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Vapor−Liquid Equilibria in Binary Systems Formed by *n*-Hexane with Alcohols

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The modified Świętosławski ebulliometer was used for the accurate determination of vapor−liquid equilibria in binary isothermal systems formed by *n*-hexane with the following: 2-butanol at (313.15, 323.15, and 333.15) K, 2-pentanol at (313.15, 323.15, 333.15, and 338.15) K, and 2-methyl-2-butanol at (313.15, 323.15, 333.15, and 338.15) K. The vapor pressures of the pure substances are also given. The experimental data have been compared with literature data (if available) of those systems and correlated by means of the Redlich−Kister, nonrandom two-liquid (NRTL), and Wilson equations.

Introduction

An enormous amount of data has been collected and correlated over the years, but the rapid advance of technology into new fields seems always to maintain a significant gap between demand and availability. Therefore, reliable and accurate vapor−liquid equilibrium (VLE) data are always needed to understand both the behavior of liquid mixtures and process engineering design.

This work is a continuation[1] of a big project concerning the accurate measurement of binary isothermal VLE data for systems formed by hydrocarbons (aliphatic, cyclic, aromatic) and organic compounds containing oxygen, nitrogen, and sulfur. The aim of the project is to deliver a very reliable, accurate VLE isothermal data at many different temperatures for systems which are not available in the literature as well as systems for which only one or two isotherms were measured or measured VLE are not reliable (small number of experimental points, lack information about the purity of pure components, or inconsistent data).

The purpose of this paper is to provide reliable and accurate isothermal binary VLE data for systems formed by *n*-hexane with the following: 2-butanol at (313.15, 323.15, and 333.15) K, 2-pentanol at (313.15, 323.15, 333.15, and 338.15) K, and 2-methyl-2-butanol at (313.15, 323.15, 333.15, and 338.15) K.

Only few VLE data for *n*-hexane + 2-butanol system have been already reported in the literature. The main sources[2−8] consist of both isobaric [from (40 to 101) kPa][2−4] and isothermal [from (298.15 to 348.15) K][4−8] data. VLE for the *n*-hexane + 2-methyl-2-butanol system has been measured only in one laboratory by Alonso et al.[9] In the literature there is a lack of VLE data for the *n*-hexane + 2-pentanol system.

Experimental Section

The modified Świętosławski ebulliometer[10] was used for the determination of both VLE data of all investigated binary systems and the boiling points of the pure components. The selection of the method for VLE measurement was imposed, as was previously,[1] by the physical properties of the mixtures investigated: the pure components were highly hygroscopic, and even a small amount of water present in the sample could considerably change the results of the vapor pressure measurements. The differences between the boiling temperatures of *n*-hexane and other components of the investigated mixtures were big, and consequently, the values of relative volatilities were high. Moreover, the experimental program was extensive, and because of this, the method chosen should provide accurate results in a relatively short time.

The selected ebulliometric method also has some other advantages.[10] It enables accurate determination of total pressure above the samples of known composition; the measurement can be isolated from the surroundings to prevent the penetration of moisture into the sample being investigated, and the time for achieving a steady state operation is short.

In our ebulliometer system,[10] the Systemteknik AB temperature meter type S1228 was used for determination of the temperature and Pfeiffer vacuum manometer TPG 251A for the measurement of the total pressure. Both instruments are subject to drift to obtain the absolute values of temperature and pressure, and that is why they were frequently recalibrated by the determination of the vapor pressure of water or benzene as a function of temperature.[11−13] The measurements have been done at constant temperature. This means that the pressure was adjusted until the desire temperature was achieved in the ebulliometer at a steady boiling condition. The pressure was measured when the readings of the pressure and the temperatures were constant within the assumed accuracy of measurement for 10 min. Such a procedure[10−13] allows for the determination of the accuracy of the measurements on the level of 0.01 K, in the case of the temperature (the thermometer resolution, 0.001 K), and 10 Pa, in the case of the pressure (the pressure gauge resolution, 1 Pa).

The ebulliometric measurements have been carried out in the following ways: (1) for pure substances: simultaneous determination of pressure, P, and temperature, T, and (2) for mixtures: simultaneous determination of P, T, and x (P, T, x method).

