

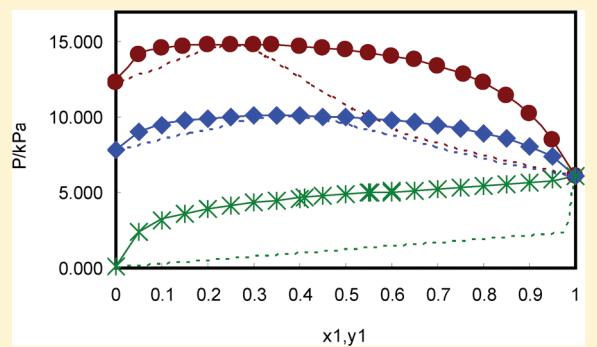
Vapor–Liquid Equilibria of Binary Mixtures Containing 2-Butanol and Hydrocarbons at 313.15 K

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ABSTRACT: The paper reports the isothermal vapor–liquid equilibria (VLE) of five binary mixtures containing 2-butanol + heptane, + 2,2,4-trimethylpentane, + dodecane, + cyclohexane, and + methylbenzene at 313.15 K. A static technique has been used for the measurements. Data reduction by Barker's method provides the parameters of G^E models. The six-parameter Margules equation, Wilson, non-random two-liquid (NRTL), and universal quasichemical activity coefficient (UNIQUAC) models have been used for the correlation of the experimental data. Good results have been obtained for all. The five investigated mixtures exhibit a positive deviation from ideality, and four of them show a maximum pressure azeotrope. Only the mixture 2-butanol + dodecane does not present an azeotrope.



INTRODUCTION

Ethers and alcohols are usually added to gasoline to improve their combustion and reduce pollution. Phase equilibrium data of oxygenated mixtures are important for predicting the vapor-phase composition that would be in equilibrium with hydrocarbon mixtures.

The first studies were focused on different ethers MTBE (methyl *tert*-butyl ether), DIPE (di-isopropyl ether), and TAME (*tert*-amyl methyl ether), and then we continue with biocompounds, those of vegetable origin, that can be considered as biofuels, ETBE (ethyl *tert*-butyl ether), or alcohols such as propanol isomers or 1-pentanol. As an example only a few papers are referenced.^{1–8}

In this paper, the vapor–liquid equilibria (VLE) data are reported for the binary systems 2-butanol + heptane, + 2,2,4-trimethylpentane, + dodecane, + cyclohexane, and + methylbenzene at 313.15 K. In a recent paper,⁹ the VLE data of the same hydrocarbons with 1-butanol at 313.15 K have been reported.

EXPERIMENTAL SECTION

Materials. 2-Butanol was an anhydrous Sigma-Aldrich product with a purity of >0.999; heptane and cyclohexane were supplied from Fluka Chemie and were of highest purity available, with a purity 0.998 and >0.999 (by gas chromatography, GC) respectively. Methylbenzene was an anhydrous Aldrich product with a purity >0.999; the other compounds (2,2,4-trimethylpentane and dodecane) were supplied from Sigma-Aldrich with a purity of >0.997. All liquids were thoroughly degassed before measurements by a modified distillation method based on the one suggested by Van Ness

and Abbott¹⁰ and kept in glass balloons equipped with leak-proof valves. In Table 1, the vapor pressures of the pure constituents measured in this work are compared with those reported in the literature as a check for complete degassing.

Apparatus and Procedure. A static VLE apparatus, consisting of an isothermal total pressure cell, has been employed for measuring the vapor–liquid equilibrium of the binary mixtures. The apparatus has been described in previous papers.^{1,2}

The sample injectors were two 100 cm³ positive displacement pumps (Ruska, model 2200-801) with a resolution of 0.01 cm³ and an estimated total uncertainty of \pm 0.03 cm³. These allowed the injection of known volumes of the pure components, previously degassed, into the cell which was immersed in a high precision water bath (Hart Scientific model 6020), assuring a stability of \pm 0.5 mK when thermostatted at 313.15 K.

