Z_{RA} constant of the modified Rackett equation (eq 2)

Registry No. MEA, 141-43-5; DEA, 111-42-2; TMSO$_2$, 126-33-0; NMP, 872-50-4; PC, 108-32-7.

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Excess Gibbs Energies and Excess Volumes of 1-Butanol–*n*-Heptane and 2-Methyl-1-propanol–*n*-Heptane Binary Systems

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Isothermal *P*–*x*–*y* and excess volume data for 1-butanol and 2-methyl-1-propanol in *n*-heptane are measured. The vapor–liquid equilibrium data were reduced according to the maximum likelihood principle. The parameters of NRTL, Wilson, and UNIQUAC equations were calculated and reported.

Introduction

In a previous paper (*1*) of this series we presented the vapor–liquid equilibrium and excess volume data of 1-butanol and 2-methyl-1-propanol in *n*-hexane. Here we carry on the study of aliphatic alcohol–alkane systems.

This article reports the results of measurements on vapor–liquid equilibria for the 1-butanol–*n*-heptane system at 333.15 and 363.15 K and for the 2-methyl-1-propanol–*n*-heptane system at 333.15 K. The experimental excess volumes at 298.15 K for both systems are reported too.

Experimental Section

***Materials*.** The 1-butanol and 2-methyl-1-propanol used in this work were Merck "pro analysis" products, with a stated minimum purity of 99.5% and 99.0%, respectively.

The *n*-heptane was "Lichrosolv" reagent from Merck with a 99.7% grade.

These materials were purified by fractional distillations under 80-kPa pressure, with an Oldershaw type, 60 real plates, column.

The measured densities and vapor pressures of purified samples are shown in Table I compared with the literature values.

***Apparatus and Procedure*.** The vapor–liquid equilibrium data were determined by using the still and the technique described previously (*2*). The temperature inside the equilibrium cell was measured by means of a Lauda digital R 42 thermometer, with a platinum resistance thermometer calibrated in the apparatus by consecutive measurements of boiling points for several pure components in the pressure range of 5–100 kP and at 298.15–373.15 K. In this case, the temperature uncertainty is $\sigma_e(T) = 0.01$ K. Pressure was measured by means of a Texas Instruments precision pressure gauge, with a fused-quartz Bourdon tube, calibrated against a mercury manometer for the range 0–101 kPa. The inaccuracy of the pressure measurements was determined as $\sigma_e(P) = 0.009$ kPa. Temperature was maintained constant by using the method described previously (*3*).

Liquid and vapor compositions were determined by densimetric analysis with an Anton Paar DMA 60 densimeter and two DMA 601 M cells. Measuring cells were thermoregulated better than 0.01 K.

The sampling of vapor and liquid phases from the ebulliometer was carried out by a recently published (*2*) technique. Compositions of both phases were analyzed continuously in the flow system.

Experimental Results and Treatments

***Excess Volume Data*.** The excess volumes were calculated for the measured densities from mixtures of known composition prepared by weighing into syringes equipped with three-way valves. The best attention was given to reduce the vapor volume and to dry the internal parts of the valve. This technique is used for preventing the partial evaporation of samples. The experimental data are given in Table II.

Equation 1, proposed by Neau (*4*) for alcohol–alkane binary systems, correlated the excess volumes calculated from density:

$$v^E/x_1x_2 = \sum_{j=1}^{m} A_jY_j \qquad (1)$$

0021-9568/84/1729-0206$01.50/0

Table I. Physical Properties of Components

compd	density at 298.15 K g cm^{-3}		vapor press., kPa			
			333.15 K		363.15 K	
	this work	lit.	this work	lit.	this work	lit.
n-heptane	0.679 49	0.67951^a	28.019	28.074^b	78.584	78.604^b
1-butanol	0.805 79	0.8058^c	8.006	7.935^d 7.867^b 7.890^c	34.163	34.205^d 34.097^b 34.188^c
2-methyl-1-propanol	0.797 94	0.7978^c	12.432	12.432^b 12.378^d 12.354^c		

[a] Reference *12*. [b] Reference *13*. [c] Reference *14*. [d] Reference *15*.