The examined samples were prepared by introducing a known mass of one substance to the ebulliometer and adding known masses of the other component. The equilibrium composition of the liquid phase in the ebulliometer was calculated from the composition of the introduced sample by means of the material balance equation.[1,10] The experimental procedures as well as a detailed description of the ebulliometer were reported previously.[1,10]

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Table 1. Parameters of the Antoine Equation (eq 1) together with Calculated (T_b^c) and Literature (NIST, T_b^l) Values of Boiling Point for All Investigated Substances

	Antoine parameters						
compound	A	B	C	T_b^c/K	T_b^l/K	ΔT/K	rmsd (P)/kPa
n-hexane	5.7662	1038.597	−65.701	341.88	341.90 ± 0.3	−0.02	0.188
2-butanol	5.8479	928.321	−130.917	372.53	372.0 ± 1.0	0.53	0.349
2-pentanol	5.6760	931.131	−139.043	392.74	392.0 ± 1.0	0.74	1.011
2-methyl-2-butanol	5.3203	744.494	−150.173	374.79	375.1 ± 0.9	−0.31	0.563

All reagents used in the investigations were supplied by Fluka with a guaranteed mass fraction greater than 99.95 % determined by gas−liquid chromatography analysis. The remaining moisture was removed by sorption on molecular sieves (AJ Wolfen Zeosorb), and to prevent further contamination, each sample was introduced into the ebulliometer by direct distillation, made just before each measurement.

Results and Discussion

Vapor pressures of the investigated four pure substances were determined as a function of temperature previously.[1,10] The obtained $P-T$ data were further correlated by the Antoine equation[14] (eq 1), and the calculated normal boiling points were compared with the values given by the National Institute of Standards and Technology (NIST).[15]

$$\log P = A - \frac{B}{T + C} \qquad (1)$$

where P is vapor pressure, kPa, T is temperature, K, and A, B, and C are Antoine's constants.

The parameters of the Antoine equation (eq 1) together with calculated and literature values of the boiling point for all investigated substances are given in Table 1. As is seen from the table, no discrepancies between data reported in the literature and those measured in this work were found.

The simultaneous (P, T, x) method without withdrawal of samples[10] was applied in this experiment. The ebulliometer was filled with a known amount of one pure compound, and a sample of the second component was added after the steady state was reached. For each experimental determination, the temperature and pressure in the apparatus and the total concentration of the sample were recorded. This procedure was repeated until the concentration of the second component reached a value higher than 0.5 mole fraction. Then the ebulliometer was filled with a known amount of the second pure compound, and the same procedure as for component one was repeated.

The vapor pressures of mixtures of different compositions were determined, and the equilibrium compositions of the liquid and vapor phases were calculated by the method described previously[1,10] using a value of 0.30 for f.

The obtained results and experimental data of temperature, pressure, and liquid-phase composition are given in Table 2 and Figures 1 to 3.

The obtained experimental data were compared with the available literature data[5−9] (see Figures 1 and 2) and correlated using the Redlich−Kister,[16] nonrandom two-liquid (NRTL),[17] and Wilson[18] equations. The minimization objective function was defined as the difference between the measured and the calculated total pressures, and for each equation the adjustable parameters were calculated using the Levenberg−Marquardt algorithm.[19] For the computation of vapor phase nonideality, the Hayden−O'Connell correlation[20] was used. The necessary auxiliary data are given in Table 3.