The cell was a cylindrical stainless steel piece with a capacity of about 180 cm³ fitted with a magnetic stirrer coupled to an external drive. An initial volume of about 50 cm³ of one component was injected into the evacuated cell, and the vapor pressure was measured. Successive injections of a second component were made over a desired composition range until the cell was nearly full. The total mass injected was determined accurately from the volumetric displacement of the pistons, the temperature of the injectors, and the known densities for the

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Table 1. Average Values of Experimental Vapor Pressures (P_i^{sat}) for the Pure Compounds Measured in This Work and Literature Values ($P_i^{\text{sat}}(\text{lit})$), Molar Volumes of Pure Liquids (V_i^L), van der Waals Molecular Volumes (r_i), Surfaces (q_i), and Second Virial Coefficients (B_{ii} , B_{ij}) Calculated by the Method of Hayden and O'Connell¹⁴ at $T = 313.15\text{ K}$ Used for the Calculations

compound	2-butanol ($i = 1$)	heptane ($i = 2$)	2,2,4-trimethylpentane ($i = 3$)	dodecane ($i = 4$)	cyclohexane ($i = 5$)	methyl benzene ($i = 6$)
$P_i^{\text{sat}}/\text{kPa}$	6.058	12.326	12.986	0.059	24.629	7.877
$P_i^{\text{sat}}(\text{lit})/\text{kPa}$	6.055 ^a	12.323 ^d	12.966 ^f	0.054 ^f	24.632 ^f	7.894 ^g
	6.048 ^b	12.331 ^e	12.981 ^h	0.059 ^k	24.630 ⁱ	7.897 ⁱ
	6.017 ^c	12.335 ^f	12.973 ⁱ	0.053 ^l	24.625 ^m	7.875 ^o
		12.334 ^g	12.960 ^j		24.560 ⁿ	7.880 ^p
$V_i^L/(\text{cm}^3 \cdot \text{mol}^{-1})^q$	94	150	169	232	111	109
$B_{11}/\text{cm}^3 \cdot \text{mol}^{-1}$	-3241.8	-1424.3	-1480.3	-2864.0	-1143.7	-1311.8
$B_{22}/\text{cm}^3 \cdot \text{mol}^{-1}$	-1424.3	-2521.3				
$B_{33}/\text{cm}^3 \cdot \text{mol}^{-1}$	-1480.3		-2716.0			
$B_{44}/\text{cm}^3 \cdot \text{mol}^{-1}$	-2864.0			-16442.0		
$B_{55}/\text{cm}^3 \cdot \text{mol}^{-1}$	-1143.7				-1554.6	
$B_{66}/\text{cm}^3 \cdot \text{mol}^{-1}$	-1311.8					-2105.7
r_i^r	3.9235	5.1742	5.8463	8.5462	4.0464	3.9228
q_i^r	3.664	4.396	5.008	7.096	3.240	2.968

^aReference 4. ^bReference 20. ^cReference 21. ^dReference 22. ^eReference 3. ^fCalculated from the Antoine equation using constants reported in ref 23.

^gReference 24. ^hCalculated from the Antoine equation using constants reported in ref 25. ⁱReference 5. ^jReference 26. ^kAdjustment of data from ref 27 using the Antoine equation. ^lCalculated from the Antoine equation using constants reported in NIST (coefficients calculated by NIST from ref 28). ^mReference 29. ⁿReference 30. ^oReference 7. ^pReference 31. ^qReference 23. ^rCalculated from ref 32.