Table II. Experimental Excess Volume Data at 298.15 K

1-butanol (1)-n-heptane (2)		2-methyl-1-propanol (1)-n-heptane (2)	
x_1°	$v^{E\circ}/(\mathrm{cm^3\ mol^{-1}})$	x_1°	$v^{E\circ}/(\mathrm{cm^3\ mol^{-1}})$
0.0454	0.110	0.0224	0.099
0.0758	0.141	0.0820	0.199
0.1017	0.164	0.0947	0.216
0.1677	0.203	0.1795	0.301
0.2472	0.219	0.2159	0.326
0.3155	0.227	0.2658	0.352
0.3710	0.222	0.2851	0.357
0.4373	0.207	0.3523	0.365
0.4898	0.182	0.3652	0.367
0.5601	0.162	0.4161	0.352
0.5783	0.158	0.4193	0.357
0.6639	0.119	0.5022	0.326
0.7213	0.089	0.5542	0.303
0.7841	0.065	0.6222	0.271
0.8194	0.051	0.6654	0.241
0.8292	0.049	0.7700	0.167
0.8763	0.029	0.8287	0.129
0.9384	0.012	0.8820	0.082
0.9740	0.006	0.9428	0.041
		0.9505	0.033

where

$$Y_j = [x_1 - 1/(1 + Dx_1)]^{j-1}$$

and where x_1 denotes the mole fraction of alcohol.

It is observed that eq 1 fits the measured excess volume data better than commonly used polynomial expansions. The calculations were performed for both systems with $D = 25$. This arbitrary value agrees with every alcohol-alkane system.

The parameters A_j of eq 1 are given in Table III with the values of root mean square deviations of excess volumes and densities:

$$\sigma(v^E) = \{\sum_{i=1}^{N} [v^E{}_i{}^\circ - v^E(x_{1i}{}^\circ, A)]^2/(N - m)\}^{1/2} \quad (2)$$

where N is the number of experimental values denoted by superscript °. $\sigma(\rho)$ was calculated in a similar way.

Vapor-Liquid Equilibrium Data. Experimental vapor-liquid equilibrium data are given in Tables IV and V with values of activity coefficients calculated according to the expression

$$\gamma_i{}^\circ = (P^\circ y_i{}^\circ / P_i{}^s x_i{}^\circ) \exp[(v_i - B_i) \times (P_i{}^s - P^\circ) + \delta_{12}(1 - y_i{}^\circ)^2 P^\circ]/RT \quad (3)$$

$$i = 1, 2$$

where

$$\delta_{12} = 2B_{12} - B_{11} - B_{22}$$

The Hayden and O'Connell method described by Prausnitz et al. (*5*) was used to rectify the liquid-phase activity coefficients. The virial coefficients are reported for each binary system and each temperature in Tables IV and V. For both systems at lowest temperature isothermal P-x data only are given for alcohol mole fractions greater than 0.90 in the liquid phase. This is due to the fact that, in this concentration range, measurements of vapor-phase compositions were distorted by partial evaporations of sampling.

The reduction of measured vapor-liquid equilibrium data was performed by using the observed deviation method (*6-8*).

The excess Gibbs energy was represented by using a Redlich-Kister polynomial:

$$g^E/(RTx_1x_2) = \sum_{j=1}^{m} A_j Y_j \quad (4)$$

where

$$Y_j = (2j - 1)(x_1 - x_2)^{j-1}$$

and where the degree of the polynomial, not fixed in advance, is chosen during the reduction as the lowest degree allowing one to avoid systematic deviations due to the model.

