon) at 162.9 K. *The Journal of Chemical Thermodynamics* **1987**, 19 (1), 35–38. [https://doi.org/10.1016/0021-9614\(87\)90159-5](https://doi.org/10.1016/0021-9614(87)90159-5).
- (378) Wu, W.; Ke, J.; Poliakov, M. Phase Boundaries of CO₂ + Toluene, CO₂ + Acetone, and CO₂ + Ethanol at High Temperatures and High Pressures. *Journal of Chemical & Engineering Data* **2006**, 51 (4), 1398–1403. <https://doi.org/10.1021/jc060099a>.
- (379) Naidoo, P.; Ramjugernath, D.; Raal, J. D. A New High-Pressure Vapour-Liquid Equilibrium Apparatus. *Fluid Phase Equilibria* **2008**, 269 (1–2), 104–112. <https://doi.org/10.1016/j.fluid.2008.05.002>.
- (380) 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 (1), 10–13.
- (381) Hong, J. H.; Kobayashi, R. Multicomponent Vapor-Liquid Equilibria Measurements for the Development of an Extractive Distillation Process for the Processing of Gas Issuing from a Carbon Dioxide/EOR Project. *Ind. Eng. Chem. Process Design Develop.* **1986**, 25, 584–589. <https://doi.org/10.1021/i200033a041>.
- (382) 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. *Industrial & Engineering Chemistry Research* **1990**, 29 (2), 295–306. <https://doi.org/10.1021/ie00098a022>.
- (383) 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 (4), 438–443.

- (384) 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 Equilibria* **1986**, *31* (3), 299–311. [https://doi.org/10.1016/0378-3812\(86\)87014-5](https://doi.org/10.1016/0378-3812(86)87014-5).
- (385) Morris, W. O.; Donohue, M. D. Vapor-Liquid Equilibria in Mixtures Containing Carbon Dioxide, Toluene, and 1-Methylnaphthalene. *Journal of Chemical & Engineering Data* **1985**, *30* (3), 259–263. <https://doi.org/10.1021/je00041a007>.
- (386) Ng, H.-J.; Robinson, D. B. Equilibrium-Phase Properties of the Toluene-Carbon Dioxide System. *Journal of Chemical & Engineering Data* **1978**, *23* (4), 325–327. <https://doi.org/10.1021/je60079a020>.
- (387) Wormald, C. J.; Eyears, J. M. Excess Molar Enthalpies and Excess Molar Volumes of $\{x\text{CO}_2 + (1-x)\text{C}_6\text{H}_5\text{CH}_3\}$ at 298.15, 304.10, and 308.15 K from 7.5 to 12.6 MPa. *The Journal of Chemical Thermodynamics* **1987**, *19* (8), 845–856. [https://doi.org/10.1016/0021-9614\(87\)90031-0](https://doi.org/10.1016/0021-9614(87)90031-0).
- (388) Cordray, D. R.; Christensen, J. J.; Izatt, R. M. The Excess Enthalpies of (Carbon Dioxide + Toluene) at 308.15, 358.15, and 573.15 K from 6.98 to 16.63 MPa. *The Journal of Chemical Thermodynamics* **1986**, *18* (7), 647–656. [https://doi.org/10.1016/0021-9614\(86\)90066-2](https://doi.org/10.1016/0021-9614(86)90066-2).
- (389) Pando, C.; Renuncio, J. A. R.; Schofield, R. S.; Izatt, R. M.; Christensen, J. J. The Excess Enthalpies of (Carbon Dioxide + Toluene) at 308.15, 385.15, and 413.15 K from 7.60 to 12.67 MPa. *The Journal of Chemical Thermodynamics* **1983**, *15* (8), 747–755. [https://doi.org/10.1016/0021-9614\(83\)90141-6](https://doi.org/10.1016/0021-9614(83)90141-6).
- (390) Christensen, J. J.; Zebolsky, D. M.; Izatt, R. M. The Excess Enthalpies of (Carbon Dioxide + Toluene) at 470.15 and 573.15 K from 7.60 to 12.67 MPa. *The Journal of Chemical Thermodynamics* **1985**, *17* (1), 1–10. [https://doi.org/10.1016/0021-9614\(85\)90025-4](https://doi.org/10.1016/0021-9614(85)90025-4).
- (391) Reaves, J. T.; Griffith, A. T.; Roberts, C. B. Critical Properties of Dilute Carbon Dioxide + Entrainer and Ethane + Entrainer Mixtures. *Journal of Chemical & Engineering Data* **1998**, *43* (4), 683–686. <https://doi.org/10.1021/je9702753>.
- (392) Zhang, H.; Liu, Z.; Han, B. Critical Points and Phase Behavior of Toluene-CO₂ and Toluene-H₂-CO₂ Mixture in CO₂-Rich Region. *The Journal of Supercritical Fluids* **2000**, *18* (3), 185–192. [https://doi.org/10.1016/S0896-8446\(00\)00081-4](https://doi.org/10.1016/S0896-8446(00)00081-4).
- (393) Jiménez-Gallegos, R.; Galicia-Luna, L. A.; Elizalde-Solis, O. Experimental Vapor-Liquid Equilibria for the Carbon Dioxide + Octane and Carbon Dioxide + Decane Systems. *Journal of Chemical & Engineering Data* **2006**, *51* (5), 1624–1628. <https://doi.org/10.1021/je060111z>.
- (394) Iwai, Y.; Hosotani, N.; Morotomi, T.; Koga, Y.; Arai, Y. High-Pressure Vapor-Liquid Equilibria for Carbon Dioxide + Linalool. *Journal of Chemical & Engineering Data* **1994**, *39* (4), 900–902. <https://doi.org/10.1021/je00016a059>.
- (395) Nagarajan, N.; Robinson, R. L. Equilibrium Phase Compositions, Phase Densities, and Interfacial Tensions for Carbon Dioxide + Hydrocarbon Systems. 2. Carbon Dioxide + n-Decane. *Journal of Chemical & Engineering Data* **1986**, *31* (2), 168–171. <https://doi.org/10.1021/je00044a012>.
- (396) Reamer, H. H.; Sage, B. H. Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the n-Decane-CO₂ System. *Journal of Chemical & Engineering Data* **1963**, *8* (4), 508–513. <https://doi.org/10.1021/je60019a010>.
- (397) Inomata, H.; Tuchiya, K.; Arai, K.; Saito, S. Measurement of Vapor-Liquid Equilibria at Elevated Temperatures and Pressures Using a Flow Type Apparatus. *Journal of Chemical Engineering of Japan* **1986**, *19* (5), 386–391. <https://doi.org/10.1252/jcej.19.386>.

- (398) 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. *Journal of Chemical & Engineering Data* **1980**, *25* (2), 138–140. <https://doi.org/10.1021/je60085a012>.
- (399) Pando, C.; Renuncio, J. A. R.; McFall, T. A.; Izatt, R. M.; Christensen, J. J. The Excess Enthalpies of (Carbon Dioxide + Decane) from 283.15 to 323.15 K at 7.58 MPa. *The Journal of Chemical Thermodynamics* **1983**, *15* (2), 173–180. [https://doi.org/10.1016/0021-9614\(83\)90157-X](https://doi.org/10.1016/0021-9614(83)90157-X).
- (400) Christensen, J. J.; Cordray, D.; Izatt, R. M. The Excess Enthalpies of (Carbon Dioxide + Decane) from 293.15 to 573.15 K at 12.50 MPa. *The Journal of Chemical Thermodynamics* **1986**, *18* (1), 53–61. [https://doi.org/10.1016/0021-9614\(86\)90043-1](https://doi.org/10.1016/0021-9614(86)90043-1).
- (401) Gurdial, G. S.; Foster, N. R.; Yun, S. L. J.; Tilly, K. D. Phase Behavior of Supercritical Fluid—Entrainer Systems. In *Supercritical Fluid Engineering Science*; 1992; Vol. 514, pp 34–45.
- (402) Gulari, Es.; Saad, H.; Bae, Y. C. Effect of Critical Phenomena on Transport Properties in the Supercritical Region. In *Supercritical Fluids*; 1987; Vol. 329, pp 2–14.
- (403) 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 CO₂ and a N-Alkane. *Fluid Phase Equilibria* **2012**, *325*, 66–70. <https://doi.org/10.1016/j.fluid.2012.04.010>.
- (404) Polikhronidi, N. G.; Batyrova, R. G.; Abdulagatov, I. M.; Stepanov, G. V. Isochoric Heat Capacity of CO₂ + N-Decane Mixtures in the Critical Region. *International Journal of Thermophysics* **2006**, *27* (3), 729–759. <https://doi.org/10.1007/s10765-006-0056-z>.
- (405) Mraw, S. C.; Hwang, S.-C.; Kobayashi, R. Vapor-Liquid Equilibrium of the Methane-Carbon Dioxide System at Low Temperatures. *Journal of Chemical & Engineering Data* **1978**, *23* (2), 135–139. <https://doi.org/10.1021/je60077a014>.
- (406) Al-Sahhaf, T. A.; Kidnay, A. J.; Sloan, E. D. Liquid + Vapor Equilibria in the Nitrogen + Carbon Dioxide + Methane System. *Industrial & Engineering Chemistry Fundamentals* **1983**, *22* (4), 372–380. <https://doi.org/10.1021/i100012a004>.
- (407) Somait, F. A.; Kidnay, A. J. Liquid-Vapor Equilibria at 270.00 K for Systems Containing Nitrogen, Methane, and Carbon Dioxide. *Journal of Chemical & Engineering Data* **1978**, *23* (4), 301–305. <https://doi.org/10.1021/je60079a019>.
- (408) 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 Equilibria* **1992**, *81*, 175–186. [https://doi.org/10.1016/0378-3812\(92\)85150-7](https://doi.org/10.1016/0378-3812(92)85150-7).
- (409) Xu, N.; Dong, J.; Wang, Y.; Shi, J. Vapor Liquid Equilibria For N₂-CH₄-CO₂ System Near Critical Region. *Huagong Xuebao* **1992**, *43* (5), 640–644.
- (410) Lee, J. I.; Mather, A. E. The Excess Enthalpy of Gaseous Mixtures of Carbon Dioxide with Methane. *The Canadian Journal of Chemical Engineering* **1972**, *50* (1), 95–100. <https://doi.org/10.1002/cjce.5450500117>.
- (411) 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. *Journal of Chemical & Engineering Data* **1982**, *27* (3), 258–264. <https://doi.org/10.1021/je00029a010>.
- (412) 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. *Journal of Chemical Engineering of Japan* **1971**, *4* (2), 113–122. <https://doi.org/10.1252/jcej.4.113>.
- (413) Mraw, S. C.; Hwang, S. C.; Kobayashi, R. The Vapor-Liquid Equilibrium of the CH₄ - CO₂ System at Low Temperatures. *GPA Research Report* **1977**, 1–18.

- (414) Hwang, S. C.; Lin, H. M.; Chappellear, P. S.; Kobayashi, R. Dew-Point Values for the Methane - Carbon Dioxide System. *GPA Research Report* **1976**, 1–14.
- (415) 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. *Journal of Chemical & Engineering Data* **1991**, *36* (2), 188–192. <https://doi.org/10.1021/je00002a014>.
- (416) 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. *Journal of Chemical & Engineering Data* **1986**, *31* (1), 26–28. <https://doi.org/10.1021/je00043a008>.
- (417) Zhang Zhanzhu; Guo Liping; Yang Xiadong; Knapp, H. Vapor And Liquid Equilibrium For Nitrogen - Ethane - Carbon Dioxide Ternary System. *Huagong Xuebao* **1999**, *50* (3), 392–398.
- (418) 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. *Journal of Chemical & Engineering Data* **1999**, *44* (5), 926–931. <https://doi.org/10.1021/je980321e>.
- (419) Brown, T. S.; Sloan, E. D.; Kidnay, A. J. Vapor-Liquid Equilibria for the Ternary System N₂ + CO₂ + n-C₄H₁₀ at 250 and 270 K. *International Journal of Thermophysics* **1994**, *15* (6), 1211–1219. <https://doi.org/10.1007/BF01458829>.
- (420) Brown, T. S.; Niesen, V. G.; Sloan, E. D.; Kidnay, A. J. Vapor-Liquid Equilibria for the Binary Systems of Nitrogen, Carbon Dioxide, and n-Butane at Temperatures from 220 to 344 K. *Fluid Phase Equilibria* **1989**, *53*, 7–14. [https://doi.org/10.1016/0378-3812\(89\)80067-6](https://doi.org/10.1016/0378-3812(89)80067-6).
- (421) Al-Sahhaf, T. A. Vapor—Liquid Equilibria for the Ternary System N₂ + CO₂ + CH₄ at 230 and 250 K. *Fluid Phase Equilibria* **1990**, *55* (1–2), 159–172. [https://doi.org/10.1016/0378-3812\(90\)85010-8](https://doi.org/10.1016/0378-3812(90)85010-8).
- (422) Yorizane, M.; Yoshimura, S.; Masuoka, H. Vapor Liquid Equilibrium at High Pressures. N₂-CO₂, H₂-CO₂ Systems. *Kagaku Kogaku* **1970**, *34* (9), 953–957. <https://doi.org/10.1252/kakoronbunshu1953.34.953>.
- (423) Zenner, G. H.; Dana, L. I. Liquid-Vapor Equilibrium Compositions of Carbon Dioxideoxygen-Nitrogen Mixtures. *Chem. Eng. Progr. Symp. Ser.* **1963**, *59* (44), 36–41.
- (424) Kaminishi, G. I.; Toriumi, T. Gas-Liquid Equilibrium under High Pressures. VI. Vapor-Liquid Phase Equilibrium in the CO₂-H₂, CO₂-N₂, and CO₂-O₂ Systems. *Kogyo Kagaku Zasshi* **1966**, *69*, 175–178.
- (425) Krichevskii, I. R.; Khazanova, N. E.; Lesnevskaya, L. S.; Sandalova, L. Yu. Liquid-Gas Equilibrium in the Nitrogen-Carbon Dioxide System under Elevated Pressures. *Khim. Promst. Moscow* **1962**, No. 3, 169–171.
- (426) 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 Equilibria* **1993**, *90* (1), 177–187. [https://doi.org/10.1016/0378-3812\(93\)85012-B](https://doi.org/10.1016/0378-3812(93)85012-B).
- (427) Lee, J. I.; Mather, A. E. Excess Enthalpy of Gaseous Mixtures of Nitrogen and Carbon Dioxide. *Journal of Chemical & Engineering Data* **1972**, *17* (2), 189–192. <https://doi.org/10.1021/je60053a042>.
- (428) Hejmadi, A. V.; Katz, D. L.; Powers, J. E. Experimental Determination of the Enthalpy of Mixing of N + CO₂ under Pressure. *The Journal of Chemical Thermodynamics* **1971**, *3* (4), 483–496. [https://doi.org/10.1016/S0021-9614\(71\)80030-7](https://doi.org/10.1016/S0021-9614(71)80030-7).
- (429) Reamer, H. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems - Volumetric and Phase Behavior of the Methane-Hydrogen Sulfide System. *Industrial & Engineering Chemistry* **1951**, *43* (4), 976–981. <https://doi.org/10.1021/ie50496a052>.

- (430) Kohn, J. P.; Kurata, F. Heterogeneous Phase Equilibria of the Methane—Hydrogen Sulfide System. *AIChE Journal* **1958**, *4* (2), 211–217. <https://doi.org/10.1002/aic.690040217>.
- (431) Barry, A. O.; Kaliaguine, S. C.; Ramalho, R. S. Excess Enthalpies of the Binary System Methane-Hydrogen Sulfide by Flow Calorimetry. *Journal of Chemical & Engineering Data* **1982**, *27* (4), 436–439. <https://doi.org/10.1021/je00030a020>.
- (432) Fall, D. J.; Luks, K. D. Phase Equilibria Behavior of the Systems Carbon Dioxide + N-Dotriacontane and Carbon Dioxide + n-Docosane. *Journal of Chemical & Engineering Data* **1984**, *29* (4), 413–417. <https://doi.org/10.1021/je00038a013>.
- (433) Tsai, F. N.; Yau, J. S. Solubility of Carbon Dioxide in N-Tetracosane and in n-Dotriacontane. *Journal of Chemical & Engineering Data* **1990**, *35* (1), 43–45. <https://doi.org/10.1021/je00059a014>.
- (434) 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 Equilibria* **1991**, *65*, 263–274. [https://doi.org/10.1016/0378-3812\(91\)87029-9](https://doi.org/10.1016/0378-3812(91)87029-9).
- (435) Segovia, J. J.; Martín, M. C.; R. Chamorro, C.; 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. This Paper Is Part of the Doctoral Thesis of J.J. Segovia.1. *Fluid Phase Equilibria* **1998**, *152* (2), 265–276. [https://doi.org/10.1016/S0378-3812\(98\)00384-7](https://doi.org/10.1016/S0378-3812(98)00384-7).
- (436) 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* (5), 527–534.
- (437) 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. *Journal of Chemical & Engineering Data* **1997**, *42* (2), 243–247. <https://doi.org/10.1021/je960301h>.
- (438) Tusel-Langer, E.; Garcia Alonso, J. M.; Villamañán Olfos, M. A.; Lichtenthaler, R. N. Excess Enthalpies of Mixtures Containing N-Heptane, Methanol and Methyl Tert-Butyl Ether (MTBE). *Journal of Solution Chemistry* **1991**, *20* (1), 153–163. <https://doi.org/10.1007/BF00651647>.
- (439) 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. *The Journal of Chemical Thermodynamics* **2013**, *62*, 111–117. <https://doi.org/10.1016/j.jct.2013.03.002>.
- (440) Carr, A. D.; Kropholler, H. W. Vapor Liquid Equilibria at Atmospheric Pressure. Binary Systems of Ethyl Acetate-Benzene, Ethyl Acetate-Toluene, and Ethyl Acetate-p-Xylene. *Journal of Chemical & Engineering Data* **1962**, *7* (1), 26–28. <https://doi.org/10.1021/je60012a007>.
- (441) Delcros, S.; Jiménez, E.; Romani, L.; Roux, A. H.; Grolier, J.-P. E.; Kehiaian, H. V. Linear Alkanoates + Aromatic Hydrocarbon Binary Mixtures: New Excess Enthalpy Measurements and DISQUAC Analysis of Thermodynamic Properties. *Fluid Phase Equilibria* **1995**, *111* (1), 71–88. [https://doi.org/10.1016/0378-3812\(95\)02838-6](https://doi.org/10.1016/0378-3812(95)02838-6).
- (442) Gmehling, J.; Meents, B. Excess Enthalpy. Ethyl Ethanoate-Toluene System. *Int. Data Ser. Sel. Data Mixtures Ser. A* **1992**, No. 3, 177.
- (443) Jiménez, E. Excess Heat Capacities and Excess Volumes of (an n-Alkylalkanoate + Heptane or Decane or Toluene). *The Journal of Chemical Thermodynamics* **1994**, *26* (8), 817–827. <https://doi.org/10.1006/jct.1994.1098>.

- (444) Steinbrecher, M.; Bittrich, H.-J. Das Isotherme Flüssigkeits-Dampf-Gleichgewicht Der Binären Systeme Zwischen Den Komponenten Tetrachlormethan, Äthylacetat Und Dioxan. *Zeitschrift für Physikalische Chemie* **1966**, *2320* (1). <https://doi.org/10.1515/zpch-1966-23228>.
- (445) Drobig, J.; Lindenau, E. A New Apparatus to Determine the Isothermal Liquid-Vapor Equilibrium. *Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg* **1966**, *8*, 144–147.
- (446) Guillen, M. D.; Gutierrez Losa, C. Excess Enthalpies and Excess Volumes of N-Hexane + and of Tetrachloromethane + Furan, + 1,4-Dioxane, + Tetrahydrofuran, and + Tetrahydropyran. *The Journal of Chemical Thermodynamics* **1978**, *10* (6), 567–576. [https://doi.org/10.1016/0021-9614\(78\)90045-9](https://doi.org/10.1016/0021-9614(78)90045-9).
- (447) Murakami, S.; Benson, G. C. An Isothermal Dilution Calorimeter for Measuring Enthalpies of Mixing. *The Journal of Chemical Thermodynamics* **1969**, *1* (6), 559–572. [https://doi.org/10.1016/0021-9614\(69\)90016-0](https://doi.org/10.1016/0021-9614(69)90016-0).
- (448) Becker, F.; Kiefer, M.; Koukol, H. Kontinuierliche Bestimmung von Mischungswärmen Durch Quasi-Isotherme Wärmeflußkalorimetrie. *Z. Phys. Chem. NF* **1972**, *80*, 29–43.
- (449) McKinnon, I.; Williamson, A. Heats of Mixing of CCl₄ with Dioxane. *Australian Journal of Chemistry* **1964**, *17* (12), 1374. <https://doi.org/10.1071/CH9641374>.
- (450) Ohta, T.; Koyabu, J.; Nagata, I. Vapor–Liquid Equilibria for the Ternary Ethanol–2-Butanone–Benzene System at 298.15 K. *Fluid Phase Equilibria* **1981**, *7* (1), 65–73. [https://doi.org/10.1016/0378-3812\(81\)87006-9](https://doi.org/10.1016/0378-3812(81)87006-9).
- (451) Diaz Peña, M.; Crespo Colin, A.; Compostizo, A. Isothermal Liquid-Vapour Equilibria 2. The Binary Systems Formed by Benzene + Acetone, + Methyl Ethyl Ketone, + Methyl Propyl Ketone, and + Methyl Isobutyl Ketone. *The Journal of Chemical Thermodynamics* **1978**, *10* (11), 1101–1106. [https://doi.org/10.1016/0021-9614\(78\)90084-8](https://doi.org/10.1016/0021-9614(78)90084-8).
- (452) Kumarkrishna Rao, V. N.; Swami, D. R.; Narasinga Rao, M. High-Pressure Vapor-Liquid Equilibria of Nonideal Solutions. II. Benzene-Methyl Ethyl Ketone System. *J. Sci. Ind. Res. Sect. B* **1957**, *16*, 195–201.
- (453) 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. *The Journal of Chemical Thermodynamics* **1977**, *9* (4), 315–323. [https://doi.org/10.1016/0021-9614\(77\)90052-0](https://doi.org/10.1016/0021-9614(77)90052-0).
- (454) 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 Equilibria* **1999**, *156* (1–2), 73–87. [https://doi.org/10.1016/S0378-3812\(99\)00033-3](https://doi.org/10.1016/S0378-3812(99)00033-3).
- (455) 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. *Journal of Chemical & Engineering Data* **2011**, *56* (5), 2256–2265. <https://doi.org/10.1021/je101250d>.
- (456) Kammerer, K.; Lichtenthaler, R. N. Excess Enthalpy HE of Binary Mixtures Containing Alkanes, Methanol and Tert-Amyl-Methyl Ether (TAME). *Thermochimica Acta* **1996**, *271*, 49–58. [https://doi.org/10.1016/0040-6031\(95\)02588-X](https://doi.org/10.1016/0040-6031(95)02588-X).
- (457) 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. *Journal of Chemical & Engineering Data* **1996**, *41* (4), 865–869. <https://doi.org/10.1021/je960078o>.

- (458) Vorenberg, D. G.; Raal, J. D.; Ramjugernath, D. Vapor-Liquid Equilibrium Measurements of MTBE and TAME with Toluene. *Journal of Chemical & Engineering Data* **2005**, *50* (1), 56–59. <https://doi.org/10.1021/je049867t>.
- (459) 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. *Collection of Czechoslovak Chemical Communications* **1979**, *44* (12), 3627–3631. <https://doi.org/10.1135/cccc19793627>.
- (460) Reich, R.; Cartes, M.; Wisniak, J.; Segura, H. Phase Equilibria in the Systems Methyl 1,1-Dimethylethyl Ether + Benzene and + Toluene. *Journal of Chemical & Engineering Data* **1998**, *43* (3), 299–303. <https://doi.org/10.1021/je970248c>.
- (461) 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. *The Journal of Chemical Thermodynamics* **1997**, *29* (7), 721–730. <https://doi.org/10.1006/jcht.1997.0198>.
- (462) Niesen, V. G.; Yesavage, V. F. Vapor-Liquid Equilibria for m-Cresol/Tetralin and Tetralin/Quinoline at Temperatures between 523 and 598 K. *Journal of Chemical & Engineering Data* **1988**, *33* (3), 253–258. <https://doi.org/10.1021/je00053a009>.
- (463) Mahmood, S.; Zhao, Q.; Kabadi, V. N. High-Temperature VLE for the Tetralin–Quinoline System. *Journal of Chemical & Engineering Data* **2001**, *46* (4), 994–999. <https://doi.org/10.1021/je000069m>.
- (464) Mollerup, J. Vapour/Liquid Equilibrium in Ethylene + Carbon Dioxide and Ethane + Carbon Dioxide. *Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases* **1975**, *71* (0), 2351. <https://doi.org/10.1039/f19757102351>.
- (465) Nagahama, K.; Konishi, H.; Hoshino, D.; Hirata, M. Binary Vapor-Liquid Equilibria Of Carbon Dioxide-Light Hydrocarbons At Low Temperature. *Journal of Chemical Engineering of Japan* **1974**, *7* (5), 323–328. <https://doi.org/10.1252/jcej.7.323>.
- (466) Bae, H. K.; Nagahama, K.; Hirata, M. Isothermal Vapor-Liquid Equilibria for the Ethylene-Carbon Dioxide System at High Pressure. *Journal of Chemical & Engineering Data* **1982**, *27* (1), 25–27. <https://doi.org/10.1021/je00027a007>.
- (467) Haselden, G. G.; Newitt, D. M.; Shah, S. M. Two-Phase Equilibrium in Binary and Ternary Systems. V. Carbon Dioxide-Ethylene. VI. Carbon Dioxide-Propylene. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* **1951**, *209* (1096), 1–14. <https://doi.org/10.1098/rspa.1951.0183>.
- (468) Wormald, C. J.; Eyeeys, J. M. Excess Molar Enthalpies of (Carbon Dioxide + Ethene) in the Liquid and near-Critical Regions. *The Journal of Chemical Thermodynamics* **2001**, *33* (7), 775–786. <https://doi.org/10.1006/jcht.2000.0778>.
- (469) Rowlinson, J. S.; Sutton, J. R.; Weston, J. F. Liquid-Vapor Equilibrium in the Ternary System Carbon Dioxide-Nitrous Oxide-Ethylene. *Proceedings* **1958**, 10–14.
- (470) 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* (6), 1594–1597.
- (471) 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 Equilibria* **2005**, *238* (1), 13–19. <https://doi.org/10.1016/j.fluid.2005.09.006>.
- (472) Reamer, H. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. Volumetric and Phase Behavior of the Propane-Carbon Dioxide System. *Industrial & Engineering Chemistry* **1951**, *43* (11), 2515–2520. <https://doi.org/10.1021/ie50503a035>.

