Isobaric Vapor−Liquid Equilibria of the Ternary System Dibutyl Ether + 1-Pentanol + Nonane

Helle Kirss, Mati Kuus, and Enn Siimer*

Department of Material Science, Tallinn University of Technology, Ehitajate tee 5, 19086 Tallinn, Estonia

Isobaric vapor−liquid equilibria (VLE) were measured for the ternary system dibutyl ether + 1-pentanol + nonane and for two constituent binaries systems, dibutyl ether + nonane and dibutyl ether + 1-pentanol, at the pressures (26.66, 53.33, 79.99, and 101.32) kPa. Boiling temperature (*T*, *x*) relations were obtained by using a semi-microebulliometer. 1-Pentanol formed a minimum boiling azeotrope with dibutyl ether. The modified Wilson model with parameters that linearly depend on temperature was used to correlate to the binary *T*, *x* data and to predict VLE in the ternary system.

Introduction

The thermodynamic information of multicomponent vapor−liquid equilibrium (VLE) is important for testing existing models not only for promoting a general understanding of interactions in solutions but also in the design of equipment for separation processes. In previous papers, we have reported VLE in eight ternary systems (and for constituent binaries): *o*-xylene + amyl acetate + nonane,[1] *o*-xylene + nonane + cyclohexanol,[2] hexan-2-one + *o*-xylene + nonane,[3] toluene + *p*-xylene + 1,2-dichloroethane,[4] toluene + ethylbenzene + chlorobenzene,[5] toluene + ethylbenzene + amyl acetate,[6] methylbutyl ketone + nonane + cyclohexanol,[7] and methylbutyl ketone + 1-pentanol + nonane.[8] In addition, we have presented experimental excess enthalpies H^E data for different ternary systems, particularly consisting of the same compounds as in the VLE investigations but also, for example, for phenols with alkanes, primary alcohols, and cyclohexanol.[9−12]

In this paper, we present VLE at pressures of (26.66, 53.33, 79.99, and 101.32) kPa for the ternary system dibutyl ether + 1-pentanol + nonane. We have not found information for VLE of this ternary system and for the binary systems dibutyl ether + nonane and dibutyl ether + 1-pentanol. For the third binary, 1-pentanol + nonane, we reported the VLE data previously, observing that a minimum boiling azeotrope exists at the molar fraction of 1-pentanol about 0.5 to 0.6.[8]

In the previous studies of ternary systems, we have not used ethers. Dibutyl ether was investigated only in the VLE experiments with isomeric alkynes.[13]

We have used our modification of the Wilson equation[2] to correlate binary VLE data and to predict ternary VLE, giving in all cases the most reliable results (compared to the UNIFAC model[14] and Wilson equation[15]). So, the modified Wilson equation was used also in the present work.

Experimental Section

Materials. Nonane and 1-pentanol used for the present measurement were the same as in our early works.[7,8] Components of 99.5 % purity before rectification were dried, dibutyl ether with Na_2SO_4 and 1-pentanol with CaO. All substances were twice fractionally distilled in a high-efficiency Teflon spinning band (rotor) column. The samples were collected and stored under argon in glass ampules. Purity, checked by gas chromatography, was greater than 99.7 % (dibutyl ether,

* Corresponding author. E-mail: enn.siimer@staff.ttu.ee.

Table 1. Densities σ, Refractive Indices n_D at 293.15 K, and Normal Boiling Temperatures T_b of Pure Components

	ρ/kg·m^{-3}		n_D		T_b/K	
component	exptl	lit	exptl	lit	exptl	lit
dibutyl ether	768.9	768.9[a]	1.3992	1.3992[a]	414.66	415.10[d]
1-pentanol	814.5	814.8[a]	1.4098	1.4100[a]	410.86	410.95[a]
nonane	717.6	717.6[c]	1.4055	1.4054[b]	423.97	423.95[a]

[a] Ref 16. [b] Ref 17. [c] Ref 18. [d] Ref 19.