Table 2. Experimental Total Pressure (P/kPa) for the Binary Systems at $T = 313.15\text{ K}$ at Various Compositions of the Liquid Phase (x_1) and the Calculated Compositions of the Vapor Phase (y_1) Using the Six-Parameter Margules Equation

x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa
2-Butanol (1) + Heptane (2)											
0.0000	0.0000	12.327	0.4999	0.3063	14.457	0.3489	0.9886	4.498	0.7504	0.9923	5.324
0.0492	0.1591	14.175	0.5500	0.3180	14.277	0.3995	0.9891	4.631	0.8008	0.9929	5.422
0.1001	0.2007	14.612	0.5498	0.3180	14.283	0.4102	0.9893	4.658	0.8508	0.9936	5.534
0.1477	0.2189	14.758	0.6001	0.3311	14.060	0.4485	0.9896	4.752	0.9003	0.9947	5.667
0.1989	0.2337	14.832	0.6004	0.3313	14.061	0.4488	0.9896	4.763	0.9505	0.9966	5.837
0.2505	0.2475	14.848	0.6502	0.3465	13.789	0.4990	0.9900	4.875	1.0000	1.0000	6.055
0.2996	0.2601	14.826	0.7005	0.3654	13.431	2-Butanol (1) + Cyclohexane (2)					
0.3397	0.2700	14.788	0.7571	0.3931	12.891	0.0000	0.0000	24.623	0.5004	0.1741	24.093
0.3998	0.2840	14.696	0.8004	0.4215	12.334	0.0498	0.0844	26.004	0.5502	0.1837	23.537
0.3999	0.2841	14.694	0.8505	0.4682	11.464	0.0999	0.1063	26.172	0.5506	0.1838	23.537
0.4495	0.2951	14.588	0.9003	0.5420	10.259	0.1501	0.1166	26.134	0.6001	0.1951	22.862
0.4500	0.2952	14.581	0.9501	0.6784	8.544	0.2002	0.1248	26.021	0.6006	0.1952	22.862
0.4993	0.3062	14.453	1.0000	1.0000	6.061	0.2499	0.1329	25.835	0.6508	0.2093	22.028
2-Butanol (1) + 2,2,4-Trimethylpentane (2)											
0.0000	0.0000	12.962	0.5003	0.2970	14.927	0.3002	0.1411	25.586	0.7009	0.2270	21.001
0.0494	0.1486	14.744	0.5497	0.3085	14.739	0.3500	0.1492	25.295	0.7508	0.2503	19.716
0.1001	0.1900	15.171	0.5506	0.3087	14.738	0.4003	0.1573	24.953	0.8007	0.2826	18.105
0.1493	0.2094	15.323	0.5954	0.3202	14.528	0.4502	0.1655	24.554	0.9001	0.4102	13.498
0.1997	0.2243	15.380	0.5997	0.3214	14.509	0.4503	0.1655	24.553	0.9497	0.5665	10.221
0.2494	0.2378	15.384	0.6519	0.3373	14.204	0.5002	0.1741	24.080	1.0000	1.0000	6.057
0.2988	0.2506	15.352	0.7006	0.3553	13.832	2-Butanol (1) + Methylbenzene (2)					
0.3493	0.2630	15.290	0.7506	0.3788	13.344	0.3002	0.1411	25.586	0.7009	0.2270	21.001
0.3992	0.2745	15.198	0.8007	0.4106	12.672	0.0000	0.0000	7.876	0.4993	0.4220	10.028
0.4003	0.2748	15.200	0.8508	0.4566	11.765	0.0494	0.1607	8.994	0.5484	0.4420	9.937
0.4496	0.2857	15.077	0.9002	0.5296	10.505	0.0986	0.2339	9.528	0.5495	0.4424	9.948
0.4504	0.2859	15.076	0.9507	0.6690	8.669	0.1492	0.2738	9.801	0.5985	0.4631	9.839
0.4997	0.2968	14.926	1.0000	1.0000	6.058	0.1991	0.2992	9.952	0.5996	0.4635	9.843
2-Butanol (1) + Dodecane (2)											
0.0000	0.0000	0.059	0.5008	0.9901	4.867	0.2485	0.3198	10.037	0.6491	0.4864	9.705
0.0500	0.9766	2.449	0.5494	0.9905	4.977	0.2985	0.3398	10.089	0.6990	0.5129	9.526
0.1006	0.9827	3.208	0.5551	0.9905	4.973	0.3486	0.3601	10.104	0.7492	0.5450	9.290
0.1490	0.9847	3.601	0.5996	0.9909	5.073	0.3983	0.3806	10.097	0.8002	0.5848	8.980
0.1989	0.9861	3.901	0.6008	0.9909	5.063	0.4485	0.4013	10.102	0.8498	0.6324	8.592
0.2489	0.9871	4.138	0.6504	0.9913	5.149	0.4487	0.4014	10.077	0.9501	0.7867	7.399
0.2986	0.9879	4.331	0.7009	0.9918	5.232	0.4983	0.4216	10.014	1.0000	1.0000	6.060