- (473) Tanaka, K.; Higashi, Y.; Akasaka, R.; Kayukawa, Y.; Fujii, K. Measurements of the Vapor–Liquid Equilibrium for the CO₂ + R290 Mixture. *Journal of Chemical & Engineering Data* **2009**, *54* (3), 1029–1033. <https://doi.org/10.1021/je800938s>.
- (474) 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. *The Journal of Chemical Thermodynamics* **1990**, *22* (8), 777–795. [https://doi.org/10.1016/0021-9614\(90\)90070-7](https://doi.org/10.1016/0021-9614(90)90070-7).
- (475) Poettmann, F. H.; Katz, D. L. Phase Behavior of Binary Carbon Dioxide-Paraffin Systems. *Industrial & Engineering Chemistry* **1945**, *37* (9), 847–853. <https://doi.org/10.1021/ie50429a017>.
- (476) Morrison, G.; Kincaid, J. M. Critical Point Measurements on Nearly Polydisperse Fluids. *AIChE Journal* **1984**, *30* (2), 257–262. <https://doi.org/10.1002/aic.690300213>.
- (477) 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. *Journal of Chemical & Engineering Data* **2013**, *58* (3), 671–676. <https://doi.org/10.1021/je301209u>.
- (478) Horstmann, S.; Fischer, K.; Gmehling, J. Experimental Determination of Critical Points of Pure Components and Binary Mixtures Using a Flow Apparatus. *Chemical Engineering & Technology* **1999**, *22* (10), 839–842. [https://doi.org/10.1002/\(SICI\)1521-4125\(199910\)22:10<839::AID-CEAT839>3.0.CO;2-L](https://doi.org/10.1002/(SICI)1521-4125(199910)22:10<839::AID-CEAT839>3.0.CO;2-L).
- (479) 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? *The Journal of Physical Chemistry B* **2002**, *106* (17), 4496–4502. <https://doi.org/10.1021/jp0129333>.
- (480) Rall, W.; Schäfer, K. Thermodynamische Untersuchungen an Flüssigen Mischsystemen von Aceton Und N-Pentan Sowie von Aceton Und n-Hexan. *Z. Elektrochem.* **1959**, *63* (9–10), 1019–1024.
- (481) Kudryavtseva, L. S.; Susarev, M. P. Liquid-Vapor Equilibria in the Systems Acetone-Hexane and Hexane-Ethyl Alcohol at 35, 45, and 55 and 760mmHg. *Zh. Prikl. Khim* **1963**, *36* (7), 1419–1424.
- (482) 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 K. *Zeitschrift für Physikalische Chemie* **1982**, *263O* (1). <https://doi.org/10.1515/zpch-1982-26317>.
- (483) 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. *Journal of Chemical & Engineering Data* **2002**, *47* (4), 849–854. <https://doi.org/10.1021/je0102917>.
- (484) Schaefer, K. Excess Enthalpies of Acetone + N-Alkane (C₃-C₆) Binary Mixtures. *Int. Data Ser. Sel. Data Mixtures Ser. A* **1978**, No. 1, 74–77.
- (485) 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. *Thermochimica Acta* **1990**, *162* (2), 291–309. [https://doi.org/10.1016/0040-6031\(90\)80350-8](https://doi.org/10.1016/0040-6031(90)80350-8).
- (486) Kay, W. B. P-T-x Diagrams in the Critical Region. Acetone-n-Alkane Systems. *The Journal of Physical Chemistry* **1964**, *68* (4), 827–831. <https://doi.org/10.1021/j100786a021>.
- (487) 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. *Journal*

- of Chemical & Engineering Data* **1986**, 31 (4), 424–430. <https://doi.org/10.1021/je00046a016>.
- (488) 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 Equilibria* **1986**, 25 (2), 137–146. [https://doi.org/10.1016/0378-3812\(86\)80011-5](https://doi.org/10.1016/0378-3812(86)80011-5).
- (489) Puri, P. S.; Polak, J.; Ruether, J. A. Vapor-Liquid Equilibriums of Acetone-Cyclohexane and Acetone-Isopropanol Systems at 25°C. *Journal of Chemical & Engineering Data* **1974**, 19 (1), 87–89. <https://doi.org/10.1021/je60060a007>.
- (490) 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 (2), 371–375.
- (491) Crespo Colin, A.; Compostizo, A.; Díaz Peña, M. Excess Gibbs Energy and Excess Volume of (Cyclohexane + 2-Propanone) and of (Cyclohexane+2-Butanone). *The Journal of Chemical Thermodynamics* **1984**, 16 (5), 497–502. [https://doi.org/10.1016/0021-9614\(84\)90208-8](https://doi.org/10.1016/0021-9614(84)90208-8).
- (492) 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 Equilibria* **2008**, 270 (1–2), 75–86. <https://doi.org/10.1016/j.fluid.2008.06.006>.
- (493) 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 Equilibria* **1995**, 106 (1–2), 139–167. [https://doi.org/10.1016/0378-3812\(94\)02630-J](https://doi.org/10.1016/0378-3812(94)02630-J).
- (494) Löwen, B.; Schulz, S. Excess Molar Enthalpies of Acetone + Water, Cyclohexane, Methanol, 1-Propanol, 2-Propanol, 1-Butanol and 1-Pentanol at 283.15, 298.15, 323.15, 343.15 and 363.15 K. *Thermochimica Acta* **1995**, 262, 69–82. [https://doi.org/10.1016/0040-6031\(95\)02278-A](https://doi.org/10.1016/0040-6031(95)02278-A).
- (495) Marongiu, B. Excess Enthalpy. 2-Propanone-Cyclohexane System. *Int. DATA Ser., Sel. Data Mixtures, Ser. A* **1987**, 1987 (1), 1–6.
- (496) Singh, P. P.; Malik, R.; Maken, S.; Acree, W. E.; Zvaigzni, A. I. Thermochemical Investigations of Associated Solutions. *Thermochimica Acta* **1990**, 165 (1), 113–127. [https://doi.org/10.1016/0040-6031\(90\)80211-G](https://doi.org/10.1016/0040-6031(90)80211-G).
- (497) Linek, J.; Wichterle, I.; Marsh, K. N. Vapor-Liquid Equilibria for N-Methyl-2-Pyrrolidone + Benzene, +Toluene, +Heptane, and +Methylcyclohexane. *Journal of Chemical & Engineering Data* **1996**, 41 (6), 1212–1218. <https://doi.org/10.1021/je9601826>.
- (498) 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-Dimethylformamide. 1. Isobaric Vapor - Liquid Equilibria. *Journal of Chemical & Engineering Data* **1997**, 42 (5), 938–942. <https://doi.org/10.1021/je970059u>.
- (499) Gupta, S. K.; Rawat, B. S.; Goswami, A. N.; Nanoti, S. M.; Krishna, R. Isobaric Vapour—Liquid Equilibria of the Systems: Benzene—Triethylene Glycol, Toluene—Triethylene Glycol and Benzene—N-Methylpyrrolidone. *Fluid Phase Equilibria* **1989**, 46 (1), 95–102. [https://doi.org/10.1016/0378-3812\(89\)80278-X](https://doi.org/10.1016/0378-3812(89)80278-X).
- (500) Letcher, T. M.; Naicker, P. K. Excess Molar Enthalpies and Excess Molar Volumes of Mixtures Containing N-Methyl-2-Pyrrolidinone and an Aromatic Hydrocarbon At T = 298.15 K And p = 0.101325 MPa. *The Journal of Chemical Thermodynamics* **1999**, 31 (12), 1585–1595. <https://doi.org/10.1006/jcht.1999.0555>.

- (501) 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. *The Journal of Chemical Thermodynamics* **2011**, *43* (5), 737–749. <https://doi.org/10.1016/j.jct.2010.12.016>.
- (502) Gmehling, J.; Meents, B. Excess Enthalpy. 1-Methyl-2-Pyrrolidinone - Benzene System. *Int. Data Ser. Sel. Data Mixtures Ser. A* **1992**, No. 3, 211.
- (503) Brown, T. S.; Kidnay, A. J.; Sloan, E. D. Vapor—Liquid Equilibria in the Carbon Dioxide-Ethane System. *Fluid Phase Equilibria* **1988**, *40* (1–2), 169–184. [https://doi.org/10.1016/0378-3812\(88\)80028-1](https://doi.org/10.1016/0378-3812(88)80028-1).
- (504) Wallis, K. P.; Clancy, P.; Zollweg, J. A.; Streett, W. B. Excess Thermodynamic Properties for $\{x\text{CO}_2 + (1 - x)\text{C}_2\text{H}_6\}$ (I): Experiment and Theory. *The Journal of Chemical Thermodynamics* **1984**, *16* (9), 811–823. [https://doi.org/10.1016/0021-9614\(84\)90028-4](https://doi.org/10.1016/0021-9614(84)90028-4).
- (505) Ohgaki, K.; Katayama, T. Isothermal Vapor-Liquid Equilibrium Data for the Ethane—Carbon Dioxide System at High Pressures. *Fluid Phase Equilibria* **1977**, *1* (1), 27–32. [https://doi.org/10.1016/0378-3812\(77\)80023-X](https://doi.org/10.1016/0378-3812(77)80023-X).
- (506) Wormald, C. J.; Eyres, J. M. Excess Molar Enthalpies and Excess Molar Volumes of $\{x\text{CO}_2 + (1 - x)\text{C}_2\text{H}_6\}$ up to 308.4 K and 11.0 MPa. *The Journal of Chemical Thermodynamics* **1988**, *20* (3), 323–331. [https://doi.org/10.1016/0021-9614\(88\)90129-2](https://doi.org/10.1016/0021-9614(88)90129-2).
- (507) Wormald, C. J.; Hodgetts, R. W. Excess Enthalpies and Volumes for (Carbon Dioxide + Ethane) At T= 291.6 K, Close to the Minimum in the Critical Locus. *The Journal of Chemical Thermodynamics* **1997**, *29* (1), 75–85. <https://doi.org/10.1006/jcht.1996.0141>.
- (508) Khazanova, N. E.; Lesnevskaya, L. S.; Zakharova, A. V. Liquid-Vapor Equilibrium in the Ethane-CO₂ System. *Khim. Promst. Moscow* **1966**, *44*, 364–365.
- (509) 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. *The Journal of Supercritical Fluids* **2008**, *44* (2), 123–138. <https://doi.org/10.1016/j.supflu.2007.11.003>.
- (510) 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.
- (511) 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. *The Journal of Chemical Thermodynamics* **1997**, *29* (12), 1481–1494. <https://doi.org/10.1006/jcht.1997.0257>.
- (512) 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. *The Journal of Chemical Thermodynamics* **2000**, *32* (4), 451–464. <https://doi.org/10.1006/jcht.2000.0611>.
- (513) Kalra, H.; Krishnana, T. R.; Robinson, D. B. Equilibrium-Phase Properties of Carbon Dioxide-Butane and Nitrogen-Hydrogen Sulfide Systems at Subambient Temperatures. *Journal of Chemical & Engineering Data* **1976**, *21* (2), 222–225. <https://doi.org/10.1021/je60069a027>.
- (514) Weber, L. A. Vapour-Liquid Equilibria Measurements for Carbon Dioxide with Normal and Isobutane from 250 to 280 K. *Cryogenics* **1985**, *25* (6), 338–342. [https://doi.org/10.1016/0011-2275\(85\)90019-0](https://doi.org/10.1016/0011-2275(85)90019-0).

- (515) Niesen, V. G. (Vapor + Liquid) Equilibria and Coexisting Densities of (Carbon Dioxide + n-Butane) at 311 to 395 K. *The Journal of Chemical Thermodynamics* **1989**, *21* (9), 915–923. [https://doi.org/10.1016/0021-9614\(89\)90150-X](https://doi.org/10.1016/0021-9614(89)90150-X).
- (516) 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. *Journal of Chemical & Engineering Data* **1985**, *30* (4), 485–491. <https://doi.org/10.1021/je00042a036>.
- (517) Pozo de Fernandez, M. E.; Zollweg, J. A.; Streett, W. B. Vapor-Liquid Equilibrium in the Binary System Carbon Dioxide + n-Butane. *Journal of Chemical & Engineering Data* **1989**, *34* (3), 324–328. <https://doi.org/10.1021/je00057a019>.
- (518) Weber, L. A. Simple Apparatus for Vapor-Liquid Equilibrium Measurements with Data for the Binary Systems of Carbon Dioxide with n-Butane and Isobutane. *Journal of Chemical & Engineering Data* **1989**, *34* (2), 171–175. <https://doi.org/10.1021/je00056a007>.
- (519) Olds, R. H.; Reamer, H. H.; Sage, B. H.; Lacey, W. N. The N-Butane–Carbon Dioxide System. *Industrial & Engineering Chemistry* **1949**, *41* (3), 475–482. <https://doi.org/10.1021/ie50471a011>.
- (520) Leu, A. D.; Robinson, D. B. Equilibrium Phase Properties of the N-Butane-Carbon Dioxide and Isobutane-Carbon Dioxide Binary Systems. *Journal of Chemical & Engineering Data* **1987**, *32* (4), 444–447. <https://doi.org/10.1021/je00050a017>.
- (521) 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 Equilibria* **2011**, *307* (1), 24–29. <https://doi.org/10.1016/j.fluid.2011.05.004>.
- (522) Murakami, S.; Amaya, K.; Fujishiro, R. Heats of Mixing for Binary Mixtures. The Energy of Hydrogen Bonding between Alcohol and Ketone Molecules. *Bulletin of the Chemical Society of Japan* **1964**, *37* (12), 1776–1780. <https://doi.org/10.1246/bcsj.37.1776>.
- (523) Kreglewski, A.; Kay, W. B. Critical Constants of Conformed Mixtures. *The Journal of Physical Chemistry* **1969**, *73* (10), 3359–3366. <https://doi.org/10.1021/j100844a035>.
- (524) 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* (2), 139–156.
- (525) Kraus, J.; Linek, J. Liquid-Vapor Equilibrium. XLVIII. Systems Acetone-Benzene, Acetone-Toluene, Benzene-Methyl Ethyl Ketone, Methyl Ethyl Ketone-Toluene, and Methyl Ethyl Ketone-Ethylbenzene. *Collection of Czechoslovak Chemical Communications* **1971**, *36* (7), 2547–2567. <https://doi.org/10.1135/cccc19712547>.
- (526) Müller, E.; Stage, H. *Experimentelle Vermessung von Dampf-Flüssigkeits-Phasengleichgewichten Dargestellt Am Beispiel Des Siedeverhaltens von Fettsäuren*; 1961.
- (527) Free, K. W.; Hutchinson, H. P. Isobaric Vapor-Liquid Equilibria for the Ternary System Acetone-Benzene-Chlorobenzene. *Journal of Chemical & Engineering Data* **1959**, *4* (3), 193–197. <https://doi.org/10.1021/je60003a001>.
- (528) Ishikawa, T.; Watari, R.; Kosakai, K.; Hirata, M. Vapor-Liquid Equilibriums of Binary Systems Containing Acetone at 760 Mm of Mercury. Acetone with Aromatic Hydrocarbons. *Mem. Fac. Technol. Tokyo Metropol. Univ.* **1971**, *21*, 1883–1896.
- (529) 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* (6), 177–182. <https://doi.org/10.1007/BF02545630>.

- (530) Kojima, K.; Tochigi, K.; Kurihara, K.; Nakamichi, M. Isobaric Vapor-Liquid Equilibria for Acetone + Chloroform + Benzene and the Three Constituent Binary Systems. *Journal of Chemical & Engineering Data* **1991**, *36* (3), 343–345. <https://doi.org/10.1021/je00003a024>.
- (531) 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. *Thermochimica Acta* **1987**, *113*, 141–150. [https://doi.org/10.1016/0040-6031\(87\)88317-X](https://doi.org/10.1016/0040-6031(87)88317-X).
- (532) Möbius, H.-H. Mischungsenthalpien Und Mischbarkeit von Aceton, Benzol Und Wasser. *Journal für Praktische Chemie* **1955**, *2* (1–2), 95–104. <https://doi.org/10.1002/prac.19550020108>.
- (533) 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. *Thermochimica Acta* **1990**, *169*, 193–201. [https://doi.org/10.1016/0040-6031\(90\)80145-O](https://doi.org/10.1016/0040-6031(90)80145-O).
- (534) Lebedeva, E. S.; Khodeeva, S. M. Phase Equilibrium and Volume Relations in the System Methylene Chloride-Ethylene. *Tr. Gos. Nauchno Issled. Proektn. Inst. Azotn. Promst. Prod. Org. Sin.* **1963**, *13*, 79–90.
- (535) 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. *Journal of Chemical & Engineering Data* **1991**, *36* (4), 436–439. <https://doi.org/10.1021/je00004a027>.
- (536) Nohka, J.; Sarashina, E.; Arai, Y.; Saito, S. Correlation Of Vapor-Liquid Equilibria For Systems Containing A Polar Component By The Bwr Equation. *Journal of Chemical Engineering of Japan* **1973**, *6* (1), 10–17. <https://doi.org/10.1252/jcej.6.10>.
- (537) Wang, X.; Wang, Y. S. Vapor-Liquid Equilibria for Nitrogen-Carbon Dioxide-Chlorodifluoromethane at Moderate Pressure. *Nanjing Huagong Xueyuan Xuebao* **1991**, *13*, 35–44.
- (538) Maslennikova, V. Ya.; Goryunova, N. P.; Tsiklis, D. S. Phase Equilibriums in the Nitrogen-Freon 12 and Nitrogen-Freon 22 Systems. *Russ. J. Phys. Chem.* **1967**, *41* (3), 383–385.
- (539) 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* (1), 87–92.
- (540) Nagata, I. Vapor-Liquid Equilibrium at Atmospheric Pressure for the Ternary System, Methyl Acetate-Chloroform-Benzene. *Journal of Chemical & Engineering Data* **1962**, *7* (3), 360–366. <https://doi.org/10.1021/je60014a012>.
- (541) 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. *Journal of Chemical & Engineering Data* **1995**, *40* (2), 361–366. <https://doi.org/10.1021/je00018a003>.
- (542) Hirobe, H. Thermochemical Studies. *J. Fac. Sci. Univ. Tokyo Sect. I* **1926**, *1* (4), 155–222.
- (543) Nagata, I.; Tamura, K.; Tokuriki, S. Excess Enthalpies and Complex Formation of Acetonitrile with Acetone, Chloroform, and Benzene. *Thermochimica Acta* **1981**, *47* (3), 315–331. [https://doi.org/10.1016/0040-6031\(81\)80110-4](https://doi.org/10.1016/0040-6031(81)80110-4).
- (544) Rastogi, R. P.; Nath, J.; Misra, R. R. Thermodynamics of Weak Interactions in Liquid Mixtures of Chloroform and Aromatic Hydrocarbons. *The Journal of Chemical Thermodynamics* **1971**, *3* (3), 307–317. [https://doi.org/10.1016/S0021-9614\(71\)80047-2](https://doi.org/10.1016/S0021-9614(71)80047-2).

- (545) 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. *Journal of Solution Chemistry* **1987**, *16* (9), 745–752. <https://doi.org/10.1007/BF00652577>.
- (546) 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.
- (547) Al-Hayan, M. N. M.; Newsham, D. M. T. Isobaric Vapour–Liquid Equilibria for Mixtures Containing Halogenated Hydrocarbons at Atmospheric Pressure: I. Binary Mixtures of Trichloromethane+ 1, 2-Dichloroethane, 1, 2-Dichloroethane+ 1, 1, 2, 2-Tetrachloroethane, Trichloromethane+ 1, 1, 2, 2-Tetrachloroethane and n-Heptane+ 1, 1, 2, 2-Tetrachloroethane. *Fluid Phase Equilibria* **1999**, *166* (1), 91–100. [https://doi.org/10.1016/S0378-3812\(99\)00297-6](https://doi.org/10.1016/S0378-3812(99)00297-6).
- (548) 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* (1), 59–78.
- (549) Góral, M.; Oracz, P.; Warycha, S. Vapour—Liquid Equilibria. IV. The Ternary System Carbon Tetrachloride—Methanol—Chloroform at 293.15 K. *Fluid Phase Equilibria* **1988**, *44* (1), 77–93. [https://doi.org/10.1016/0378-3812\(88\)80104-3](https://doi.org/10.1016/0378-3812(88)80104-3).
- (550) Rulewicz, G.; Schuberth, H.; Leibnitz, E. Untersuchungen Über Das Dampf-Flüssigkeits-Phasengleichgewicht Des Systems Methylenchlorid/Chloroform/Tetrachlorkohlenstoff Bei 45°C Unter Verwendung Einer Gaschromatographischen Analysenmethode. *Journal für Praktische Chemie* **1968**, *37* (3–4), 122–136. <https://doi.org/10.1002/prac.19680370303>.
- (551) Krauze, R.; Serwinski, M. Liquid-Vapor Equilibrium in He System Chloroform-Carbon Tetrachloride. *Zesz. Nauk. Politech. Lodz. Chem.* **1973**, *24*, 53–63.
- (552) Siddiqi, M. A.; Lucas, K. Excess Enthalpy of the System Chloroform + Carbon Tetrachloride and a Thermodynamic Evaluation of Its State Dependence. *Fluid Phase Equilibria* **1984**, *16* (1), 87–98. [https://doi.org/10.1016/0378-3812\(84\)85023-2](https://doi.org/10.1016/0378-3812(84)85023-2).
- (553) 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 Equilibria* **2013**, *360*, 293–297. <https://doi.org/10.1016/j.fluid.2013.09.056>.
- (554) 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. *Journal of Chemical & Engineering Data* **2008**, *53* (9), 2193–2196. <https://doi.org/10.1021/jc800505y>.
- (555) Kleiber, M. Vapor-Liquid Equilibria of Binary Refrigerant Mixtures Containing Propylene or R134a. *Fluid Phase Equilibria* **1994**, *92*, 149–194. [https://doi.org/10.1016/0378-3812\(94\)80046-4](https://doi.org/10.1016/0378-3812(94)80046-4).
- (556) Bobbo, S.; Fedele, L.; Camporese, R.; Stryjek, R. VLE Measurements and Modeling for the Strongly Positive Azeotropic R32+propane System. *Fluid Phase Equilibria* **2002**, *199* (1–2), 175–183. [https://doi.org/10.1016/S0378-3812\(01\)00798-1](https://doi.org/10.1016/S0378-3812(01)00798-1).
- (557) 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 Equilibria* **2003**, *211* (2), 273–287. [https://doi.org/10.1016/S0378-3812\(03\)00237-1](https://doi.org/10.1016/S0378-3812(03)00237-1).

- (558) 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. *Journal of Chemical & Engineering Data* **2003**, *48* (2), 317–323. <https://doi.org/10.1021/je020115d>.
- (559) 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. *Industrial & Engineering Chemistry Research* **2001**, *40* (21), 4610–4614. <https://doi.org/10.1021/ie010215x>.
- (560) Higashi, Y. Experimental Determination of the Critical Locus for the Difluoromethane (R32) and Propane (R290) System. *Fluid Phase Equilibria* **2004**, *219* (1), 99–103. <https://doi.org/10.1016/j.fluid.2004.02.004>.
- (561) 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. *Journal of Chemical & Engineering Data* **2006**, *51* (4), 1411–1414. <https://doi.org/10.1021/je0601107>.
- (562) Kordikowski, A.; Poliakoff, M. Acoustic Probing of Phase Equilibria in Near-Critical Fluids. *Fluid Phase Equilibria* **1998**, *150–151*, 493–499. [https://doi.org/10.1016/S0378-3812\(98\)00296-9](https://doi.org/10.1016/S0378-3812(98)00296-9).
- (563) Baginskii, V. A.; Zakharov, N. D.; Lapardin, N. I. Study and Calculation of the Liquid-Vapor Phase Equilibrium of Mixtures of Refrigerants. *Issled. Teplofiz. Svoistv Rab. Veshchestv i Protsessov Teploobmena v Kholod. Tekhn., L.* **1989**, *9*, 9–15.
- (564) 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* (22), 10–18.
- (565) 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 Equilibria* **2010**, *290* (1–2), 121–126. <https://doi.org/10.1016/j.fluid.2009.09.008>.
- (566) Bobbo, S.; Fedele, L.; Camporese, R.; Stryjek, R. Hydrogen-Bonding of HFCs with Dimethyl Ether: Evaluation by Isothermal VLE Measurements. *Fluid Phase Equilibria* **2002**, *199* (1–2), 153–160. [https://doi.org/10.1016/S0378-3812\(01\)00813-5](https://doi.org/10.1016/S0378-3812(01)00813-5).
- (567) 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). *Journal of Chemical & Engineering Data* **2004**, *49* (4), 750–755. <https://doi.org/10.1021/je030156p>.
- (568) Kubic, W. L.; Stein, F. P. An Experimental and Correlative Study of the Vapor-Liquid Equilibria of the Tetrafluoromethane-Chlorotrifluoromethane System. *Fluid Phase Equilibria* **1981**, *5* (3–4), 289–304. [https://doi.org/10.1016/0378-3812\(80\)80062-8](https://doi.org/10.1016/0378-3812(80)80062-8).
- (569) 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 Equilibria* **2008**, *268* (1–2), 68–73. <https://doi.org/10.1016/j.fluid.2008.04.002>.
- (570) 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 Equilibria* **2013**, *354*, 109–113. <https://doi.org/10.1016/j.fluid.2013.06.031>.
- (571) Kriebel, M. Liquid-Vapor Phase Equilibria of the Binary System Difluoromonochloromethane (R 22)-Difluorodichloromethane (R 12). *Kaeltetechnik* **1967**, *19* (1), 8–14.

