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Isobaric vapour–liquid equilibrium for the binary systems of 2-butanol with some halohydrocarbons at 40.0 and 101.3 kPa

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Abstract

Isobaric vapour–liquid equilibrium at 40.0 and 101.3 kPa is reported for the binary systems 2-butanol with chlorocyclohexane, chlorobenzene, bromocyclohexane and bromobenzene. Some of the studied systems show minimum temperature azeotropes. The VLE results were thermodynamically consistent and correlated with the Margules, van Laar, Wilson, NRTL and UNIQUAC equations. Predictions with the UNIFAC and ASOG methods were also made. © 1997 Elsevier Science B.V.

Keywords: ASOG; 2-Butanol; Halohydrocarbons; UNIFAC; VLE

1. Introduction

The present paper reports experimental data of the isobaric vapour–liquid equilibrium for the binary systems 2-butanol with chlorocyclohexane, chlorobenzene, bromocyclohexane and bromobenzene at two different pressures (40.0 and 101.3 kPa). This study is a continuation of our research project on vapour–liquid equilibrium for mixtures containing butanols and halogenated hydrocarbons [1,2]. We have found two references for vapour–liquid equilibrium measurements of 2-butanol with chlorobenzene [3,4] but no references for the remaining systems studied.

The VLE results have been checked for the thermodynamic consistency and the activity coefficients have been correlated with the following models: Margules [5], van Laar [6], Wilson [7], NRTL [8] and UNIQUAC [9].

The experimental results were used to test the prediction capability of two group contribution methods: UNIFAC [10] and ASOG [11]. These predictive methods play an important role in order to make a quick investigation of many mixtures.

2. Experimental

2.1. Materials

The liquids used were 2-butanol and chlorocyclohexane (better than 99 mol%) obtained from Aldrich, chlorobenzene and bromobenzene (better than 99.5 mol%) and bromocyclohexane (better than 99 mol%) provided by Fluka. Liquids were used without further purification, 2-butanol was dried over

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Table 1
Physical properties (densities at 298.15 K and normal boiling points) of the pure compounds

Compound	ρ/kg m^{-3}		T_b/K	
	Exptl.	Lit.	Exptl.	Lit.
2-Butanol	802.40	802.41	372.65	372.662
Chlorocyclohexane	993.23	—	415.76	—
Chlorobenzene	1101.00	1100.9	404.82	404.837
Bromocyclohexane	1328.9	—	438.88	—
Bromobenzene	1488.18	1488.20	429.01	429.058

activated molecular sieve type 0.3 nm from Merck. The purity of the materials was checked by GLC. The physical properties of the chemicals, densities and normal boiling points, appear together published values from Riddick et al.[12] in Table 1.

2.2. Measurements

The vapour–liquid equilibrium measurements were carried out in a still (Labodest model) manufactured by Fischer (Germany). It is an all-glass dynamic recirculating still, equipped with a Cottrell pump. The equilibrium temperatures were measured to an accuracy of ± 0.01 K by means of a thermometer (model F25) from Automatic Systems Laboratories. The pressure in the still was measured with a pressure transducer Druck PDCR 110/W (pressure indicator DPI201) with an accuracy of ± 0.1 kPa. Liquid- and vapour-phase compositions were determined by measuring their densities at 298.15 K with an Anton Paar DMA-58 vibrating tube densimeter that was previously calibrated at atmospheric pressure with doubly distilled water and dry air. Prior to this, density-calibration curves for these systems were obtained by Artigas et al. [13]. The estimated uncertainty in the determination of both liquid- and vapour-phase mole fractions is ± 0.0001.

3. Experimental results

Table 2 shows the vapour–liquid equilibrium data (T, x_1, and y_1) and the calculated activity coefficients at 40.0 and 101.3 kPa. In Figs. 1–4 the T–x_1–y_1 diagrams are represented. The systems present positive deviation from ideality.