Table 3. Parameters of the Models Used for the Binary Systems at $T = 313.15\text{ K}$ together with the Root-Mean-Square Deviation of Pressure (rms ΔP), Maximum Value of Deviation (max ΔP), Azeotropic Mole Fractions of 1-Butanol ($x_{1,\text{az}}$), and Azeotropic Pressure (P_{az})

	Margules (6p)	Margules (4p)	Margules (3p)	Wilson	NRTL	UNIQUAC
2-Butanol (1) + Heptane (2)						
A_{12}	2.6541	2.4677	2.2904	0.1558	1.0956	1.2535
A_{21}	1.6683	1.6254	1.7716	0.4576	1.8927	0.4450
λ_{12}	4.0377	2.0794	1.2180			
λ_{21}	0.9459	0.5380	1.2180			
η_{12}	4.7641					
η_{21}	1.1760					
α					0.5705	
rms $\Delta P/\text{kPa}$	0.005	0.037	0.087	0.086	0.044	0.199
max $\Delta P/\text{kPa}$	0.008	0.115	0.295	0.263	0.139	0.550
$x_{1,\text{az}}$	0.2505	0.2505	0.2505	0.2505	0.2505	0.2505
P_{az}/kPa	14.849	14.871	14.854	14.819	14.865	14.742
2-Butanol (1) + 2,2,4-Trimethylpentane (2)						
A_{12}	2.6043	2.4239	2.2544	0.1670	1.1033	1.3359
A_{21}	1.6740	1.6345	1.7714	0.4509	1.8436	0.4098
λ_{12}	3.8907	2.0047	1.1859			
λ_{21}	0.9314	0.5526	1.1859			
η_{12}	4.5735					
η_{21}	1.1009					
α					0.5747	
rms $\Delta P/\text{kPa}$	0.007	0.036	0.086	0.091	0.045	0.209
max $\Delta P/\text{kPa}$	0.024	0.113	0.283	0.268	0.140	0.548
$x_{1,\text{az}}$	0.2494	0.2494	0.2494	0.2494	0.2494	0.2494
P_{az}/kPa	15.389	15.409	15.383	15.343	15.400	15.248
2-Butanol (1) + Dodecane (2)						
A_{12}	2.6696	2.4885	2.3656	0.1997	1.6724	1.4220
A_{21}	2.2335	2.1082	2.2824	0.2818	1.8515	0.3713
λ_{12}	4.1729	2.2759	1.7313			
λ_{21}	1.7678	0.9060	1.7313			
η_{12}	5.3987					
η_{21}	1.1462					
α					0.5644	
rms $\Delta P/\text{kPa}$	0.010	0.040	0.062	0.103	0.039	0.209
max $\Delta P/\text{kPa}$	0.014	0.095	0.201	0.289	0.105	0.639
2-Butanol (1) + Cyclohexane (2)						
A_{12}	2.6546	2.4469	2.2407	0.1242	0.8316	1.1971
A_{21}	1.3713	1.3289	1.5294	0.5994	1.9527	0.4829
λ_{12}	4.2567	2.0853	1.1142			
λ_{21}	0.6122	0.2743	1.1142			
η_{12}	5.3261					
η_{21}	0.8543					
α					0.5718	
rms $\Delta P/\text{kPa}$	0.007	0.081	0.202	0.117	0.095	0.313
max $\Delta P/\text{kPa}$	0.009	0.174	0.412	0.224	0.182	0.546
$x_{1,\text{az}}$	0.0999	0.0999	0.0999	0.0999	0.0999	0.0999
P_{az}/kPa	26.166	26.052	25.829	25.972	26.033	25.666
2-Butanol (1) + Methylbenzene (2)						
A_{12}	1.8516	1.8649	1.8726	0.2851	0.4534	0.8928
A_{21}	1.7836	1.6109	1.6038	0.5109	0.3398	0.7907
λ_{12}	0.8365	1.1855	1.2254			
λ_{21}	3.1796	1.2626	1.2254			
η_{12}	-1.6355					
η_{21}	5.4730					
α					0.7263	
rms $\Delta P/\text{kPa}$	0.006	0.022	0.021	0.079	0.022	0.110
max $\Delta P/\text{kPa}$	0.008	0.060	0.064	0.252	0.077	0.318
$x_{1,\text{az}}$	0.3486	0.3486	0.3486	0.3983	0.3486	0.3983
P_{az}/kPa	10.105	10.117	10.116	10.122	10.106	10.127