- (572) 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* (5), 58–67.
- (573) 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. [https://doi.org/10.1016/0378-3812\(94\)02644-G](https://doi.org/10.1016/0378-3812(94)02644-G).
- (574) Geller, Z. I.; Chaikovskii, V. F.; Egorov, A. V. Heats of Mixing of Freons. *Teplofiz. Svoist. Zhidk.* **1973**, 148–152.
- (575) Geller, Z. I.; Chaikovskii, V. F.; Egorov, A. V. Heats of Mixing of Freons 112 and 115 with Freon 22. *Kholod. Tekh.* **1971**, *48* (8), 29–30.
- (576) 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* (1), 31–36. <https://doi.org/10.1021/je00035a012>.
- (577) Siddiqi, M. A.; Lucas, K. The Excess Enthalpy of (Tetrachloromethane + Carbon Disulphide) and (Tetrachloromethane + Dichloromethane) over a Range of Temperatures and Pressures. *The Journal of Chemical Thermodynamics* **1983**, *15* (12), 1181–1187. [https://doi.org/10.1016/0021-9614\(83\)90009-5](https://doi.org/10.1016/0021-9614(83)90009-5).
- (578) Bissell, T. G.; Williamson, A. G. Vapour Pressures and Excess Gibbs Energies of N-Hexane and of n-Heptane + Carbon Tetrachloride and + Chloroform at 298.15 K. *The Journal of Chemical Thermodynamics* **1975**, *7* (2), 131–136. [https://doi.org/10.1016/0021-9614\(75\)90260-8](https://doi.org/10.1016/0021-9614(75)90260-8).
- (579) Kudryavtseva, L. S.; Susarev, M. P. Liquid-Vapor Equilibrium in Systems Chloroform-Hexane and Acetone-Chloroform. *J. Appl. Chem. USSR* **1963**, *36* (6), 1231–1237.
- (580) Brzostowski, W.; Verhoeve, L. Thermodynamic Properties of Mixtures of Hexane and Chloroform. *Rocz. Chem.* **1968**, *42*, 507–515.
- (581) Ortega, J.; Placido, J. Excess Enthalpies of Trichloromethane + N-Alkanes. Measurement and Comparison with the DISQUAC Model. *Int. Electron. J. Phys. Chem. Data* **1995**, *1* (1), 59–68.
- (582) Bissell, T. G.; Okafor, G. E.; Williamson, A. G. Enthalpies and Volumes of Mixing of Alkanes with Carbon Tetrachloride, Chloroform, and Methylene Chloride at 25 °C. *The Journal of Chemical Thermodynamics* **1971**, *3* (3), 393–399. [https://doi.org/10.1016/S0021-9614\(71\)80056-3](https://doi.org/10.1016/S0021-9614(71)80056-3).
- (583) Sharma, B. R.; Pundeer, G. S.; Singh, P. P. Thermodynamics of Weak Interactions: Excess Enthalpies and Excess Gibbs Free Energies of Mixing. *Thermochimica Acta* **1975**, *11* (2), 105–114. [https://doi.org/10.1016/0040-6031\(75\)80013-X](https://doi.org/10.1016/0040-6031(75)80013-X).
- (584) 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* (3), 217–237.
- (585) 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* (9), 1355–1359. <https://doi.org/10.1051/jcp/1973701355>.
- (586) Shatas, J. P.; Abbott, M. M.; Van Ness, H. C. Excess Thermodynamic Functions for Ternary Systems. II. Chloroform-Ethanol-n-Heptane at 50°C. *Journal of Chemical & Engineering Data* **1975**, *20* (4), 406–409. <https://doi.org/10.1021/je60067a020>.
- (587) 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. *Journal of Chemical & Engineering Data* **1986**, *31* (4), 389–390. <https://doi.org/10.1021/je00046a005>.

- (588) Tenn, F. G.; Missen, R. W. A Study of the Condensation of Binary Vapors of Miscible Liquids: Part I: The Equilibrium Relations. *The Canadian Journal of Chemical Engineering* **1963**, *41* (1), 12–14. <https://doi.org/10.1002/cjce.5450410105>.
- (589) 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. *Canadian Journal of Chemistry* **1986**, *64* (10), 1966–1968. <https://doi.org/10.1139/v86-325>.
- (590) Tsang, C. Y.; Streett, W. B. Vapor-Liquid Equilibrium in the System Carbon Dioxide/Dimethyl Ether. *Journal of Chemical & Engineering Data* **1981**, *26* (2), 155–159. <https://doi.org/10.1021/je00024a018>.
- (591) Jonasson, A.; Persson, O.; Fredenslund, A. High Pressure Solubility of Carbon Dioxide and Carbon Monoxide in Dimethyl Ether. *Journal of Chemical & Engineering Data* **1995**, *40* (1), 296–300. <https://doi.org/10.1021/je00017a066>.
- (592) Laursen, T.; Rasmussen, P.; Andersen, S. I. VLE and VLLE Measurements of Dimethyl Ether Containing Systems. *J. Chem. Eng. Data* **2002**, *47* (2), 198–202. <https://doi.org/10.1021/je010154+>.
- (593) Ferrell, J. K.; Rousseau, R. W.; Bass, D. G. *The Solubility of Acid Gases in Methanol*; 1979; pp 1–40.
- (594) 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 Equilibria* **2013**, *356*, 223–228. <https://doi.org/10.1016/j.fluid.2013.07.050>.
- (595) Sobocinski, D. P.; Kurata, F. Heterogeneous Phase Equilibria of the Hydrogen Sulfide–Carbon Dioxide System. *AIChE Journal* **1959**, *5* (4), 545–551. <https://doi.org/10.1002/aic.690050425>.
- (596) Bierlein, J. A.; Kay, W. B. Phase-Equilibrium Properties of System Carbon Dioxide–Hydrogen Sulfide. *Industrial & Engineering Chemistry* **1953**, *45* (3), 618–624. <https://doi.org/10.1021/ie50519a043>.
- (597) Wagner, Z.; Pavliček, J. Vapour-Liquid Equilibrium in the Carbon Dioxide—Ethyl Acetate System at High Pressure. *Fluid Phase Equilibria* **1994**, *97*, 119–126. [https://doi.org/10.1016/0378-3812\(94\)85010-0](https://doi.org/10.1016/0378-3812(94)85010-0).
- (598) Chrisochoou, A.; Schaber, K.; Bolz, U. Phase Equilibria for Enzyme-Catalyzed Reactions in Supercritical Carbon Dioxide. *Fluid Phase Equilibria* **1995**, *108* (1–2), 1–14. [https://doi.org/10.1016/0378-3812\(95\)02696-C](https://doi.org/10.1016/0378-3812(95)02696-C).
- (599) 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. *The Journal of Chemical Thermodynamics* **2012**, *51*, 59–64. <https://doi.org/10.1016/j.jct.2012.02.034>.
- (600) 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. *The Journal of Supercritical Fluids* **2006**, *37* (3), 323–332. <https://doi.org/10.1016/j.supflu.2005.10.007>.
- (601) 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. *Journal of Chemical & Engineering Data* **2014**, *59* (10), 3205–3219. <https://doi.org/10.1021/je5002494>.
- (602) Reiff, W.-E.; Roth, H.; Lucas, K. Phase Equilibria in the Binary System Carbon Disulfide–Carbon Dioxide. *Fluid Phase Equilibria* **1992**, *73* (3), 323–338. [https://doi.org/10.1016/0378-3812\(92\)80016-3](https://doi.org/10.1016/0378-3812(92)80016-3).

- (603) Wormald, C. J.; Hodgetts, R. W. Measurements of HmE for $\{x\text{CO}_2+(1-x)\text{CS}_2\}$ in the Liquid Region up to $T=300.15$ K and $P=7.5$ MPa. *Fluid Phase Equilibria* **2003**, *204* (2), 303–308. [https://doi.org/10.1016/S0378-3812\(02\)00266-2](https://doi.org/10.1016/S0378-3812(02)00266-2).
- (604) 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 Equilibria* **2012**, *318*, 77–82. <https://doi.org/10.1016/j.fluid.2012.01.020>.
- (605) Im, J.; Kim, M.; Lee, J.; Kim, H. Vapor–Liquid Equilibria of Binary Carbon Dioxide + Alkyl Carbonate Mixture Systems. *Journal of Chemical & Engineering Data* **2004**, *49* (2), 243–245. <https://doi.org/10.1021/je034089a>.
- (606) 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* (1), 11–16.
- (607) 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. *Journal of Chemical & Engineering Data* **2005**, *50* (4), 1419–1424. <https://doi.org/10.1021/je050089u>.
- (608) 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 Equilibria* **2011**, *307* (1), 72–77. <https://doi.org/10.1016/j.fluid.2011.05.005>.
- (609) Hou, Y.; Chen, X.; Ren, S.; Song, Z.; Wu, W. Phase Behavior, Densities, and Isothermal Compressibility of (Carbon Dioxide + Dimethyl Carbonate). *Journal of Chemical & Engineering Data* **2010**, *55* (4), 1580–1587. <https://doi.org/10.1021/je900691n>.
- (610) Huamin, S. Solubility Of Carbon Monoxide In Methanol And Carbon Dioxide Under High Pressure. *Huaxue Gongcheng* **1991**, *19* (6), 61–69.
- (611) Kaminishi, G.-I.; Arai, Y.; Saito, S.; Maeda, S. Vapor-Liquid Equilibria For Binary And Ternary Systems Containing Carbon Dioxide. *Journal of Chemical Engineering of Japan* **1968**, *1* (2), 109–116. <https://doi.org/10.1252/jcej.1.109>.
- (612) Christiansen, L. J.; Fredenslund, A.; Gardner, N. Gas-Liquid Equilibria of the CO₂-CO and CO₂-CH₄-CO Systems. In *Advances in Cryogenic Engineering*; 1995; pp 309–319.
- (613) Fredenslund, A.; Sather, G. A. Gas-Liquid Equilibrium of the Oxygen-Carbon Dioxide System. *Journal of Chemical & Engineering Data* **1970**, *15* (1), 17–22. <https://doi.org/10.1021/je60044a024>.
- (614) Chueh, P. L.; Muirbrook, N. K.; Prausnitz, J. M. Multicomponent Vapor-Liquid Equilibria at High Pressures: Part II. Thermodynamic Analysis. *AIChE Journal* **1965**, *11* (6), 1097–1102. <https://doi.org/10.1002/aic.690110625>.
- (615) Muirbrook, N. K.; Prausnitz, J. M. Multicomponent Vapor-Liquid Equilibria at High Pressures: Part I. Experimental Study of the Nitrogen—Oxygen—Carbon Dioxide System at 0°C. *AIChE Journal* **1965**, *11* (6), 1092–1096. <https://doi.org/10.1002/aic.690110624>.
- (616) Booth, H. S.; Carter, J. M. The Critical Constants of Carbon Dioxide-Oxygen Mixtures. *The Journal of Physical Chemistry* **1930**, *34* (12), 2801–2825. <https://doi.org/10.1021/j150318a013>.
- (617) Kim, C. N.; Park, Y. M. Vapor–Liquid Equilibrium of HFC-32/134a And HFC-125/134a Systems. *Int. J. Thermophys.* **1999**, *20* (2), 519–530. <https://doi.org/10.1023/A:1022605104490>.
- (618) Kobayashi, M.; Nishiumi, H. Vapor–Liquid Equilibria for the Pure, Binary and Ternary Systems Containing HFC32, HFC125 and HFC134a. *Fluid Phase Equilibria* **1998**, *144* (1–2), 191–202. [https://doi.org/10.1016/S0378-3812\(97\)00257-4](https://doi.org/10.1016/S0378-3812(97)00257-4).

- (619) Nishiumi, H.; Ohno, T. High Pressure Vapor-Liquid Equilibria and Critical Loci for the HFC125-HFC134a System. *Korean Journal of Chemical Engineering* **2000**, *17* (6), 668–671. <https://doi.org/10.1007/BF02699115>.
- (620) Kato, R.; Nishiumi, H. Vapor–Liquid Equilibria and Critical Loci of Binary and Ternary Systems Composed of CH₂F₂, C₂HF₅ and C₂H₂F₄. *Fluid Phase Equilibria* **2006**, *249* (1–2), 140–146. <https://doi.org/10.1016/j.fluid.2006.07.017>.
- (621) 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.
- (622) 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 Equilibria* **1991**, *63* (1–2), 151–156. [https://doi.org/10.1016/0378-3812\(91\)80027-S](https://doi.org/10.1016/0378-3812(91)80027-S).
- (623) Nishiumi, H.; Komatsu, M.; Yokoyama, T.; Kohmatsu, S. Two- and Three-Phase Equilibria and Critical Locus for the System of HCFC22-HFC134a. *Fluid Phase Equilibria* **1993**, *83*, 109–117. [https://doi.org/10.1016/0378-3812\(93\)87013-Q](https://doi.org/10.1016/0378-3812(93)87013-Q).
- (624) Chung, E.-Y.; Kim, M. S. Vapor–Liquid Equilibria for the Difluoromethane (HFC-32) + 1,1,1,2-Tetrafluoroethane (HFC-134a) System. *Journal of Chemical & Engineering Data* **1997**, *42* (6), 1126–1128. <https://doi.org/10.1021/je970071m>.
- (625) 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 Equilibria* **2006**, *249* (1–2), 97–103. <https://doi.org/10.1016/j.fluid.2006.09.017>.
- (626) 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* (3), 801–808. <https://doi.org/10.1023/A:1015407205188>.
- (627) Weber, L. A.; Silva, A. M. Design of a High-Pressure Ebulliometer, with Vapor-Liquid Equilibrium Results for the Systems CHF₂ Cl + CF₃ CH₃ and CF₃ CH₂ F + CH₂F₂. *International Journal of Thermophysics* **1996**, *17* (4), 873–888. <https://doi.org/10.1007/BF01439194>.
- (628) 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 + CH₃CH₂ and in Their Binary Subsystems. *The Journal of Physical Chemistry B* **1997**, *101* (30), 5853–5862. <https://doi.org/10.1021/jp9630611>.
- (629) 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* (5), 613–618.
- (630) Tillner-Roth, R. An Experimental Study of the Thermodynamic Properties of the Refrigerant Mixture: {1,1,1,2-Tetrafluoroethane (R 134a) + 1,1-Difluoroethane (R 152a)}. *The Journal of Chemical Thermodynamics* **1993**, *25* (12), 1419–1441. <https://doi.org/10.1006/jcht.1993.1144>.
- (631) Engelmann, K.; Bittrich, H. J. Estimation of Isothermal Mixing Functions from Isobaric Liquid-Vapor Equilibriums. *Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg* **1969**, *11*, 213–218.
- (632) Engelmann, K.; Bittrich, H. J. Isobaric Liquid-Vapor Equilibriums of the System Diethylamine-Ethyl Acetate, Diethylamine-1,4-Dioxane and Ethyl Acetate-1,4-Dioxane at Reduced Pressures. *Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg* **1966**, *8*, 289–291.

- (633) Engelmann, K.; Bittrich, H. J. Isobaric Liquid-Vapor Equilibriums of the Systems Diethylamine/Ethyl Acetate, Diethylamine/1,4-Dioxane, and Ethyl Acetate/1,4-Dioxane at 760 Mm. *Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg* **1966**, *8*, 148–153.
- (634) Comelli, F.; Francesconi, R.; Ottani, S. Isothermal Vapor–Liquid Equilibria of Dimethyl Carbonate + Diethyl Carbonate in the Range (313.15 to 353.15) K. *Journal of Chemical & Engineering Data* **1996**, *41* (3), 534–536. <https://doi.org/10.1021/je950287t>.
- (635) Luo, H.-P.; Xiao, W.-D.; Zhu, K.-H. Isobaric Vapor–Liquid Equilibria of Alkyl Carbonates with Alcohols. *Fluid Phase Equilibria* **2000**, *175* (1–2), 91–105. [https://doi.org/10.1016/S0378-3812\(00\)00444-1](https://doi.org/10.1016/S0378-3812(00)00444-1).
- (636) 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. *Journal of Chemical & Engineering Data* **1995**, *40* (4), 811–814. <https://doi.org/10.1021/je00020a016>.
- (637) 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. *Journal of Chemical & Engineering Data* **1996**, *41* (4), 736–740. <https://doi.org/10.1021/je950298m>.
- (638) 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* (4), 297–309.
- (639) Noles, J. R.; Zollweg, J. A. Isothermal Vapor-Liquid Equilibrium for Dimethyl Ether + Sulfur Dioxide. *Fluid Phase Equilibria* **1991**, *66* (3), 275–289. [https://doi.org/10.1016/0378-3812\(91\)85061-X](https://doi.org/10.1016/0378-3812(91)85061-X).
- (640) Glowka, S.; Zawisza, A. C. Liquid-Vapor Equilibriums and Thermodynamic Functions of Methyl Ethyl Ether-Sulfur Dioxide System up to 300.Deg. and 77.81 Atm. *Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques* **1970**, *18* (9), 555–560.
- (641) Feng Yaosheng; Li, C.; Shou, Z. Vapor-Liquid Equilibrium for Trifluoromethane and Chlorodifluoromethane. *Huaxue Gongcheng* **1984**, *12* (3), 41–47.
- (642) Roth, H.; Peters-Gerth, P.; Lucas, K. Experimental Vapor-Liquid Equilibria in the Systems R 22-R 23, R 22-Co₂, Cs₂-R 22, R 23-Co₂, Cs₂-R 23 and Their Correlation by Equations of State. *Fluid Phase Equilibria* **1992**, *73* (1–2), 147–166. [https://doi.org/10.1016/0378-3812\(92\)85045-A](https://doi.org/10.1016/0378-3812(92)85045-A).
- (643) Gerrits, G. C. On P_x-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.
- (644) Sameshima, J. On The System Acetone—Ethyl Ether. *Journal of the American Chemical Society* **1918**, *40* (10), 1482–1503. <https://doi.org/10.1021/ja02243a002>.
- (645) Litvinov, N. D. Isothermal Equilibrium of Vapor and Liquid in Systems of Three Fully Miscible Liquids. *Zh. Fiz. Khim.* **1952**, *26* (10), 1405–1412.
- (646) Zawidzki, J. von. Über Die Dampfdrücke Binärer Flüssigkeitsgemische. *Zeitschrift für Physikalische Chemie* **1900**, *35U* (1). <https://doi.org/10.1515/zpch-1900-3514>.
- (647) 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. *Journal de Chimie Physique* **1964**, *61*, 1231–1233. <https://doi.org/10.1051/jcp/1964611231>.
- (648) Bittrich, H. J.; Rodrigues, L. F. T. G. Dampf-Flüssigkeit-Gleichgewichte Der Mischungen von Triethylamin Mit Tetrahydrofuran Und 1,4-Dioxan. *Zeitschrift für Physikalische Chemie* **1988**, *269O* (1). <https://doi.org/10.1515/zpch-1988-26997>.
- (649) 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. *Journal of Solution Chemistry* **1994**, 23 (2), 153–166. <https://doi.org/10.1007/BF00973543>.
- (650) Ahlers, S. Systematische Messung Thermodynamischer Daten Für Das System Thiophen - Sulfolan Zur Erweiterung Der Gruppenbeitragsmethode Modified UNIFAC (Dortmund), Universität Oldenburg, 2009.
- (651) Geier, K.; Bittrich, H.-J. Zur Thermodynamik Der Flüssig-Dampf-Gleichgewichte Der Binären Systeme n-Hexan/Benzol, Cyclohexan/Benzol Und Tetrahydrofuran Mit n-Hexan, Cyclohexan, Benzol Und Dimethylformamid. *Zeitschrift für Physikalische Chemie* **1979**, 2600 (1). <https://doi.org/10.1515/zpch-1979-26094>.
- (652) Conti, G.; Gianni, P.; Matteoli, E. Excess Enthalpies and Excess Heat Capacities of (N,N-Dimethylformamide + Tetrahydrofuran + Cyclohexane) at the Temperature 298.15 K. *The Journal of Chemical Thermodynamics* **1994**, 26 (12), 1249–1257. <https://doi.org/10.1006/jcht.1994.1142>.
- (653) Shealy, G. S.; Sandler, S. I. Vapor-Liquid Equilibrium for Four Mixtures Containing N,N-Dimethylformamide. *Journal of Chemical & Engineering Data* **1985**, 30 (4), 455–459. <https://doi.org/10.1021/je00042a026>.
- (654) Venkatesu, P.; Ramadevi, R. S.; Prabhakara Rao, M. V.; Prasad, D. H. L. Excess Molar Enthalpies of N,N-Dimethylformamide with Chloroethanes and Acetates at 298.15 K. *Journal of Chemical & Engineering Data* **2000**, 45 (4), 515–517. <https://doi.org/10.1021/je990286r>.
- (655) Reamer, H. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. n-Butane-Water System in the Two-Phase Region. *Industrial & Engineering Chemistry* **1952**, 44 (3), 609–615. <https://doi.org/10.1021/ie50507a049>.
- (656) Danneil, A.; Tödheide, K.; Franck, E. U. Verdampfungsgleichgewichte Und Kritische Kurven in Den Systemen Äthan/Wasser Und n-Butan/Wasser Bei Hohen Drücken. *Chemie Ingenieur Technik - CIT* **1967**, 39 (13), 816–822. <https://doi.org/10.1002/cite.330391309>.
- (657) Lancaster, N. M.; Wormald, C. J. Excess Molar Enthalpies for {xH₂O + (1 - x)C₃H₆} (g), {xH₂O + (1 - x)C₃H₈} (g), and {xH₂O + (1 - x)C₄H₁₀} (g). *The Journal of Chemical Thermodynamics* **1986**, 18 (6), 545–550. [https://doi.org/10.1016/0021-9614\(86\)90137-0](https://doi.org/10.1016/0021-9614(86)90137-0).
- (658) 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. *The Journal of Supercritical Fluids* **2004**, 30 (2), 145–153. <https://doi.org/10.1016/j.supflu.2003.09.002>.
- (659) Reamer, H. H.; Olds, R. H.; Sage, B. H.; Lacey, W. N. Phase Equilibria in Hydrocarbon Systems. n-Butane–Water System in Three-Phase Region. *Industrial & Engineering Chemistry* **1944**, 36 (4), 381–383. <https://doi.org/10.1021/ie50412a024>.
- (660) 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. *Chemical Engineering Communications* **1995**, 140 (1), 41–72. <https://doi.org/10.1080/00986449608936454>.
- (661) 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.
- (662) Thompson, W. H.; Snyder, J. R. Mutual Solubilities of Benzene and Water. Equilibria in the Two Phase Liquid - Liquid Region. *Journal of Chemical & Engineering Data* **1964**, 9 (4), 516–520. <https://doi.org/10.1021/je60023a013>.
- (663) Wormald, C. J.; Lancaster, N. M.; Sowden, C. J. Benzene–Water Association Excess Molar Enthalpy and Second Virial Cross-Coefficients for (Benzene–Water)(g) and

- (Cyclohexane–Water)(g). *Journal of the Chemical Society, Faraday Transactions* **1997**, 93 (10), 1921–1926. <https://doi.org/10.1039/a608259i>.
- (664) Wormald, C. J.; Slater, J. Excess Enthalpies for (Water + Benzene) in the Liquid and Supercritical Regions at T= 503 K to T= 592 K and P= 16.4 MPa. *The Journal of Chemical Thermodynamics* **1996**, 28 (6), 627–636. <https://doi.org/10.1006/jcht.1996.0059>.
- (665) 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. *Journal of Chemical & Engineering Data* **2006**, 51 (5), 1629–1633. <https://doi.org/10.1021/je060112r>.
- (666) 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. *Journal of Chemical & Engineering Data* **1990**, 35 (1), 63–66. <https://doi.org/10.1021/je00059a020>.
- (667) McFall, T. A.; Post, M. E.; Christensen, J. J.; Izatt, R. M. The Excess Enthalpies of Eight (Ethane + Alcohol) Mixtures at 298.15 K. *The Journal of Chemical Thermodynamics* **1981**, 13 (5), 441–446. [https://doi.org/10.1016/0021-9614\(81\)90051-3](https://doi.org/10.1016/0021-9614(81)90051-3).
- (668) Ott, J. B.; Lemon, L. R.; Sipowska, J. T.; Brown, P. R. Excess Enthalpies and Excess Volumes for (Ethane + Propan-1-ol) at the Temperatures (298.15, 323.15, and 348.15) K and at the Pressures (5, 10, 12.5, and 15) MPa. *The Journal of Chemical Thermodynamics* **1995**, 27 (9), 1033–1045. <https://doi.org/10.1006/jcht.1995.0108>.
- (669) Kodama, D.; Tanaka, H.; Kato, M. High Pressure Phase Equilibrium for Ethane + 1-Propanol at 314.15 K. *Journal of Chemical & Engineering Data* **2001**, 46 (5), 1280–1282. <https://doi.org/10.1021/je010077i>.
- (670) Lam, D. H.; Jangkamolkulchai, A.; Luks, K. D. Liquid-Liquid-Vapor Phase Equilibrium Behavior of Certain Binary Ethane + n-Alkanol Mixtures. *Fluid Phase Equilibria* **1990**, 59 (3), 263–277. [https://doi.org/10.1016/0378-3812\(90\)80003-T](https://doi.org/10.1016/0378-3812(90)80003-T).
- (671) Reamer, H. H.; Sage, B. H. Phase Behavior in the Nitrogen-Ammonia System. *Journal of Chemical & Engineering Data* **1959**, 4 (4), 303–305. <https://doi.org/10.1021/je60004a005>.
- (672) Lindroos, A. E.; Dodge, B. F. Phase-Equilibria at High Pressures; the System Nitrogen-Ammonia at Pressures above 1000 Atmospheres. *Chem. Eng. Progr. Symp. Ser.* **1952**, 48 (3), 10–17.
- (673) Naumowicz-Węglińska, E.; Wóycicki, W. Excess Enthalpies of Gaseous Mixtures Containing Ammonia 2. (Ammonia + Nitrogen) and (Ammonia + Methane). *The Journal of Chemical Thermodynamics* **1986**, 18 (11), 1047–1052. [https://doi.org/10.1016/0021-9614\(86\)90019-4](https://doi.org/10.1016/0021-9614(86)90019-4).
- (674) 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 Equilibria* **2007**, 252 (1–2), 162–174. <https://doi.org/10.1016/j.fluid.2006.12.018>.
- (675) Goodman, J. B.; Krase, N. W. Solubility of Nitrogen in Water at High Pressures and Temperatures. *Industrial & Engineering Chemistry* **1931**, 23 (4), 401–404. <https://doi.org/10.1021/ie50256a015>.
- (676) Rigby, M.; Prausnitz, J. M. Solubility of Water in Compressed Nitrogen, Argon, and Methane. *The Journal of Physical Chemistry* **1968**, 72 (1), 330–334. <https://doi.org/10.1021/j100847a064>.
- (677) Maslennikova, V. Ya.; Vdovina, N. A.; Tsiklis, D. S. Solubility of Water in Compressed Nitrogen. *Russ. J. Phys. Chem.* **1971**, 45 (9), 1354–1354.

