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Vapor–Liquid Equilibria of 1-Propanol or 2-Propanol with 2,2,4-Trimethylpentane at 101.3 kPa

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Isobaric vapor–liquid equilibria were measured for 1-propanol or 2-propanol with 2,2,4-trimethylpentane at 101.3 kPa in an equilibrium still with circulation of both the vapor and liquid phases. The results were best correlated with the Wilson equation.

Introduction

In the present study, vapor–liquid equilibria (VLE) were measured for 1-propanol + 2,2,4-trimethylpentane and 2-propanol + 2,2,4-trimethylpentane, at 101.3 kPa of pressure using a vapor and liquid recirculating still (*1*). For 1-propanol + 2,2,4-trimethylpentane, one set of data is available in the literature (*2*), but these data are not consistent according to the results of a thermodynamic consistency test by using the Kojima method (*3*). New reliable data seem, therefore, to be required for this system. No VLE data have been reported previously for 2-propanol + 2,2,4-trimethylpentane.

Experimental Section

Materials. 2,2,4-Trimethylpentane, 1-propanol, and 2-propanol were special grade reagents, supplied by the Junsei Chemical Co. Ltd. 1-Propanol and 2-propanol were used after water was reduced with molecular sieves having a pore diameter of 0.3 nm. Gas-chromatographic analysis on all three materials indicated that each had a purity of at least 99.9 mole %. Table 1 compares some of the measured properties with literature values.

Procedure. The equilibrium still (*1*) was a modified Rogalski–Malanowski (*4*) still with a provision for vapor and liquid circulation. The still had a total capacity of about 100 cm³. The pressure *P* in the still was measured by a Fortin-type mercury barometer. Since the barometric pressure changed slightly, the experimental temperatures were corrected to 101.3 kPa. The equilibrium temperature *T* was measured with a calibrated platinum resistance thermometer with an accuracy of ±0.03 K.

Analysis. The equilibrium composition of the samples was determined using a Shimadzu gas chromatograph, type GC-14A, equipped with a flame ionization detector. The column packing was PEG-20M (10% polyethylene glycol on chromosorb W-AW 60/80). The relationship between peak area and composition was determined from analysis of samples of known composition. The accuracy of liquid, x_i, and vapor, y_i, mole fractions was estimated as ±0.002.

Table 1. Normal Boiling Points, T_b, and Densities, ρ, of the Materials Used

	T_b/K		ρ(298.15 K)/(g·cm^{-3})	
material	exptl	lit. (*17*)	exptl	lit. (*17*)
1-propanol	370.26	370.301	0.799 65	0.799 60
2-propanol	355.42	355.392	0.780 86	0.781 26
2,2,4-trimethylpentane	372.40	372.388	0.687 64	0.687 81

Table 2. Antoine Constants of Materials Used[a] (*18*)

material	*A*	*B*	*C*
1-propanol	6.870 65	1438.587	−74.598
2-propanol	6.866 34	1360.183	−75.557
2,2,4-trimethylpentane	5.927 51	1252.340	−53.060

[a] $\log(P/\text{kPa}) = A - B/[(T/\text{K}) + C]$.

Table 3. Isobaric Vapor–Liquid Equilibrium Data: Temperature, *T*, Liquid Phase, x_1, and Vapor Phase, y_1, Mole Fractions, and Activity Coefficients, γ_i, for 1-Propanol (1) + 2,2,4-Trimethylpentane (2) at 101.3 kPa

T/K	x_1	y_1	γ_1	γ_2
360.931	0.0915	0.3242	5.1255	1.0231
359.620	0.1428	0.3646	3.8829	1.0598
358.731	0.1986	0.3893	3.0852	1.1188
358.553	0.2266	0.4018	2.8093	1.1419
358.190	0.2874	0.4200	2.3475	1.2151
358.038	0.3060	0.4291	2.2655	1.2339
357.879	0.3727	0.4412	1.9238	1.3429
357.930	0.4071	0.4482	1.7851	1.4012
357.931	0.4680	0.4588	1.5888	1.5321
357.979	0.5548	0.4789	1.3952	1.7614
358.076	0.6117	0.4893	1.2874	1.9743
358.211	0.6330	0.4962	1.2545	2.0530
358.973	0.7373	0.5468	1.1494	2.5277
359.233	0.7594	0.5595	1.1297	2.6635
359.837	0.8078	0.5808	1.0757	3.1203
361.729	0.8779	0.6658	1.0513	3.7206
362.879	0.9076	0.7020	1.0247	4.2489
365.457	0.9505	0.8035	1.0133	4.8856