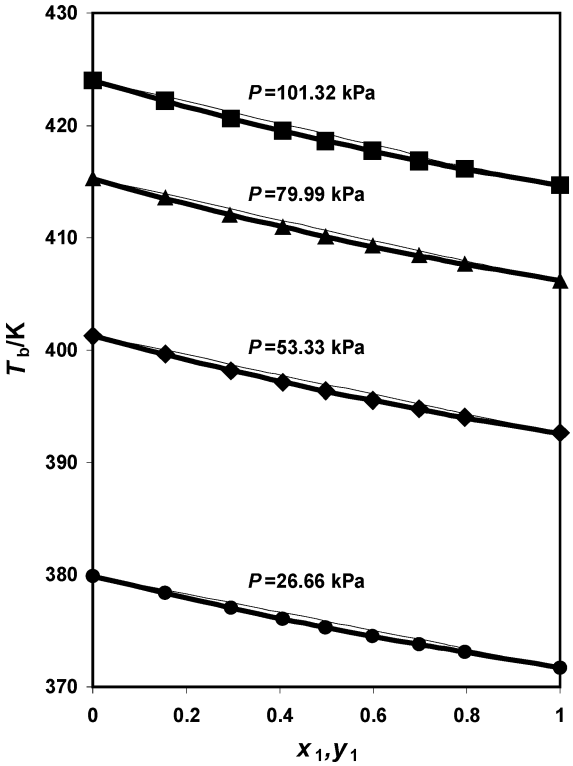

Figure 1. Experimental boiling temperature T_b−x_1 diagrams for dibutyl ether + nonane at pressures: ●, 26.66 kPa; ◆, 53.33 kPa; ▲, 79.99 kPa; and ■, 101.32 kPa. Calculated by the modified Wilson equation[2] curves: T_b−x_1 (bold lines), T_b−y_1 (thin lines).

10.1021/je060237w CCC: $30.25
Published on Web 08/26/2006

Table 2. Isobaric Vapor−Liquid Equilibrium Data: Liquid Phase Mole Fraction x_1 and Boiling Temperatures T in Binary Systems

	T/K			
x_1	P = 26.66 kPa	P = 53.33 kPa	P = 79.99 kPa	P = 101.32 kPa
	Dibutyl Ether (1) + Nonane (2)			
0.000	379.88	401.28	415.26	423.97
0.155	378.33	399.66	413.53	422.20
0.295	376.95	398.15	412.00	420.59
0.406	376.05	397.15	410.92	419.55
0.498	375.26	396.36	410.08	418.59
0.599	374.53	395.54	409.23	417.78
0.698	373.82	394.76	408.39	416.78
0.796	373.07	394.00	407.66	416.09
1.000	371.73	392.61	406.15	414.66
	Dibutyl Ether (1) + 1-Pentanol (2)			
0.000	375.63	392.70	403.80	410.86
0.150	371.73	389.74	401.29	408.48
0.284	369.62	388.03	399.92	407.29
0.390	368.79	387.44	399.48	406.94
0.486	368.19	387.07	399.30	406.88
0.594	367.98	387.09	399.53	407.22
0.698	368.04	387.36	400.03	407.93
0.798	368.59	388.43	401.41	409.57
0.898	369.62	389.90	403.20	411.48
1.000	371.73	392.61	406.15	414.66
	1-Pentanol (1) + Nonane (2)[a]			
0.000				423.97
0.150				412.69
0.189				410.93
0.267				408.61
0.401				406.89
0.501				406.15
0.605				405.95
0.693				406.00
0.803				406.58
0.900				408.03
1.000				410.86

[a] Experimental data at the pressures (26.66, 53.33, and 79.99) kPa are reported.[8]

Table 3. Coefficients for the Antoine Vapor-Pressure Equation (eq 1)

component	A_1	B_i	C_1	temperature region/K
dibutyl ether	13.9161	3178.040	−72.8469	370 to 415
1-pentanol	13.2675	2277.432	−147.537	375 to 415
nonane	13.8546	3224.816	−74.824	375 to 425

1-pentanol) and 99.8 % nonane. Measured densities, refractive indices, and normal boiling temperatures are compared with the literature values in Table 1.

Apparatus and Procedure. The boiling temperature−liquid composition (T, x) results were obtained at constant pressure in a semi-microebulliometer with a volume of liquid about 1 mL. A detail description of the apparatus and procedure has been reported previously.[1] Boiling temperature of the liquid was measured by a specially manufactured thermistor. The liquid mixtures were prepared by mass. The uncertainties in the boiling temperature, pressure, and liquid mole fraction were estimated to be less than 0.05 K, 13 Pa, and 5×10^{-4}, respectively.