- (678) Wiebe, R.; Gaddy, V. L.; Heinss, C. Solubility of Nitrogen in Water at 25°C from 25 to 1000 Atmospheres. *Industrial & Engineering Chemistry* **1932**, 24 (8), 927–927. <https://doi.org/10.1021/ie50272a023>.
- (679) Gillespie, P. C.; Wilson, G. M. Vapor-Liquid Equilibrium Data on Water-Substitute Gas Components: N₂-H₂O, H₂-H₂O, CO-H₂O, H₂-CO-H₂O, and H₂S-H₂O. *GPA Research Report* **1980**, 1–34.
- (680) Wiebe, R.; Gaddy, V. L.; Heins, C. The Solubility of Nitrogen in Water at 50, 75 and 100° from 25 to 1000 Atmospheres. *Journal of the American Chemical Society* **1933**, 55 (3), 947–953. <https://doi.org/10.1021/ja01330a011>.
- (681) Maslennikova, V. Ya. Solubility of Nitrogen in Water. *Tr. Gos. Nauchno Issled. Proektn. Inst. Azotn. Promst. Prod. Org. Sin.* **1971**, 12, 82–87.
- (682) Richards, P.; Wormald, C. J.; Yerlett, T. K. The Excess Enthalpy of (Water + Nitrogen) Vapour and (Water + n-Heptane) Vapour. *The Journal of Chemical Thermodynamics* **1981**, 13 (7), 623–628. [https://doi.org/10.1016/0021-9614\(81\)90032-X](https://doi.org/10.1016/0021-9614(81)90032-X).
- (683) Wormald, C. J.; Colling, C. N. Excess Enthalpies for (Water + Nitrogen)(g) up to 698.2 K and 12.6 MPa. *The Journal of Chemical Thermodynamics* **1983**, 15 (8), 725–737. [https://doi.org/10.1016/0021-9614\(83\)90139-8](https://doi.org/10.1016/0021-9614(83)90139-8).
- (684) Prokhorova, V. M.; Tsiklis, D. S. Vapor– Vapor Equilibrium in the System Nitrogen– Water. *Zh. Fiz. Khim.* **1970**, 44 (8), 2069–2070.
- (685) Siedler, R.; Grote, L.; Kauert, E.; Werner, U.; Bittrich, H. J. Zur Thermodynamik Der Binären Systeme von Benzol Mit Diäthylamin Und Triäthylamin. *Zeitschrift für Physikalische Chemie* **1969**, 2410 (1). <https://doi.org/10.1515/zpch-1969-24127>.
- (686) 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**, No. 1, 60–64.
- (687) Dehmelt, Ch.; Finke, M.; Bittrich, H. J. Untersuchungen Zur Zwischenmolekularen Wechselwirkung in Systemen von Diäthylamin Mit Aromatischen Komponenten. *Zeitschrift für Physikalische Chemie* **1974**, 2550 (1). <https://doi.org/10.1515/zpch-1974-25533>.
- (688) Ruffine, L. Équilibres de Phases à Basse Température de Systèmes Complexes CO₂ - Hydrocarbures Légers - Méthanol - Eau : Mesures et Modélisation, 2005.
- (689) 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. *Industrial & Engineering Chemistry Research* **2005**, 44 (22), 8387–8392. <https://doi.org/10.1021/ie0506365>.
- (690) Ohgaki, K.; Sano, F.; Katayama, T. Isothermal Vapor-Liquid Equilibrium Data for Binary Systems Containing Ethane at High Pressures. *Journal of Chemical & Engineering Data* **1976**, 21 (1), 55–58. <https://doi.org/10.1021/je60068a016>.
- (691) Ishihara, K.; Tanaka, H.; Kato, M. Phase Equilibrium Properties of Ethane+methanol System at 298.15 K. *Fluid Phase Equilibria* **1998**, 144 (1–2), 131–136. [https://doi.org/10.1016/S0378-3812\(97\)00251-3](https://doi.org/10.1016/S0378-3812(97)00251-3).
- (692) Ma, Y. Hua.; Kohn, J. P. Multiphase and Volumetric Equilibria of the Ethane-Methanol System at Temperatures between -40° and 100°C. *Journal of Chemical & Engineering Data* **1964**, 9 (1), 3–5. <https://doi.org/10.1021/je60020a002>.
- (693) Sipowska, J. T.; Graham, R. C.; Neely, B. J.; Ott, J. B.; Izatt, R. M. Excess Enthalpies for (Ethane + Methanol) at 298.15 and 348.15 K and 7.5 and 15 MPa, and at 323.15 K at 7.5, 10, and 15 MPa. *The Journal of Chemical Thermodynamics* **1989**, 21 (10), 1085–1093. [https://doi.org/10.1016/0021-9614\(89\)90095-5](https://doi.org/10.1016/0021-9614(89)90095-5).
- (694) 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. *The*

- Canadian Journal of Chemical Engineering* **1992**, 70 (2), 330–334. <https://doi.org/10.1002/cjce.5450700217>.
- (695) Galivel-Solastiouk, F.; Laugier, S.; Richon, D. Vapor-Liquid Equilibrium Data for the Propane-Methanol and Propane-Methanol-Carbon Dioxide System. *Fluid Phase Equilibria* **1986**, 28 (1), 73–85. [https://doi.org/10.1016/0378-3812\(86\)85069-5](https://doi.org/10.1016/0378-3812(86)85069-5).
- (696) 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. *Journal of Chemical & Engineering Data* **2004**, 49 (3), 426–429. <https://doi.org/10.1021/je0340506>.
- (697) Sipowska, J. T.; Ott, J. B.; Woolley, A. T.; Marchant, B. G.; Gruskiewicz, M. S. Excess Enthalpies for (Propane + Methanol) at the Pressure 5 MPa and the Temperatures (253.15, 258.15, 263.15, and 273.15) K. The Effect of Water as an Impurity on the (Liquid + Liquid) Equilibria in (Propane + Methanol). *The Journal of Chemical Thermodynamics* **1993**, 25 (8), 999–1004. <https://doi.org/10.1006/jcht.1993.1095>.
- (698) Sipowska, J. T.; Ott, J. B.; Neely, B. J.; Izatt, R. M. Excess Enthalpies for (Propane + Methanol) at the Temperatures (298.15, 323.15, 348.15, and 373.15) K and Pressures (5, 10, and 15) MPa, and at 363.15K and (5 and 15) MPa. *The Journal of Chemical Thermodynamics* **1991**, 23 (6), 551–559. [https://doi.org/10.1016/S0021-9614\(05\)80098-9](https://doi.org/10.1016/S0021-9614(05)80098-9).
- (699) 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 (11), 1654–1658.
- (700) Brown, I.; Smith, F. Liquid-Vapour Equilibria. IX. The Systems n-Propanol + Benzene and n-Butanol + Benzene at 45°C. *Australian Journal of Chemistry* **1959**, 12 (3), 407. <https://doi.org/10.1071/CH9590407>.
- (701) Strubl, K.; Svoboda, V.; Holub, R.; Pick, J. Liquid-Vapour Equilibrium in the Benzene-n-Propanol System. *Collection of Czechoslovak Chemical Communications* **1975**, 40 (6), 1647–1656. <https://doi.org/10.1135/cccc19751647>.
- (702) Hiaki, T.; Tochigi, K.; Kojima, K. Measurement of Vapor-Liquid Equilibria and Determination of Azeotropic Point. *Fluid Phase Equilibria* **1986**, 26 (1), 83–102. [https://doi.org/10.1016/0378-3812\(86\)85006-3](https://doi.org/10.1016/0378-3812(86)85006-3).
- (703) Shouyu Wang; Chenpu Zao. VLE Data for Benzene-n-Propanol-Lithium Chloride System. *Huaxue Gongcheng* **1991**, 19 (2), 72–76.
- (704) 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 (1), 51–65.
- (705) Chao, J. P.; Dai, M. Studies on Thermodynamic Properties of Binary Systems Containing Alcohols. VII. Temperature Dependence of Excess Enthalpies for n-Propanol + Benzene An. *Thermochimica Acta* **1988**, 123, 285–291. [https://doi.org/10.1016/0040-6031\(88\)80032-7](https://doi.org/10.1016/0040-6031(88)80032-7).
- (706) 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 (10), 549–552.
- (707) Skaates, J. M.; Kay, W. B. The Phase Relations of Binary Systems That Form Azeotropes. *Chemical Engineering Science* **1964**, 19 (7), 431–444. [https://doi.org/10.1016/0009-2509\(64\)85070-3](https://doi.org/10.1016/0009-2509(64)85070-3).
- (708) Iguchi, A. Vapor-Liquid Equilibria at 25°C for Binary Systems between Alcohols and Hydrocarbons. *Kagaku Sochi* **1978**, 20 (3), 66–68.

- (709) Smith, V. C.; Robinson, R. L. Vapor-Liquid Equilibria at 25°C in the Binary Mixtures Formed by Hexane, Benzene, and Ethanol. *Journal of Chemical & Engineering Data* **1970**, *15* (3), 391–395. <https://doi.org/10.1021/je60046a005>.
- (710) Tamir, A.; Apelblat, A.; Wagner, M. A New Device for Measuring Isothermal Vapor - Liquid Equilibria. *Fluid Phase Equilibria* **1981**, *6* (3–4), 237–259. [https://doi.org/10.1016/0378-3812\(81\)85007-8](https://doi.org/10.1016/0378-3812(81)85007-8).
- (711) 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* (11), 2397–2402.
- (712) 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* (5), 719–730.
- (713) Stokes, R. H.; Burfitt, C. Enthalpies of Dilution and Transfer of Ethanol in Non-Polar Solvents. *The Journal of Chemical Thermodynamics* **1973**, *5* (5), 623–631. [https://doi.org/10.1016/S0021-9614\(73\)80003-5](https://doi.org/10.1016/S0021-9614(73)80003-5).
- (714) 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* (2), 141–145.
- (715) Missopolinou, D.; Tzivintzelis, I.; Panayiotou, C. Excess Enthalpies of Binary Mixtures of 2-Ethoxyethanol with Four Hydrocarbons at 298.15, 308.15, and 318.15K. *Fluid Phase Equilibria* **2006**, *245* (2), 89–101. <https://doi.org/10.1016/j.fluid.2006.04.016>.
- (716) 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.
- (717) 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. *Journal of Chemical & Engineering Data* **1997**, *42* (5), 871–874. <https://doi.org/10.1021/je9700479>.
- (718) Neau, E.; Blanc, C.; Bares, D. Les Fonctions Thermodynamiques d'excès Du Binaire 2 Propanol-Isooctane. *Journal de Chimie Physique* **1973**, *70*, 843–849. <https://doi.org/10.1051/jcp/1973700843>.
- (719) 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. *The Journal of Chemical Thermodynamics* **2012**, *45* (1), 83–89. <https://doi.org/10.1016/j.jct.2011.09.007>.
- (720) 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* (4), 179–189.
- (721) 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. *The Journal of Chemical Thermodynamics* **2012**, *47*, 260–266. <https://doi.org/10.1016/j.jct.2011.10.025>.
- (722) 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. *Journal of Chemical & Engineering Data* **1994**, *39* (3), 602–604. <https://doi.org/10.1021/je00015a047>.
- (723) 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. *Journal of Chemical & Engineering Data* **2010**, *55* (1), 513–518. <https://doi.org/10.1021/je900327x>.

- (724) Heintz, A. The Pressure Dependence of the Excess Enthalpy of Mixtures of Isopropanol with Heptane and Isooctane up to 553 Bar. *Berichte der Bunsengesellschaft für physikalische Chemie* **1981**, 85 (9), 632–635. <https://doi.org/10.1002/bbpc.19810850905>.
- (725) 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. *Journal of Chemical & Engineering Data* **2007**, 52 (4), 1401–1407. <https://doi.org/10.1021/jc700092d>.
- (726) 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. *Journal of Chemical & Engineering Data* **2012**, 57 (3), 982–987. <https://doi.org/10.1021/jc201284y>.
- (727) Araujo, M. E.; Maciel, M. R. W.; Francesconi, A. Z. Excess Gibbs Free Energies of (Hexane + Butan-2-ol) and of (Cyclohexane + Butan-2-ol) at the Temperatures (323.15, 338.15, and 348.15) K. *The Journal of Chemical Thermodynamics* **1993**, 25 (11), 1295–1299. <https://doi.org/10.1006/jcht.1993.1129>.
- (728) Gascón, I.; Artigas, H.; Cea, P.; Domínguez, M.; Royo, F. M. Isobaric Vapour-Liquid Equilibrium of Ternary Mixtures Cyclohexane (or n -Hexane) Plus 1,3-Dioxolane Plus 2-Butanol at 40.0 and 101.3 KPa. *Physics and Chemistry of Liquids* **2003**, 41 (1), 1–13. <https://doi.org/10.1080/00319100290032703>.
- (729) 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. *Journal of Chemical & Engineering Data* **1998**, 43 (4), 658–661. <https://doi.org/10.1021/jc9800205>.
- (730) French, H. T. Thermodynamic Functions for the Systems 1-Butanol, 2-Butanol, and 2-Butanol + Cyclohexane. *Journal of Solution Chemistry* **1983**, 12 (12), 869–887. <https://doi.org/10.1007/BF00643927>.
- (731) 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. *Collection of Czechoslovak Chemical Communications* **1983**, 48 (12), 3482–3494. <https://doi.org/10.1135/cccc19833482>.
- (732) 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.
- (733) 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. *The Journal of Chemical Thermodynamics* **1988**, 20 (5), 539–544. [https://doi.org/10.1016/0021-9614\(88\)90081-X](https://doi.org/10.1016/0021-9614(88)90081-X).
- (734) 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 Equilibria* **2004**, 220 (1), 41–46. <https://doi.org/10.1016/j.fluid.2003.12.004>.
- (735) Gmehling, J.; Meents, B. Excess Enthalpy. 1-Propanol - Hexane System. *Int. Data Ser. Sel. Data Mixtures Ser. A* **1992**, No. 3, 158.
- (736) Mato, M. M.; Cebreiro, S. M.; Verdes, P. V.; Legido, J. L.; Paz Andrade, M. I. Thermodynamic Properties of the Ternary System MTBE+1-Propanol+hexane: Application of Different Group Contribution Models and Empirical Methods. *Journal of Thermal Analysis and Calorimetry* **2005**, 80 (2), 303–309. <https://doi.org/10.1007/s10973-005-0651-4>.

- (737) Brown, I.; Fock, W.; Smith, F. Heats of Mixing. V. Systems of n-Alcohols with n-Hexane. *Australian Journal of Chemistry* **1964**, *17* (10), 1106. <https://doi.org/10.1071/CH9641106>.
- (738) 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. *The Journal of Supercritical Fluids* **2012**, *71*, 26–44. <https://doi.org/10.1016/j.supflu.2012.07.008>.
- (739) 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 Equilibria* **1982**, *8* (1), 55–73. [https://doi.org/10.1016/0378-3812\(82\)80005-8](https://doi.org/10.1016/0378-3812(82)80005-8).
- (740) Ratcliff, G. A.; Chao, K. C. Prediction of Thermodynamic Properties of Polar Mixtures by a Group Solution Model. *The Canadian Journal of Chemical Engineering* **1969**, *47* (2), 148–153. <https://doi.org/10.1002/cjce.5450470208>.
- (741) 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.
- (742) Seo, J.; Lee, J.; Kim, H. Measurement and Correlation of Vapor–Liquid Equilibria for the 2-Propanol + n-Hexane System near the Critical Region. *Journal of Chemical & Engineering Data* **2003**, *48* (4), 856–859. <https://doi.org/10.1021/je025604s>.
- (743) Van Ness, H. C.; Soczek, C. A.; Kochar, N. K. Thermodynamic Excess Properties for Ethanol-n-Heptane. *Journal of Chemical & Engineering Data* **1967**, *12* (3), 346–351. <https://doi.org/10.1021/je60034a015>.
- (744) 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. *Journal of Chemical & Engineering Data* **2001**, *46* (2), 229–233. <https://doi.org/10.1021/je000212b>.
- (745) 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. *Journal of Chemical & Engineering Data* **1994**, *39* (4), 785–788. <https://doi.org/10.1021/je00016a033>.
- (746) Grosse-Wortmann, H.; Jost, W.; Wagner, H. Gg. Kalorimetrische Messungen Am System Äthanol - Cyclohexan - n-Heptan. *Zeitschrift für Physikalische Chemie* **1966**, *49* (1_2), 74–93. https://doi.org/10.1524/zpch.1966.49.1_2.074.
- (747) 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* (1), 11.
- (748) Mier, W.; Oswald, G.; Tusel-Langer, E.; Lichtenthaler, R. N. Excess Enthalpy HE of Binary Mixtures Containing Alkanes, Ethanol and Ethyl-Tert. Butyl Ether (ETBE). *Berichte der Bunsengesellschaft für physikalische Chemie* **1995**, *99* (9), 1123–1130. <https://doi.org/10.1002/bbpc.199500043>.
- (749) Tanaka, R.; Toyama, S.; Murakami, S. Heat Capacities of {xC_nH_{2n}+1OH + (1 – x)C₇H₁₆} for n = 1 to 6 at 298.15 K. *The Journal of Chemical Thermodynamics* **1986**, *18* (1), 63–73. [https://doi.org/10.1016/0021-9614\(86\)90044-3](https://doi.org/10.1016/0021-9614(86)90044-3).
- (750) Iguchi, A. Excess Molal Specific Heat of Nonelectrolyte Solutions. *Kagaku Sochi* **1977**, *19*, 64–65.
- (751) Mier, W.; Lichtenthaler, R. N.; Roux, A. H.; Grolier, J.-P. E. Excess Molar Heat Capacities C_{E,p,m} and Excess Molar Volumes V_{E,m} of {x₁CH₃(CH₂)₅CH₃ + X₂CH₃C(CH₃)₂CH₂CH(CH₃)CH₃ + X₃CH₃C(CH₃)₂OC₂H₅ + (1 - X₁ - X₂ - X₃)C₂H₅OH}(l) I. Binary and Quaternary Mixtures. *The Journal of Chemical Thermodynamics* **1994**, *26* (12), 1323–1334. <https://doi.org/10.1006/jcht.1994.1151>.

- (752) Fortier, J.-L.; Benson, G. C. Excess Heat Capacities of Binary Liquid Mixtures Determined with a Picker Flow Calorimeter. *The Journal of Chemical Thermodynamics* **1976**, *8* (5), 411–423. [https://doi.org/10.1016/0021-9614\(76\)90061-6](https://doi.org/10.1016/0021-9614(76)90061-6).
- (753) Klesper, I. Messung Der Spezifischen Wärmen Binärer Flüssigkeitsgemische. *Zeitschrift für Physikalische Chemie* **1966**, *51* (1_2), 1–12. https://doi.org/10.1524/zpch.1966.51.1_2.001.
- (754) 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. *The Journal of Supercritical Fluids* **2010**, *55* (2), 545–553. <https://doi.org/10.1016/j.supflu.2010.10.022>.
- (755) 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. *The Journal of Chemical Thermodynamics* **2014**, *74*, 161–168. <https://doi.org/10.1016/j.jct.2014.01.025>.
- (756) Scheller, M.; Schuberth, H.; Könnecke, H. G. Ergebnisse von Dampf-Flüssigkeits-Phasengleichgewichtsuntersuchungen Am System n-Hexan/Methylcyclohexan/Methanol Bei 60°C. *Journal für Praktische Chemie* **1969**, *311* (6), 974–982. <https://doi.org/10.1002/prac.19693110616>.
- (757) 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 Equilibria* **1996**, *122* (1–2), 207–222. [https://doi.org/10.1016/0378-3812\(96\)03037-3](https://doi.org/10.1016/0378-3812(96)03037-3).
- (758) 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 Equilibria* **2001**, *180* (1–2), 59–69. [https://doi.org/10.1016/S0378-3812\(00\)00510-0](https://doi.org/10.1016/S0378-3812(00)00510-0).
- (759) Andreoli-Ball, L.; Patterson, D.; Costas, M.; Cáceres-Alonso, M. Heat Capacity and Corresponding States in Alkan-1-Ol–n-Alkane Systems. *Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases* **1988**, *84* (11), 3991. <https://doi.org/10.1039/f19888403991>.
- (760) Costas, M.; Patterson, D. Self-Association of Alcohols in Inert Solvents. Apparent Heat Capacities and Volumes of Linear Alcohols in Hydrocarbons. *Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases* **1985**, *81* (3), 635. <https://doi.org/10.1039/f19858100635>.
- (761) 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. *Journal of Chemical & Engineering Data* **2001**, *46* (6), 1635–1637. <https://doi.org/10.1021/je010146t>.
- (762) de Loos, Th. W.; Poot, W.; de Swaan Arons, J. Vapour-Liquid Equilibria and Critical Phenomena in Methanol + n-Alkane Systems. *Fluid Phase Equilibria* **1988**, *42*, 209–227. [https://doi.org/10.1016/0378-3812\(88\)80060-8](https://doi.org/10.1016/0378-3812(88)80060-8).
- (763) 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. *Journal of Chemical & Engineering Data* **2003**, *48* (6), 1610–1613. <https://doi.org/10.1021/je034127q>.
- (764) Zawisza, A. High-Pressure Liquid-Vapour Equilibria, Critical State, and $p(V_m, T, x)$ to 448.15 K and 4.053 MPa for $\{xC_6H_{14} + (1-x)CH_3OH\}$. *The Journal of Chemical Thermodynamics* **1985**, *17* (10), 941–947. [https://doi.org/10.1016/0021-9614\(85\)90007-2](https://doi.org/10.1016/0021-9614(85)90007-2).

- (765) Toghiani, H.; Toghiani, R. K.; Viswanath, D. S. Vapor-Liquid Equilibria for the Methanol-Benzene and Methanol-Thiophene Systems. *Journal of Chemical & Engineering Data* **1994**, *39* (1), 63–67. <https://doi.org/10.1021/je00013a018>.
- (766) Strubl, K.; Svoboda, V.; Holub, R. Liquid-Vapour Equilibrium. LV. The System Methanol-Benzene. *Collection of Czechoslovak Chemical Communications* **1972**, *37* (11), 3522–3531. <https://doi.org/10.1135/cccc19723522>.
- (767) Scatchard, G.; Wood, S. E.; Mochel, J. M. Vapor-Liquid Equilibrium. VI. Benzene-Methanol Mixtures. *Journal of the American Chemical Society* **1946**, *68* (10), 1957–1960. <https://doi.org/10.1021/ja01214a024>.
- (768) Butcher, K. L.; Medani, M. S. Thermodynamic Properties of Methanol-Benzene Mixtures at Elevated Temperatures. *Journal of Applied Chemistry* **2007**, *18* (4), 100–107. <https://doi.org/10.1002/jctb.5010180402>.
- (769) Battler, J. R.; Rowley, R. L. Excess Enthalpies between 293 and 323 K for Constituent Binaries of Ternary Mixtures Exhibiting Partial Miscibility. *The Journal of Chemical Thermodynamics* **1985**, *17* (8), 719–732. [https://doi.org/10.1016/0021-9614\(85\)90101-6](https://doi.org/10.1016/0021-9614(85)90101-6).
- (770) Vesely, F.; Hynek, V.; Svoboda, V.; Holub, R. Isothermal Calorimeter for Measuring Endothermic Heats of Mixing. *Collect. Czech. Chem. Commun.* **1974**, *39* (2), 355–365. <https://doi.org/10.1135/cccc19740355>.
- (771) Williamson, A. G.; Scott, R. L. Heats of Mixing of Non-Electrolyte Solutions. I. Ethanol + Benzene and Methanol + Benzene. *J. Phys. Chem.* **1960**, *64*, 440–442. <https://doi.org/10.1021/j100833a015>.
- (772) Hudson, J. W.; Van Winkle, M. Multicomponent Vapor-Liquid Equilibria in Systems of Mixed Positive and Negative Deviations. *Journal of Chemical & Engineering Data* **1969**, *14* (3), 310–318. <https://doi.org/10.1021/je60042a025>.
- (773) Triday, J.; Andrade, A.; Aguirre Ode, F. Isobaric Study of the Binary Systems Formed by Thiophene or Benzene with Light Alcohols. *Scientia Valparaiso* **1978**, *43*, 1–24.
- (774) Strubl, K.; Voňka, P.; Svoboda, V.; Holub, R. Liquid-Vapour Equilibrium LVI. Correlation of the Benzene-Methanol Systems. *Collection of Czechoslovak Chemical Communications* **1973**, *38* (2), 468–476. <https://doi.org/10.1135/cccc19730468>.
- (775) 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* (12), 2711–2716.
- (776) 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 Journal of Chemical Engineering* **2000**, *17* (5), 510–515. <https://doi.org/10.1007/BF02707158>.
- (777) Duran-Valencia, C.; Pointurier, G.; Valtz, A.; Guilbot, P.; Richon, D. Vapor-Liquid Equilibrium (VLE) Data for the Carbon Dioxide (CO₂) + 1,1,1,2-Tetrafluoroethane (R134a) System at Temperatures from 252.95 K to 292.95 K and Pressures up to 2 MPa. *Journal of Chemical & Engineering Data* **2002**, *47* (1), 59–61. <https://doi.org/10.1021/je010075y>.
- (778) Silva-Oliver, G.; Galicia-Luna, L. A. Vapor-Liquid Equilibria for Carbon Dioxide + 1,1,1,2-Tetrafluoroethane (R-134a) Systems at Temperatures from 329 to 354 K and Pressures Upto 7.37 MPa. *Fluid Phase Equilibria* **2002**, *199* (1–2), 213–222. [https://doi.org/10.1016/S0378-3812\(01\)00816-0](https://doi.org/10.1016/S0378-3812(01)00816-0).
- (779) 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. *The Journal of Supercritical Fluids* **2008**, *44* (3), 279–283. <https://doi.org/10.1016/j.supflu.2007.09.025>.

