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Glossary

C	molar concentration, mol cm^{-3}
d	liquid density, g cm^{-3}
H	Henry's constant, atm
L	Ostwald coefficient
P	total pressure, atm
P^S	vapor pressure of pure liquid or liquid mixture, atm
p	partial pressure, atm
v	molar volume, cm^3 mol^{-1}
x	mole fraction
$\kappa(L)$	excess quantity of gas solubility defined in eq 4
Φ	volume fraction

Subscripts

A, B	solvents of A and B, respectively
R	gas component
R,mix	R in mixed solvents
R,α	R in pure solvent of α
α	pure solvent of A or B

Superscripts

E	excess quantity
G	gas phase
L	liquid phase

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Vapor–Liquid Equilibrium Data for the Systems 2-Propanol–Isopropylbenzene, Allyl Alcohol–Isopropylbenzene, 2-Methoxyethanol–Isopropylbenzene, and 2-Ethoxyethanol–Isopropylbenzene

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Vapor–liquid equilibrium data were obtained experimentally for the binary systems, 2-propanol–isopropylbenzene, allyl alcohol–isopropylbenzene, 2-methoxyethanol–isopropylbenzene, and 2-ethoxyethanol–isopropylbenzene at 760 mmHg pressure. Vapor-phase nonideality was taken into account to calculate the activity coefficients. The data were found to be thermodynamically consistent by the application of the tests of Herington, Norrish-Twigg, and Black. The correlations of Wilson and NRTL fit the activity coefficient–composition data well.

Isobaric vapor–liquid equilibrium data for the binary systems 2-propanol–isopropylbenzene, allyl alcohol–isopropylbenzene, 2-methoxyethanol–isopropylbenzene, and 2-ethoxyethanol–isopropylbenzene were obtained at 760 ± 2 mmHg pressure using a vapor recirculating type equilibrium still reported earlier (*8*). The wide boiling systems, 2-propanol–isopropylbenzene and allyl alcohol–isopropylbenzene formed no azeotropes as has been reported in literature (*6*), whereas the systems 2-methoxyethanol–isopropylbenzene and 2-ethoxyethanol–isopropylbenzene formed minimum boiling azeotropes. The azeotropic conditions for these systems are 122.2 °C and 79.5 mol % 2-methoxyethanol and 133.1 °C and 73.5 mol % 2-ethoxyethanol, respectively, whereas the values reported in the literature (*6*) are 122.4 °C and 81.5 mol % 2-methoxyethanol and 133.2 °C and 73.1 mol % 2-ethoxyethanol, respectively.

Experimental Section

2-Methoxyethanol and 2-ethoxyethanol were purified as described earlier (*8*). 2-Propanol obtained from British Drug Houses was initially dried by refluxing for about 4 h with pure quicklime. Allyl alcohol obtained from Riedel was refluxed for 4 h with chemically pure anhydrous potassium carbonate. Isopropylbenzene obtained from British Drug Houses was kept overnight in contact with pure magnesium sulfate for preliminary drying. These were finally purified by distillation as described earlier for 2-methoxyethanol and 2-ethoxyethanol. The details of apparatus and the experimental procedure used for obtaining the vapor–liquid equilibrium data have been described earlier (*8*). The refractive index method was used for the analysis of the equilibrium samples.

Results and Discussion

The activity coefficients were calculated using eq 1 and 2 described earlier (*8*). Table I gives the vapor–liquid equilibrium data along with activity coefficients for these systems.

On the basis of the recommendations made elsewhere (*7*, *11*), the pure component properties were chosen. For isopropylbenzene, the vapor pressures were estimated by the RPME equation (*9*, *10*), second virial coefficients by the Pitzer–Curl correlation (*15*), and liquid molar volumes by the surface tension method (*4*). For allyl alcohol, the Thek–Stiel equation (*17*, *18*) was used to estimate the vapor pressures and the O'Connell–Prausnitz correlation (*14*) for estimating second virial

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Table I. Vapor-Liquid Equilibrium Data at 760 ± 2 mmHg Pressure