Table 2. VLE Measurements for the 2-Butanol (1) + *n*-Hexane (2) System at (313.15 to 333.15) K, the 2-Pentanol (1) + *n*-Hexane (2) System at (313.15 to 338.15) K, and the 2-Methyl-2-butanol (1) + *n*-Hexane (2) System at (313.15 to 338.15) K

Experimental Data

2-butanol (1) + *n*-hexane (2)

P/kPa	x_1	P/kPa	x_1	P/kPa	x_1
T = 313.15 K		T = 323.15 K		T = 333.15 K	
37.04	0.0000	53.91	0.0000	76.32	0.0000
38.24	0.1113	55.95	0.1090	79.65	0.1068
37.55	0.2089	55.04	0.2046	78.87	0.2009
36.97	0.2763	54.27	0.2710	77.47	0.2667
36.53	0.3351	53.61	0.3294	76.15	0.3247
35.93	0.3953	52.83	0.3894	75.47	0.3843
35.15	0.4642	51.67	0.4580	74.03	0.4523
35.14	0.4644	51.67	0.4581	72.20	0.5160
34.16	0.5292	50.32	0.5225	69.83	0.5741
33.13	0.5971	48.62	0.5895	67.71	0.6146
33.11	0.5976	48.60	0.5898	62.00	0.6929
31.89	0.6564	46.95	0.6475	54.32	0.7988
30.39	0.7125	44.00	0.7025	48.93	0.8480
27.71	0.7726	40.60	0.7614	41.87	0.8940
25.25	0.8226	37.64	0.8108	34.39	0.9299
22.44	0.8746	33.67	0.8620	30.17	0.9557
5.83	1.0000	29.20	0.9108	26.13	0.9735
		23.84	0.9478	21.91	0.9885
		10.48	1.0000	18.20	1.0000

2-pentanol (1) + *n*-hexane (2)

P/kPa	x_1	P/kPa	x_1	P/kPa	x_1	P/kPa	x_1
T = 313.15 K		T = 323.15 K		T = 333.15 K		T = 338.15 K	
37.04	0.0000	53.91	0.0000	76.32	0.0000	89.92	0.0000
36.48	0.0852	53.19	0.0841	75.43	0.0827	88.95	0.0813
36.41	0.1038	52.99	0.1026	75.09	0.1010	88.40	0.0994
36.13	0.1293	52.67	0.1278	74.57	0.1260	88.01	0.1243
35.44	0.1762	51.65	0.1742	73.68	0.1720	86.81	0.1704
34.83	0.2285	50.56	0.2258	71.73	0.2233	85.27	0.2219
34.43	0.2728	49.73	0.2698	70.65	0.2669	83.47	0.2802
33.93	0.2877	48.67	0.3143	69.97	0.2815	81.57	0.3096
33.80	0.3176	47.31	0.3601	68.93	0.3110	81.04	0.3288
32.97	0.3372	45.68	0.4282	68.29	0.3303	80.31	0.3548
32.80	0.3637	45.66	0.4285	66.99	0.3564	78.81	0.3875
32.00	0.3965	44.31	0.4889	65.56	0.3889	78.79	0.3870
31.69	0.4312	42.47	0.5520	62.45	0.4841	73.45	0.4815
30.90	0.4482	42.46	0.5523	62.46	0.4844	70.71	0.5436
30.89	0.4485	39.60	0.6181	60.04	0.5466	66.12	0.6082
30.57	0.4931	36.11	0.6821	60.02	0.5471	66.11	0.6089
29.26	0.5565	33.40	0.7326	56.00	0.6121	60.73	0.6745
29.25	0.5569	28.80	0.8012	51.27	0.6780	48.80	0.7865
27.93	0.6234	24.20	0.8617	41.01	0.7920	42.05	0.8436
25.64	0.6923	19.77	0.9102	35.43	0.8506	34.73	0.8904
23.64	0.7407	4.16	1.0000	29.04	0.8976	18.15	0.9780
19.35	0.8099			7.57	1.0000	9.99	1.0000
16.00	0.8709						
2.13	1.0000						

2-methyl-2-butanol (1) + *n*-hexane (2)