- (780) 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 + 1,1,1,2,3,3,3-Hexafluoropropane (HFC-236ea). *Journal of Chemical & Engineering Data* **2004**, *49* (6), 1615–1621. <https://doi.org/10.1021/je0499723>.
- (781) Valtz, A.; Coquelet, C.; Baba-Ahmed, A.; Richon, D. Vapor–Liquid Equilibrium Data for the CO₂ + 1,1,1,2,3,3,3-Heptafluoropropane (R227ea) System at Temperatures from 276.01 to 367.30 K and Pressures up to 7.4 MPa. *Fluid Phase Equilibria* **2003**, *207* (1–2), 53–67. [https://doi.org/10.1016/S0378-3812\(02\)00326-6](https://doi.org/10.1016/S0378-3812(02)00326-6).
- (782) 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). *Journal of Chemical & Engineering Data* **2010**, *55* (11), 4999–5003. <https://doi.org/10.1021/je100583z>.
- (783) Chevalier, J. L. Systèmes Binaires Chloroforme-Éthers Aliphatiques - III. — Équilibres Liquide-Vapeur. *Journal de Chimie Physique et de Physico-Chimie Biologique* **1969**, *66*, 1457–1466.
- (784) Becker, F.; Kiefer, M. Heat of Mixing and Formation of Compounds in Binary Liquid Systems. III. Ether-Chloroform Systems. *Z. Naturforsch. Sec. A* **1971**, *26*, 1040–1046.
- (785) 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 Equilibria* **2007**, *251* (1), 59–62. <https://doi.org/10.1016/j.fluid.2006.10.017>.
- (786) Chevalier, J.-L.; Bares, D. Systèmes Binaires Chloroforme-Éthers Aliphatiques - I. — Chaleurs de Mélange à 25 °C. *Journal de Chimie Physique* **1969**, *66*, 1448–1452. <https://doi.org/10.1051/jcp/196966s21448>.
- (787) Stein, F. Paul.; Adams, R. A. Vapor-Liquid Equilibria for Carbon Dioxide-Difluoromethane System. *Journal of Chemical & Engineering Data* **1971**, *16* (2), 146–149. <https://doi.org/10.1021/je60049a015>.
- (788) Rivollet, F.; Chapoy, A.; Coquelet, C.; Richon, D. Vapor–Liquid Equilibrium Data for the Carbon Dioxide (CO₂) + Difluoromethane (R32) System at Temperatures from 283.12 to 343.25 K and Pressures up to 7.46 MPa. *Fluid Phase Equilibria* **2004**, *218* (1), 95–101. <https://doi.org/10.1016/j.fluid.2003.12.002>.
- (789) Diefenbacher, A.; Türk, M. (Vapour+liquid) Equilibria of Binary Mixtures of CO₂, CH₂F₂, CHF₃, and SF₆. *The Journal of Chemical Thermodynamics* **2002**, *34* (9), 1361–1375. [https://doi.org/10.1016/S0021-9614\(02\)00123-4](https://doi.org/10.1016/S0021-9614(02)00123-4).
- (790) 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* (1), 128–132. <https://doi.org/10.1021/je049789+>.
- (791) 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 Equilibria* **2005**, *232* (1–2), 44–49. <https://doi.org/10.1016/j.fluid.2005.02.013>.
- (792) Im, J.; Lee, G.; Kim, H. Vapor–Liquid Equilibria of the Difluoromethane + Dimethyl Ether and 1,1,1,2-Tetrafluoroethane + Dimethyl Ether Systems. *Journal of Chemical & Engineering Data* **2006**, *51* (3), 1126–1129. <https://doi.org/10.1021/je060028b>.
- (793) Valtz, A.; Coquelet, C.; Richon, D. Vapor–Liquid Equilibrium Data for the Sulfur Dioxide (SO₂) + Difluoromethane (R32) System at Temperatures from 288.07 to 403.16 K and at Pressures up to 7.31 MPa. *International Journal of Thermophysics* **2004**, *25* (6), 1695–1711. <https://doi.org/10.1007/s10765-004-7730-9>.

- (794) Rao, M. R.; Rao, K. V. K.; Rao, C. V. Vapour-Liquid Equilibria of Ethyl Acetate-Trichloroethylene System. *Journal of Applied Chemistry* **1957**, 7 (12), 666–671. <https://doi.org/10.1002/jctb.5010071205>.
- (795) Valtz, A.; Coquelet, C.; Richon, D. Vapor–Liquid Equilibrium Data for the Sulfur Dioxide (SO₂) + 1,1,1,2,3,3,3-Heptafluoropropane (R227ea) System at Temperatures from 288.07 to 403.19 K and Pressures up to 5.38 MPa. *Fluid Phase Equilibria* **2004**, 220 (1), 75–82. <https://doi.org/10.1016/j.fluid.2004.02.016>.
- (796) Noles, J. R.; Zollweg, J. A. Vapor-Liquid Equilibrium for Chlorodifluoromethane + Dimethyl Ether from 283 to 395 K at Pressures to 5.0 MPa. *Journal of Chemical & Engineering Data* **1992**, 37 (3), 306–310. <https://doi.org/10.1021/je00007a008>.
- (797) Im, J.; Lee, G.; Lee, J.; Kim, H. (Vapour+liquid) Equilibria of the {pentafluoroethane (HFC-125)+dimethyl Ether (DME)} System. *The Journal of Chemical Thermodynamics* **2006**, 38 (12), 1510–1514. <https://doi.org/10.1016/j.jct.2006.04.009>.
- (798) 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 Equilibria* **1998**, 147 (1–2), 215–228. [https://doi.org/10.1016/S0378-3812\(98\)00235-0](https://doi.org/10.1016/S0378-3812(98)00235-0).
- (799) 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 Equilibria* **2000**, 174 (1–2), 3–12. [https://doi.org/10.1016/S0378-3812\(00\)00413-1](https://doi.org/10.1016/S0378-3812(00)00413-1).
- (800) 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. *The Journal of Chemical Thermodynamics* **1998**, 30 (8), 1041–1046. <https://doi.org/10.1006/jcht.1998.0369>.
- (801) 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 (12), 2764–2766.
- (802) Siddiqi, M. A.; Lucas, K. The Excess Enthalpy of Methyl iodide + Carbon Disulphide, Methyl iodide + Dichloromethane and Dichloromethane + Carbon Disulphide over a Range of Temperatures and Pressures. *Fluid Phase Equilibria* **1985**, 20, 297–304. [https://doi.org/10.1016/0378-3812\(85\)90048-2](https://doi.org/10.1016/0378-3812(85)90048-2).
- (803) Röck, H.; Schröder, W. Dampf-Flüssigkeits-Gleichgewichtsmessungen Im System Azeton-Chloroform. *Z. Phys. Chem. NF* **1957**, 11, 41–55. https://doi.org/10.1524/zpch.1957.11.1_2.041.
- (804) 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.
- (805) Beckmann, E.; Faust, O. Die Dampfspannung Der Aceton-Chloroformgemische in Abhängigkeit von Der Temperatur. *Zeitschrift für Physikalische Chemie* **1914**, 89U (1). <https://doi.org/10.1515/zpch-1914-8917>.
- (806) 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. *Physics and Chemistry of Liquids* **2003**, 41 (3), 283–301. <https://doi.org/10.1080/0031910021000044456>.
- (807) 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.

- (808) Kulanek, M.; Bittrich, H. J. Heat of Solution of the System Acetone-Chloroform. *Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg* **1962**, *4* (2), 139–141.
- (809) 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. *Journal of Chemical & Engineering Data* **1975**, *20* (4), 403–405. <https://doi.org/10.1021/je60067a019>.
- (810) 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. *The Journal of Supercritical Fluids* **2014**, *94*, 17–29. <https://doi.org/10.1016/j.supflu.2014.06.014>.
- (811) Ohta, T.; Asano, H.; Nagata, I. Thermodynamic Study of Complex Formation in Four Binary Liquid Mixtures Containing Chloroform. *Fluid Phase Equilibria* **1980**, *4* (1–2), 105–114. [https://doi.org/10.1016/0378-3812\(80\)80008-2](https://doi.org/10.1016/0378-3812(80)80008-2).
- (812) Nagata, I. Isobaric Vapor-Liquid Equilibria for the Ternary System Chloroform-Methanol-Ethyl Acetate. *Journal of Chemical & Engineering Data* **1962**, *7* (3), 367–373. <https://doi.org/10.1021/je60014a013>.
- (813) Ortega, J. Excess Enthalpy. Trichloromethane-Ethyl Methanoate System. *Int. Data Ser. Sel. Data Mixtures Ser. A* **1993**, *21* (1), 40.
- (814) Fang, W.; Yu, Q.; Lin, R.; Zong, H. Vapor Heat Capacities of Some Polar–Polar Binary Systems. *Thermochimica Acta* **2000**, *352–353*, 19–23. [https://doi.org/10.1016/S0040-6031\(99\)00431-1](https://doi.org/10.1016/S0040-6031(99)00431-1).
- (815) Haase, R.; Tillmann, W. Negative Values of the Entropy of Mixing. *Z. Phys. Chem. Munich* **1992**, *175*, 209–216.
- (816) Suri, S. K.; Maheshwari, R. C. Molar Excess Enthalpies of Arsenic Tribromide + Benzene, +cyclohexane, and +tetrachloromethane at 313.15 K. *The Journal of Chemical Thermodynamics* **1980**, *12* (12), 1191–1192. [https://doi.org/10.1016/S0021-9614\(80\)80013-9](https://doi.org/10.1016/S0021-9614(80)80013-9).
- (817) van Ness, H. C.; Abbott, M. M. Excess Enthalpy. Trichloromethane (Chloroform)-Oxolane (Tetrahydrofuran) System. *Int. Data Ser. Sel. Data Mixtures Ser. A* **1974**, *1974* (1), 67.
- (818) 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. *Thermochimica Acta* **1981**, *44* (1), 77–87. [https://doi.org/10.1016/0040-6031\(81\)80273-0](https://doi.org/10.1016/0040-6031(81)80273-0).
- (819) Beath, L. A.; Williamson, A. G. Thermodynamics of Ether Solutions I. Enthalpies of Mixing of Ethers with Carbon Tetrachloride and with Chloroform. *The Journal of Chemical Thermodynamics* **1969**, *1* (1), 51–57. [https://doi.org/10.1016/0021-9614\(69\)90036-6](https://doi.org/10.1016/0021-9614(69)90036-6).
- (820) Becker, F.; Kiefer, M. Kontinuierliche Bestimmung von Mischungswärmen Durch Isotherme Enthalpietitation. *Zeitschrift für Naturforschung A* **1969**, *24* (1). <https://doi.org/10.1515/zna-1969-0103>.
- (821) Nagata, I.; Hayashida, H. Vapor-Liquid Equilibrium Data For The Ternary Systems: Methyl Acetate-2-Propanol-Benzene And Methyl Acetate-Chloroform-Benzene. *Journal of Chemical Engineering of Japan* **1970**, *3* (2), 161–166. <https://doi.org/10.1252/jcej.3.161>.
- (822) 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* (2), 85–96.
- (823) 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. *The Journal of Chemical Thermodynamics* **2006**, 38 (11), 1432–1437. <https://doi.org/10.1016/j.jct.2006.01.010>.
- (824) 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. *Thermochimica Acta* **1995**, 258, 109–115. [https://doi.org/10.1016/0040-6031\(94\)02236-H](https://doi.org/10.1016/0040-6031(94)02236-H).
- (825) 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. *Journal of Chemical & Engineering Data* **1995**, 40 (3), 645–646. <https://doi.org/10.1021/je00019a024>.
- (826) 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.
- (827) Ortega, J. Excess Enthalpy. 1,1,2,2-Tetrachloroethane - Ethyl Ethanoate System. *International DATA Series, Selected Data on Mixtures, Series A: Thermodynamic Properties of Non-Reacting Binary Systems of Organic Substances* **1991**, 4, 249.
- (828) 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). *The Journal of Chemical Thermodynamics* **1992**, 24 (8), 823–827. [https://doi.org/10.1016/S0021-9614\(05\)80227-7](https://doi.org/10.1016/S0021-9614(05)80227-7).
- (829) Nagata, I.; Kawamura, Y.; Asano, H.; Fujiwara, K.; Ogasawara, Y. Excess Enthalpies for Binary Mixtures of Chloroform with Alcohols. *Z. Phys. Chem. Leipzig* **1978**, 259 (6), 1109–1116.
- (830) 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. *Journal of Chemical & Engineering Data* **1995**, 40 (1), 332–335. <https://doi.org/10.1021/je00017a073>.
- (831) Iloukhani, H. Excess Molar Enthalpies for Binary Mixtures with Trichloroethylene + Alkan-1-Ols (C3–C8) at 298.15 K. *Journal of Chemical & Engineering Data* **1997**, 42 (4), 802–804. <https://doi.org/10.1021/je970024u>.
- (832) 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. *Journal of Chemical & Engineering Data* **1996**, 41 (1), 89–92. <https://doi.org/10.1021/je950163g>.
- (833) 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 (5), 425–433. <https://doi.org/10.1023/A:1010396430848>.
- (834) Harris, H. G. Vapor-Liquid Equilibria in Binary Hydrocarbon - Polar Solvent Systems, University of California, Berkeley, 1968.
- (835) Desplanches, H.; Chevalier, J.-L.; Llinas, R. Étude Thermodynamique de Solutions d'acétonitrile et d'hydrocarbures Acétyléniques. *Journal de Chimie Physique* **1977**, 74, 259–265. <https://doi.org/10.1051/jcp/1977740259>.
- (836) Nagata, I. Vapor-Liquid Equilibria for the Ternary System 2-Propanol-Chloroform-Benzene at 50°C. *Journal of Chemical & Engineering Data* **1985**, 30 (1), 80–82. <https://doi.org/10.1021/je00039a027>.
- (837) Hanumantharao, G.; Subbarao, B. V. ISOBARIC VAPOR-LIQUID-EQUILIBRIA-CHLOROFORM-ISOPROPANOL, TERTIARY BUTANOL-TOLUENE AND TERTIARY BUTANOL-TRICHLOROETHYLENE SYSTEMS. *INDIAN JOURNAL OF TECHNOLOGY* **1974**, 12 (7), 292–295.

- (838) Zudkevitch, D.; Lindrud, M.; Chu, Y.-Z. Vapor–Liquid Equilibria for Ethanol + Hept-1-Yne and Butyric Acid + Butyric Anhydride. *Journal of Chemical & Engineering Data* **1999**, *44* (3), 393–397. <https://doi.org/10.1021/je980210f>.
- (839) 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 Equilibria* **1990**, *61* (1–2), 111–119. [https://doi.org/10.1016/0378-3812\(90\)90008-B](https://doi.org/10.1016/0378-3812(90)90008-B).
- (840) Scatchard, G.; Raymond, C. L. Vapor–Liquid Equilibrium. II. Chloroform–Ethanol Mixtures at 35, 45 and 55°. *Journal of the American Chemical Society* **1938**, *60* (6), 1278–1287. <https://doi.org/10.1021/ja01273a002>.
- (841) Roeck, H.; Schroeder, W. Beitrag Zur Kenntnis Des Konzentrationsverlaufs Thermodynamischer Mischungsfunctionen. *Z. Phys. Chem. NF* **1956**, *9*, 277–284.
- (842) Bourrelly, V.; Chevalier, J.-L. Appareil Pour La Détermination Rapide Des Équilibres Isothermes Liquide-Vapeur. *Journal de Chimie Physique* **1968**, *65*, 1561–1564. <https://doi.org/10.1051/jcp/1968651561>.
- (843) 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.
- (844) 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. *Journal of Chemical & Engineering Data* **2008**, *53* (11), 2642–2648. <https://doi.org/10.1021/je800548t>.
- (845) 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. *Journal of Chemical & Engineering Data* **1984**, *29* (2), 181–183. <https://doi.org/10.1021/je00036a026>.
- (846) Campbell, A. N.; Kartzmark, E. M.; Gieskes, J. M. T. M. Vapor–Liquid Equilibria, Densities, And Refractivities In The System Acetic Acid – Chloroform – Water At 25 °C. *Canadian Journal of Chemistry* **1963**, *41* (2), 407–429. <https://doi.org/10.1139/v63-059>.
- (847) Conti, J. J.; Othmer, D. F.; Gilmont, R. Composition of Vapors from Boiling Binary Solutions. Systems Containing Formic Acid, Acetic Acid, Water, and Chloroform. *Journal of Chemical & Engineering Data* **1960**, *5* (3), 301–307. <https://doi.org/10.1021/je60007a019>.
- (848) Campbell, A. N.; Gieskes, J. M. T. M. The Isobaric Boiling Points Of The System: Acetic Acid – Chloroform – Water At A Pressure Of 760 Mm Hg. *Canadian Journal of Chemistry* **1964**, *42* (1), 186–189. <https://doi.org/10.1139/v64-032>.
- (849) 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* (4), 26–32.
- (850) Ratkovics, F. Adiabatic Calorimeter for Determining Heats of Mixing. *Magy. Kem. Foly.* **1971**, *77* (10), 499–502.
- (851) 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. *Journal of Chemical & Engineering Data* **1980**, *25* (1), 29–32. <https://doi.org/10.1021/je60084a016>.
- (852) Fenclova, D.; Dohnal, V. Excess Gibbs Energy. Bromochloro-1,1,1-Trifluoroethane - Methanol System. *Int. Data Ser. Sel. Data Mixtures Ser. A* **1993**, *21* (2), 100.
- (853) Costas, M. Excess Heat Capacity. Bromochloro-1,1,1-Trifluoroethane - Methanol System. *Int. Data Ser. Sel. Data Mixtures Ser. A* **1993**, *21* (2), 158.
- (854) 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. *Journal of Chemical & Engineering Data* **1994**, 39 (1), 134–139. <https://doi.org/10.1021/je00013a038>.
- (855) Venkatesulu, D.; Rao, M. V. P.; Veeranna, D. Excess Enthalpies of 2-Alkoxyethanols with Trichloroethylene and Tetrachloroethylene at 298.15 K. *Thermochimica Acta* **1994**, 242, 33–39. [https://doi.org/10.1016/0040-6031\(94\)85006-2](https://doi.org/10.1016/0040-6031(94)85006-2).
- (856) Lazarte, M.; Gómez Marigliano, A. C.; Sólamo, 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. *Journal of Solution Chemistry* **2004**, 33 (12), 1549–1563. <https://doi.org/10.1007/s10953-004-1393-9>.
- (857) Nagata, I.; Kawamura, Y. Excess Thermodynamic Functions and Complex Formation in Binary Liquid Mixtures Containing Acetonitrile. *Fluid Phase Equilibria* **1979**, 3 (1), 1–11. [https://doi.org/10.1016/0378-3812\(79\)80023-0](https://doi.org/10.1016/0378-3812(79)80023-0).
- (858) Mato, F.; Sanchez, M. Liquid-Vapor Equilibriums of Binary Mixtures of Acetonitrile. *Anales de la Real Sociedad Espanola de Fisica y Quimica, Serie B: Quimica* **1967**, 63, 1–11.
- (859) Handa, Y. P.; Jones, D. E. Molar Excess Enthalpies of Acetonitrile + Chloroform and of Acetonitrile + Chloroform-D1 at 298 K. *Canadian Journal of Chemistry* **1977**, 55 (16), 2977–2979. <https://doi.org/10.1139/v77-414>.
- (860) 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. *The Journal of Chemical Thermodynamics* **1983**, 15 (8), 721–724. [https://doi.org/10.1016/0021-9614\(83\)90138-6](https://doi.org/10.1016/0021-9614(83)90138-6).
- (861) Zegers, H. C.; Somsen, G. Volumes and Heat Capacities of Mixtures of Dimethylformamide with Several Dialkylacetamides. *Fluid Phase Equilibria* **1984**, 18 (3), 299–311. [https://doi.org/10.1016/0378-3812\(84\)85013-X](https://doi.org/10.1016/0378-3812(84)85013-X).
- (862) Nagata, I. Isothermal (Vapour + Liquid) Equilibria of Propan-1-Ol + Acetonitrile and + Trichloromethane and of (Propan-1-Ol + Acetonitrile + Trichloromethane). *The Journal of Chemical Thermodynamics* **1985**, 17 (11), 1017–1022. [https://doi.org/10.1016/0021-9614\(85\)90086-2](https://doi.org/10.1016/0021-9614(85)90086-2).
- (863) Wang Shouyu; Cai Shuxing. VLE Data for Chloroform - n-Propanol and Its System Containing Salt. *Huaxue Gongcheng* **1994**, 22 (5), 36–40.
- (864) Ortega, J. Excess Enthalpy. 1,1,2,2-Tetrachloroethane - Propyl Methanoate System. *International DATA Series, Selected Data on Mixtures, Series A: Thermodynamic Properties of Non-Reacting Binary Systems of Organic Substances* **1991**, 4, 248.
- (865) Zel'venskii, Ya. D. The Solubility of Carbon Dioxide in Water under Pressure. *Zh. Khim. Prom.* **1937**, 14, 1250–1257.
- (866) 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. *The Journal of Supercritical Fluids* **2013**, 73, 87–96. <https://doi.org/10.1016/j.supflu.2012.11.011>.
- (867) Gillespie, P. C.; Wilson, G. M. Vapor-Liquid and Liquid-Liquid Equilibria: Water - Methane, Water - Carbon Dioxide, Water - Hydrogen Sulfide, Water - n-Pentane, Water - Methane - n-Pentane. *GPA Research Report* **1982**, 1–73.
- (868) 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. *Journal of Chemical & Engineering Data* **2012**, 57 (7), 1928–1932. <https://doi.org/10.1021/je3000958>.
- (869) 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. *The Journal of Supercritical Fluids* **2010**, 52 (1), 142–150. <https://doi.org/10.1016/j.supflu.2009.10.005>.
- (870) 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. *The Journal of Supercritical Fluids* **2011**, 56 (2), 125–129. <https://doi.org/10.1016/j.supflu.2010.12.003>.
- (871) King, M. B.; Mubarak, A.; Kim, J. D.; Bott, T. R. The Mutual Solubilities of Water with Supercritical and Liquid Carbon Dioxides. *The Journal of Supercritical Fluids* **1992**, 5 (4), 296–302. [https://doi.org/10.1016/0896-8446\(92\)90021-B](https://doi.org/10.1016/0896-8446(92)90021-B).
- (872) Zaalishvili, S. D. Solubility of Carbon Dioxide from Its Mixtures with Hydrogen and Nitrogen in Water under Pressure. *Zh. Fiz. Khim.* **1940**, 14 (3), 413–417.
- (873) Dohrn, R.; Büinz, A. P.; Devlieghere, F.; Thelen, D. Experimental Measurements of Phase Equilibria for Ternary and Quaternary Systems of Glucose, Water, CO₂ and Ethanol with a Novel Apparatus. *Fluid Phase Equilibria* **1993**, 83, 149–158. [https://doi.org/10.1016/0378-3812\(93\)87017-U](https://doi.org/10.1016/0378-3812(93)87017-U).
- (874) D'souza, R.; Patrick, J. R.; Teja, A. S. High Pressure Phase Equilibria in the Carbon Dioxide - n-Hexadecane and Carbon Dioxide - Water Systems. *The Canadian Journal of Chemical Engineering* **1988**, 66 (2), 319–323. <https://doi.org/10.1002/cjce.5450660221>.
- (875) Briones, J. A.; Mullins, J. C.; Thies, M. C.; Kim, B.-U. Ternary Phase Equilibria for Acetic Acid-Water Mixtures with Supercritical Carbon Dioxide. *Fluid Phase Equilibria* **1987**, 36, 235–246. [https://doi.org/10.1016/0378-3812\(87\)85026-4](https://doi.org/10.1016/0378-3812(87)85026-4).
- (876) Bamberger, A.; Sieder, G.; Maurer, G. High-Pressure (Vapor+liquid) Equilibrium in Binary Mixtures of (Carbon Dioxide+water or Acetic Acid) at Temperatures from 313 to 353 K. *The Journal of Supercritical Fluids* **2000**, 17 (2), 97–110. [https://doi.org/10.1016/S0896-8446\(99\)00054-6](https://doi.org/10.1016/S0896-8446(99)00054-6).
- (877) 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 Equilibria* **1998**, 141, 179–206. [https://doi.org/10.1016/S0378-3812\(97\)00210-0](https://doi.org/10.1016/S0378-3812(97)00210-0).
- (878) Takenouchi, S.; Kennedy, G. C. The Binary System H₂O-CO₂ at High Temperatures and Pressures. *American Journal of Science* **1964**, 262 (9), 1055–1074. <https://doi.org/10.2475/ajs.262.9.1055>.
- (879) 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. *Journal of Chemical & Engineering Data* **1981**, 26 (4), 388–391. <https://doi.org/10.1021/je00026a012>.
- (880) Tödheide, K.; Franck, E. U. Das Zweiphasengebiet Und Die Kritische Kurve Im System Kohlendioxid–Wasser Bis Zu Drucken von 3500 Bar. *Zeitschrift für Physikalische Chemie* **1963**, 37 (5_6), 387–401. https://doi.org/10.1524/zpch.1963.37.5_6.387.
- (881) 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. *The Journal of Supercritical Fluids* **2005**, 36 (1), 23–30. <https://doi.org/10.1016/j.supflu.2005.03.006>.
- (882) Xuemin Chen; 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. *Journal of Solution Chemistry* **1992**, 21 (8), 825–848. <https://doi.org/10.1007/BF00651511>.
- (883) Wormald, C. J.; Lancaster, N. M.; Sellars, A. J. The Excess Molar Enthalpies of {xH₂O + (1 - x)CO}(g) and {xH₂O + (1 - x)CO₂}(g) at High Temperatures and Pressures. *The*

- Journal of Chemical Thermodynamics* **1986**, 18 (2), 135–147. [https://doi.org/10.1016/0021-9614\(86\)90128-X](https://doi.org/10.1016/0021-9614(86)90128-X).
- (884) Guo, L.; Wu, X.-H.; Zheng, D.-X.; Deng, W. Measurement and Correlation of Vapor–Liquid Equilibrium for the Carbon Dioxide + 1-Butoxy Butane System. *Journal of Chemical & Engineering Data* **2010**, 55 (1), 476–478. <https://doi.org/10.1021/jc900231r>.
- (885) Secuianu, C.; Ferouiu, V.; Geană, D. Phase Behavior for Carbon Dioxide+ethanol System: Experimental Measurements and Modeling with a Cubic Equation of State. *The Journal of Supercritical Fluids* **2008**, 47 (2), 109–116. <https://doi.org/10.1016/j.supflu.2008.08.004>.
- (886) Day, C.-Y.; Chang, C. J.; Chen, C.-Y. Phase Equilibrium of Ethanol + CO₂ and Acetone + CO₂ at Elevated Pressures. *Journal of Chemical & Engineering Data* **1996**, 41 (4), 839–843. <https://doi.org/10.1021/jc960049d>.
- (887) 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 (3), 9–15.
- (888) Tanaka, H.; Kato, M. Vapor-Liquid Equilibrium Properties of Carbon Dioxide + Ethanol Mixture at High Pressures. *JOURNAL OF CHEMICAL ENGINEERING OF JAPAN* **1995**, 28 (3), 263–266. <https://doi.org/10.1252/jcej.28.263>.
- (889) 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. *The Journal of Supercritical Fluids* **2010**, 55 (2), 682–689. <https://doi.org/10.1016/j.supflu.2010.10.016>.
- (890) 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 Equilibria* **2001**, 185 (1–2), 219–230. [https://doi.org/10.1016/S0378-3812\(01\)00472-1](https://doi.org/10.1016/S0378-3812(01)00472-1).
- (891) Brandt, L. Einsatz Überkritischer Fluide Für Die Trenntechnik. *Thesis* **2011**, 1–128.
- (892) 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. *Journal of Chemical & Engineering Data* **2000**, 45 (2), 265–271. <https://doi.org/10.1021/jc990187d>.
- (893) Yi-Ling Tian; Ming Han; Li Chen; Ji-Jun Feng; Ying Qin. Study on Vapor-Liquid Phase Equilibria for CO₂-C₂H₅OH System. *Wuli Huaxue Xuebao* **2001**, 17 (2), 155–160.
- (894) 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 (3), 157–164.
- (895) 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. *The Journal of Chemical Thermodynamics* **1996**, 28 (11), 1303–1317. <https://doi.org/10.1006/jcht.1996.0115>.
- (896) Cordray, D. R.; Izatt, R. M.; Christensen, J. J.; Oscarson, J. L. The Excess Enthalpies of (Carbon Dioxide + Ethanol) at 308.15, 325.15, 373.15, 413.15, and 473.15 K from 5.00 to 14.91 MPa. *The Journal of Chemical Thermodynamics* **1988**, 20 (6), 655–663. [https://doi.org/10.1016/0021-9614\(88\)90016-X](https://doi.org/10.1016/0021-9614(88)90016-X).
- (897) 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 (4), 469–472.