Table 2
Experimental VLE data at the indicated pressure

T/K	x_1	y_1	γ_1	γ_2
2-Butanol(1) + chlorocyclohexane(2) at 40.0 kPa				
372.83	0.0432	0.3216	3.000	1.002
370.17	0.0617	0.3911	2.813	1.004
361.20	0.1581	0.5795	2.287	1.064
357.10	0.2787	0.6827	1.802	1.093
354.82	0.3936	0.7299	1.498	1.208
353.52	0.5005	0.7698	1.312	1.314
352.51	0.5844	0.7893	1.202	1.504
351.49	0.6874	0.8244	1.115	1.735
350.67	0.7980	0.8682	1.047	2.082
350.05	0.8995	0.9197	1.011	2.614
349.93	0.9415	0.9452	0.998	3.080
349.83	0.9640	0.9610	0.995	3.576
2-Butanol(1) + chlorocyclohexane(2) at 101.3 kPa				
403.66	0.0542	0.3183	2.204	0.990
399.20	0.0788	0.4039	2.184	1.006
393.65	0.1317	0.5227	1.993	1.002
387.85	0.2101	0.6234	1.783	1.033
383.08	0.3244	0.7138	1.542	1.063
380.25	0.4239	0.7582	1.377	1.153
378.37	0.5221	0.7928	1.245	1.265
376.53	0.6365	0.8301	1.139	1.448
374.96	0.7589	0.8730	1.061	1.719
373.60	0.8815	0.9258	1.016	2.139
372.95	0.9516	0.9647	1.004	2.546
2-Butanol(1) + chlorobenzene(2) at 40.0 kPa				
363.99	0.0680	0.3227	2.657	1.009
357.73	0.1622	0.4912	2.171	1.052
354.67	0.2655	0.5859	1.794	1.091
352.67	0.3821	0.6466	1.496	1.192
351.59	0.4812	0.6830	1.314	1.325
350.72	0.5846	0.7215	1.185	1.503
350.13	0.6924	0.7678	1.092	1.730
349.67	0.8037	0.8283	1.036	2.040
349.57	0.8506	0.8582	1.018	2.222
349.50	0.9071	0.9015	1.006	2.489
349.55	0.9432	0.9346	1.001	2.698
2-Butanol(1) + chlorobenzene(2) at 101.3 kPa				
395.27	0.0587	0.2855	2.265	0.989
388.32	0.1343	0.4529	1.959	1.009
384.02	0.2136	0.5534	1.761	1.027
380.10	0.3260	0.6375	1.513	1.097
377.45	0.4465	0.6975	1.322	1.211
376.17	0.5410	0.7363	1.204	1.326
374.65	0.6608	0.7880	1.112	1.515
373.65	0.7815	0.8471	1.047	1.752
372.83	0.8960	0.9135	1.014	2.138
372.70	0.9445	0.9486	1.003	2.391
372.65	0.9882	0.9880	1.000	2.630

Table 2 (Continued)

T/K	x_1	y_1	γ_1	γ_2
2-Butanol(1) + bromocyclohexane(2) at 40.0 kPa				
394.95	0.0208	0.2793	2.611	1.004
392.95	0.0256	0.3261	2.633	1.005
386.58	0.0461	0.4662	2.553	1.001
377.43	0.0882	0.6206	2.411	1.018
370.07	0.1508	0.7316	2.161	1.009
365.95	0.1967	0.7776	2.053	1.031
361.47	0.2922	0.8268	1.747	1.084
357.27	0.4066	0.8661	1.556	1.181
355.22	0.5149	0.8880	1.370	1.313
354.22	0.5898	0.8973	1.260	1.483
353.06	0.6764	0.9147	1.176	1.638
352.35	0.7645	0.9254	1.084	2.028
351.53	0.8298	0.9403	1.051	2.324
350.76	0.9088	0.9565	1.009	3.263
2-Butanol(1) + bromocyclohexane(2) at 101.3 kPa				
428.05	0.0257	0.2517	1.966	1.010
419.53	0.0545	0.4307	1.949	0.992
412.75	0.0792	0.5305	1.964	1.014
406.55	0.1150	0.6292	1.895	0.996
395.77	0.1973	0.7478	1.786	1.035
388.08	0.3109	0.8261	1.585	1.064
384.37	0.4011	0.8591	1.439	1.122
381.21	0.5031	0.8849	1.311	1.230
379.05	0.5929	0.8998	1.216	1.408
377.48	0.6786	0.9163	1.141	1.574
375.92	0.7737	0.9356	1.079	1.817
375.47	0.8309	0.9475	1.033	2.014
374.80	0.8734	0.9579	1.017	2.209
374.15	0.9127	0.9676	1.006	2.524
373.51	0.9418	0.9779	1.008	2.642
2-Butanol(1) + bromobenzene(2) at 40.0 kPa				
386.95	0.0244	0.2577	2.635	1.032
382.70	0.0373	0.3833	2.945	1.000
376.19	0.0693	0.5186	2.677	1.008
369.75	0.1164	0.6303	2.440	1.025
365.15	0.1718	0.7119	2.219	1.009
360.56	0.2806	0.7763	1.771	1.072
357.86	0.3661	0.8075	1.573	1.163
355.92	0.4610	0.8319	1.393	1.289
354.35	0.5737	0.8560	1.229	1.486
352.91	0.6886	0.8836	1.123	1.742
351.76	0.7957	0.9109	1.052	2.129
351.06	0.8667	0.9341	1.020	2.483
350.60	0.9174	0.9533	1.003	2.894
2-Butanol(1) + bromobenzene(2) at 101.3 kPa				
420.71	0.0247	0.2309	2.239	0.984
413.62	0.0486	0.3835	2.262	0.980
408.21	0.0714	0.4669	2.164	1.012
392.15	0.2164	0.7193	1.747	1.022
387.84	0.2895	0.7752	1.610	1.036
382.53	0.4197	0.8343	1.418	1.112
380.05	0.5154	0.8598	1.293	1.225
378.62	0.5958	0.8787	1.199	1.334
376.76	0.6976	0.9029	1.122	1.521
375.59	0.7750	0.9217	1.073	1.717
374.57	0.8515	0.9404	1.033	2.052
373.71	0.9056	0.9601	1.022	2.227
373.19	0.9440	0.9740	1.013	2.492
372.83	0.9716	0.9854	1.008	2.794