P/kPa	x_1	P/kPa	x_1	P/kPa	x_1	P/kPa	x_1
T = 313.15 K		T = 323.15 K		T = 333.15 K		T = 338.15 K	
37.04	0.0000	53.91	0.0000	76.32	0.0000	89.92	0.0000
37.31	0.0503	54.35	0.0499	76.96	0.0484	90.73	0.0479
36.87	0.1265	53.83	0.1260	76.37	0.1219	90.13	0.1204
34.91	0.2466	52.63	0.1899	75.21	0.1863	89.15	0.1849
34.23	0.2935	51.19	0.2462	73.79	0.2433	87.17	0.2419
33.23	0.3432	50.00	0.2929	72.20	0.2901	86.00	0.2886
32.21	0.4127	48.27	0.3418	70.11	0.3385	82.93	0.3367
32.21	0.4129	45.81	0.4092	66.94	0.4039	79.45	0.4014
30.74	0.5408	44.72	0.4765	66.91	0.4042	79.43	0.4017
30.73	0.5410	44.69	0.4768	57.98	0.5772	69.01	0.5735
29.29	0.5976	41.76	0.5317	57.95	0.5776	69.00	0.5733
27.07	0.6612	40.29	0.5867	54.57	0.6338	65.01	0.6295
25.07	0.7151	40.27	0.5870	49.11	0.7532	59.09	0.7484
21.91	0.7714	37.39	0.6432	44.57	0.8093	53.63	0.8038
19.60	0.8280	35.27	0.7035	40.11	0.8543	48.47	0.8483
5.69	1.0000	33.28	0.7625	34.21	0.8961	41.95	0.8901
		29.92	0.8204	29.87	0.9245	36.87	0.9193
		26.53	0.8674	24.77	0.9595	31.13	0.9563
		22.29	0.9097	21.33	0.9820	27.07	0.9807
		19.51	0.9367	17.87	1.0000	22.87	1.0000
		10.41	1.0000				

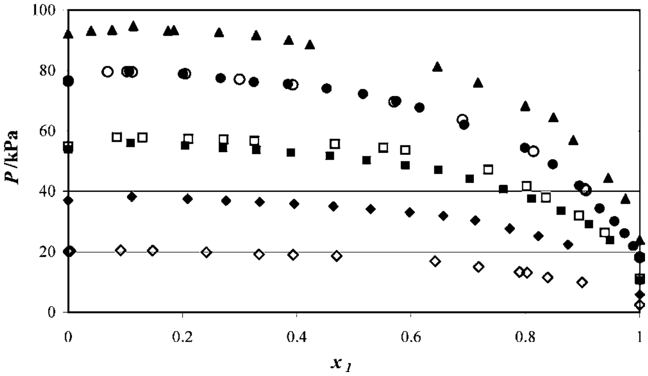

Figure 1. Comparison of the experimental isothermal $P-x$ data with the literature data for the 2-butanol (1) + *n*-hexane (2) system. ◆, $T = 313.15$ K; ■, $T = 323.15$ K; ●, $T = 333.15$ K; ◇, $T = 298.15$ K from ref 7; ○, $T = 333.15$ from ref 6; □, $T = 323.15$ from ref 8; ▲ $T = 338.15$ from ref 8.

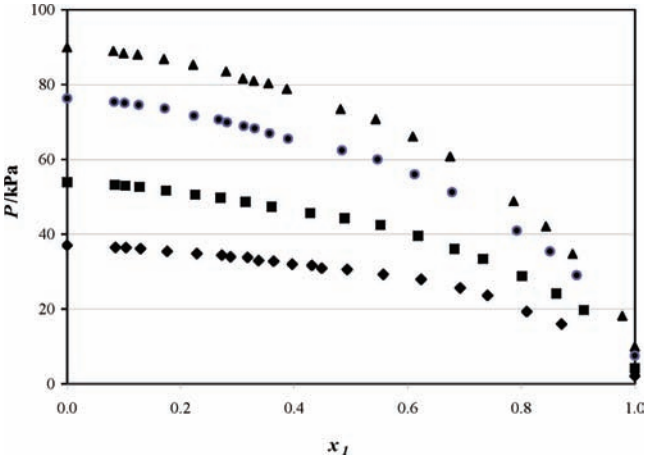

Figure 2. Experimental isothermal $P-x$ data for the 2-pentanol (1) + *n*-hexane (2) system. ◆, $T = 313.15$ K; ■, $T = 323.15$ K; ●, $T = 333.15$ K; ▲, $T = 338.15$ K.