Results and Discussion

The activity coefficients γ_i were calculated from

$$\phi_i P y_i = \gamma_i P_i^\circ x_i \phi_i^\circ \exp[V_i(P - P_i^\circ)/RT] \qquad (1)$$

where ϕ_i and ϕ_i°, the fugacity coefficients of component *i* in the mixture and pure vapor, respectively, were evaluated by using the second virial coefficients obtained by the Hayden–O'Connell method (*5*). The vapor pressures of the pure components, P_i°, were obtained using the Antoine equation constants (Table 2). The liquid molar volumes V_i were calculated from the Rackett equation as modified by Spencer and Danner (*6*).

The VLE data for 1-propanol (1) + 2,2,4-trimethylpentane (2) and 2-propanol (1) + 2,2,4-trimethylpentane (2) are reported in Tables 3 and 4 along with the activity coefficients calculated using eq 1. Both binary systems form a minimum boiling azeotrope. The azeotropic points were determined

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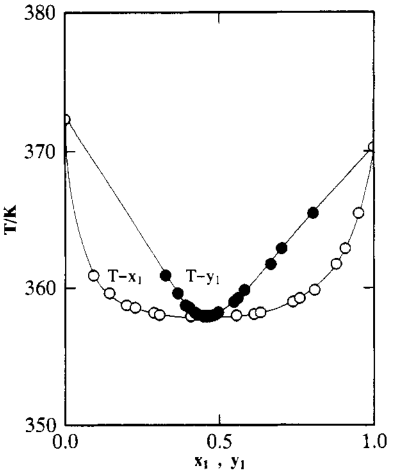

Figure 1. Temperature–composition diagram for 1-propanol (1) + 2,2,4-trimethylpentane (2): (○, ●) this work, (—) Wilson equation.

Table 4. Isobaric Vapor–Liquid Equilibrium Data: Temperature, *T*, Liquid Phase, x_1, and Vapor Phase, y_1, Mole Fractions, and Activity Coefficients, γ_i, for 2-Propanol (1) + 2,2,4-Trimethylpentane (2) at 101.3 kPa

T/K	x_1	y_1	γ_1	γ_2
357.846	0.0737	0.3824	4.7941	1.0046
354.737	0.1209	0.4529	3.8858	1.0307
353.435	0.1573	0.4847	3.3577	1.0546
352.092	0.2155	0.5135	2.7339	1.1155
351.640	0.2393	0.5234	2.5537	1.1433
351.116	0.2900	0.5479	2.2501	1.1821
350.537	0.3575	0.5685	1.9366	1.2706
350.042	0.4553	0.5910	1.6111	1.4442
349.797	0.4953	0.5994	1.5164	1.5390
349.751	0.5370	0.6039	1.4116	1.6615
349.584	0.5994	0.6226	1.3118	1.8410
349.632	0.6518	0.6415	1.2398	2.0109
349.740	0.6913	0.6538	1.1858	2.1844
349.810	0.7311	0.6632	1.1339	2.4356
349.903	0.7651	0.6773	1.1020	2.6657
350.100	0.7970	0.6981	1.0813	2.8714
350.543	0.8444	0.7358	1.0559	3.2404
351.521	0.9010	0.7999	1.0336	3.7566
352.839	0.9469	0.8725	1.0177	4.3050

on the basis of the experimental VLE data, and are x_1(AZ) = 0.458 and T(AZ) = 357.89 K for 1-propanol (1) + 2,2,4-trimethylpentane (2) and x_1(AZ) = 0.635 and T(AZ) = 349.58 K for 2-propanol (1) + 2,2,4-trimethylpentane (2).