Results and Discussion

The experimental values of the boiling temperature measurements for the binary systems dibutyl ether + nonane and dibutyl ether + 1-pentanol at four pressures (26.66, 53.33, 79.99, and 101.32) kPa are reported in Table 2. Table 2 also includes VLE experiments for the 1-pentanol + nonane system at 101.32 kPa. Data at other pressures were reported in our previous work.[8] The boiling temperature−composition diagram for the binary systems dibutyl ether + nonane and dibutyl ether + 1-pentanol at pressures of (26.66, 53.33, 79.99, and 101.32) kPa are presented in Figure 1 and in Figure 2. The vapor phase was calculated, considering it to be ideal.

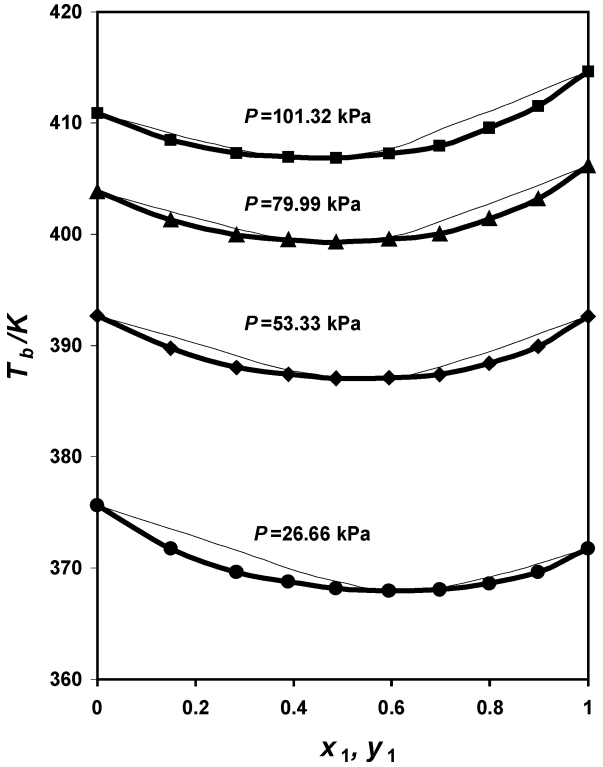

Figure 2. Experimental boiling temperature T_b−x_1 diagrams for dibutyl ether + 1-pentanol at pressures: ●, 26.66 kPa; ◆, 53.33 kPa; ▲, 79.99 kPa; and ■, 101.32 kPa. Calculated by the modified Wilson equation[2] curves: T_b−x_1 (bold lines), T_b−y_1 (thin lines).

The vapor pressure of pure components P_i^0 was calculated by the Antoine equation:

$$\ln(P_i^0/\text{kPa}) = A_i - \frac{B_i}{T/\text{K} + C_i} \quad (1)$$

where A_i, B_i, and C_i and the used temperature regions are reported in Table 3. The values of coefficients the Antoine equation are calculated by our experimental values of the boiling temperature of all components at pressures of (26.66, 53.33, 79.99, and 101.32) kPa.

The T, x data for the binary systems were fitted with the Wilson equation,[15] defined as

$$\ln \gamma_i = -\ln(x_i - \Lambda_{ik}x_k) + x_k\left[\frac{\Lambda_{ik}}{x_i + \Lambda_{ik}x_k} - \frac{\Lambda_{ki}}{x_k + \Lambda_{ki}x_i}\right] \quad (2)$$

where γ_i is the activity coefficient of component i in the liquid phase. We have used the modified form of the Wilson model,[2] considering the linear dependence of the parameters $\lambda_{ij}-\lambda_{ii} = m_i + n_iT$ on temperature. In this case, the coefficients Λ_{ik} and Λ_{ki} can be simply expressed as (see ref 2):

$$\Lambda_{ik} = \exp\left[a_{ik} + \frac{b_{ik}}{T}\right] \quad (3)$$

$$\Lambda_{ki} = \exp\left[a_{ki} + \frac{b_{ki}}{T}\right] \quad (4)$$

including in the parameters a_{ik} and b_{ik} molar volumes of components. The parameters a_{ik} and b_{ik} were calculated by the