The results of correlation ($D(P)$ and DR(P), the absolute and relative root-mean-square deviations of total pressure, respectively) for all investigated equations are shown in Table 4.

$$D(P) = \left[\frac{\sum_{i=1}^{n}(P_i^{\text{exp}} - P_i^{\text{cal}})^2}{n - m}\right]^{0.5} \tag{2}$$

$$\text{DR}(P) = \left[\frac{\sum_{i=1}^{n}\left(\frac{P_i^{\text{exp}} - P_i^{\text{cal}}}{P_i^{\text{exp}}}\right)^2}{n - m}\right]^{0.5} \tag{3}$$

where P_i^{exp} and P_i^{cal} are the experimental and calculated total pressures, respectively, n is the number of experimental data points, and m is the number of adjustable parameters.

The experimental VLE data for 2-butanol + *n*-hexane agree very well with the Hanson and Van Winkle data.[6] There is no discrepancy between these data obtained for $T = 333.15$ K[6] and our data measured for the same temperature (Figure 1). However, there is a slight discrepancy between our data and Araujo et al.[8] data measured for $T = 323.15$ K (Figure 1). The literature data lay a little bit higher in the region rich in 2-butanol. It is difficult to make a deeper conclusion concerning this fact because, besides the another set of Araujo et al.[8] data for $T = 338.15$, there is a lack of other reliable experimental data at higher temperatures for this system. Only one other set of 2-butanol + *n*-hexane isothermal data given in the literature[7] describes the VLE for $T = 298.15$. The data lay below our experiment, so we can compare only the shape and tendency of those and our data. Looking at Figure 1, it is seen that not only the data for $T = 298.15$ K[7] but also the data for $T = 338.15$ K[8] are in good correlation with our data for $T = (313.15$ to $333.15)$ K. It is worth pointing out that the experimental data were obtained by the use of the same experimental procedure,[10] and the data obtained for the series of binary systems of 1-alkohols with cyclohexane agreed very well with all available literature data.[1]

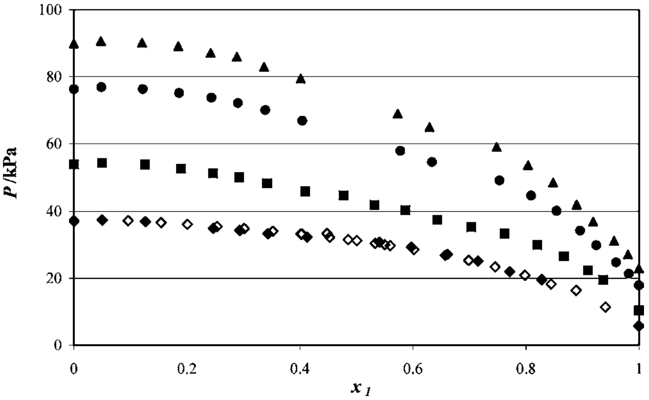

Figure 3. Comparison of the experimental isothermal $P-x$ data with the literature data for the 2-methyl-2-butanol (1) + hexane (2) system. ◆, $T = 313.15$ K; ■, $T = 323.15$ K; ●, $T = 333.15$ K; ▲, $T = 338.15$ K; ◇, $T = 313.15$ K from ref 9.

Table 3. Parameters for the Hayden−O'Connell Correlation[a]

compound	T_c/K	P_c/kPa	μ/D	RD/Å	η
n-hexane	507.43	3012.00	0.00	3.812	0.2635
2-butanol	536.00	4200.00	1.66	3.182	0.2580
2-pentanol	560.30	3700.10	1.70	3.634	0.2435
2-methyl-2-butanol	543.70	3700.10	1.68	3.641	0.2476

[a] T_c is the critical temperature; P_c, critical pressure; μ, dipole moment; RD, mean radius of gyration; η, association parameter.

In the literature, there is only one available set of VLE data for the 2-methyl-2-butanol + *n*-hexane system,[9] and our experimental VLE data fully agree with the these data. There is no discrepancy between our data measured for $T = 313.15$ K and Alonso et al. data[9] measured for the same temperature (Figure 3).