- (898) Yeo, S.-D.; Park, S.-J.; Kim, J.-W.; Kim, J.-C. Critical Properties of Carbon Dioxide + Methanol, + Ethanol, + 1-Propanol, and + 1-Butanol. *Journal of Chemical & Engineering Data* **2000**, *45* (5), 932–935. <https://doi.org/10.1021/je000104p>.
- (899) Mejía, A.; Segura, H.; Cartes, M. Vapor–Liquid Equilibria and Interfacial Tensions of the System Ethanol + 2-Methoxy-2-Methylpropane. *Journal of Chemical & Engineering Data* **2010**, *55* (1), 428–434. <https://doi.org/10.1021/je9004068>.
- (900) 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. *Journal of Chemical & Engineering Data* **1996**, *41* (4), 718–723. <https://doi.org/10.1021/je950323o>.
- (901) Letcher, T. M.; Govender, P. U. Excess Molar Enthalpies of an Alkanol + a Branched Chain Ether at the Temperature 298.15 K. *Journal of Chemical & Engineering Data* **1995**, *40* (4), 997–1000. <https://doi.org/10.1021/je00020a060>.
- (902) 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* (1), 251–254. <https://doi.org/10.1023/A:1020634507355>.
- (903) 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 Equilibria* **2010**, *296* (1), 37–41. <https://doi.org/10.1016/j.fluid.2010.02.012>.
- (904) 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.
- (905) 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 Equilibria* **2002**, *198* (2), 229–237. [https://doi.org/10.1016/S0378-3812\(01\)00766-X](https://doi.org/10.1016/S0378-3812(01)00766-X).
- (906) Gutiérrez, J. E.; Bejarano, A.; Fuente, J. C. de la. Measurement and Modeling of High-Pressure (Vapour+liquid) Equilibria of (CO₂+alcohol) Binary Systems. *The Journal of Chemical Thermodynamics* **2010**, *42* (5), 591–596. <https://doi.org/10.1016/j.jct.2009.11.015>.
- (907) 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. *Journal of Chemical & Engineering Data* **2003**, *48* (6), 1407–1412. <https://doi.org/10.1021/je020214r>.
- (908) 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.* **1978**, *52* (5), 1149–1152.
- (909) 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 Equilibria* **2002**, *194–197*, 919–928. [https://doi.org/10.1016/S0378-3812\(01\)00704-X](https://doi.org/10.1016/S0378-3812(01)00704-X).
- (910) Brunner, E.; Hültenschmidt, W.; Schlichthärle, G. Fluid Mixtures at High Pressures IV. Isothermal Phase Equilibria in Binary Mixtures Consisting of (Methanol + Hydrogen or Nitrogen or Methane or Carbon Monoxide or Carbon Dioxide). *The Journal of Chemical Thermodynamics* **1987**, *19* (3), 273–291. [https://doi.org/10.1016/0021-9614\(87\)90135-2](https://doi.org/10.1016/0021-9614(87)90135-2).
- (911) Li, N.; Ma, P.; Xia, S. Determination of Solubility of Carbon Monoxide in Methanol-Dimethyl Carbonate under High Pressure. *Shiyou Huagong* **2005**, *34* (1), 60–64.

- (912) 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.
- (913) Secuianu, C.; Feroiu, V.; Geană, D. Measurements and Modeling of High-Pressure Phase Behavior of the Carbon Dioxide + Pentan-1-ol Binary System. *Journal of Chemical & Engineering Data* **2011**, *56* (12), 5000–5007. <https://doi.org/10.1021/jc200867n>.
- (914) Secuianu, C.; Feroiu, V.; Geană, D. High-Pressure Vapour-Liquid Equilibria of Carbon Dioxide + 1-Pentanol System. Experimental Measurements and Modelling. *Revista de Chimie-Bucharest* **2007**, *58* (12), 1176–1181.
- (915) Staby, A.; Mollerup, J. Measurement of Mutual Solubilities of 1-Pentanol and Supercritical Carbon Dioxide. *The Journal of Supercritical Fluids* **1993**, *6* (1), 15–19. [https://doi.org/10.1016/0896-8446\(93\)90005-1](https://doi.org/10.1016/0896-8446(93)90005-1).
- (916) 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 Equilibria* **2002**, *200* (1), 161–172. [https://doi.org/10.1016/S0378-3812\(02\)00024-9](https://doi.org/10.1016/S0378-3812(02)00024-9).
- (917) Bittrich, H. J.; Kauer, E. Thermodynamics of the System Diethylamine-Triethylamine. I. The Liquid-Vapor Equilibrium. *Z. Phys. Chem. Leipzig* **1962**, *219* (3–4), 224–238.
- (918) Bittrich, H. J.; Kulanek, M.; Duering, G. Thermodynamics of the System Diethylamine-Triethylamine. Enthalpies of Mixing at 14, 18, and 25°. *Z. Phys. Chem. Leipzig* **1962**, *219*, 387–395.
- (919) 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* (3), 249–265.
- (920) Kauer, E.; Grote, L.; Bittrich, H.-J. Zur Thermodynamik Des Systems Diäthylamin-Triäthylamin. IV. *Zeitschrift für Physikalische Chemie* **1966**, *2320* (1). <https://doi.org/10.1515/zpch-1966-23231>.
- (921) 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. *Journal of Chemical & Engineering Data* **1999**, *44* (3), 405–410. <https://doi.org/10.1021/jc980248s>.
- (922) 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 Equilibria* **2001**, *180* (1–2), 235–245. [https://doi.org/10.1016/S0378-3812\(01\)00349-1](https://doi.org/10.1016/S0378-3812(01)00349-1).
- (923) 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. *Journal of Chemical & Engineering Data* **1999**, *44* (6), 1169–1174. <https://doi.org/10.1021/jc990095o>.
- (924) 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 Equilibria* **1999**, *156* (1–2), 161–171. [https://doi.org/10.1016/S0378-3812\(99\)00026-6](https://doi.org/10.1016/S0378-3812(99)00026-6).
- (925) Davolio, F.; Pedrosa, G. C.; Katz, M. Vapor-Liquid Equilibrium for the p-Dioxane-Acetonitrile System at 298.15 K. *Journal of Chemical & Engineering Data* **1981**, *26* (1), 26–27. <https://doi.org/10.1021/jc00023a011>.
- (926) Francesconi, R.; Comelli, F. Excess Thermodynamic Properties for the Binary System 1,4-Dioxane-Acetonitrile at 40.Degree.C. *Journal of Chemical & Engineering Data* **1988**, *33* (2), 80–83. <https://doi.org/10.1021/jc00052a004>.

- (927) 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. *The Journal of Chemical Thermodynamics* **1991**, *23* (5), 421–429. [https://doi.org/10.1016/S0021-9614\(05\)80130-2](https://doi.org/10.1016/S0021-9614(05)80130-2).
- (928) Song, H. J.; Zhang, H. T.; Ying, W. Y. Study on Vapor-Liquid Equilibrium for Dimethyl Ether/Methanol Binary System. *Tianranqi Huagong* **2005**, *30* (6), 67–71.
- (929) 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. *Journal of Chemical & Engineering Data* **1984**, *29* (3), 324–329. <https://doi.org/10.1021/je00037a030>.
- (930) 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 Equilibria* **1988**, *44* (2), 195–209. [https://doi.org/10.1016/0378-3812\(88\)80111-0](https://doi.org/10.1016/0378-3812(88)80111-0).
- (931) 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. *Journal of Chemical & Engineering Data* **2007**, *52* (5), 1814–1818. <https://doi.org/10.1021/je700174h>.
- (932) Hong, J. H.; Kobayashi, R. Vapor—Liquid Equilibrium Studies for the Carbon Dioxide—Methanol System. *Fluid Phase Equilibria* **1988**, *41* (3), 269–276. [https://doi.org/10.1016/0378-3812\(88\)80011-6](https://doi.org/10.1016/0378-3812(88)80011-6).
- (933) 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. *Journal of Chemical & Engineering Data* **1976**, *21* (1), 53–55. <https://doi.org/10.1021/je60068a015>.
- (934) 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. *Journal of Chemical Engineering of Japan* **1975**, *8* (2), 89–92. <https://doi.org/10.1252/jcej.8.89>.
- (935) 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 Equilibria* **1997**, *131* (1–2), 243–258. [https://doi.org/10.1016/S0378-3812\(96\)03208-6](https://doi.org/10.1016/S0378-3812(96)03208-6).
- (936) 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* (1), 16–20. <https://doi.org/10.2963/jjtp.10.16>.
- (937) 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* (10), 2502–2505.
- (938) Leu, A.-D.; Chung, S. Y.-K.; Robinson, D. B. The Equilibrium Phase Properties of (Carbon Dioxide + Methanol). *The Journal of Chemical Thermodynamics* **1991**, *23* (10), 979–985. [https://doi.org/10.1016/S0021-9614\(05\)80178-8](https://doi.org/10.1016/S0021-9614(05)80178-8).
- (939) Zhu Hu-Gang; Tian Yi-Ling; Chen Li; Feng Ji-Jun; Fu Hua-Feng. Studies on Vapor-Liquid Phase Equilibria for SCF CO₂+ CH₃OH and SCF CO₂+ C₂H₅OH Systems. *Gaodeng Xuexiao Huaxue Xuebao* **2002**, *23* (8), 1588–1591.
- (940) 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* (1), 161–164. <https://doi.org/10.1021/je980191+>.
- (941) 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* (2), 64–69. <https://doi.org/10.2963/jjtp.12.64>.
- (942) Christensen, J. J.; Cordray, D. R.; Oscarson, J. L.; Izatt, R. M. The Excess Enthalpies of Four (Carbon Dioxide + an Alkanol) Mixtures from 308.15 to 573.15 K at 7.50 to 12.50

- MPa. *The Journal of Chemical Thermodynamics* **1988**, *20* (7), 867–875. [https://doi.org/10.1016/0021-9614\(88\)90076-6](https://doi.org/10.1016/0021-9614(88)90076-6).
- (943) 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. Leipzig* **1992**, *44* (2), 64–66.
- (944) 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. *Industrial & Engineering Chemistry Chemical & Engineering Data Series* **1958**, *3* (1), 72–81. <https://doi.org/10.1021/i460003a016>.
- (945) 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. *Journal of Chemical & Engineering Data* **1975**, *20* (3), 271–275. <https://doi.org/10.1021/je60066a007>.
- (946) 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. *Journal of Chemical & Engineering Data* **2010**, *55* (12), 5701–5706. <https://doi.org/10.1021/je100614r>.
- (947) 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. *Journal of Chemical & Engineering Data* **1998**, *43* (4), 638–645. <https://doi.org/10.1021/je980012o>.
- (948) Ortega, J. Excess Enthalpy. Ethanol-Ethyl Ethanoate System. *Int. Data Ser. Sel. Data Mixtures Ser. A* **1995**, *23* (3), 161.
- (949) Zhang, R.; Yan, W.; Wang, X.; Lin, R. Molar Excess Enthalpies of Ethyl Acetate+alkanols at T=298.15K, P=10.0MPa. *Thermochimica Acta* **2005**, *429* (2), 155–161. <https://doi.org/10.1016/j.tca.2005.03.009>.
- (950) Rajendran, M.; Renganarayanan, S.; Madhavan, P. R.; Srinivasan, D. Effect Of Dissolved Inorganic Salts On The Vapor-Liquid Equilibria And Enthalpy Of Mixing Of The Methanol-Ethyl Acetate System. *Chemical Engineering Communications* **1988**, *74* (1), 179–193. <https://doi.org/10.1080/00986448808940458>.
- (951) 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 Equilibria* **2007**, *262* (1–2), 271–279. <https://doi.org/10.1016/j.fluid.2007.09.014>.
- (952) 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. *Journal of Chemical & Engineering Data* **2013**, *58* (2), 357–363. <https://doi.org/10.1021/je300994y>.
- (953) 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* (3), 199–201. <https://doi.org/10.1002/bbpc.19510550307>.
- (954) Park, W. K. Vapor-Liquid Equilibria of Ester-Alcohol Systems. III. *Hwahak Konghak* **1971**, *9* (4), 181–190.
- (955) 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. *Industrial & Engineering Chemistry Research* **2010**, *49* (19), 9548–9558. <https://doi.org/10.1021/ie101165r>.
- (956) 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* (1), 8B-12B.

- (957) Gordon, A. R.; Hornibrook, E. J. Liquid-Vapor Equilibrium for the System Ethanol - Diethyl - Ether. *Can. J. Res. Sect. B* **1946**, *24*, 263–267.
- (958) Villamañan, M. A.; Casanova, C.; Roux, A. H.; Grolier, J.-P. E. Calorimetric Investigation of the Interactions between Oxygen and Hydroxyl Groups in (Alcohol+ether) at 298.15 K. *The Journal of Chemical Thermodynamics* **1982**, *14* (3), 251–258. [https://doi.org/10.1016/0021-9614\(82\)90015-5](https://doi.org/10.1016/0021-9614(82)90015-5).
- (959) Kortüm, G.; Valent, V. Thermodynamische Mischungseffekte Der Systeme Wasser(1)-1,4-Dioxan(2) Und Methanol(1)-1,4-Dioxan(2); Ein Vergleich. *Berichte der Bunsengesellschaft für physikalische Chemie* **1977**, *81* (8), 752–761. <https://doi.org/10.1002/bbpc.19770810811>.
- (960) 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* (2), 139–166.
- (961) 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. *The Journal of Chemical Thermodynamics* **2003**, *35* (10), 1657–1669. [https://doi.org/10.1016/S0021-9614\(03\)00150-2](https://doi.org/10.1016/S0021-9614(03)00150-2).
- (962) 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* (11), 2405–2410.
- (963) 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. *Journal of Chemical & Engineering Data* **1999**, *44* (5), 948–954. <https://doi.org/10.1021/jc990078z>.
- (964) Singh, P. P.; Verma, D. V.; Arora, P. S. Thermodynamics of Binary Methanol Solutions. *Thermochimica Acta* **1976**, *15* (3), 267–280. [https://doi.org/10.1016/0040-6031\(76\)85080-0](https://doi.org/10.1016/0040-6031(76)85080-0).
- (965) Gmehling, J. VLE Data for the Design of Separation Processes. *AIChE Symp. Ser.* **1985**, *81* (244), 121–129.
- (966) 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 Journal of Chemical Engineering* **2008**, *25* (5), 1160–1164. <https://doi.org/10.1007/s11814-008-0191-2>.
- (967) 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. *Journal of Chemical & Engineering Data* **1996**, *41* (6), 1455–1458. <https://doi.org/10.1021/jc960179m>.
- (968) 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. *The Journal of Chemical Thermodynamics* **2013**, *58*, 330–339. <https://doi.org/10.1016/j.jct.2012.11.005>.
- (969) Fárková, J.; Linek, J.; Wichterle, I. Isothermal Vapour-Liquid Equilibria and Excess Volumes in the Methanol-Aliphatic Ether Systems. *Fluid Phase Equilibria* **1995**, *109* (1), 53–65. [https://doi.org/10.1016/0378-3812\(95\)02710-V](https://doi.org/10.1016/0378-3812(95)02710-V).
- (970) Piñeiro, Á. Excess Volumes and Isobaric Heat Capacities of Diisopropyl Ether with Several Alkanols at 298.15K. *Fluid Phase Equilibria* **2004**, *216* (2), 245–256. <https://doi.org/10.1016/j.fluid.2003.11.003>.

- (971) Toghiani, R. K.; Toghiani, H.; Venkateswarlu, G. Vapor-Liquid Equilibria for Methyl Tert-Butyl Ether + Methanol and Tert-Amyl Methyl Ether + Methanol. *Fluid Phase Equilibria* **1996**, *122* (1–2), 157–168. [https://doi.org/10.1016/0378-3812\(96\)03043-9](https://doi.org/10.1016/0378-3812(96)03043-9).
- (972) Loras, S.; Aucejo, A.; Muñoz, R.; Wisniak, J. Azeotropic Behavior in the System Methanol + Methyl 1,1-Dimethylethyl Ether. *Journal of Chemical & Engineering Data* **1999**, *44* (2), 203–208. <https://doi.org/10.1021/jc9801563>.
- (973) Wang, Y.; Tong, A.; Su, Y.; Yang, Z. Isobaric Vapor-Liquid Equilibrium for the System MTBE-Methanol. *Shiyou Huagong* **1989**, *18* (7), 442–446.
- (974) Westerholt, A. Weiterentwicklung Der Gruppenbeitragszustandsgleichung VTPR Zur Beschreibung Der TAME-Synthese Und Spaltung Durch Systematische Messung Fehlender Phasengleichgewichtsdaten Und Anpassung Der Erforderlichen Parameter. *Master's Thesis* **2010**, 1–113.
- (975) 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* (3), 146–152.
- (976) Mertl, I. Liquid-Vapour Equilibrium. II. Phase Equilibria in the Ternary System Ethyl Acetate-Ethanol-Water. *Collection of Czechoslovak Chemical Communications* **1972**, *37* (2), 366–374. <https://doi.org/10.1135/cccc19720366>.
- (977) Pavliček, 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 Equilibria* **2012**, *328*, 61–68. <https://doi.org/10.1016/j.fluid.2012.05.016>.
- (978) Li, Q.; Zhang, J.; Lei, Z.; Zhu, J.; Xing, F. Isobaric Vapor-Liquid Equilibrium for Ethyl Acetate + Ethanol + 1-Ethyl-3-Methylimidazolium Tetrafluoroborate. *Journal of Chemical & Engineering Data* **2009**, *54* (2), 193–197. <https://doi.org/10.1021/jc800175s>.
- (979) Susial, P.; Rodriguez-Henriquez, J. J.; Sosa-Rosario, A.; Rios-Santana, R. Vapor-Liquid Equilibrium of Ethyl Acetate + C_nH_{2n+1}OH (N= 1,2,3) Binary Systems at 0.3 MPa. *Chinese Journal of Chemical Engineering* **2012**, *20* (4), 723–730. [https://doi.org/10.1016/S1004-9541\(11\)60241-3](https://doi.org/10.1016/S1004-9541(11)60241-3).
- (980) 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. *JOURNAL OF CHEMICAL ENGINEERING OF JAPAN* **2011**, *44* (3), 155–163. <https://doi.org/10.1252/jcej.10we176>.
- (981) 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 Equilibria* **1997**, *134* (1–2), 239–253. [https://doi.org/10.1016/S0378-3812\(97\)00015-0](https://doi.org/10.1016/S0378-3812(97)00015-0).
- (982) Wen-jun, F.; Qing-sen, Y.; Rui-sen, L.; Han-xing, Z. Vapor Heat Capacity of Binary and Ternary Systems. *Thermochimica Acta* **1997**, *299* (1–2), 43–47. [https://doi.org/10.1016/S0040-6031\(97\)00135-4](https://doi.org/10.1016/S0040-6031(97)00135-4).
- (983) Hu, T.; Qin, Z.; Wang, G.; Hou, X.; Wang, J. Critical Properties of the Reacting Mixture in the Esterification of Acetic Acid with Ethanol. *Journal of Chemical & Engineering Data* **2004**, *49* (6), 1809–1814. <https://doi.org/10.1021/jc049771z>.
- (984) Pierotti, G. J.; Deal, C. H.; Derr, E. L. Activity Coefficients and Molecular Structure. *Industrial & Engineering Chemistry* **1959**, *51* (1), 95–102. <https://doi.org/10.1021/ie50589a048>.
- (985) Im, J. N.; Park, S. S.; Lee, H. O. Isothermal Vapor-Liquid Equilibrium for the Binary System Acetone-Water by the Total Pressure Method. *Korean Chemical Engineering Research* **1974**, *12* (3), 179–187.

- (986) 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. In *Thermodynamic Behavior of Electrolytes in Mixed Solvents*; 1976; Vol. 155, pp 303–317.
- (987) Lieberwirth, I.; Schuberth, H. Das Isotherme Dampf-Flüssigkeits-Phasengleichgewichtsverhalten Des Systems Aceton/Wasser Bei 35° C. *Zeitschrift für Physikalische Chemie* **1979**, *2600* (1). <https://doi.org/10.1515/zpch-1979-26090>.
- (988) Sokolova, E. P.; Morachevskii, A. G. Thermodynamic Properties of the Acetone-Water System. *Vestn Lenin U. Fiz. Kh* **1967**, No. 16, 110–115.
- (989) Griswold, J.; Wong, S. Y. Phase-Equilibria in the Acetone-Methanol-Water System from 100° into the Critical Region. *Chemical Engineering Progress Symposium Series* **1952**, *48* (3), 18–34.
- (990) Verhoeve, L.; De Schepper, H. The Vapour-Liquid Equilibria of the Binary, Ternary and Quaternary Systems Formed by Acetone, Methanol, Propan-2-ol, and Water. *Journal of Applied Chemistry and Biotechnology* **2007**, *23* (8), 607–619. <https://doi.org/10.1002/jctb.5020230807>.
- (991) Ochi, K.; Kojima, K. Vapor-Liquid Equilibria for the System Acetone + Methanol + Water. *Kagaku Kogaku* **1971**, *35*, 583–586. <https://doi.org/10.1252/kakoronbunshu1953.35.583>.
- (992) Kojima, K.; Tochigi, K.; Seki, H.; Watase, K. Determination of Vapor-Liquid Equilibria from Boiling Point Curves. *Kagaku Kogaku* **1968**, *32*, 149–153. <https://doi.org/10.1252/kakoronbunshu1953.32.149>.
- (993) Othmer, D. F.; Chudgar, M. M.; Levy, S. L. Binary and Ternary Systems of Acetone, Methyl Ethyl Ketone, and Water. *Industrial & Engineering Chemistry* **1952**, *44* (8), 1872–1881. <https://doi.org/10.1021/ie50512a042>.
- (994) French, H. T. Excess Enthalpies of (Acetone + Water) at 278.15, 288.15, 298.15, 308.15, 318.15, and 323.15 K. *The Journal of Chemical Thermodynamics* **1989**, *21* (8), 801–809. [https://doi.org/10.1016/0021-9614\(89\)90026-8](https://doi.org/10.1016/0021-9614(89)90026-8).
- (995) Costas, M.; Patterson, D. Heat Capacities of Water + Organic-Solvent Mixtures. *Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases* **1985**, *81* (10), 2381. <https://doi.org/10.1039/f19858102381>.
- (996) 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. *Journal of Chemical & Engineering Data* **2013**, *58* (5), 1280–1287. <https://doi.org/10.1021/je400065j>.
- (997) 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 Equilibria* **2008**, *270* (1–2), 62–68. <https://doi.org/10.1016/j.fluid.2008.06.004>.
- (998) 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 Equilibria* **2007**, *258* (2), 131–139. <https://doi.org/10.1016/j.fluid.2007.06.005>.
- (999) Chao, J.-P.; Dai, M. Studies of Thermodynamic Properties of Binary Mixtures Containing an Alcohol. *Thermochimica Acta* **1991**, *179*, 257–264. [https://doi.org/10.1016/0040-6031\(91\)80355-M](https://doi.org/10.1016/0040-6031(91)80355-M).
- (1000) Iñárrrea, J.; Valero, J.; Pérez, P.; Gracia, M.; Gutiérrez Losa, C. HmE and VmE of Some (Butanone or Dipropylether + an Alkanol) Mixtures. *The Journal of Chemical Thermodynamics* **1988**, *20* (2), 193–199. [https://doi.org/10.1016/0021-9614\(88\)90154-1](https://doi.org/10.1016/0021-9614(88)90154-1).