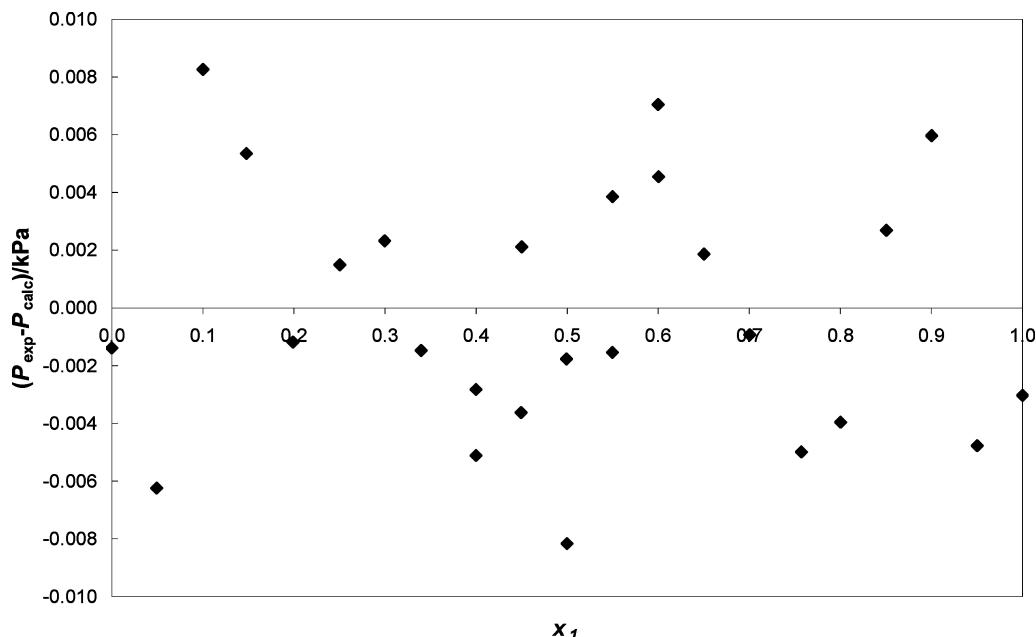


Figure 1. Pressure residuals defined as differences between experimental and calculated pressures using the six-parameter Margules equation as a function of the liquid composition (x_1) for the system 2-butanol (1) + heptane (2).

pure components. This resulted in uncertainties in mole fraction of ± 0.0001 .

Experimental values of total vapor pressure for the binary mixtures were obtained in two overlapping runs starting from opposite ends of the composition range.