The parameters A_j in eq 4 and the experimental uncertainties on densities $\sigma_e(\rho)$ and on the temperature $\sigma_e(T)$ were estimated according to the maximum likelihood principle. The precision on molar fractions corresponding to the $\sigma_e(\rho)$ values is about $\sigma_e(x) = 0.0002$ for the alcohol side and $\sigma_e(x) = 0.00045$ for the hydrocarbon side. The experimental uncertainty on pressure was fixed to the value $\sigma_e(P) = 0.009$ kPa according to the calibration of the manometer used.

The thermodynamic consistency of experimental values was checked by fitting the vapor-liquid equilibrium data to eq 4 for the appropriate number of parameters. The reduction was performed by minimizing an objective function S, the form of

Table III. Excess Volumes at 298.15 K, Parameters of Eq 1 ($D = 25$), and Values of Mean Square Deviation in v^E and ρ

	1-butanol (1)-n-heptane (2)	2-methyl-1-propanol (1)-n-heptane (2)
$A_j \pm \sigma(A_j)/(\mathrm{cm^3\ mol^{-1}})$	1.396 78 ± 0.011 04	2.054 53 ± 0.011 46
	−1.959 81 ± 0.049 47	−1.999 81 ± 0.074 71
	1.213 89 ± 0.150 60	0.824 37 ± 0.262 80
	−0.566 59 ± 0.139 07	−1.335 76 ± 0.356 95
		2.909 67 ± 0.846 11
		−1.905 75 ± 0.683 59
$\sigma(\rho)/(\mathrm{g\ cm^{-3}})$	0.00002	0.00002
$\sigma(v^E)/(\mathrm{cm^3\ mol^{-1}})$	0.00280	0.00277

Table IV. Experimental Vapor-Liquid Equilibrium Data for the System 1-Butanol (1)-n-Heptane (2)

333.15 K					363.15 K				
x_1°	y_1°	P°/kPa	$\ln \gamma_1^\circ$	$\ln \gamma_2^\circ$	x_1°	y_1°	P°/kPa	$\ln \gamma_1^\circ$	$\ln \gamma_2^\circ$
0.0000	0.0000	28.019			0.0000	0.0000	78.584		
0.0672	0.1163	30.515	1.8817	0.0296	0.0299	0.0815	83.537	1.8949	0.0038
0.1288	0.1401	30.731	1.4230	0.0777	0.0610	0.1310	86.466	1.6870	0.0141
0.1748	0.1513	30.720	1.1937	0.1186	0.1086	0.1716	88.497	1.4002	0.0407
0.2211	0.1602	30.635	1.0127	0.1631	0.1637	0.1987	89.331	1.1439	0.0805
0.2565	0.1662	30.527	0.8972	0.1991	0.1937	0.2097	89.486	1.0306	0.1050
0.2978	0.1726	30.371	0.7803	0.2436	0.2507	0.2267	89.415	0.8488	0.1561
0.3525	0.1805	30.108	0.6476	0.3067	0.3064	0.2410	89.079	0.7049	0.2114
0.3943	0.1863	29.891	0.5597	0.3593	0.3556	0.2523	88.561	0.5956	0.2646
0.4322	0.1915	29.640	0.4870	0.4094	0.4064	0.2641	87.846	0.4993	0.3233
0.4829	0.1988	29.278	0.4011	0.4819	0.4716	0.2791	86.696	0.3923	0.4069
0.5609	0.2118	28.560	0.2898	0.6049	0.5101	0.2884	85.853	0.3367	0.4604
0.6030	0.2198	28.071	0.2372	0.6787	0.5589	0.3011	84.560	0.2732	0.5331
0.6376	0.2275	27.528	0.1963	0.7409	0.6056	0.3150	83.016	0.2196	0.6077
0.7060	0.2477	26.173	0.1291	0.8744	0.6476	0.3289	81.368	0.1758	0.6809
0.7595	0.2698	24.770	0.0866	0.9917	0.6996	0.3500	78.758	0.1284	0.7779
0.8014	0.2941	23.301	0.0583	1.0895	0.7465	0.3743	75.770	0.0923	0.8731
0.8488	0.3345	21.152	0.0333	1.2086	0.7589	0.3816	74.798	0.0824	0.8993
0.8776	0.3708	19.473	0.0207	1.2828	0.7992	0.4105	71.374	0.0574	0.9899
0.9130	0.4366	16.964	0.0074	1.3783	0.8572	0.4710	64.760	0.0286	1.1322
0.9372		14.935			0.9245	0.5980	53.745	0.0087	1.3150
0.9555		13.147			0.9608	0.7278	45.451	0.0021	1.4198
0.9620		12.480			0.9830	0.8547	39.385	0.0005	1.4898
1.0000	1.0000	8.006			1.0000	1.0000	34.163		
$B_{11} = -3241\ \mathrm{cm^3\ mol^{-1}}$ $B_{22} = -2111\ \mathrm{cm^3\ mol^{-1}}$ $B_{12} = -1384\ \mathrm{cm^3\ mol^{-1}}$					$B_{11} = -1803\ \mathrm{cm^3\ mol^{-1}}$ $B_{22} = -1640\ \mathrm{cm^3\ mol^{-1}}$ $B_{12} = -1101\ \mathrm{cm^3\ mol^{-1}}$				