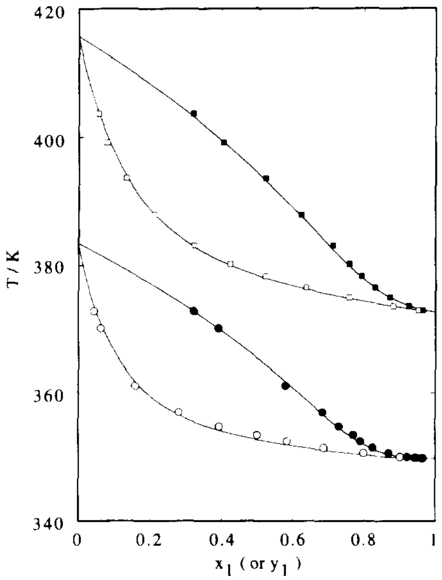

Fig. 1. T–x_1–y_1 diagram for 2-butanol(1) + chlorocyclohexane(2): (○,●) exptl. data at 40.0 kPa; (□,■) exptl. data at 101.3 kPa; (———) Wilson equation.

The activity coefficients of the components in the liquid phase γ_i were calculated, taking into account the non-ideality of the vapour phase, from the following equations:

$$\gamma_i = \frac{y_i P}{x_i P_i^0}\exp\left[\frac{(B_{ii}-V_i^0)(P-p_i^0)+(1-y_i)^2 P\delta_{ij}}{RT}\right] \qquad (1)$$

$$\delta_{ij} = 2B_{ij} - B_{ii} - B_{jj} \qquad (2)$$

where x^i and y^i are the liquid- and vapour-phase

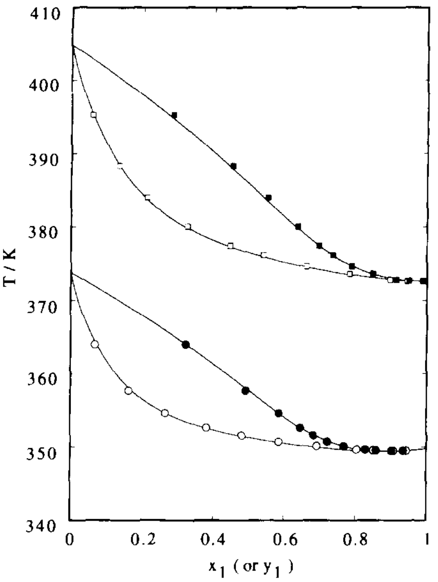

Fig. 2. T–x_1–y_1 diagram for 2-butanol(1) + chlorobenzene(2): (○,●) exptl. data at 40.0 kPa; (□,■) exptl. data at 101.3 kPa; (———) Wilson equation.