Table 4. Values of $(\lambda_{ij}-\lambda_{ii})/R$ (the Wilson equation[15]), a_{ij}, b_{ij} (the modified Wilson equation[2]), Standard Deviations (σP; eq 5), and Mean Relative Errors (δP; eq 6) of Calculated Pressure for Binary Systems

	dibutyl ether (1) + nonane (2)	dibutyl ether (1) + 1-pentanol (2)	1-pentanol (1) + nonane (2)
Wilson Equation			
$[(\lambda_{12}-\lambda_{11})/R]$ J·mol^{-1}	173.4	2772.0	4102.2
$[(\lambda_{21}-\lambda_{22})/R]$ J·mol^{-1}	−31.8	−174.6	920.7
σP/kPa	0.113	0.591	0.747
100 δP	0.122	0.977	1.056
Modified Wilson Equation			
a_{12}	0.84780	−1.09362	5.23968
b_{12}/K	−213.164	279.212	−2429.40
a_{21}	−1.34622	2.94678	−2.75089
b_{21}/K	370.112	−1335.51	818.942
σP/kPa	0.086	0.283	0.546
100 δP	0.092	0.330	0.609

Table 5. Azeotropic Boiling Temperatures (T_{az}) and Composition (x_1^{az}) of the Binary System Dibutyl Ether (1) + 1-Pentanol (2) versus Pressure (P)

P/kPa	T_{az}/K	x_1^{az}
26.66	368.0	0.638
53.33	387.1	0.535
79.99	399.3	0.471
101.32	406.9	0.434

Newton iteration method. Standard deviation was calculated using

$$\sigma(P) = [\sum_{1}^{N} (P_{calc} - P_{exptl})^2/(N-n)]^{1/2} \quad (5)$$

where P_{calc} and P_{exptl} are the calculated and experimental values of the total pressure, respectively; N is the number of experimental points; and n is the number of parameters in correlation models (in determining parameters a_{ik} and b_{ik}, n is equal to 4). The mean relative error between experimental and calculated pressure is defined as

$$\delta P = \frac{1}{N}\sum^{N} |(P_{exptl} - P_{calc})/P_{exptl}| \times 100 \quad (6)$$

The T, x data of the binary systems were fitted with the two-parameter Wilson model[15] and with our modified Wilson model.[2] The parameters of both models were calculated as unified values for all boiling temperatures at each of four experimental pressures and are presented in Table 4. Additionally Table 4 contains standard deviation and mean relative error of pressure calculation. As seen in Table 4, the modified Wilson equation can correlate experimental data better.

In the previous work,[8] we presented the coefficients of the Wilson equation[15] and the modified Wilson model[2] for the binary 1-pentanol + nonane system. In the present paper, we have recalculated these values considering the experimental data at (26.66, 53.33, and 79.99) kPa[8] together with the data at 101.32 kPa (see Table 2).

The binary dibutyl ether + 1-pentanol system exhibits a minimum boiling azeotrope. The azeotropic points have been determined from the function

$$\alpha_{12} = \frac{y_1/y_2}{x_1/x_2} \quad (7)$$

where y_i is the mole fraction of component i in the vapor phase, calculated by the modified Wilson equation and solving for $\alpha_{12} = 1$. Azeotropic compositions x_1^{az}, boiling temperatures T_{az}, and pressures are presented in Table 5.

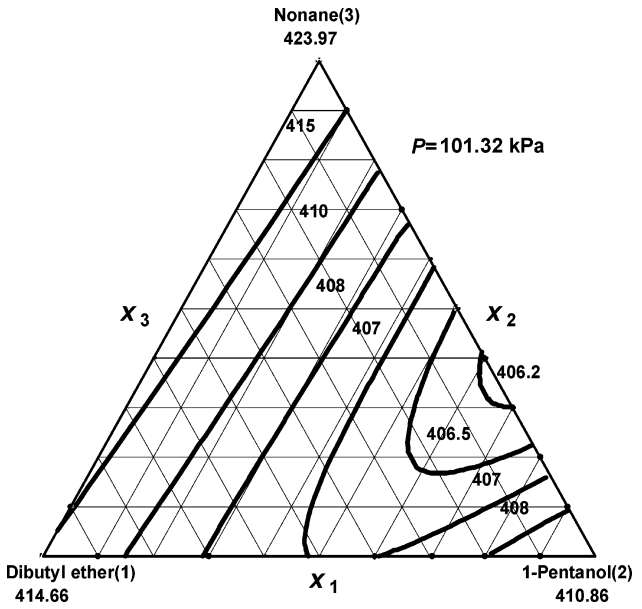

Figure 3. Calculated by the modified Wilson equation[2] boiling temperature isotherms for the dibutyl ether (1) + 1-pentanol (2) + nonane (3) at 101.32 kPa.