The temperature was measured with a calibrated platinum resistance thermometer (SDL model 5385/100) and an ac resistance bridge (ASL model F250) with a resolution of 1 mK and an estimated overall uncertainty of ± 10 mK. The measurement of pressure was done indirectly through a differential pressure cell and indicator (Ruska models 2413-705 and 2416-11, respectively). Air was used on the reference side of the differential pressure cell, and the pressure required to obtain a null indication was measured with a fused quartz Bourdon pressure gauge (Texas Instruments model 801). The overall uncertainty of the pressure was estimated to be ± 5 Pa.

RESULTS AND CORRELATIONS

Data reduction for the binary was done by Barker's method¹¹ according to well-established procedures.^{12,13}

The nonideality of the vapor phase was taken into account with the virial equation of state, truncated after the second term. The pure component and interaction second virial coefficients (B_{ij}) were calculated by the Hayden and O'Connell method¹⁴ using the parameters given by Dymond and Smith.¹⁵

Binary systems have been correlated by the up to six-parameter Margules equation:¹⁶

$$\begin{aligned} G^E/RT = & [A_{ji}x_i + A_{ij}x_j - (\lambda_{ji}x_i + \lambda_{ij}x_j)x_i x_j \\ & + (\eta_{ji}x_i + \eta_{ij}x_j)x_i^2 x_j^2]x_i x_j \end{aligned} \quad (1)$$

where parameters A_{ij} , A_{ji} , λ_{ij} , λ_{ji} , η_{ij} , and η_{ji} were obtained by regression of the binary data. Also the Wilson,¹⁷ NRTL,¹⁸ and UNIQUAC¹⁹ models have been used for fitting the binary

systems, whose expressions for the excess Gibbs energy are given by

$$G^E/RT = -\sum_i x_i \ln \left(\sum_j x_j A_{ij} \right) \quad (2)$$

$$G^E/RT = \sum_i x_i \left(\sum_j A_{ji} G_{ji} x_j / \sum_k G_{ki} x_k \right) \quad (3)$$

$$\begin{aligned} G^E/RT = & \sum_i x_i \ln(\varphi_i/x_i) + (z/2) \sum_i q_i x_i \ln(\vartheta_i/q_i) \\ & - \sum_i q_i x_i \ln \left(\sum_j \vartheta_j A_{ji} \right) \end{aligned} \quad (4)$$

where $G_{ji} = \exp(-\alpha_{ji}A_{ji})$; $\alpha_{ji} = 0.3$; $\vartheta_i = q_i x_i / \sum_j q_j x_j$; $\varphi_i = r_i x_i / \sum_j r_j x_j$ and $z = 10$.

The adjustable parameters are A_{ij} and A_{ji} and also α_{ji} of the NRTL model.

Table 2 gives experimental values of total pressure and the corresponding compositions of the liquid and vapor phases for the five binary systems; the vapor phase composition was calculated using the six-parameter Margules equation.

The results of data correlation for all of the binary systems are summarized in Table 3. This table contains the adjustable parameter values, the root-mean-square of the difference between the experimental and the calculated pressures (rms ΔP), and the maximum value of these pressure residuals (max ΔP) (both are indicators of the quality of the agreement with data), which have been obtained, using Barker's method, for the different models.

As an example, Figure 1 reports the plot of the pressure residuals ($P_{\text{exp}} - P_{\text{calc}}$) as a function of the liquid mole fraction of the alcohol (x_1) for the binary system (2-butanol (1) + *n*-heptane (2)), where the pressures were calculated using the six-parameter Margules equation; it can be seen how the residuals scatter around the zero value. The same behavior has been observed for the other investigated binary mixtures.