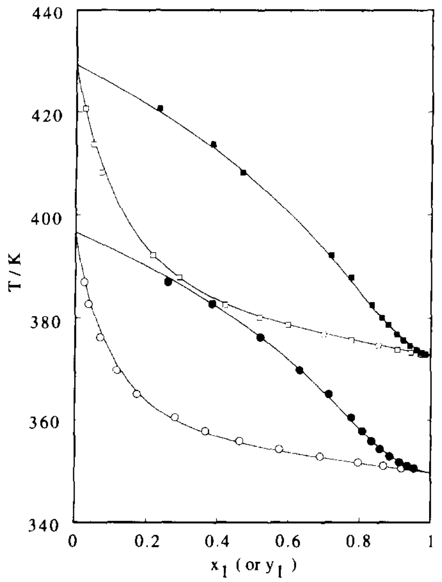

Fig. 4. T–x_1–y_1 diagram for 2-butanol(1) + bromobenzene(2): (○,●) exptl. data at 40.0 kPa; (□,■) exptl. data at 101.3 kPa; (———) Wilson equation.

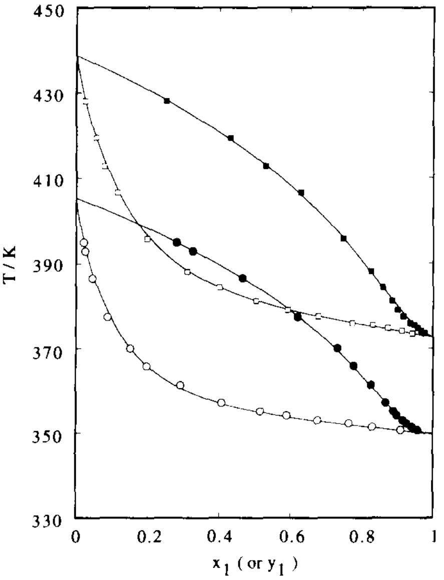

Fig. 3. T–x_1–y_1 diagram for 2-butanol(1) + bromocyclohexane(2): (○,●) exptl. data at 40.0 kPa; (□,■) exptl. data at 101.3 kPa; (———) Wilson equation.

Table 3
Constants of Antoine's equation for vapour pressures of the pure compounds (temperature in °C, pressure in kPa)

Compound	*A*	*B*	*C*
2-Butanol	6.35457	1171.891	169.955
Chlorocyclohexane	5.73540	1235.480	188.647
Chlorobenzene	6.30963	1556.6	230
Bromocyclohexane	6.1293	1568.129	214.459
Bromobenzene	6.37912	1688.4	230

compositions, P the total pressure, p the vapour pressures of the pure compounds calculated by using the Antoine equation, the constants are given in Table 3, B_{ii} are the second virial coefficients, B_{ij} are the cross second virial coefficient calculated using the Amdur–Mason equation [14], and V_i^0 are the molar volumes of the saturated liquids calculated using the Yen and Woods method [15].

Antoine's constants for 2-butanol, chlorobenzene and bromobenzene were obtained from Riddick et al. [12] for chlorocyclohexane were taken from Gmehling et al. [16], and those for bromocyclohexane were obtained from our own vapour-pressure measurements [1]. The second virial coefficients for 2-butanol were obtained from TRC-tables [17] and for the halogenated compounds were estimated by the Redlich–Kwong equation [18].

Table 4
Results of the thermodynamic consistency test. Average deviation ΔP and Δy

System	P/kPa	ΔP/kPa	Δy
2-Butanol +			
chlorocyclohexane	40.0	0.4	0.0038
	101.3	0.7	0.0018
chlorobenzene	40.0	0.2	0.0040
	101.3	0.5	0.0017
bromocyclohexane	40.0	0.5	0.0028
	101.3	0.9	0.0025
bromobenzene	40.0	0.6	0.0055
	101.3	0.6	0.0032

Table 5
Correlation parameters, average deviations ΔT and Δy, and activity coefficients at infinite dilution