Table V. Experimental Vapor-Liquid Equilibrium Data for the System 2-Methyl-1-propanol (1)-n-Heptane (2) at 333.15 K

x_1°	y_1°	P°/kPa	$\ln \gamma_1^\circ$	$\ln \gamma_2^\circ$
0.0000	0.0000	28.019		
0.0595	0.1535	31.892	1.8894	0.0216
0.0943	0.1796	32.448	1.6019	0.0450
0.1419	0.2011	32.793	1.3159	0.0830
0.1999	0.2196	32.928	1.0645	0.1337
0.2643	0.2358	32.908	0.8552	0.1963
0.3095	0.2462	32.831	0.7378	0.2438
0.3546	0.2553	32.687	0.6333	0.2951
0.4516	0.2766	32.257	0.4507	0.4190
0.5045	0.2855	31.881	0.3669	0.4940
0.5539	0.2966	31.475	0.2937	0.5710
0.5966	0.3078	30.980	0.2455	0.6403
0.6179	0.3435	30.728	0.2206	0.6784
0.6747	0.3317	29.870	0.1606	0.7850
0.7265	0.3533	28.836	0.1145	0.8915
0.7810	0.3847	27.368	0.0751	1.0132
0.8691	0.4692	23.750	0.0255	1.2422
0.9004		21.845		
0.9506		17.776		
0.9740		15.399		
1.0000	1.0000	12.432		
$B_{11} = -2495\ \mathrm{cm^3\ mol^{-1}}$ $B_{22} = -2111\ \mathrm{cm^3\ mol^{-1}}$ $B_{12} = -1222\ \mathrm{cm^3\ mol^{-1}}$				

which is given in Appendix A. The weighting factors (expressions 3a and 4a, Appendix A) of the objective function S were calculated with the values of the experimental uncertainties estimated according to the maximum likelihood principle.

The weighted root mean square deviation (WRMSD) found in this way should be equal to 1 for perfectly consistent data; a value close to 2 would indicate that there are systematic errors of the same magnitude as random errors in measurements.

Results of vapor-liquid equilibrium data reduction are given in Table VI together with the estimates of experimental uncertainties of densities $\sigma_e(\rho)$, temperature $\sigma_e(T)$, and pressure $\sigma_e(P)$.

Vapor-liquid equilibrium data were fitted to UNIQUAC, Wilson, and NRTL models; the corresponding expressions are given in Appendix B. The model parameters were estimated by minimizing the objective function S (expression 1a, Appendix A). They are reported in Table VII together with the values of standard deviations on pressure and vapor composition calculated by using the following expressions:

$$100DP/P = (100/N) \sum_{i=1}^{N} |\Delta P_i|/P_i \tag{5}$$

$$100Dy = (100/N) \sum_{i=1}^{N} |\Delta y_{1i}| \tag{6}$$

Table VI. Results of Vapor-Liquid Equilibrium Data Reduction

	1-butanol (1)-n-heptane (2)		2-methyl-1-propanol (1)-n-heptane (2) at 333.15 K
	333.15 K	363.15 K	
$A_j \pm \sigma(A_j)$	1.760 63 ± 0.000 53	1.596 46 ± 0.000 27	1.715 44 ± 0.000 61
	−0.092 06 ± 0.000 46	−0.062 48 ± 0.000 26	−0.080 60 ± 0.000 57
	0.046 80 ± 0.000 70	0.039 12 ± 0.000 39	0.048 31 ± 0.000 93
	−0.017 36 ± 0.000 99	−0.013 72 ± 0.000 52	−0.014 31 ± 0.001 06
	0.013 47 ± 0.001 40	0.006 72 ± 0.000 41	0.010 51 ± 0.001 88
	−0.015 78 ± 0.000 93	−0.002 68 ± 0.000 46	−0.014 44 ± 0.000 98
	0.005 98 ± 0.001 19		0.004 86 ± 0.001 44
$\sigma_e(\rho) \pm \sigma(\sigma_e(\rho))/(\mathrm{g\ cm^{-3}})$	0.000 037 ± 0.000 007	0.000 034 ± 0.000 005	0.000 045 ± 0.000 01
$\sigma_e(T) \pm \sigma(\sigma_e(T))/\mathrm{K}$	0.008 9 ± 0.003 4	0.008 0 ± 0.002 0	0.01 ± 0.004
$\sigma_e(P)/\mathrm{kPa}$	0.009	0.009	0.009
WRMSD	1.37	1.55	1.74

Table VII. Parameters of the Most Usual Models Estimated from Vapor–Liquid Equilibrium Data

	1-butanol (1)–*n*-heptane (2)			2-methyl-1-propanol (1)–*n*-heptane (2)		
	parameters	100*DP*/*P*	100*Dy*	parameters	100*DP*/*P*	100*Dy*
			NRTL			
333.15 K	$C_{21} = 642.225$ $C_{12} = 327.552$ $\alpha = 0.52442$	0.46	0.23	$C_{21} = 614.876$ $C_{12} = 343.720$ $\alpha = 0.55530$	0.33	0.25
363.15 K	$C_{21} = 564.165$ $C_{12} = 331.756$ $\alpha = 0.56285$	0.16	0.15			
			Wilson			
333.15 K	$\Lambda_{12} = 0.12954$ $\Lambda_{21} = 0.42804$	0.30	0.21	$\Lambda_{12} = 0.15216$ $\Lambda_{21} = 0.46908$	0.38	0.37
363.15 K	$\Lambda_{12} = 0.21329$ $\Lambda_{21} = 0.47877$	0.33	0.23			
			UNIQUAC			
333.15 K	$A_{21} = 1372.35$ $A_{12} = -203.87$	0.37	0.16	$A_{21} = 1430.87$ $A_{12} = -205.58$	0.25	0.18
363.15 K	$A_{21} = 1224.64$ $A_{12} = -224.78$	0.56	0.38			

Table VIII. Temperature-Dependent NRTL Parameters Estimated from Vapor–Liquid Equilibrium and Heat of Mixing Data for 1-Butanol (1)–*n*-Heptane (2)

C_{21}/K	$787.470 - 2.5667(T - 273.15)$
C_{12}/K	$335.690 - 0.1445(T - 273.15)$
α	$0.52251 + 0.000211(T - 273.15)$
100*DP*/*P*	0.31
100*Dy*	0.16

In Table VIII are reported the NRTL temperature-dependent parameters for the 1-butanol–*n*-heptane system, estimated from the vapor–liquid equilibrium measurements and heat of mixing data. H^E data used in this study were measured by Nguyen and Ratcliff at 288.15 and 328.15 K (*9*), and by Savini et al. at 303.15 and 318.15 K (*10*). The heat of mixing data were weighted assuming that experimental uncertainties are equal to $\sigma(H^E) = 0.01H^E$.