The results were tested for thermodynamic consistency by using the point test of Fredenslund et al. (*7*) and of Van Ness et al. (*8*) and the area test of Herington (*9*) and of Redlich and Kister (*10*) as described by Gmehling and Onken (*11*). In addition, the results were checked by the Kojima (*3*) method, which permits the overall check of the data by combining three tests, namely, the point test, the area test, and the infinite dilution test. The results of the three consistency tests indicate that the results for both systems are thermodynamically consistent.

The activity coefficients were correlated with the Wilson (*12*), modified Wilson (*13*), nonrandom two-liquid (NRTL) (*14*), and UNIQUAC (*15*) equations (see ref 11, Vol. I, Part 1). The parameters in each of these equations are obtained by using the Marquardt method (*16*). The sum of the squares of relative deviations in temperature and vapor composition was minimized during optimization of the parameters.

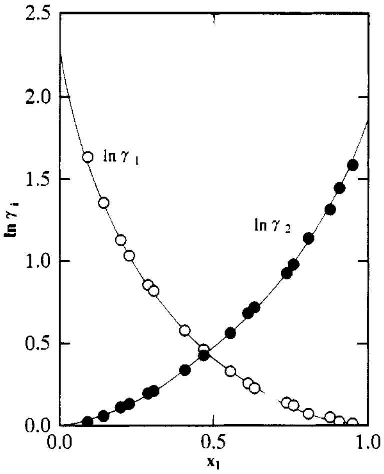

Figure 2. Activity coefficient–liquid composition diagram for 1-propanol (1) + 2,2,4-trimethylpentane (2): (○, ●) this work, (—) Wilson equation.

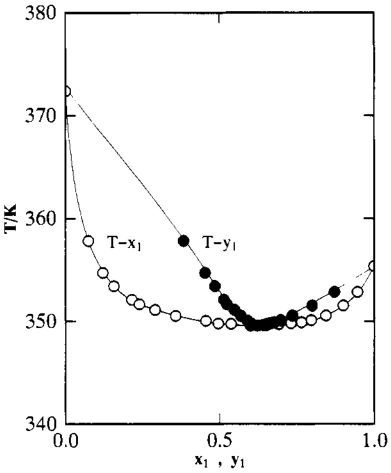

Figure 3. Temperature–composition diagram for 2-propanol (1) + 2,2,4-trimethylpentane (2): (○, ●) this work, (—) Wilson equation.

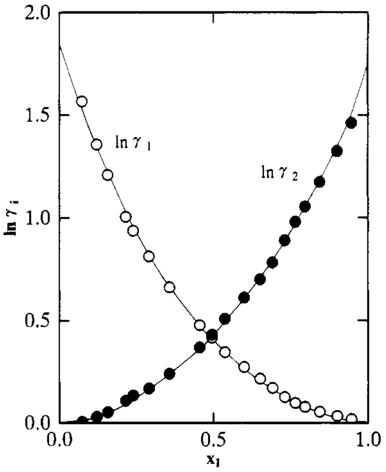

Figure 4. Activity coefficient–liquid composition diagram for 2-propanol (1) + 2,2,4-trimethylpentane (2): (○, ●) this work, (—) Wilson equation.

For 1-propanol (1) + 2,2,4-trimethylpentane (2), the Wilson equation yielded the lowest mean deviations between the experimental and calculated temperatures, 0.07 K, and vapor compositions, 0.003 mole fraction. The Wilson parameters for this system were found to be

$$\lambda_{12} - \lambda_{11} = 1716.698\ \text{J·mol}^{-1} \quad \lambda_{12} - \lambda_{22} = 142.541\ \text{J·mol}^{-1}$$

The results for the system 2-propanol (1) + 2,2,4-trimethylpentane (2) were also correlated using the Wilson equation with the parameters

$$\lambda_{12} - \lambda_{11} = 1439.950\ \mathrm{J{\cdot}mol^{-1}} \quad \lambda_{12} - \lambda_{22} = 198.623\ \mathrm{J{\cdot}mol^{-1}}$$

Absolute average deviations of 0.004 in mole fraction and 0.07 K in temperature were observed. The calculated results using the Wilson equation are shown by solid lines in Figures 1–4.

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