The system dibutyl ether + nonane has a relatively weak deviation from ideality. It seems that dibutyl ether has quite a weak ether group that cannot form hydrogen bonds with hydroxyl groups of 1-pentanol, especially at higher temperatures. Dibutyl ether is similar to an aliphatic hydrocarbon. 1-Pentanol as a typical primary alcohol is strongly self-associated; adding an inert solvent (nonane, dibutyl ether) to alcohol, some dissociation of the 1-pentanol takes place. In our VLE experiments, the formation of a minimum boiling azeotrope with dibutyl ether was observed at pressures of (26.66, 53.33, and 79.99) kPa.[8] The experiments at 101.32 kPa, presented in this paper, showed that x_1^{az} was equal to 0.646 and that $T_{az} = 405.95$ K, in good agreement with the literature data.[20−22]

The isobaric VLE data for the ternary system are given in Table 6. Experimental T, x values are presented together with calculated values of activity coefficients, vapor compositions, excess Gibbs energy, temperatures, and total pressures predicted by the modified Wilson equation using the binary parameters (3 × 4 parameters) from Table 4. For example, the values of activity coefficients in the ternary systems can be calculated from eq 8 as

$$\gamma_i = \exp\left[1 - \ln(\sum_{j=1}^{3} x_j\Lambda_{ij}) - \sum_{k=1}^{3} \frac{x_k\Lambda_{ki}}{\sum_{j=1}^{3} x_j\Lambda_{jk}}\right] \quad (8)$$

and the Gibbs energy G^E can be expressed as

$$G^E = -RT[\sum_{i=1}^{3} x_i \ln \sum_{j=1}^{3} x_j\Lambda_{ij}] \quad (9)$$

where x_i is the mole fraction of component i.

In Figure 3, the predicted boiling temperature isotherms for the ternary system dibutyl ether (1) + 1-pentanol (2) + nonane (3) at 101.32 kPa are presented on the Gibbs triangle. As seen from Figure 3, a ternary azeotrope was not detected; the ternary

Table 6. Experimental Vapor−Liquid Equilibria Data, Liquid Mole Fractions x_1 and x_2, Boiling Temperature T_{exptl} for the Ternary System Dibutyl Ether (1) + 1-Pentanol (2) + Nonane (3) at Four Pressures and Values Calculated by the Modified Wilson Equation[2] Activity Coefficients (γ_1, γ_2, and γ_3), Vapor Mole Fractions (y_1 and y_2), Excess Gibbs Energy (G^E), Pressure (P_{calcd}), Boiling Temperature (T_{calcd}), and Differences in Pressure (ΔP) and Boiling Temperature (ΔT)[a]