Conclusion

It can be observed in Figure 1 that the replacement of 1-butanol with 2-methyl-1-propanol decreases the excess Gibbs energy by 32 J mol^{-1} for $x_1 = 0.5$. In the previous paper (*1*), we had observed the same difference for the binary systems including the same alcohols and the *n*-hexane. Van Ness et al. (*11*) have measured the 1-propanol and 2-propanol with heptane systems at 303.15 K; the difference between the excess Gibbs energies was 3l J mol^{-1} for $x_1 = 0.5$. So it seems that the branching of a "methyl group" on an alcohol slightly decreases the excess Gibbs energy.

Appendix A

The *T*–*P*–*x*–*y* data are reduced by minimizing the objective function *S* of the form

$$S = \sum_{i=1}^{N} (a_i \Delta P_i + b_i \Delta y_{1i})^2 \qquad (1a)$$

where

$$\Delta P = P^\circ - P(x_1^\circ, A) \qquad \Delta y_1 = y_1^\circ - y_1(x_1^\circ, A) \qquad (2a)$$

$$a = -\overline{\delta P\,\delta y_1}/\sigma(P)D^{1/2} \qquad b = \sigma(P)/D^{1/2} \qquad (3a)$$

$$D = \sigma^2(P)\,\sigma^2(y_1) - \overline{\delta P\,\delta y_1}^2 \qquad (4a)$$

If the vapor mole fraction is not measured, $a = 1/\sigma(P)$, $b = 0$.

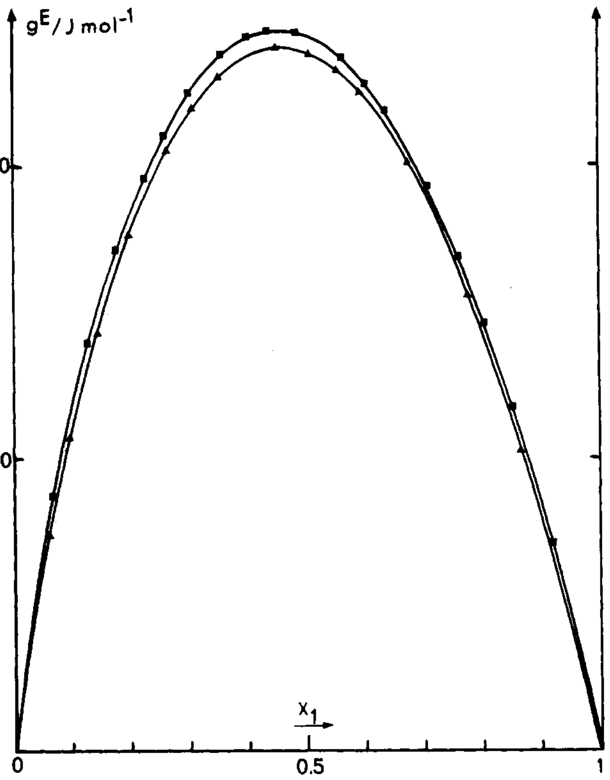

Figure 1. Plot of g^E as a function of composition for the 1-butanol (1)–*n*-heptane (2) (■) and 2-methyl-1-propanol (1)–*n*-heptane (2) (▲) systems at 333.15 K.

The variances and the covariances are expressed by the following relations:

$$\sigma^2(P) = \sigma_e^2(P) + (\partial P/\partial x_1)_T^2(\partial x_1/\partial \rho)_T^2\sigma_e^2(\rho) + (\partial P/\partial T)_{x_1}^2\sigma_e^2(T) \qquad (5a)$$

$$\sigma^2(y_1) = [(\partial y_1/\partial \rho)_T^2 + (\partial y_1/\partial x_1)_T^2(\partial x_1/\partial \rho)_T^2]\sigma_e^2(\rho) + (\partial y_1/\partial T)_{x_2}^2\sigma_e^2(T) \qquad (6a)$$

$$\overline{\delta P\,\delta y_1} = (\partial P/\partial x_1)_T(\partial y_1/\partial x_1)(\partial x_1/\partial \rho)_T^2\sigma_e^2(\rho) + (\partial P/\partial T)_{x_1}\sigma_e^2(T) \qquad (7a)$$