- (1001) Nagata, I.; Ohta, T.; Nakagawa, S. Excess Gibbs Free Energies And Heats Of Mixing For Binary Alcoholic Liquid Mixtures. *Journal of Chemical Engineering of Japan* **1976**, 9 (4), 276–281. <https://doi.org/10.1252/jcej.9.276>.
- (1002) Nagata, I.; Tago, O.; Takahashi, T. Heats of Mixing for Binary Methyl Ethyl Ketone, Methyl Acetate-Alcohol Systems. *Chemical engineering* **1970**, 34 (10), 1107-1112,a.1. <https://doi.org/10.1252/kakoronbunshu1953.34.1107>.
- (1003) Pikkarainen, L. Excess Enthalpies of Binary Solvent Mixtures of 2-Butanone with Aliphatic Alcohols. *Thermochimica Acta* **1987**, 114 (2), 239–244. [https://doi.org/10.1016/0040-6031\(87\)80044-8](https://doi.org/10.1016/0040-6031(87)80044-8).
- (1004) 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 (7), 1475–1478.
- (1005) Lee, M.-J.; Hu, C.-H. Isothermal Vapor-Liquid Equilibria for Mixtures of Ethanol, Acetone, and Diisopropyl Ether. *Fluid Phase Equilibria* **1995**, 109 (1), 83–98. [https://doi.org/10.1016/0378-3812\(95\)02705-J](https://doi.org/10.1016/0378-3812(95)02705-J).
- (1006) 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. *Journal of Chemical & Engineering Data* **1987**, 32 (3), 357–362. <https://doi.org/10.1021/je00049a021>.
- (1007) 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 Equilibria* **2005**, 231 (1), 99–108. <https://doi.org/10.1016/j.fluid.2005.01.007>.
- (1008) 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), 1–7.
- (1009) Lien, P.-J.; Lin, H.; Lee, M.-J. Excess Molar Enthalpies for Binary Mixtures of Ethanol + Acetone, + Octane, + Cyclohexane and 1-Propanol + Acetone, + Octane, + Heptane at 323.15 K. *Journal of Chemical & Engineering Data* **2003**, 48 (2), 359–361. <https://doi.org/10.1021/je020149l>.
- (1010) 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 Equilibria* **1981**, 6 (1–2), 113–139. [https://doi.org/10.1016/0378-3812\(81\)80007-6](https://doi.org/10.1016/0378-3812(81)80007-6).
- (1011) 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 Equilibria* **1986**, 28 (1), 13–37. [https://doi.org/10.1016/0378-3812\(86\)85066-X](https://doi.org/10.1016/0378-3812(86)85066-X).
- (1012) 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. *Industrial & Engineering Chemistry Research* **2010**, 49 (13), 6176–6183. <https://doi.org/10.1021/ie901702h>.
- (1013) 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. *Journal of Chemical & Engineering Data* **2013**, 58 (6), 1717–1723. <https://doi.org/10.1021/je400138m>.
- (1014) 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 Equilibria* **2014**, 383, 182–187. <https://doi.org/10.1016/j.fluid.2014.10.011>.
- (1015) Campbell, A. N.; Kartzmark, E. M. Thermodynamic and Other Properties of Methanol + Acetone, Carbon Disulphide + Acetone, Carbon Disulphide + Methanol, and Carbon Disulphide + Methanol + Acetone. *The Journal of Chemical Thermodynamics* **1973**, 5 (2), 163–172. [https://doi.org/10.1016/S0021-9614\(73\)80076-X](https://doi.org/10.1016/S0021-9614(73)80076-X).

- (1016) Schmelzer, J.; Quitzsd, K. Isobare Flüssigkeit-Dampfgleichgewichte Der Binären Systeme Benzol-Äthylendiamin Und Wasser-Äthylendiamin. *Zeitschrift für Physikalische Chemie* **1973**, *2520* (1). <https://doi.org/10.1515/zpch-1973-25231>.
- (1017) Rivenq, F. Ebulliometry of Water-Ethylenediamine Mixtures. *Bull. Soc. Chim. Fr.* **1963**, 8–9, 1606–1608.
- (1018) 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.
- (1019) Bahlmann, M. Evaluation and revision of the modified UNIFAC (Dortmund) approach for alcohol systems. Master, Universität Oldenburg, Germany, 2010.
- (1020) 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* (2), 181–183.
- (1021) Marongiu, B.; Ferino, I.; Monaci, R.; Solinas, V.; Torrazza, S. Thermodynamic Properties of Aqueous Non-Electrolyte Mixtures. Alkanols + Water Systems. *Journal of Molecular Liquids* **1984**, *28* (4), 229–247. [https://doi.org/10.1016/0167-7322\(84\)80027-6](https://doi.org/10.1016/0167-7322(84)80027-6).
- (1022) Lee, M.-J.; Tsai, L.-H.; Hong, G.-B.; Lin, H. Multiphase Coexistence for Aqueous Systems with Amyl Alcohol and Amyl Acetate. *Industrial & Engineering Chemistry Research* **2002**, *41* (13), 3247–3252. <https://doi.org/10.1021/ie0105371>.
- (1023) 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. *Canadian Journal of Chemistry* **1970**, *48* (16), 2457–2465. <https://doi.org/10.1139/v70-417>.
- (1024) 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 Equilibria* **2000**, *171* (1–2), 207–218. [https://doi.org/10.1016/S0378-3812\(00\)00364-2](https://doi.org/10.1016/S0378-3812(00)00364-2).
- (1025) Kay, W. B.; Donham, W. E. Liquid-Vapour Equilibria in the Iso-Butanol—n-Butanol, Methanol—n-Butanol and Diethyl Ether—n-Butanol Systems. *Chemical Engineering Science* **1955**, *4* (1), 1–16. [https://doi.org/10.1016/0009-2509\(55\)85001-4](https://doi.org/10.1016/0009-2509(55)85001-4).
- (1026) Stokes, R. H. Excess Enthalpies of (Butan-1-ol + Methanol) at 278.15, 298.15, and 318.15 K. *The Journal of Chemical Thermodynamics* **1988**, *20* (11), 1349–1352. [https://doi.org/10.1016/0021-9614\(88\)90172-3](https://doi.org/10.1016/0021-9614(88)90172-3).
- (1027) Ogawa, H.; Murakami, S. Excess Volumes, Isentropic Compressions, and Isobaric Heat Capacities for Methanol Mixed with Other Alkanols at 25°C. *Journal of Solution Chemistry* **1987**, *16* (4), 315–326. <https://doi.org/10.1007/BF00646123>.
- (1028) Wright, E. H. M.; Akhtar, B. A. Soluble Surface Films of Short-Chain Monocarboxylic Acids on Organic and Aqueous Substrates. *Journal of the Chemical Society B: Physical Organic* **1970**, 151. <https://doi.org/10.1039/j29700000151>.
- (1029) Miyamoto, S.; Nakamura, S.; Iwai, Y.; Arai, Y. Measurement of Isothermal Vapor–Liquid Equilibria for Binary and Ternary Systems Containing Monocarboxylic Acid. *Journal of Chemical & Engineering Data* **2001**, *46* (5), 1225–1230. <https://doi.org/10.1021/je0003849>.
- (1030) 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 Equilibria* **1998**, *153* (1), 113–134. [https://doi.org/10.1016/S0378-3812\(98\)00409-9](https://doi.org/10.1016/S0378-3812(98)00409-9).
- (1031) Zhao, J.; Bao, J.; Hu, Y. Excess Molar Enthalpies of (an Alkanol + a Carboxylic Acid) at 298.15 K Measured with a Picker Calorimeter. *The Journal of Chemical*

- Thermodynamics* **1989**, *21* (8), 811–818. [https://doi.org/10.1016/0021-9614\(89\)90027-X](https://doi.org/10.1016/0021-9614(89)90027-X).
- (1032) Kooner, Z.; Fenby, D. Vapour Pressure Study of the Deuterium Exchange Reaction in Methanol-Ethanol Systems: Equilibrium Constant Determination. *Australian Journal of Chemistry* **1980**, *33* (9), 1943. <https://doi.org/10.1071/CH9801943>.
- (1033) Hall, D. J.; Mash, C. J.; Pemberton, R. C. *Vapor Liquid Equilibria for the Systems Water-Methanol, Water-Ethanol, Methanol-Ethanol, and Water-Methanol-Ethanol at 298.15 K Determined by a Rapid Transpiration Method*; 1979; pp 1–13.
- (1034) Oh, S.-K.; Campbell, S. W. Total Pressure Measurements for Copper(II) Chloride + Methanol + Ethanol at 303.15 K. *Journal of Chemical & Engineering Data* **1995**, *40* (2), 504–508. <https://doi.org/10.1021/je00018a033>.
- (1035) Butcher, K. L.; Robinson, W. I. An Apparatus for Determining High-Pressure Liquid-Vapour Equilibrium Data. I. The Methanol-Ethanol System. *Journal of Applied Chemistry* **2007**, *16* (10), 289–292. <https://doi.org/10.1002/jctb.5010161003>.
- (1036) 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 Equilibria* **1998**, *146* (1–2), 139–153. [https://doi.org/10.1016/S0378-3812\(98\)00227-1](https://doi.org/10.1016/S0378-3812(98)00227-1).
- (1037) Pflug, H. D.; Pope, A. E.; Benson, G. C. Heats of Mixing of Normal Alcohols at 25.Deg. *Journal of Chemical & Engineering Data* **1968**, *13* (3), 408–410. <https://doi.org/10.1021/je60038a032>.
- (1038) Trampe, D. M.; Eckert, C. A. Calorimetric Measurement of Partial Molar Excess Enthalpies at Infinite Dilution. *Journal of Chemical & Engineering Data* **1991**, *36* (1), 112–118. <https://doi.org/10.1021/je00001a033>.
- (1039) Geiseler, G.; Sühnel, K.; Quitzsch, K. Exzeßeigenschaften Der Binären Mischsysteme Aus Den Isomeren Butanolen. *Zeitschrift für Physikalische Chemie* **1973**, *2540* (1). <https://doi.org/10.1515/zpch-1973-25425>.
- (1040) Quitzsch, K.; Köhler, S.; Taubert, K.; Geiseler, G. Isobare Flüssigkeit-Dampf-Gleichgewichte Der „quasi-Idealen” Binären Systeme n-Butanol/Sek.-Butanol Und n-Butanol/Tert.-Butanol. *Journal für Praktische Chemie* **1969**, *311* (3), 429–437. <https://doi.org/10.1002/prac.19693110312>.
- (1041) Murakami, S.; Benson, G. C. Thermodynamic Properties of Some Isomeric Butyl Alcohol Mixtures. *Bulletin of the Chemical Society of Japan* **1973**, *46* (1), 74–79. <https://doi.org/10.1246/bcsj.46.74>.
- (1042) 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 Equilibria* **2013**, *338*, 128–134. <https://doi.org/10.1016/j.fluid.2012.11.004>.
- (1043) Gay, L. Distillation and Rectification of Complex Mixtures. II. *Chim. Ind. Genie Chim.* **1927**, *18* (2), 187–203.
- (1044) Udovenko, V. V.; Frid, Ts. B. Heats of Vaporization of Binary Mixtures. II. *Zh. Fiz. Khim.* **1948**, *22*, 1135–1145.
- (1045) 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* (6), 749–754.
- (1046) 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 Equilibria* **1997**, *132* (1–2), 205–213. [https://doi.org/10.1016/S0378-3812\(97\)00027-7](https://doi.org/10.1016/S0378-3812(97)00027-7).
- (1047) Yamamoto, H.; Fukase, K.; Shibata, J. Vapor–Liquid Equilibria for Alcohol + Alcohol + Sodium Iodide at 298.15 K. *Journal of Chemical & Engineering Data* **1996**, *41* (5), 1066–1070. <https://doi.org/10.1021/je9600966>.

- (1048) 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 (10), 1118–1123.
- (1049) Gultekin, N. Vapor-Liquid Equilibria at 1 Atm for Ternary and Quaternary Systems Composed of Acetone, Methanol, 2-Propanol, and 1-Propanol. *Journal of Chemical & Engineering Data* **1990**, 35 (2), 132–136. <https://doi.org/10.1021/je00060a010>.
- (1050) Khurma, J. R.; Fenby, D. V. Thermochemical Study of Deuterium Exchange Reactions in Water-Alcohol and Alcohol-Alcohol Systems. *The Journal of Physical Chemistry* **1979**, 83 (19), 2443–2447. <https://doi.org/10.1021/j100482a004>.
- (1051) Wilson, T. A. The Total and Partial Vapor Pressures of Aqueous Ammonia Solutions. *Univ. Illinois Eng. Exp. Stand. Bull.* **1925**, 146.
- (1052) 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 (256), 97–127.
- (1053) Inomata, H.; Ikawa, N.; Arai, K.; Saito, S. Vapor-Liquid Equilibria for the Ammonia-Methanol-Water System. *Journal of Chemical & Engineering Data* **1988**, 33 (1), 26–29. <https://doi.org/10.1021/je00051a010>.
- (1054) Clifford, I. I.; Hunter, E. The System Ammonia–Water at Temperatures up to 150°C. and at Pressures up to Twenty Atmospheres. *The Journal of Physical Chemistry* **1932**, 37 (1), 101–118. <https://doi.org/10.1021/j150343a014>.
- (1055) Rizvi, S. S. H.; Heidemann, R. A. Vapor-Liquid Equilibria in the Ammonia-Water System. *Journal of Chemical & Engineering Data* **1987**, 32 (2), 183–191. <https://doi.org/10.1021/je00048a017>.
- (1056) Chu, J. C.; Getty, R. J.; Brennecke, L. F.; Paul, R. *Distillation Equilibrium Data*; 1950.
- (1057) 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.
- (1058) Sakabe, A.; Arai, D.; Miyamoto, H.; Uematsu, M. Measurements of the Critical Parameters for $\{x\text{NH}_3+(1-x)\text{H}_2\text{O}\}$ with $X=(0.9098,0.7757,0.6808)$. *The Journal of Chemical Thermodynamics* **2008**, 40 (10), 1527–1530. <https://doi.org/10.1016/j.jct.2008.05.017>.
- (1059) Polikhronidi, N. G.; Abdulagatov, I. M.; Batyrova, R. G.; Stepanov, G. V. PVT Measurements of Water-Ammonia Refrigerant Mixture in the Critical and Supercritical Regions. *International Journal of Refrigeration* **2009**, 32 (8), 1897–1913. <https://doi.org/10.1016/j.ijrefrig.2009.07.008>.
- (1060) Sassen, C. L.; Van Kwartel, R. A. C.; Van der Kooi, H. J.; De Swaan Arons, J. Vapor-Liquid Equilibria for the System Ammonia + Water up to the Critical Region. *Journal of Chemical & Engineering Data* **1990**, 35 (2), 140–144. <https://doi.org/10.1021/je00060a013>.
- (1061) Tyvina, T. N.; Naumova, A. A.; Fokina, V. V. Liquid-Gas Equilibrium in an Acetonitrile-Ammonia System. *J. Appl. Chem. USSR* **1979**, 52 (11), 2458–2460.
- (1062) Ewert, M. Theory of Concentrated Solutions. XIII. Aqueous Solutions of Organic Compounds. *Bull. Soc. Chim. Belg.* **1936**, 45, 493–515.
- (1063) Aucejo, A.; Loras, S.; Monton, J. B. Isobaric Vapor-Liquid Equilibria of Prop-2-En-1-Ol (Allyl Alcohol) + Water System at 30, 60, and 100 KPa. *ELDATA: The International Electronic Journal of Physico-Chemical Data* **1996**, 2 (1), 1–4.
- (1064) Weller, R.; Schubert, H.; Leibnitz, E. Phasengleichgewichtsmessungen. IV. Die Phasengleichgewichte Dampfförmig/Flüssig Des Systems Phenol/n-Butylacetat/Wasser

- Bei 44,4°C. *Journal für Praktische Chemie* **1963**, 21 (5–6), 234–249. <https://doi.org/10.1002/prac.19630210502>.
- (1065) 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.
- (1066) 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 (6), 393–399.
- (1067) von Erichsen, L.; Dobbert, E. The Mutual Solubility Behavior of Alkylphenols and Water. *Brennstoff-Chemie* **1955**, 21–22, 338–345.
- (1068) Schuermann, E.; Diederichs, R. Heats of Mixing of Phenol-Water Systems. *Ber. Bunsen-Ges. Phys. Chem.* **1964**, 68 (5), 429–434.
- (1069) Ferguson, J. B. The System Water-Phenol. *The Journal of Physical Chemistry* **1926**, 31 (5), 757–763. <https://doi.org/10.1021/j150275a013>.
- (1070) 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. *Journal of the American Chemical Society* **1937**, 59 (12), 2481–2488. <https://doi.org/10.1021/ja01291a001>.
- (1071) 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. *The Journal of Chemical Thermodynamics* **1972**, 4 (3), 469–476. [https://doi.org/10.1016/0021-9614\(72\)90031-6](https://doi.org/10.1016/0021-9614(72)90031-6).
- (1072) Kozub, N.; Schuberth, H.; Leibnitz, E. Phasengleichgewichtsuntersuchungen Dampfförmig-Flüssig Am System Methanol/Methylformiat Unter Verwendung Einer Gaschromatographischen Analysenmethode. *Journal für Praktische Chemie* **1962**, 17 (5–6), 282–292. <https://doi.org/10.1002/prac.19620170505>.
- (1073) Sundberg, A. T.; Uusi-Kyyny, P.; Pakkanen, M.; Alopaeus, V. Vapor–Liquid Equilibrium for Methoxymethane + Methyl Formate, Methoxymethane + Hexane, and Methyl Formate + Methanol. *Journal of Chemical & Engineering Data* **2011**, 56 (5), 2634–2640. <https://doi.org/10.1021/je200140m>.
- (1074) Zeng, J.; Fu, C.; Hu, W. L. Study on the VLE for Methyl Formate-Methanol System. *Tianranqi Huagong* **2000**, 25 (5), 54–56.
- (1075) 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. $\{x\text{HCO}_2(\text{CH}_2)_i\text{CH}_3 + (1-x)\text{C}_j\text{H}_{2j+1}\text{OH}\}$ ($i = 0$ to 3 and $j = 1$ and 2). *The Journal of Chemical Thermodynamics* **1992**, 24 (8), 809–814. [https://doi.org/10.1016/S0021-9614\(05\)80225-3](https://doi.org/10.1016/S0021-9614(05)80225-3).
- (1076) Linek, J.; Wichterle, I.; Marsh, K. N. Vapor–Liquid Equilibria for Water + Diacetone Alcohol, Ethyl Methanoate + Water, and Ethyl Methanoate + Phenol. *Journal of Chemical & Engineering Data* **1996**, 41 (6), 1219–1222. <https://doi.org/10.1021/je960183y>.
- (1077) 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). *Industrial & Engineering Chemistry Research* **2001**, 40 (24), 5831–5838. <https://doi.org/10.1021/ie010444j>.
- (1078) 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. *Journal of Chemical & Engineering Data* **1976**, 21 (3), 310–313. <https://doi.org/10.1021/je60070a020>.

- (1079) 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 Equilibria* **1998**, *146* (1–2), 351–370. [https://doi.org/10.1016/S0378-3812\(98\)00193-9](https://doi.org/10.1016/S0378-3812(98)00193-9).
- (1080) 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 Equilibria* **1997**, *131* (1–2), 197–212. [https://doi.org/10.1016/S0378-3812\(96\)03230-X](https://doi.org/10.1016/S0378-3812(96)03230-X).
- (1081) 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* (10), 151–153.
- (1082) Cerdeiriña, C. A.; Tovar, C. A.; González, D.; Carballo, E.; Romani, L. Thermodynamics of the Nitromethane + 1-Butanol System near the Upper Critical Point. *Fluid Phase Equilibria* **2001**, *179* (1–2), 101–115. [https://doi.org/10.1016/S0378-3812\(00\)00485-4](https://doi.org/10.1016/S0378-3812(00)00485-4).
- (1083) 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). *The Journal of Chemical Thermodynamics* **1991**, *23* (2), 169–174. [https://doi.org/10.1016/S0021-9614\(05\)80294-0](https://doi.org/10.1016/S0021-9614(05)80294-0).
- (1084) Rebelo, L. P. N.; Najdanovic-Visak, V.; Visak, Z. P.; Nunes da Ponte, M.; Troncoso, J.; Cerdeiriña, C. A.; Romani, L. Two Ways of Looking at Prigogine and Defay's Equation. *Physical Chemistry Chemical Physics* **2002**, *4* (11), 2251–2259. <https://doi.org/10.1039/b200292b>.
- (1085) 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* (1), 65–69.
- (1086) Scatchard, George.; Wilson, G. M. Vapor-Liquid Equilibrium. XIII. The System Water-Butyl Glycol from 5 to 85°. *Journal of the American Chemical Society* **1964**, *86* (2), 133–137. <https://doi.org/10.1021/ja01056a004>.
- (1087) Chiavone-Filho, O.; Proust, P.; Rasmussen, P. Vapor-Liquid Equilibria for Glycol Ether + Water Systems. *Journal of Chemical & Engineering Data* **1993**, *38* (1), 128–131. <https://doi.org/10.1021/je00009a031>.
- (1088) Escobedo-Alvarado, G. N.; Sandler, S. I. Vapor-Liquid Equilibrium of Two Aqueous Systems That Exhibit Liquid-Liquid Phase Separation. *Journal of Chemical & Engineering Data* **1999**, *44* (2), 319–322. <https://doi.org/10.1021/je980228q>.
- (1089) 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. *Chemical Physics* **1992**, *165* (1), 31–39. [https://doi.org/10.1016/0301-0104\(92\)80040-3](https://doi.org/10.1016/0301-0104(92)80040-3).
- (1090) Onken, U. Die Thermodynamischen Funktionen Des Systems Wasser/Butylglykol. *Z. Elektrochem.* **1959**, *63* (2), 321–327.
- (1091) 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. *Journal of Chemical & Engineering Data* **1994**, *39* (2), 399–403. <https://doi.org/10.1021/je00014a048>.
- (1092) Dobson, H. J. E. CCCXCVII.—The Partial Pressures of Aqueous Ethyl Alcohol. *J. Chem. Soc., Trans.* **1925**, *127* (0), 2866–2873. <https://doi.org/10.1039/CT9252702866>.
- (1093) Pemberton, R. C.; Mash, C. J. Thermodynamic Properties of Aqueous Non-Electrolyte Mixtures II. Vapour Pressures and Excess Gibbs Energies for Water + Ethanol at 303.15 to 363.15 K Determined by an Accurate Static Method. *The Journal of Chemical*