t, °C	x_1	y_1	γ_1	γ_2	t, °C	x_1	y_1	γ_1	γ_2
System 2-Propanol (1)-Isopropylbenzene (2)									
83.1	0.968	0.985	0.985	3.954	89.1	0.515	0.900	1.351	1.399
83.3	0.952	0.978	0.987	3.765	91.3	0.400	0.885	1.580	1.200
83.7	0.920	0.968	0.995	3.396	93.6	0.316	0.871	1.811	1.086
84.4	0.868	0.954	1.012	2.853	97.8	0.222	0.840	2.160	1.020
85.4	0.781	0.936	1.062	2.282	101.1	0.176	0.820	2.367	0.967
86.3	0.702	0.923	1.127	1.945	105.1	0.142	0.775	2.436	1.015
88.0	0.580	0.908	1.260	1.549	111.7	0.105	0.716	2.485	0.990
					115.6	0.088	0.674	2.496	0.984
System Allyl Alcohol (1)-Isopropylbenzene (2)									
97.2	0.964	0.972	1.000	3.838	103.6	0.406	0.854	1.673	0.996
97.3	0.944	0.958	1.001	3.768	105.6	0.332	0.835	1.877	0.940
97.9	0.872	0.922	1.023	2.991	108.0	0.260	0.815	2.151	0.878
98.4	0.808	0.905	1.061	2.402	111.0	0.200	0.800	2.495	0.801
99.1	0.736	0.887	1.114	2.032	114.0	0.172	0.785	2.599	0.754
99.7	0.666	0.881	1.198	1.656	118.3	0.119	0.726	3.032	0.790
101.1	0.558	0.866	1.344	1.340	121.7	0.106	0.695	2.958	0.782
102.4	0.482	0.862	1.482	1.127	125.0	0.091	0.610	2.747	0.892
					127.4	0.076	0.524	2.629	0.996
System 2-Methoxyethanol (1)-Isopropylbenzene (2)									
123.9	0.974	0.960	0.999	3.227	122.5	0.718	0.758	1.116	1.919
123.0	0.925	0.902	1.015	2.884	123.0	0.648	0.733	1.176	1.675
123.0	0.922	0.900	1.017	2.833	123.8	0.550	0.700	1.293	1.438
122.6	0.877	0.856	1.029	2.616	124.8	0.474	0.663	1.382	1.339
122.4	0.820	0.814	1.053	2.321	126.3	0.371	0.630	1.602	1.178
122.3	0.849	0.835	1.045	2.468	127.6	0.304	0.596	1.785	1.117
122.2	0.823	0.815	1.056	2.366	129.9	0.226	0.544	2.044	1.064
122.3	0.773	0.786	1.082	2.134	132.4	0.176	0.488	2.198	1.045
					135.1	0.136	0.432	2.323	1.026
System 2-Ethoxyethanol (1)-Isopropylbenzene (2)									
134.8	0.966	0.954	0.990	2.204	133.2	0.746	0.746	1.053	1.650
134.5	0.938	0.918	0.989	2.144	133.2	0.727	0.732	1.061	1.617
134.0	0.902	0.878	1.000	2.013	133.2	0.671	0.696	1.092	1.520
133.7	0.867	0.842	1.008	1.933	133.6	0.592	0.650	1.146	1.396
133.3	0.818	0.797	1.022	1.837	134.3	0.502	0.604	1.226	1.271
133.2	0.841	0.817	1.021	1.900	135.0	0.410	0.565	1.376	1.153
133.1	0.809	0.788	1.029	1.834	136.5	0.323	0.510	1.508	1.091
133.2	0.779	0.765	1.033	1.755	138.3	0.246	0.445	1.641	1.053
133.2	0.747	0.744	1.048	1.665	140.1	0.186	0.388	1.796	1.027
					142.5	0.133	0.306	1.847	1.027

Table II. Data Fit in Correlations

	Wilson		NRTL	
System	Constants[a]	RMS dev in y_1	Constants[a]	RMS dev in y_1
2-Propanol (1)-isopropylbenzene (2)	$\Lambda_{12} = 0.4706$ $\Lambda_{21} = 0.3701$	0.037	$\tau_{12} = 0.9878$ $\tau_{21} = 0.7351$	0.037
Allyl alcohol (1)-isopropylbenzene (2)	$\Lambda_{12} = 0.3990$ $\Lambda_{21} = 0.3245$	0.037	$\tau_{12} = 1.1071$ $\tau_{21} = 0.9102$	0.038
2-Methoxyethanol (1)-isopropylbenzene (2)	$\Lambda_{12} = 0.4813$ $\Lambda_{21} = 0.4766$	0.010	$\tau_{12} = 0.7554$ $\tau_{21} = 0.7059$	0.010
2-Ethoxyethanol (1)-isopropylbenzene (2)	$\Lambda_{12} = 0.5470$ $\Lambda_{21} = 0.6505$	0.008	$\tau_{12} = 0.4338$ $\tau_{21} = 0.5886$	0.008

[a] Constants obtained by minimizing ln (γ_1/γ_2) function.

coefficients, and the liquid molar volumes were estimated using the surface tension method (*4*). For 2-propanol, vapor pressures were calculated by the Ambrose-Townsend correlation (*1*), second virial coefficients by the O'Connell-Prausnitz correlation, and liquid molar volumes by the surface tension method. For 2-methoxyethanol and 2-ethoxyethanol, the pure component properties were estimated, as mentioned earlier (*8*). Thermodynamic consistency tests of Herington (*5*), Black (*2*, *3*), and Norrish-Twigg (*13*) were well satisfied by the data for all the systems. The activity coefficient-composition data above 0.1 mole fraction of the low boiling components are well represented by the correlation of Wilson (*19*) and NRTL (*16*). The constants in these correlations were evaluated by using the nonlinear least-squares method illustrated by Nagahama et al. (*12*) minimizing the ln (γ_1/γ_2) function. The value of the nonrandom constant, α_{12}, in the NRTL correlation was taken to be 0.47. Table II gives the root mean square deviations in vapor composition along with the constants for the correlating equations.

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