The weighted root mean square deviation is

$$\mathrm{WRMSD} = [S/(N + n - m)]^{1/2} \tag{8a}$$

Appendix B

The parameters given in Tables VII and VIII were calculated for the following models:

NRTL

$$g^{\mathrm{E}}/R = x_1x_2\left[\frac{\delta_{21}C_{21}}{x_1 + \delta_{21}x_2} + \frac{\delta_{12}C_{12}}{\delta_{12}x_1 + x_2}\right] \tag{1b}$$

where

$$\delta_{21} = \exp(-\alpha C_{21}/T) \qquad \delta_{12} = \exp(-\alpha C_{12}/T) \tag{2b}$$

UNIQUAC

$$g^{\mathrm{E}} = g^{\mathrm{E}}(\text{combinatorial}) + g^{\mathrm{E}}(\text{residual}) \tag{3b}$$

$$\frac{g^{\mathrm{E}}(\text{combinatorial})}{RT} = x_1 \ln\frac{\phi_1}{x_1} + x_2 \ln\frac{\phi_2}{x_2} + \frac{z}{2}\left(q_1x_1 \ln\frac{\theta_1}{\phi_1} + q_2x_2 \ln\frac{\theta_2}{\phi_2}\right) \tag{4b}$$

$$\frac{g^{\mathrm{E}}(\text{residual})}{RT} = -q_1x_1 \ln(\theta_1' + \theta_2'\delta_{21}) - q_2x_2 \ln(\theta_2' + \theta_1'\delta_{12}) \tag{5b}$$

$$\phi_1 = x_1r_1/(x_1r_1 + x_2r_2)$$

$$\theta_1 = x_1q_1/(x_1q_1 + x_2q_2)$$

$$\theta_1' = x_1q_1'/(x_1q_1' + x_2q_2') \tag{6b}$$

$$\ln \delta_{21} = -A_{21}/T \qquad \ln \delta_{12} = -A_{12}/T \tag{7b}$$

with

$$z = 10$$

For n-heptane

$$r = 5.17 \qquad q = q' = 4.40$$

For 1-butanol

$$r = 3.45 \qquad q = 3.05 \qquad q' = 0.85 \tag{8b}$$

For 2-methyl-1-propanol

$$r = 3.45 \qquad q = 3.05 \qquad q' = 0.79$$

Wilson

$$g^{\mathrm{E}}/RT = -x_1 \ln(x_1 + \Lambda_{12}x_2) - x_2 \ln(x_2 + \Lambda_{21}x_1) \tag{9b}$$

Glossary

A_j	parameters of polynomial model
A_{ij}	parameters of UNIQUAC model
B_{ij}	second virial coefficients
C_{ij}	parameters of NRTL model
H^{E}	excess enthalpy
m	number of polynomial parameters A_j
N	total number of measurements
n	number of measurements of vapor-phase compositions
P	total vapor pressure
P_i^{s}	saturated vapor pressure of pure component i
S	objective function
T	temperature
v_i	molar volume of component i
x_i	liquid mole fraction of component i
y_i	vapor mole fraction of component i

Greek Letters

α	parameters of NRTL model
γ_i	activity coefficient of component i
Λ_{ij}	parameters of Wilson model
ρ	density of pure liquid or liquid mixture
σ_{e}	experimental uncertainty
σ	root of resulting variance

Superscripts

E	excess property
°	experimental measured value

Subscripts

1, 2	molecular species (1 normally refers to alcohol, and 2 to alkane)

Registry No. 1-Butanol, 71-36-3; 2-methyl-1-propanol, 78-83-1; n-heptane, 142-82-5.

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Received for review March 16, 1983. Accepted October 12, 1983.