Equation	A_{12}	A_{21}	ΔT/K	Δy	γ_1^∞	γ_2^∞
2-Butanol(1) + chlorocyclohexane(2) at 40.0 kPa						
Margules	1.1552 [a]	1.2575 [a]	0.38	0.0055	3.17	3.52
van Laar	1.1531 [a]	1.2626 [a]	0.39	0.0056	3.17	3.53
Wilson	2793.7903 [b]	1534.1436 [b]	0.36	0.0041	3.13	3.63
NRTL ($\alpha_{12} = 0.3$)	2166.0674 [b]	1812.1200 [b]	0.39	0.0051	3.07	3.53
UNIQUAC	63.8819 [b]	1052.0995 [b]	0.40	0.0054	3.05	3.50
2-Butanol(1) + chlorocyclohexane(2) at 101.3 kPa						
Margules	0.8717	1.0241	0.24	0.0017	2.39	2.78
van Laar	0.8751	1.0302	0.23	0.0017	2.40	2.80
Wilson	2228.9361	1277.9882	0.20	0.0025	2.35	2.83
NRTL	2154.6666	1145.5630	0.21	0.0025	2.34	2.79
UNIQUAC	115.7826	788.2122	0.22	0.0026	2.32	2.78
2-Butanol(1) + chlorobenzene(2) at 40.0 kPa						
Margules	1.1430	1.0852	0.11	0.0039	3.14	2.96
van Laar	1.1441	1.0855	0.11	0.0039	3.14	2.96
Wilson	2590.1622	1331.4383	0.11	0.0027	3.14	3.02
NRTL	1349.4399	2286.1559	0.12	0.0027	3.06	2.96
UNIQUAC	337.3006	616.6042	0.12	0.0029	3.06	2.95
2-Butanol(1) + chlorobenzene(2) at 101.3 kPa						
Margules	0.9247	0.9673	0.22	0.0026	2.52	2.63
van Laar	0.9243	0.9681	0.21	0.0026	2.52	2.63
Wilson	2092.9843	1351.4175	0.19	0.0020	2.50	2.65
NRTL	1581.2130	1659.8796	0.20	0.0022	2.46	2.63
UNIQUAC	624.5661	207.4680	0.20	0.0023	2.47	2.63
2-Butanol(1) + bromocyclohexane(2) at 40.0 kPa						
Margules	0.9833	1.3960	0.29	0.0031	2.67	4.04
van Laar	0.9942	1.4659	0.29	0.0028	2.70	4.33
Wilson	2001.0192	2638.6577	0.30	0.0023	2.62	4.59
NRTL	3620.7258	615.8109	0.30	0.0027	2.61	4.24
UNIQUAC	704.5464	360.1318	0.32	0.0031	2.58	4.17

The thermodynamic consistency of the experimental results was checked using the van Ness method [19], described by Fredenslund et al. [20] using a third-order Legendre polynomial for the excess free energies. According to this test, experimental data are considered consistent if the average deviation in y (Δy) is smaller than 0.01. All systems satisfy this condition, as one can see in Table 4.

The activity coefficients were correlated with the Margules, van Laar, Wilson, NRTL and UNIQUAC equation. Estimation of parameters for all equations was based on minimization, using a non-linear regression procedure [21], of an objective function F in

Table 5 (Continued)

Equation	A_{12}	A_{21}	ΔT/K	Δy	γ_1^∞	γ_2^∞
2-Butanol(1) + bromocyclohexane(2) at 101.3 kPa						
Margules	0.7213	1.1599	0.22	0.0026	2.06	3.19
van Laar	0.7537	1.1989	0.22	0.0032	2.12	3.32
Wilson	1518.8544	2261.3454	0.19	0.0023	2.07	3.32
NRTL	3723.6971	−83.5130	0.19	0.0021	2.07	3.24
UNIQUAC	860.3092	39.9343	0.19	0.0019	2.06	3.22
2-Butanol(1) + bromobenzene(2) at 40.0 kPa						
Margules	1.0930	1.2466	0.31	0.0058	2.98	3.48
van Laar	1.0954	1.2521	0.31	0.0059	2.99	3.50
Wilson	2268.5393	1962.6717	0.29	0.0049	2.92	3.61
NRTL	2171.5520	1718.9366	0.29	0.0047	2.89	3.46
UNIQUAC	700.0281	296.3169	0.30	0.0048	2.90	3.44
2-Butanol(1) + bromobenzene(2) at 101.3 kPa						
Margules	0.8338	1.0559	0.24	0.0034	2.30	2.87
van Laar	0.8376	1.0695	0.22	0.0033	2.31	2.91
Wilson	1644.7918	1896.8726	0.25	0.0049	2.26	2.93
NRTL	2501.2301	849.8153	0.26	0.0050	2.24	2.89
UNIQUAC	1207.8638	−318.5724	0.24	0.0046	2.25	2.91