DISCUSSION

The six-parameter Margules equation leads to the best correlation results for the binary systems measured in this work: the root-mean-square deviation (rms) of the pressure is 5 Pa for (2-butanol + heptane), 7 Pa for (2-butanol + 2,2,4-trimethylpentane), 10 Pa for (2-butanol + dodecane), 7 Pa for (2-butanol + cyclohexane), and 6 Pa for (2-butanol + methylbenzene), and the maximum deviations are (8, 24, 14, 9, and 8) Pa, respectively. The other models give higher values of the root-mean-square deviations, and the NRTL model with three parameters gives the best results of them with values of the rms pressure deviations of 44 Pa for (2-butanol + heptane), 45 Pa for (2-butanol + 2,2,4-trimethylpentane), 39 Pa for (2-butanol + dodecane), 95 Pa for (2-butanol + cyclohexane), and 22 Pa for (2-butanol + methylbenzene). For the binary mixture (2-butanol + cyclohexane), there are some data in the literature³⁰ which give lower values for the pressure than the calculated by the six-parameter Margules equation, and the rms pressure residual is 548 Pa; also the pure cyclohexane vapor pressure is lower than the values of this work and the literature as is shown in Table 1.

All of the investigated systems show an azeotropic behavior except (2-butanol + dodecane) as have been represented in Figures 2

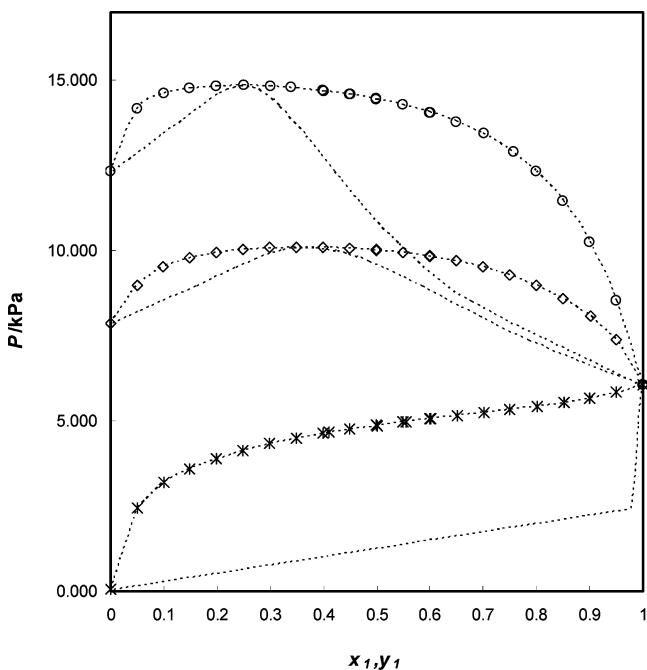


Figure 2. Total pressure at $T = 313.15$ K for the binary systems as a function of the liquid (x_1) and vapor composition (y_1): \circ , 2-butanol (1) + heptane (2); $*$, 2-butanol (1) + dodecane (2); \diamond , 2-butanol (1) + methylbenzene (2). Symbols represent the experimental points; lines are the calculations using the six-parameter Margules equation.

and 3. The azeotropic molar fractions of 2-butanol ($x_{1,\text{az}}$) and the azeotropic pressure (P_{az}) calculated by the different models at $T = 313.15$ K are reported in Table 3. The systems present a maximum pressure azeotrope, and the highest effect is obtained for the mixture containing cyclohexane.

Finally, the excess molar Gibbs energy (G^E) for the binary systems has been calculated. Figure 4 shows the values of G^E , calculated by the six-parameter Margules equation, as a function