experimental data			calculated values									
x_1	x_2	T_{exptl}/K	γ_1	γ_2	γ_3	y_1	y_2	G^E/J·mol^{-1}	P_{calcd}/kPa	ΔP/kPa	T_{calcd}/K	ΔT/K
						$P = 26.66$ kPa						
0.331	0.332	368.19	1.0662	1.6067	1.2843	0.3184	0.3904	805.0	26.01	−0.66	368.80	0.61
0.238	0.238	368.79	1.0011	2.0067	1.1549	0.2207	0.3610	740.4	25.90	−0.77	369.52	0.73
0.118	0.118	371.17	0.9676	2.9791	1.0433	0.1137	0.2926	485.5	26.24	−0.42	371.58	0.41
0.751	0.166	368.90	1.0237	1.9224	1.1500	0.6984	0.2369	422.2	26.51	−0.16	369.05	0.15
0.140	0.574	368.13	1.2735	1.2096	1.6890	0.1619	0.5110	896.8	25.79	−0.88	368.93	0.80
0.554	0.276	368.22	1.0602	1.6580	1.2492	0.5258	0.3324	642.2	26.24	−0.42	368.62	0.40
0.240	0.120	370.78	0.9773	2.7660	1.0544	0.2310	0.2722	463.8	26.17	−0.50	371.26	0.48
0.378	0.188	369.24	0.9994	2.1388	1.1228	0.3527	0.3078	592.3	26.12	−0.55	369.77	0.53
0.282	0.566	368.32	1.2996	1.1916	1.7214	0.3304	0.4937	783.0	26.16	−0.51	368.78	0.46
0.207	0.414	368.08	1.1098	1.4531	1.3841	0.2073	0.4398	916.5	25.91	−0.76	368.78	0.70
0.121	0.242	369.27	0.9866	2.0762	1.1428	0.1111	0.3834	798.8	26.24	−0.43	369.67	0.40
0.207	0.689	369.14	1.4790	1.0917	2.0542	0.2831	0.5695	663.9	26.28	−0.39	369.49	0.35
0.548	0.178	369.28	1.0115	2.0359	1.1338	0.5116	0.2743	513.4	26.45	−0.21	369.48	0.20
0.325	0.513	368.36	1.2392	1.2482	1.6090	0.3604	0.4656	797.7	26.39	−0.28	368.62	0.26
0.727	0.091	370.25	1.0014	2.3224	1.0756	0.6938	0.1668	279.9	26.53	−0.13	370.38	0.13
0.107	0.298	368.75	1.0098	1.8371	1.2017	0.0993	0.4104	894.0	26.06	−0.60	369.31	0.56
						$P = 53.33$ kPa						
0.331	0.332	387.35	1.0432	1.5699	1.2551	0.2958	0.4289	773.9	52.76	−0.57	387.65	0.30
0.238	0.238	388.33	0.9920	1.9218	1.1320	0.2090	0.3918	705.6	52.69	−0.64	388.68	0.35
0.118	0.118	391.82	0.9755	2.6616	1.0336	0.1119	0.3028	449.1	53.38	0.25	391.68	−0.14
0.751	0.166	388.79	1.0170	1.7767	1.1461	0.6803	0.2555	386.6	53.14	−0.19	388.90	0.11
0.140	0.574	386.68	1.2123	1.2130	1.6311	0.1427	0.5595	892.8	52.61	−0.72	387.05	0.37
0.554	0.276	387.74	1.0434	1.5893	1.2344	0.4983	0.3643	603.4	53.10	−0.23	387.87	0.13
0.240	0.120	391.33	0.9819	2.4857	1.0446	0.2266	0.2835	432.2	53.35	0.01	391.32	−0.01
0.378	0.188	389.23	0.9943	2.0020	1.1076	0.3392	0.3308	558.8	53.19	−0.14	389.31	0.08
0.282	0.566	387.10	1.2423	1.1879	1.6794	0.2947	0.5422	764.2	53.31	−0.03	387.11	0.01
0.207	0.414	387.07	1.0748	1.4424	1.3418	0.1884	0.4846	894.7	52.91	−0.42	387.29	0.22
0.121	0.242	388.86	0.9792	1.9962	1.1175	0.1049	0.4156	761.4	53.56	0.23	388.74	−0.12
0.207	0.689	387.57	1.4021	1.0916	2.0095	0.2475	0.6171	653.9	53.38	0.05	387.54	−0.03
0.548	0.178	389.31	1.0052	1.8935	1.1237	0.4947	0.2949	480.5	53.59	0.26	389.17	−0.14
0.325	0.513	387.12	1.1907	1.2403	1.5713	0.3251	0.5125	773.8	53.42	0.08	387.08	−0.04
0.727	0.091	390.80	1.0001	2.0704	1.0759	0.6848	0.1747	258.7	53.56	0.23	390.67	−0.13
0.107	0.298	387.93	0.9941	1.7979	1.1691	0.0923	0.4487	861.6	53.05	−0.29	388.08	0.15
						$P = 79.99$ kPa						
0.331	0.332	399.90	1.0313	1.5368	1.2337	0.2860	0.4468	743.5	79.53	−0.47	400.08	0.18
0.238	0.238	401.16	0.9890	1.8508	1.1170	0.2049	0.4037	673.2	79.45	−0.55	401.37	0.21
0.118	0.118	405.31	0.9813	2.4476	1.0281	0.1121	0.3016	419.9	80.59	0.59	405.07	−0.24
0.751	0.166	401.91	1.0135	1.6839	1.1462	0.6736	0.2617	360.5	79.88	−0.12	401.96	0.05
0.140	0.574	398.74	1.1769	1.2116	1.5847	0.1335	0.5848	877.5	79.42	−0.58	398.96	0.22
0.554	0.276	400.51	1.0343	1.5392	1.2216	0.4864	0.3783	572.0	79.92	−0.08	400.54	0.03
0.240	0.120	404.77	0.9858	2.2991	1.0387	0.2263	0.2837	406.4	80.32	0.32	404.64	−0.13
0.378	0.188	402.30	0.9928	1.9034	1.0972	0.3348	0.3385	530.3	80.15	0.15	402.24	−0.06
0.207	0.414	399.40	1.0563	1.4273	1.3112	0.1799	0.5065	867.8	79.79	−0.21	399.48	0.08
0.207	0.689	399.44	1.3546	1.0903	1.9629	0.2298	0.6418	639.4	80.17	0.17	399.38	−0.06
0.548	0.178	402.41	1.0025	1.7976	1.1157	0.4888	0.3020	454.3	80.63	0.63	402.16	−0.25
0.325	0.513	399.30	1.1622	1.2317	1.5383	0.3079	0.5363	748.8	80.29	0.29	399.19	−0.11
0.727	0.091	404.16	0.9997	1.9216	1.0747	0.6826	0.1760	243.1	80.38	0.38	404.00	−0.16
0.107	0.298	400.54	0.9879	1.7549	1.1480	0.0897	0.4654	827.4	80.05	0.05	400.52	−0.02
						$P = 101.32$ kPa						
0.331	0.332	407.73	1.0252	1.5130	1.2197	0.2815	0.4552	720.9	100.81	−0.53	407.90	0.17
0.238	0.238	409.22	0.9880	1.8018	1.1077	0.2034	0.4084	649.4	100.82	−0.51	409.39	0.17
0.118	0.118	413.86	0.9851	2.3144	1.0250	0.1127	0.2983	399.6	102.29	0.96	413.54	−0.32
0.751	0.166	410.13	1.0116	1.6277	1.1435	0.6711	0.2641	343.1	101.27	−0.07	410.15	0.02
0.140	0.574	406.26	1.1567	1.2093	1.5533	0.1288	0.5986	862.7	100.80	−0.53	406.42	0.16
0.554	0.276	408.50	1.0294	1.5066	1.2127	0.4810	0.3847	550.1	101.33	−0.00	408.50	0.00
0.240	0.120	413.23	0.9884	2.1839	1.0352	0.2269	0.2816	388.4	101.90	0.56	413.04	−0.19
0.378	0.188	410.45	0.9926	1.8402	1.0907	0.3335	0.3408	510.2	101.53	0.19	410.39	−0.06
0.207	0.414	407.05	1.0465	1.4148	1.2916	0.1758	0.5175	846.3	101.05	−0.28	407.14	0.09
0.207	0.689	406.84	1.3260	1.0890	1.9278	0.2204	0.6553	627.2	101.51	0.18	406.79	−0.05
0.548	0.178	410.71	1.0013	1.7370	1.1102	0.4868	0.3043	435.9	102.48	1.15	410.33	−0.38
0.325	0.513	406.95	1.1456	1.2250	1.5148	0.2989	0.5490	729.3	101.86	0.52	406.79	−0.16
0.727	0.091	412.59	0.9996	1.8340	1.0735	0.6823	0.1755	232.6	102.00	0.67	412.36	−0.23
0.107	0.298	408.47	0.9854	1.7220	1.1352	0.0886	0.4729	801.0	101.63	0.29	408.38	−0.09