The correlation results (Table 4) show that, depending on the equation used, the relative root-mean-square deviation of total pressure has varied from (0.80 to 2.96) %. The best correlation results, for 2-pentanol + *n*-hexane systems (DR(P) = (0.84 to 1.43) %, Table 4), have been obtained for the use of the NRTL[17] equation and for 2-methyl-2-butanol + *n*-hexane and 2-butanol + *n*-hexane by the use of the Redlich−Kister[16] equation with four adjustable parameters. The worst (sometimes almost three times) correlation results for all of the investigated systems have been obtained by the use of the Wilson[18] equation. It is worth noticing that the difference between results given by the Redlich−Kister[16] and the NRTL[17] equations is very small, but both as well as another equation based on the local composition concept (the Wilson[18] equation) cannot be used for accurate correlation of these systems. The obtained results again[1] confirmed the opinion that in the case of highly associating systems good correlation can be achieved only by the use of models providing an extra term and taking into account association (usually an extra adjustable parameter).[21]

Table 4. Results of Correlation ($D(P)$ and DR(P), the Absolute and Relative Root-Mean-Square Deviations of Total Pressure, Respectively) of the Experimental VLE Isothermal Data for All of the Investigated Systems

		equation					
		NRTL[17]		Wilson[18]		Redlich−Kister[16] (four parameters)	
system	T/K	$D(P)$/kPa	DR(P)/%	$D(P)$/kPa	DR(P)/%	$D(P)$/kPa	DR(P)/%
2-butanol + *n*-hexane	313.15	0.452	1.393	0.644	1.985	0.301	0.928
	323.15	0.524	1.074	1.086	2.225	0.495	1.014
	333.15	0.491	1.070	0.641	1.489	0.473	1.098
2-pentanol + *n*-hexane	313.15	0.340	1.403	0.528	2.178	0.394	1.624
	323.15	0.426	1.074	0.879	2.215	0.532	1.341
	333.15	0.468	0.842	1.144	2.058	0.650	1.169
	338.15	0.447	1.147	0.992	2.437	0.541	1.329
2-methyl-2-butanol + *n*-hexane	313.15	0.468	1.653	0.631	2.229	0.393	1.388
	323.15	0.497	1.167	1.262	2.961	0.347	0.814
	333.15	0.466	1.452	0.752	2.343	0.257	0.801
	338.15	0.752	1.806	0.939	2.256	0.408	0.980

Note Added after Print Publication: In the original version of this article that was published on the Web on November 23, 2009, two files were inadvertently included as Supporting Information. In the corrected version that was reposted on April 15, 2010, these files and the Supporting Information Available paragraph have been removed.

Literature Cited

(1) Gierycz, P.; Kosowski, A.; Swietlik, R. Vapour-liquid equilibria in binary systems formed by cyclohexane with alcohols. *J. Chem. Eng. Data* **2009**, DOI: 10.1021/je900050z.

(2) Domínguez, M.; Martin, S.; Artigas, H.; López, M. C.; Royo, F. M. Isobaric Vapor-Liquid Equilibrium for the Binary Mixtures (2-Butanol + *n*-Hexane) and (2-Butanol + 1-Butylamine) and for the Ternary System (2-Butanol + *n*-Hexane + 1-Butylamine) at 101.3 kPa. *J. Chem. Eng. Data* **2002**, *47*, 405–410.

(3) Domínguez, M.; Mainar, A. M.; Pardo, J.; Santafé, J.; Urieta, J. S. Experimental data, correlation and prediction of isobaric VLE for the ternary mixture (2-butanol + n-hexane + 1-chlorobutane) at 101.3 kPa. *Fluid Phase Equilib.* **2003**, *211*, 179–188.

(4) Prasad, T. E. V.; Kumar, B. S.; Naveen, P. G.; Prasad, V. V. J.; Prasad, D. H. L. Boiling temperature measurements on the binary mixtures of n-hexane with some aliphatic alcohols. *Phys. Chem. Liq.* **2003**, *41*, 39–43.

(5) Uusi-Kyyny, P.; Pokki, J. P.; Laakkonen, M.; Aittamaa, J.; Liukkonen, S. Vapor Liquid Equilibrium for the Binary Systems 2-Methylpentane + 2-Butanol at 329.2 K and n-Hexane + 2-Butanol at 329.2 and 363.2 K with a Static Apparatus. *Fluid Phase Equilib.* **2002**, *201*, 343–358.