- Thermodynamics* **1978**, *10* (9), 867–888. [https://doi.org/10.1016/0021-9614\(78\)90160-X](https://doi.org/10.1016/0021-9614(78)90160-X).
- (1094) 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. *Journal of Chemical & Engineering Data* **2006**, *51* (4), 1220–1225. <https://doi.org/10.1021/jc050537y>.
- (1095) Kurihara, K.; Minoura, T.; Takeda, K.; Kojima, K. Isothermal Vapor-Liquid Equilibria for Methanol + Ethanol + Water, Methanol + Water, and Ethanol + Water. *Journal of Chemical & Engineering Data* **1995**, *40* (3), 679–684. <https://doi.org/10.1021/je00019a033>.
- (1096) 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 Equilibria* **1986**, *31* (3), 283–298. [https://doi.org/10.1016/0378-3812\(86\)87013-3](https://doi.org/10.1016/0378-3812(86)87013-3).
- (1097) Barr-David, F.; Dodge, B. F. Vapor-Liquid Equilibrium at High Pressures. The Systems Ethanol-Water and 2-Propanol-Water. *Journal of Chemical & Engineering Data* **1959**, *4* (2), 107–121. <https://doi.org/10.1021/je60002a003>.
- (1098) 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 Equilibria* **2011**, *308* (1–2), 135–141. <https://doi.org/10.1016/j.fluid.2011.06.009>.
- (1099) Jones, C. A.; Schoenborn, E. M.; Colburn, A. P. Equilibrium Still for Miscible Liquids. *Industrial & Engineering Chemistry* **1943**, *35* (6), 666–672. <https://doi.org/10.1021/ie50402a009>.
- (1100) Hughes, H. E.; Maloney, J. O. Application of Radioactive Tracers to Diffusional Operations. Binary and Ternary Equilibrium Data. *Chem. Eng. Progr.* **1952**, *48* (4), 192–200.
- (1101) Bloom, C. H.; Clump, C. W.; Koeckert, A. H. Simultaneous Measurement of Vapor-Liquid Equilibria and Latent Heats of Vaporization. *Industrial & Engineering Chemistry* **1961**, *53* (10), 829–832. <https://doi.org/10.1021/ie50622a029>.
- (1102) Stabnikov, V. N.; Matyushev, B. Z.; Protsyuk, T. B.; Yushchenko, N. M. Equilibrium in the Ethyl Alcohol-Water System at Atmospheric Pressure. *Pishch. Promst. Kiev* **1972**, *15*, 49–56.
- (1103) Otsuki, H.; Williams, F. C. Effect of Pressure on Vapor-Liquid Equilibria for the System Ethyl Alcohol-Water. *Chem. Eng. Progr. Symp. Ser.* **1953**, *49*, 55–67.
- (1104) 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. **1999**, *44* (4), 701–714. <https://doi.org/10.1021/je980303x>.
- (1105) Ott, J. B.; Stouffer, C. E.; Cornett, G. V.; Woodfield, B. F.; Wirthlin, R. C.; Christensen, J. J.; Deiters, U. K. Excess Enthalpies for (Ethanol + Water) at 298.15 K and Pressures of 0.4, 5, 10, and 15 MPa. *The Journal of Chemical Thermodynamics* **1986**, *18* (1), 1–12. [https://doi.org/10.1016/0021-9614\(86\)90036-4](https://doi.org/10.1016/0021-9614(86)90036-4).
- (1106) Ott, J. B.; Cornett, G. V.; Stouffer, C. E.; Woodfield, B. F.; Guanquan, C.; Christensen, J. J. Excess Enthalpies of (Ethanol+water) at 323.15, 333.15, 348.15, and 373.15 K and from 0.4 to 15 MPa. *The Journal of Chemical Thermodynamics* **1986**, *18* (9), 867–875. [https://doi.org/10.1016/0021-9614\(86\)90121-7](https://doi.org/10.1016/0021-9614(86)90121-7).
- (1107) 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. *The Journal of Chemical Thermodynamics* **1987**, *19* (4), 337–348. [https://doi.org/10.1016/0021-9614\(87\)90115-7](https://doi.org/10.1016/0021-9614(87)90115-7).
- (1108) Wormald, C. J.; Lloyd, M. J. Excess Enthalpies for (Water + Ethanol) At T = 398 K To T = 548 K And p = 15 MPa. *The Journal of Chemical Thermodynamics* **1996**, *28* (6), 615–626. <https://doi.org/10.1006/jcht.1996.0058>.
- (1109) Benson, G. C.; D'Arcy, P. J. Excess Isobaric Heat Capacities of Water-n-Alcohol Mixtures. *Journal of Chemical & Engineering Data* **1982**, *27* (4), 439–442. <https://doi.org/10.1021/jc00030a021>.
- (1110) Ogawa, H.; Murakami, S. Excess Isobaric Heat Capacities for Water + Alkanol Mixtures at 298.15 K. *Thermochimica Acta* **1986**, *109* (1), 145–154. [https://doi.org/10.1016/0040-6031\(86\)85016-X](https://doi.org/10.1016/0040-6031(86)85016-X).
- (1111) Grolier, J.-P. E.; Wilhelm, E. Excess Volumes and Excess Heat Capacities of Water + Ethanol at 298.15 K. *Fluid Phase Equilibria* **1981**, *6* (3–4), 283–287. [https://doi.org/10.1016/0378-3812\(81\)85011-X](https://doi.org/10.1016/0378-3812(81)85011-X).
- (1112) Bazaev, A. R.; Abdulagatov, I. M.; Bazaev, E. A.; Abdurashidova, A. (P,v,T,x) Measurements of $\{(1-x)\text{H}_2\text{O}+x\text{C}_2\text{H}_5\text{OH}\}$ Mixtures in the near-Critical and Supercritical Regions. *The Journal of Chemical Thermodynamics* **2007**, *39* (3), 385–411. <https://doi.org/10.1016/j.jct.2006.08.002>.
- (1113) Vierk, A.-L. Experimentelle Untersuchungen an Den Zweistoffsystemen: Wasser-Acetonitril, Wasser-Dioxan, Äthanol-Acetonitril Und Cyclohexan-Dioxan. *Zeitschrift für anorganische Chemie* **1950**, *261* (5–6), 283–296. <https://doi.org/10.1002/zaac.19502610504>.
- (1114) 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* (5), 678–683.
- (1115) 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. *Journal of Chemical Engineering of Japan* **1978**, *11* (3), 167–172. <https://doi.org/10.1252/jcej.11.167>.
- (1116) Szydłowski, J.; Szykuła, M. Isotope Effect on Miscibility of Acetonitrile and Water. *Fluid Phase Equilibria* **1999**, *154* (1), 79–87. [https://doi.org/10.1016/S0378-3812\(98\)00438-5](https://doi.org/10.1016/S0378-3812(98)00438-5).
- (1117) Stokes, R. H. Excess Partial Molar Enthalpies for (Acetonitrile + Water) from 278 to 318 K. *The Journal of Chemical Thermodynamics* **1987**, *19* (9), 977–983. [https://doi.org/10.1016/0021-9614\(87\)90044-9](https://doi.org/10.1016/0021-9614(87)90044-9).
- (1118) Nakamura, M.; Tamura, K.; Murakami, S. Isotope Effects on Thermodynamic Properties: Mixtures of $x(\text{D}_2\text{O or H}_2\text{O}) + (1 - x)\text{CH}_3\text{CN}$ at 298.15 K. *Thermochimica Acta* **1995**, *253*, 127–136. [https://doi.org/10.1016/0040-6031\(94\)02086-4](https://doi.org/10.1016/0040-6031(94)02086-4).
- (1119) Schedemann, A. Weiterentwicklung von Thermodynamischen Vorhersagemethoden Als Grundlage Für Die Lösungsmittelauswahl Bei Der Flüssig-Flüssig-Extraktion Und Der Absorption, 2013.
- (1120) Acosta, J.; Arce, A.; Rodil, E.; Soto, A. A Thermodynamic Study on Binary and Ternary Mixtures of Acetonitrile, Water and Butyl Acetate. *Fluid Phase Equilibria* **2002**, *203* (1–2), 83–98. [https://doi.org/10.1016/S0378-3812\(02\)00171-1](https://doi.org/10.1016/S0378-3812(02)00171-1).
- (1121) 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. *Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases* **1978**, *74* (0), 1159. <https://doi.org/10.1039/f19787401159>.

- (1122) 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. *Thermochimica Acta* **1981**, *46* (3), 295–301. [https://doi.org/10.1016/0040-6031\(81\)80328-0](https://doi.org/10.1016/0040-6031(81)80328-0).
- (1123) Jinyan Fu; Kun Wang; Ying Hu. Studies on the Vapor-Liquid Equilibrium and Vapor-Liquid-Liquid Equilibrium for a Methanol-Methyl Methacrylate-Water Ternary System (I) Three Different Binary Systems. *Huagong Xuebao* **1988**, *39* (1), 64–76.
- (1124) 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 Equilibria* **2010**, *299* (1), 32–41. <https://doi.org/10.1016/j.fluid.2010.08.018>.
- (1125) McGlashan, M. L.; Williamson, A. G. Isothermal Liquid-Vapor Equilibria for System Methanol-Water. *Journal of Chemical & Engineering Data* **1976**, *21* (2), 196–199. <https://doi.org/10.1021/je60069a019>.
- (1126) Yao, J.; Li, H.; Han, S. Vapor-Liquid Equilibrium Data for Methanol-Water-NaCl at 45°C. *Fluid Phase Equilibria* **1999**, *162* (1–2), 253–260. [https://doi.org/10.1016/S0378-3812\(99\)00204-6](https://doi.org/10.1016/S0378-3812(99)00204-6).
- (1127) Dulitskaya, K. A. Vapor Pressure of Binary Systems. I. *Zh. Obshch. Khim.* **1945**, *15* (1–2), 9–21.
- (1128) Nagatani, M.; Fujino, K. Measurement of Isothermal Vapor-Liquid Equilibria for Methanol-Water System. *Fukuoka Daigaku Kogaku Shuho* **2000**, *64*, 147–152.
- (1129) 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* (2), 230–233.
- (1130) Schröder, W. Messungen von Siedegleichgewichten Bei Überdruck: Messungen von Siedegleichgewichten Bei Überdruck. *Chemie Ingenieur Technik* **1958**, *30* (8), 523–525. <https://doi.org/10.1002/cite.330300809>.
- (1131) 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.
- (1132) 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. *Journal of Chemical & Engineering Data* **2012**, *57* (10), 2696–2701. <https://doi.org/10.1021/je300613v>.
- (1133) 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* (7), 1582–1586.
- (1134) Hirata, M.; Suda, S. Vapor-Liquid Equilibrium under Pressurized Conditions; Experimental Apparatus and Methanol-Water System. *Kagaku Kogaku* **1967**, *31* (8), 759–766. <https://doi.org/10.1252/kakoronbunshu1953.31.759>.
- (1135) Bose, E. Remarks on Thermochemical Statement of Julius Thomsens. *Phys. Z.* **1906**, *7* (14), 503–505.
- (1136) Cochran, S. W.; Holste, J. C.; Marsh, K. N.; Gammon, B. E.; Hall, K. R. Enthalpies of Water + Methanol Mixtures between 180 K and 320 K. *Fluid Phase Equilibria* **1993**, *88*, 171–181. [https://doi.org/10.1016/0378-3812\(93\)87110-M](https://doi.org/10.1016/0378-3812(93)87110-M).
- (1137) Tomaszkiwicz, I.; Randzio, Stanisław. 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. *Thermochimica Acta* **1986**, *103* (2), 281–289. [https://doi.org/10.1016/0040-6031\(86\)85164-4](https://doi.org/10.1016/0040-6031(86)85164-4).

- (1138) 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* (6), 631–666. <https://doi.org/10.1023/A:1021759810070>.
- (1139) 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. *Journal of Solution Chemistry* **1980**, *9* (12), 931–938. <https://doi.org/10.1007/BF00646404>.
- (1140) Bazaev, A. R.; Abdulagatov, I. M.; Magee, J. W.; Bazaev, E. A.; Ramazanova, A. E.; Abdurashidova, A. A. PVTx Measurements for a H₂O + Methanol Mixture in the Subcritical and Supercritical Regions. *International Journal of Thermophysics* **2004**, *25* (3), 805–838. <https://doi.org/10.1023/B:IJOT.0000034238.64651.32>.
- (1141) Sazonov, V. P. Isothermal Liquid-Liquid-Vapor Equilibrium of Nitromethane - Isopropanol - Water. *Zh. Prikl. Khim.* **1986**, *59* (7), 1451–1456.
- (1142) Udovenko, V. V.; Mazanko, T. F. Liquid-Vapor Equilibrium in the Propan-2-Ol - Water and Propan-2-Ol - Benzene Systems. *Zhurnal Fizicheskoi Khimii* **1967**, *41*, 1615–1620.
- (1143) Sada, E.; Morisue, T. ISOTHERMAL VAPOR-LIQUID EQUILIBRIUM DATA OF ISOPROPANOL-WATER SYSTEM. *Journal of Chemical Engineering of Japan* **1975**, *8* (3), 191–195. <https://doi.org/10.1252/jcej.8.191>.
- (1144) Wu, H. S.; Hagewiesche, D.; Sandler, S. I. Vapor—Liquid Equilibria of 2-Propanol + Water + N,N-Dimethyl Formamide. *Fluid Phase Equilibria* **1988**, *43* (1), 77–89. [https://doi.org/10.1016/0378-3812\(88\)80073-6](https://doi.org/10.1016/0378-3812(88)80073-6).
- (1145) Wilson, A.; Simons, E. L. Vapor-Liquid Equilibria. 2-Propanol - Water System. *Industrial & Engineering Chemistry* **1952**, *44* (9), 2214–2219. <https://doi.org/10.1021/ie50513a063>.
- (1146) Marzal, P.; Montón, J. B.; Rodrigo, M. A. Isobaric Vapor—Liquid Equilibria of the Water + 2-Propanol System at 30, 60, and 100 KPa. *Journal of Chemical & Engineering Data* **1996**, *41* (3), 608–611. <https://doi.org/10.1021/je9503113>.
- (1147) Arce, A.; Arce, A.; Martínez-Ageitos, J.; Rodil, E.; Soto, A. (Vapour+liquid) Equilibrium of (DIPE+IPA+water) at 101.32kPa. *The Journal of Chemical Thermodynamics* **2003**, *35* (6), 871–884. [https://doi.org/10.1016/S0021-9614\(03\)00018-1](https://doi.org/10.1016/S0021-9614(03)00018-1).
- (1148) 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. *Computers and Chemical Engineering* **2013**, *50*, 139–151. <https://doi.org/10.1016/j.compchemeng.2012.11.006>.
- (1149) Robinson, D. B.; Peng, D.-Y. The Characterization of the Heptanes and Heavier Fractions for the GPA Peng–Robinson Programs (RR-28). *Research Report of the GPA* **1978**, 1–36.
- (1150) 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 Equilibria* **2019**, *485*, 264–269. <https://doi.org/10.1016/j.fluid.2018.12.007>.
- (1151) 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 Equilibria* **1997**, *139* (1–2), 155–170. [https://doi.org/10.1016/S0378-3812\(97\)00168-4](https://doi.org/10.1016/S0378-3812(97)00168-4).
- (1152) Kontogeorgis, G. M.; Privat, R.; Jaubert, J.-N. Taking Another Look at the van Der Waals Equation of State—Almost 150 Years Later. *Journal of Chemical & Engineering Data* **2019**. <https://doi.org/10.1021/acs.jced.9b00264>.

- (1153) 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 Equilibria* **2004**, *224* (2), 285–304. <https://doi.org/10.1016/j.fluid.2004.06.059>.
- (1154) Vitu, S.; Privat, R.; Jaubert, J.-N.; Mutelet, F. Predicting the Phase Equilibria of CO₂ + Hydrocarbon Systems with the PPR78 Model (PR EoS and k_{ij} Calculated through a Group Contribution Method). *Journal of Supercritical Fluids* **2008**, *45* (1), 1–26. <https://doi.org/10.1016/j.supflu.2007.11.015>.
- (1155) Jaubert, J.-N.; Privat, R.; Mutelet, F. Predicting the Phase Equilibria of Synthetic Petroleum Fluids with the PPR78 Approach. *AIChE Journal* **2010**, *56* (12), 3225–3235. <https://doi.org/10.1002/aic.12232>.
- (1156) 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. *Journal of Supercritical Fluids* **2013**, *75*, 58–71. <https://doi.org/10.1016/j.supflu.2012.12.014>.
- (1157) Xu, X.; Jaubert, J.-N.; Privat, R.; Arpentinier, P. Prediction of Thermodynamic Properties of Alkyne-Containing Mixtures with the E-PPR78 Model. *Industrial & Engineering Chemistry Research* **2017**, *56* (28), 8143–8157. <https://doi.org/10.1021/acs.iecr.7b01586>.
- (1158) 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 CO₂ and Fatty Acids. *Industrial and Engineering Chemistry Research* **1999**, *38* (12), 5011–5018. <https://doi.org/10.1021/ie990544d>.
- (1159) 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 Equilibria* **2010**, *295* (1), 26–37. <https://doi.org/10.1016/j.fluid.2010.03.037>.
- (1160) 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 Equilibria* **2002**, *200* (2), 411–429. [https://doi.org/10.1016/S0378-3812\(02\)00048-1](https://doi.org/10.1016/S0378-3812(02)00048-1).
- (1161) Holderbaum, T.; Gmehling, J. PSRK: A Group Contribution Equation of State Based on UNIFAC. *Fluid Phase Equilibria* **1991**, *70* (2–3), 251–265. [https://doi.org/10.1016/0378-3812\(91\)85038-V](https://doi.org/10.1016/0378-3812(91)85038-V).
- (1162) Ahlers, J.; Gmehling, J. Development of an Universal Group Contribution Equation of State. *Fluid Phase Equilibria* **2001**, *191* (1–2), 177–188. [https://doi.org/10.1016/S0378-3812\(01\)00626-4](https://doi.org/10.1016/S0378-3812(01)00626-4).
- (1163) Ahlers, J.; Gmehling, J. Development of a Universal Group Contribution Equation of State. 2. Prediction of Vapor–liquid Equilibria for Asymmetric Systems. *Industrial & Engineering Chemistry Research* **2002**, *41* (14), 3489–3498. <https://doi.org/10.1021/ie020047o>.
- (1164) Jaubert, J.-N.; Borg, P.; Coniglio, L.; Barth, D. Phase Equilibria Measurements and Modeling of EPA and DHA Ethyl Esters in Supercritical Carbon Dioxide. *Journal of Supercritical Fluids* **2001**, *20* (2), 145–155. [https://doi.org/10.1016/S0896-8446\(01\)00062-6](https://doi.org/10.1016/S0896-8446(01)00062-6).
- (1165) Louli, V.; Pappa, G.; Boukouvalas, C.; Skouras, S.; Solbraa, E.; Christensen, K. O.; Voutsas, E. Measurement and Prediction of Dew Point Curves of Natural Gas Mixtures. *Fluid Phase Equilibria* **2012**, *334*, 1–9. <https://doi.org/10.1016/j.fluid.2012.07.028>.

- (1166) Privat, R.; Jaubert, J.-N. PPR78, a Thermodynamic Model for the Prediction of Petroleum Fluid Phase Behaviour. In *JEPP 2011 - 37th Conference on Phase Equilibria*; 2011. <https://doi.org/10.1051/jepp/20110011>.
- (1167) Novak, N.; Louli, V.; Skouras, S.; Voutsas, E. Prediction of Dew Points and Liquid Dropouts of Gas Condensate Mixtures. *Fluid Phase Equilibria* **2018**, *457*, 62–73. <https://doi.org/10.1016/j.fluid.2017.10.024>.
- (1168) Mathias, P. M.; Copeman, T. W. Extension of the Peng-Robinson Equation of State to Complex Mixtures: Evaluation of the Various Forms of the Local Composition Concept. *Fluid Phase Equilibria* **1983**, *13*, 91–108. [https://doi.org/10.1016/0378-3812\(83\)80084-3](https://doi.org/10.1016/0378-3812(83)80084-3).
- (1169) Petropoulou, E.; Pappa, G. D.; Voutsas, E. Modelling of Phase Equilibrium of Natural Gas Mixtures Containing Associating Compounds. *Fluid Phase Equilibria* **2017**, *433*, 135–148. <https://doi.org/10.1016/j.fluid.2016.10.028>.
- (1170) Petropoulou, E. G.; Voutsas, E. C. Thermodynamic Modeling and Simulation of Natural Gas Dehydration Using Triethylene Glycol with the UMR-PRU Model. *Ind. Eng. Chem. Res.* **2018**, *57* (25), 8584–8604. <https://doi.org/10.1021/acs.iecr.8b01627>.
- (1171) Koulocheris, V.; Louli, V.; Panteli, E.; Skouras, S.; Voutsas, E. Modelling of Hydrogen Vapor-Liquid Equilibrium with Oil & Gas Components. *Fluid Phase Equilibria* **2019**, *494*, 125–134. <https://doi.org/10.1016/j.fluid.2019.04.010>.
- (1172) Twu, C. H.; Coon, J. E.; Cunningham, J. R. A New Generalized Alpha Function for a Cubic Equation of State Part 2. Redlich-Kwong Equation. *Fluid Phase Equilibria* **1995**, *105* (1), 61–69. [https://doi.org/10.1016/0378-3812\(94\)02602-W](https://doi.org/10.1016/0378-3812(94)02602-W).
- (1173) Plakia, A.; Pappa, G.; Voutsas, E. Modeling of CO₂ Solubility in Aqueous Alkanolamine Solutions with an Extended UMR-PRU Model. *Fluid Phase Equilibria* **2018**, *478*, 134–144. <https://doi.org/10.1016/j.fluid.2018.09.013>.
- (1174) Chen, C.-C.; Britt, H. I.; Boston, J. F.; Evans, L. B. Local Composition Model for Excess Gibbs Energy of Electrolyte Systems. Part I: Single Solvent, Single Completely Dissociated Electrolyte Systems. *AIChE J.* **1982**, *28* (4), 588–596. <https://doi.org/10.1002/aic.690280410>.
- (1175) Fredenslund, A.; Jones, R. L.; Prausnitz, J. M. Group-Contribution Estimation of Activity Coefficients in Nonideal Liquid Mixtures. *AIChE J.* **1975**, *21* (6), 1086–1099. <https://doi.org/10.1002/aic.690210607>.
- (1176) Compernelle, S.; Ceulemans, K.; Müller, J.-F. Influence of Non-Ideality on Condensation to Aerosol. *Atmos. Chem. Phys.* **2009**, *9* (4), 1325–1337. <https://doi.org/10.5194/acp-9-1325-2009>.
- (1177) H. K. Hansen; Coto, B.; Kuhlman, B. *UNIFAC with Lineary Temperature-Dependent Group-Interaction Parameters*; Internal SEP 9212; Institut for Kemiteknik, Danmarks Tekniske Universitet: Lyngby, Denmark, 1992.
- (1178) Fischer, K.; Gmehling, J. Further Development, Status and Results of the PSRK Method for the Prediction of Vapor-Liquid Equilibria and Gas Solubilities. *Fluid Phase Equilibria* **1995**, *112* (1), 1–22. [https://doi.org/10.1016/0378-3812\(95\)02792-D](https://doi.org/10.1016/0378-3812(95)02792-D).
- (1179) Gmehling, J.; Li, J.; Fischer, K. Further Development of the PSRK Model for the Prediction of Gas Solubilities and Vapor-Liquid Equilibria at Low and High Pressures II. *Fluid Phase Equilibria* **1997**, *141* (1–2), 113–127. [https://doi.org/10.1016/S0378-3812\(97\)00204-5](https://doi.org/10.1016/S0378-3812(97)00204-5).
- (1180) Horstmann, S.; Fischer, K.; Gmehling, J. PSRK Group Contribution Equation of State: Revision and Extension III. *Fluid Phase Equilibria* **2000**, *167* (2), 173–186. [https://doi.org/10.1016/S0378-3812\(99\)00333-7](https://doi.org/10.1016/S0378-3812(99)00333-7).
- (1181) Horstmann, S.; Jabłoniec, A.; Krafczyk, J.; Fischer, K.; Gmehling, J. PSRK Group Contribution Equation of State: Comprehensive Revision and Extension IV, Including

- Critical Constants and α -Function Parameters for 1000 Components. *Fluid Phase Equilibria* **2005**, 227 (2), 157–164. <https://doi.org/10.1016/j.fluid.2004.11.002>.
- (1182) Abrams, D. S.; Prausnitz, J. M. Statistical Thermodynamics of Liquid Mixtures: A New Expression for the Excess Gibbs Energy of Partly or Completely Miscible Systems. *AIChE J.* **1975**, 21 (1), 116–128. <https://doi.org/10.1002/aic.690210115>.
- (1183) Xu, X.; Privat, R.; Jaubert, J.-N. *Evaluation of PSRK Model with a New Benchmark Database.*; Internal Communication; Université de Lorraine: Nancy, France, 2021.
- (1184) Gmehling, J. From UNIFAC to Modified UNIFAC to PSRK with the Help of DDB. *Fluid Phase Equilibria* **1995**, 107 (1), 1–29. [https://doi.org/10.1016/0378-3812\(95\)02720-Y](https://doi.org/10.1016/0378-3812(95)02720-Y).
- (1185) Hansen, H. K.; Rasmussen, P.; Fredenslund, A.; Schiller, M.; Gmehling, J. Vapor-Liquid Equilibria by UNIFAC Group Contribution. 5. Revision and Extension. *Ind. Eng. Chem. Res.* **1991**, 30 (10), 2352–2355. <https://doi.org/10.1021/ie00058a017>.
- (1186) Lin, S.-T.; Sandler, S. I. A Priori Phase Equilibrium Prediction from a Segment Contribution Solvation Model. *Ind. Eng. Chem. Res.* **2002**, 41 (5), 899–913. <https://doi.org/10.1021/ie001047w>.

Résumé

Résumé

Les modèles thermodynamiques sont au cœur des outils de modélisation en génie des procédés qui fournissent, d'une part, la description, tant qualitative que quantitative des équilibres de phase des mélanges complexes, et d'autres part, une mesure des propriétés énergétiques (enthalpies, entropies, capacités thermiques) nécessaires à l'établissement des bilans énergétique et exergetique. Ce travail s'intéresse en particulier aux équations d'état issues de la théorie statistique des fluides associés (SAFT) appliquées aux corps purs. Notre objectif principal est de proposer des méthodes de paramétrage universelles et systématiques de ces modèles incluant, en particulier, les paramètres d'association qui traduisent, pour l'essentiel, l'influence que les liaisons hydrogène présentes dans un fluide pur exercent sur ses propriétés thermodynamiques.

En utilisant une des variantes les plus populaires de la famille SAFT (le modèle PC-SAFT), nous avons cherché quelles sont les propriétés expérimentales les plus pertinentes à considérer pour régresser les paramètres de corps purs ($m, \sigma, \epsilon/k$) qui suffisent à décrire les composés non associés. Nous avons montré que seules la pression de vapeur saturante et la densité du liquide s'avèrent strictement nécessaires pour obtenir une description fiable de la thermodynamique d'un corps pur non associé (i.e., de ses propriétés d'équilibre de phases et de ses propriétés énergétiques). Ce travail a produit également une base de données de paramètres pour 1800 corps purs, répartis en 1252 espèces non associées et 548 espèces auto-associées (traitées comme des espèces non-associées). En utilisant ce paramétrage, nous avons pu décrire avec précision plus de 70 % de tous les composés, et parmi eux, près de 60 % des composés auto-associés ont été correctement représentés.

L'influence du terme d'association sur les performances de l'équation d'état a ensuite été étudiée pour une famille de molécules fortement associées: les alcools linéaires. Ceci nous a permis de tirer trois conclusions majeures : 1) le terme d'association améliore nettement l'efficacité des modèles SAFT dans le cas des molécules associées ; 2) dans l'éventualité où les mêmes paramètres d'association sont utilisés pour l'ensemble des composés de la famille, des données de pression de vapeur saturante et de densité du liquide suffisent pour estimer les paramètres d'association et 3) si l'on opte pour des paramètres d'association spécifiques à chaque constituant, des données de propriétés dérivées doivent être incluses dans la régression (par exemple, la capacité thermique du liquide).

Dans une seconde partie, nous exposons une méthodologie pour l'évaluation des performances d'équations d'état des mélanges au développement duquel nous avons participé, ainsi que son application au modèle UMR-PRU.

Abstract

Thermodynamic models are at the heart of modeling tools in process engineering that provide, on the one hand, the description, both qualitative and quantitative, of phase equilibria of complex mixtures, and on the other hand, a measure of energetic properties (enthalpies, entropies, heat capacities) necessary to establish energy and exergy balances. This work is particularly interested in the equations of state from the statistical associating fluid theory (SAFT) applied to pure compounds. Our main objective is to propose universal and systematic parameterization methods for these models including, in particular, the association parameters which essentially reflect the influence that hydrogen bonds have on the thermodynamic properties of a pure fluid.

Using one of the most popular variants of the SAFT family (the PC-SAFT model), we have investigated which experimental properties are most relevant to consider when regressing the pure body parameters ($m, \sigma, \epsilon/k$) that are sufficient to describe the non-associated compounds. We have shown that only the saturating vapor pressure and the density of the liquid are found to be strictly necessary to obtain a reliable description of the thermodynamics of a non-associated pure body (i.e., its phase equilibrium properties and energy properties). This work has also produced a database of parameters for 1800 pure bodies, divided into 1252 non-associated species and 548 self-associated species (treated as non-associated species). Using this parameterization, we were able to accurately describe over 70% of all compounds, and of these, nearly 60% of the self-associated compounds were correctly represented.

The influence of the association term on the performance of the equation of state was then studied for a family of strongly associated molecules: the linear alcohols. This allowed us to draw three major conclusions: 1) the association term significantly improves the efficiency of SAFT models for associated molecules; 2) in the event that the same association parameters are used for all compounds in the family, saturation vapor pressure and liquid density data are sufficient to estimate the association parameters and 3) if component-specific association parameters are chosen, derived property data must be included in the regression (e.g., liquid heat capacity).

In a second part, we present a methodology for the evaluation of the performance of equations of state of mixtures in the development of which we participated, and its application to the UMR-PRU model.