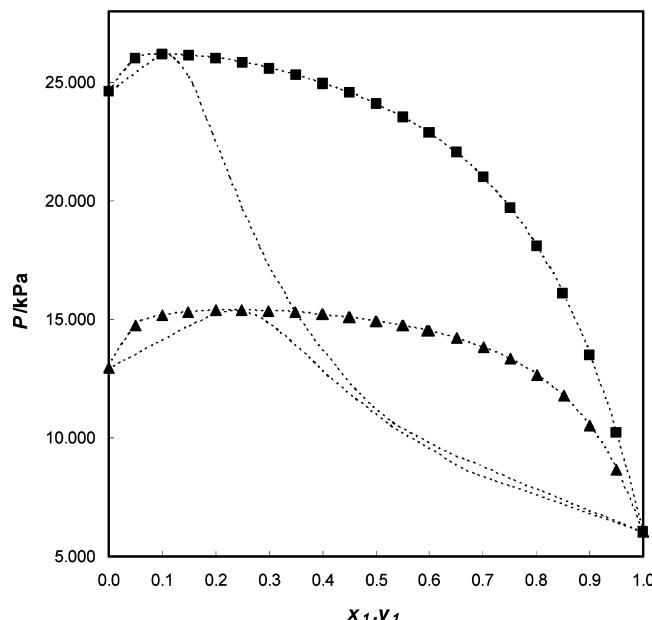


Figure 3. Total pressure at $T = 313.15$ K of the binary systems as a function of the liquid (x_1) and vapor composition (y_1): \blacktriangle , 2-butanol (1) + 2,2,4-trimethylpentane (2); \blacksquare , 2-butanol (1) + cyclohexane (2). Symbols represent the experimental points; lines are the calculations using the six-parameter Margules equation.

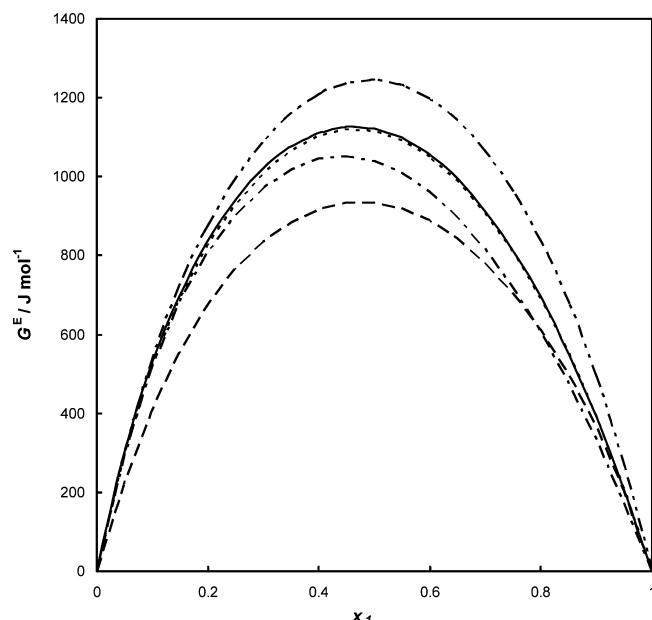


Figure 4. Excess molar Gibbs energy calculated using the six-parameter Margules equation as a function of the molar fraction of the liquid phase (x_1) for binary systems at $T = 313.15$ K: —, 2-butanol (1) + heptane; ---, 2-butanol (1) + 2,2,4-trimethylpentane (2); - - -, 2-butanol (1) + dodecane; - · -, 2-butanol (1) + cyclohexane; - · - · -, 2-butanol (1) + benzene.

of the liquid mole fraction. The five binary systems measured exhibit a high positive deviation from ideality. As expected, this effect is stronger for 2-butanol (1) + dodecane (2). Indeed, the G^E values for the composition of 2-butanol $x_1 = 0.45$ or $x_1 = 0.50$ vary with the change of the chain of hydrocarbon: $1246 \text{ J}\cdot\text{mol}^{-1}$ (dodecane) $> 1127 \text{ J}\cdot\text{mol}^{-1}$ (heptane) $> 1119 \text{ J}\cdot\text{mol}^{-1}$

(2,2,4-trimethylpentane) $> 1052 \text{ J}\cdot\text{mol}^{-1}$ (cyclohexane) $> 935 \text{ J}\cdot\text{mol}^{-1}$ (methylbenzene); this order of the hydrocarbons is the same than the observed for the mixtures with 1-butanol, which presented slightly higher values of the maximum.⁹

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Notes

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