[a] Mean relative absolute error (δP) is 0.81 %, and standard deviation (σP) is 0.51 kPa.

system is characterized by quite considerable positive deviation from ideal behavior.

Literature Cited

(1) Kirss, H.; Siimer, E.; Kuus, M.; Kudryavtseva, L. Isobaric vapor−liquid equilibria in the system *o*-xylene + amyl acetate + nonane. *J. Chem. Eng. Data* **2001**, *46*, 147−150.

(2) Siimer, E.; Kirss, H.; Kuus, M.; Kudryavtseva, L. Isobaric vapor−liquid equilibrium for the ternary system *o*-xylene + nonane + cyclohexanol. *J. Chem. Eng. Data* **2002**, *47*, 52−55.

(3) Siimer, E.; Kirss, H.; Kuus, M.; Kudryavtseva, L. Isobaric vapour−liquid equilibria of the ternary system hexan-2-one + *o*-xylene + nonane. *Proc. Est. Acad. Sci., Chem.* **2002**, *51*, *1*, 19−28.

(4) Kirss, H.; Kuus, M.; Siimer, E.; Kudryavtseva, L. Isobaric vapor−liquid equilibria of the ternary system toluene + *p*-xylene + 1,2-dichloroethane. *Proc. Est. Acad. Sci., Chem.* **2002**, *51*, *4*, 215−224.

(5) Kuus, M.; Kirss, H.; Siimer, E.; Kudryavtseva, L. Thermodynamics of ternary liquid mixtures containing toluene, ethylbenzene, and chlorobenzene. *J. Chem. Eng. Data* **2003**, *48*, 898−903.