[a] Dimensionless
[b] Joules per mole

terms of experimental and calculated γ_i values. The function F [22] for a binary system can be stated as:

$$F = \sum_{i=1}^{i=N} \left[\left(\frac{\gamma_1^{\text{exptl}} - \gamma_1^{\text{cal}}}{\gamma_1^{\text{exptl}}} \right)^2 + \left(\frac{\gamma_2^{\text{exptl}} - \gamma_2^{\text{cal}}}{\gamma_2^{\text{exptl}}} \right)^2 \right]_i \tag{3}$$

where N is the number of experimental data. These adjustable parameters, A_{12} and A_{21}, see definitions in Gmehling et al. [16], along with the average deviation in T (ΔT), the average deviation in y (Δy) and the activity coefficients at infinite dilution are listed in Table 5. The average deviation in temperature is less than 0.4 K and in vapour composition is less than 0.01. It can be concluded that all equations show a good performance in correlating the activity coefficients.

Our VLE results for the system 2-butanol with chlorobenzene at 101.3 kPa compare reasonably well with those of Rao et al. [3] ($\Delta T = 0.61$ K, $\Delta y = 0.0122$).

Some of the systems show minimum temperature azeotropes. VLE calculations using the Wilson equation were employed to obtain y_1–x_1 and T–x_1–y_1 diagrams from experimental VLE data. By means of these diagrams the precise location of the azeotropes were determined establishing the following conditions to the azeotropic point:

Table 6
Composition ($x_{1(\text{az})}$) and boiling temperature ($T_{(\text{az})}$) of the azeotropic mixtures

System	P/kPa	$x_{1(\text{az})}$	$T_{(\text{az})}$/K
2-Butanol +			
chlorocyclohexane	40.0	0.968	349.7
chlorobenzene	40.0	0.882	349.4
	101.3	0.988	372.6

$$y_1 = x_1 \quad \left(\frac{\partial T}{\partial x_1}\right)_P = 0 \quad \left(\frac{\partial T}{\partial y_1}\right)_P = 0 \tag{4}$$

Information about composition and boiling temperature of the azeotropes is summarized in Table 6.

4. VLE predictions

In this work the UNIFAC and ASOG methods were used to predict the vapour–liquid equilibrium of the systems studied. The temperature and vapour-phase composition obtained experimentally were compared

Table 7
VLE predictions, average deviations ΔT and Δy

System	P/kPa	UNIFAC		ASOG	
		ΔT/K	Δy	ΔT/K	Δy
2-Butanol +					
chlorocyclohexane	40.0	1.17	0.0162	0.42	0.0103
	101.3	0.81	0.0101	0.92	0.0103
chlorobenzene	40.0	0.53	0.0149	0.76	0.0178
	101.3	0.45	0.0120	0.46	0.0152
bromocyclohexane	40.0	2.30	0.0190	4.59	0.0368
	101.3	1.96	0.0153	6.15	0.0386
bromobenzene	40.0	0.15	0.0046	2.21	0.0187
	101.3	0.64	0.0057	2.26	0.0149

with the theoretical predictions obtained using UNIFAC and ASOG methods, in Table 7 the average deviations in temperature and vapour-phase composition are given.

The major error appears in the prediction with the ASOG method of the system 2-butanol + bromocyclohexane, for the rest of the systems the predictions obtained with the two methods can be considered acceptable. Similar behaviour was noted in our previous works with 1-butanol[1] and 2-methyl-1-propanol[2].

5. Symbols

A_{12}, A_{21}	adjustable parameters for VLE correlation equations
B_{ii}	second virial coefficient of component i ($m^3\,mol^{-1}$)
B_{ij}	cross second virial coefficient ($m^3\,mol^{-1}$)
F	objective function
N	number of experimental data
P	total pressure (Pa)
p	vapour pressure of component i (Pa)
R	gas constant (= 8.314 J K^{-1} mol^{-1})
T	temperature (K)
T_b	normal boiling point (K)
V	molar volume of component i ($m^3\,mol^{-1}$)
x_i	mole fraction of component i in the liquid phase
y_i	mole fraction of component i in the vapour phase

6. Greek letters

α_{12}	nonrandomness parameter in the NRTL equation
Δ	average deviation
γ_i	activity coefficient of component i
γ_i^{∞}	activity coefficient of component i at infinite dilution
ρ	density (kg m^{-3})

7. Subscripts

az	azeotropic
i	component i

8. Superscripts

cal	calculated quantity
exptl	experimental quantity

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