(6) Hanson, D. O.; Van Winkle, M. Alteration of the Relative Volatility of n-Hexane 4-Hexene. by Oxygenated and Chlorinated Solvents. *J. Chem. Eng. Data* **1967**, *12*, 319–325.

(7) Rodriguez, V.; Pardo, J.; López, M. C.; Royo, F. M.; Uriela, J. Vapor pressures of binary mixtures of hexane + 1-butanol, + 2-butanol, + 2-methyl-1-propanol, or + 2-methyl-2-propanol at 298.15 K S. *J. Chem. Eng. Data* **1993**, *38*, 350–352.

(8) Araujo, M. E.; Maciel, M. R. W.; Francesconi, A. Z. Excess Gibbs free energies of (hexane + butan-2-ol) and of (cyclohexane + butan-2-ol) at the temperatures (323.15, 338.15, and 348.15) K. *J. Chem. Thermodyn.* **1993**, *25*, 1295–1299.

(9) Alonso, C.; Montero, E. A.; Chamorro, C. R.; Segovia, J. J.; Martin, M. C.; Villamanan, M. A. Vapour-liquid equilibrium of octane-enhancing additives in gasolines 2. Total pressure data and g^E for binary and ternary mixtures containing tert-amylmethyl ether (TAME), tert-amyl alcohol (TAOH) and n-hexane. *Fluid Phase Equilib.* **2001**, *182*, 241–255.

(10) Gierycz, P.; Kosowski, A.; Świetlik, R. Modified Ebulliometer for the Accurate Determination of Vapour-Liquid Equilibrium. *Pol. J. Chem.* **2009**, *83*, 325–337.

(11) Rogalski, M.; Rybakiewicz, K.; Malanowski, S. Rapid and accurate method for determination of vapour-liquid equilibrium. *Ber. Bunsen Ges.* **1977**, *81*, 1070–1081.

(12) Rogalski, M.; Malanowski, S. Ebuliometers modified for the accurate determination of vapour-liquid equilibrium. *Fluid Phase Equilib.* **1980**, *5*, 97–112.

(13) Gierycz, P.; Rogalski, M.; Malanowski, S. Vapour-liquid equilibria in binary systems formed by N-methylpyrrolidone with hydrocarbons and hydroxyl derivatives. *Fluid Phase Equilib.* **1985**, *22*, 107–122.

(14) Bittrich, H. J. *Modellierung von Phasegleichgewichten als Grundlage von Stoffrennprozessen*; Akademie Verlag: Berlin, 1981.

(15) NIST Chemistry WebBook. http://webbook.nist.gov (accessed April 24, 2009).

(16) Redlich, O.; Kister, A. Algebraic Representation of Thermodynamic Properties and the Classification of Solutions. *Ind. Eng. Chem.* **1948**, *40*, 345–348.

(17) Renon, M.; Prausnitz, J. M. Local Compositions in Thermodynamic Excess Functions for Liquid Mixtures. *AIChE J.* **1968**, *14*, 135–144.

(18) Wilson, G. M. Vapour-Liquid Equilibrium XI. A New Expression for the Excess Free Energy of Mixing. *J. Am. Chem. Soc.* **1964**, *86*, 127–130.

(19) Marquardt, D. An Algorithm for Least-squares Estimation of Nonlinear Parameters. *SIAM J. Appl. Math.* **1963**, *11*, 431–441.

(20) Prausnitz, J. M.; Anderson, T. F.; Grens, E. A., II; Eckert, C. A.; Hsieh, R.; O'Connell, J. P. *Computer Calculations for Multicomponent Vapor-Liquid and Liquid-Liquid Equilibria*; Prentice-Hall: Englewood Cliffs, New York, 1980.

(21) Gierycz, P. Comparison and Verification of Methods for Correlation and Prediction of VLE in Multicomponent Systems. *Pol. J. Chem.* **1996**, *70*, 1373–1401.

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