(6) Kirss, H.; Kuus, M.; Siimer, E. Isobaric vapor−liquid equilibria of the ternary system toluene + ethylbenzene + amyl acetate. *J. Chem. Eng. Data* **2004**, *49*, 465−467.

(7) Kirss, H., Kuus, M., Siimer, E. Isobaric vapor−liquid equilibria of the ternary system methylbutyl ketone + nonane + cyclohexanol. *J. Chem. Eng. Data* **2005**, *50*, 309−311.

(8) Kirss, H.; Siimer, E.; Kuus, M. Isobaric vapor−liquid equilibria of ternary system methylbutyl ketone + 1-pentanol + nonane. *J. Chem. Eng. Data* **2006**, *51*, 153−156.

(9) Kirss, H., Kudryavtseva, L., Kuus, M., Siimer, E. Excess enthalpies for ternary mixtures phenol−3-methylphenol−1-hexanol, 3-methylphenol−1-hexanol−cyclohexanol and their constituent binaries at 318.15 K. *Chem. Eng. Commun.* **1996**, *146*, 139−147.

(10) Kirss, H.; Kuus, M.; Siimer, E.; Kudryavtseva, L. Excess enthalpies of 3-methylphenol−*n*-heptane, 3-methylphenol−phenol−*n*-heptane and 3-methylphenol−1-hexanol−*n*-heptane at 318.15 K. *Chem. Eng. Commun.* **1997**, *162*, 15−22.

(11) Siimer, E.; Kirss, H.; Kuus, M.; Kudryavtseva, L. Excess enthalpies for the systems *o*-xylene + cyclohexanol + nonane at 298.15 K and 318.5 K and 3-methylphenol + 1-hexanol + heptane at 298.15 K and for constituent binaries. *J. Chem. Eng. Data* **1997**, *42*, 619−622.

(12) Kuus, M.; Kirss, H.; Siimer, E.; Kudryavtseva, L. Excess enthalpies for the systems *o*-xylene + cyclohexanol + phenol and *o*-xylene + cyclohexanol + 1,3-butanediol at 318.15 K. *J. Chem. Eng. Data* **1998**, *43*, 351−353.

(13) Kirss, H.; Siimer, E.; Kudryavtseva, L. Isobaric vapor-liquid equilibria in the mixtures of 1-heptyne + butanal, 1-octyne + 3-octyne, + ethylbenzene and + dibutyl ether, 2-octyne + dibutyl ether and 1-butanol, 3-octyne + 1-octene. *Thermochim. Acta* **1993**, *228*, 283−289.

(14) Gmehling, J.; Rasmussen, P.; Fredenslund, A. Vapor−liquid equilibria by UNIFAC group contribution. Revision and extension II. *Ind. Eng., Proces Des. Dev.* **1982**, *211*, 118−127.

(15) Wilson, G. M. Vapor-liquid equilibrium. XI. A new expression excess free energy of mixing. *J. Am. Chem. Soc.* **1964**, *86*, 127−130.

(16) Dean, J. *Lange's Handbook of Chemistry*, 14th ed.; McGraw-Hill: New York, 1992.

(17) Riddick, J. A.; Bunge, W. B.; Sakano, T. K. *Techniques of Chemistry*, Vol. II. Organic Solvents, 4th ed,; John Wiley&Sons: New York, 1986.

(18) Thermodynamic Research Center. *TRC Databases for Chemistry and Engineering: Thermodynamic Tables, version 1996-2S*; Texas A&M University System: College Station, TX, 1966.

(19) Greune, G.; Kehlen, H. Fluessigkeits-Dampf-Gleichgewicht von Butanol-Butylaether-Mischungen. *Z. Phys. Chem. (Leipzig)* **1977**, *258*, 912−924.

(20) Seymour, K. M.; Carmichael, R. H. An empirical correlation among azeotropic data. *Ind. Eng. Chem., Fundam.* **1977**, *16*, 200−207.

(21) Roekens, E. I. L.; Verhoeye, L. A. I. Azeotropic data for the systems formed by representatives of the homologous series of alkanes and alcohols. *J. Appl. Chem. Biotechnol.* **1976**, *26*, 595−610.

(22) Kushner, T. M.; Shleinikova, M. B.; Ryazanova, A. V.; Bakhvalov, L. A.; Serafimov, L. A. Azeotropy in aliphatic alcohol−paraffinic hydrocarbon systems at atmospheric pressure. *Zh. Fiz. Khim.* **1981**, *55*, 1511.

Received for review May 29, 2006. Accepted July 16, 2006.

JE060237W