Isothermal VLE and V^E at 303.15 K for the Binary and Ternary Mixtures of Di-isopropyl Ether (DIPE) + 1-Propanol + 2,2,4-Trimethylpentane

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Isothermal vapor−liquid equilibrium (VLE) data at 303.15 K are reported for the binary systems of di-isopropyl ether (DIPE) + 1-propanol, DIPE + 2,2,4-trimethylpentane, and 1-propanol + 2,2,4-trimethylpentane and also for the ternary system of DIPE + 1-propanol + 2,2,4-trimethylpentane by using headspace gas chromatography. Additionally, the excess molar volumes (V^E) at 303.15 K for the same systems were also determined by measured densities. The experimental binary and ternary VLE data were correlated with G^E model equations and the V^E were correlated with the Redlich−Kister equation for binary systems and the Cibulka equation for ternary system, respectively.

Introduction

The addition of fuel oxygenates to gasoline raises combustion temperatures and improves engine efficiencies. The results are lower levels of carbon monoxide and unburned hydrocarbons in auto exhaust. Today, methyl *tert*-butyl ether (MTBE) dominates the market, but the insufficient supply of this ether increases the interest in heavier ethers. Di-isopropyl ether (DIPE) could be a suitable gasoline additive.[1] Among other ether compounds, ethyl *tert*-butyl ether (ETBE) and *tert*-amyl methyl ether (TAME) have been used as oxygenates in gasoline. We have reported the phase equilibria and mixture properties systematically for new candidate materials of alternative additives and energy.[2−5]

In this work, the isothermal vapor−liquid equilibrium (VLE) data are reported at 303.15 K for the binary systems of DIPE + 1-propanol, DIPE + 2,2,4-trimethylpentane, and 1-propanol + 2,2,4-trimethylpentane and for the ternary system of DIPE + 1-propanol + 2,2,4-trimethylpentane by using headspace gas chromatography (HSGC). While the experimental binary VLE data were correlated using Margules, van Laar, Wilson, nonrandom, two-liquid (NRTL), and UNIQUAC equations, the ternary VLE data were correlated with Wilson, NRTL, and UNIQUAC models. Additionally, densities (ρ) at 303.15 K for the same binary and ternary systems were measured by using a digital vibrating tube densimeter. The excess molar volumes (V^E) were calculated from directly measured pure and mixture densities, and these V^E data were correlated with the Redlich−Kister polynomial for binary data and the Cibulka equation for ternary data, respectively.

Experimental Section

Materials. The chemicals of analytical commercial grade of high-purity were used in this work. Before the measurement, all the chemicals were dried using molecular sieves with a pore diameter of 0.4 nm. The purity of the chemicals was checked by gas chromatograph and by comparing the density with reported values in the literatures. Purity of all the samples was more than 99.9 wt % by gas chromatographic analysis. The measured densities of the samples are summarized in Table 1 with Antoine constants and critical properties of the pure substances.

Apparatus and Procedure. HSGC was used for the measurement of isothermal VLE data for all the binary and ternary

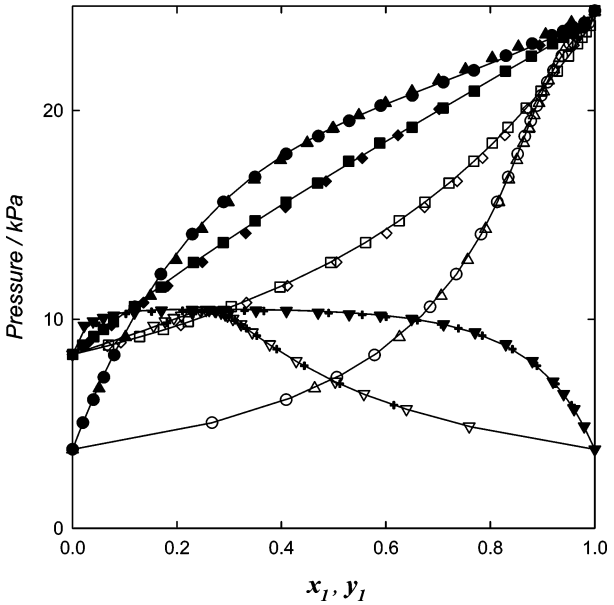

Figure 1. VLE for the three binary systems of DIPE, 1-propanol, and 2,2,4-trimethylpentane at 303.15 K: filled symbols, liquid phase; open symbols, vapor phase; ●, DIPE (1) + 1-propanol (2); ▲, DIPE (1) + 1-propanol (2) by Villamañán et al.;[8] ■, DIPE (1) + 2,2,4-trimethylpentane (2); ♦, DIPE (1) + 2,2,4-trimethylpentane (2) by Wichterle;[9] +, 1-propanol (1) + 2,2,4-trimethylpentane (2) by Hiaki et al.;[10] ▼, 1-propanol (1) + 2,2,4-trimethylpentane (2) from previous work.[7] Solid curves were calculated from G^E model equation.

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Table 1. Densities, Refractive Indices, Antoine Constants, and Critical Properties of Pure Components

	ρ at 298.15 K		Antoine constants[a]			critical properties[a]		
chemicals	present study	literature value	*A*	*B*	*C*	*Tc*/(K)	*Pc*/(kPa)	*Vc*/(cm^3·mol^{-1})
DIPE	0.71873	0.71870[b]	6.84953	1139.34	218.742	500.00	2877.63	386.00
1-propanol	0.79981	0.79970[a]	7.74887	1440.74	198.800	536.70	5167.58	218.50
2,2,4-trimethyl pentane	0.68781	0.68774[b]	6.96602	1339.49	229.033	543.80	2569.60	468.00

[a] Ref 14. [b]Ref 15.

Table 2. Isothermal VLE for Binary Systems of DIPE (1) + 1-Propanol (2) and DIPE (1) + 2,2,4-Trimethylpentane (2) at 303.15 K

P_{cal}/kPa	x_1	y_1	γ_1	γ_2	P_{cal}/kPa	x_1	y_1	γ_1	γ_2
	DIPE + 1-propanol					DIPE + 2,2,4-trimethylpentane			
5.05	0.0199	0.2671	2.782	1.001	8.76	0.0197	0.0692	1.264	1.001
6.15	0.0399	0.409	2.587	1.003	9.17	0.0410	0.1284	1.181	1.003
7.22	0.0601	0.5061	2.499	1.005	9.51	0.0590	0.1741	1.153	1.004
8.29	0.0799	0.5783	2.464	1.006	9.89	0.0786	0.2217	1.145	1.005
10.60	0.1192	0.6847	2.498	1.005	10.61	0.1188	0.3040	1.115	1.008
12.16	0.1694	0.7346	2.165	1.030	12.72	0.2316	0.4944	1.115	1.007
14.07	0.2294	0.7822	1.970	1.053	11.55	0.1696	0.3974	1.111	1.008
15.62	0.2891	0.8133	1.804	1.087	13.67	0.2886	0.5611	1.091	1.015
16.81	0.3495	0.8343	1.648	1.134	14.72	0.3497	0.6255	1.081	1.019
17.91	0.409	0.8524	1.533	1.185	15.61	0.4087	0.6747	1.058	1.033
18.77	0.4708	0.8659	1.417	1.260	16.52	0.4695	0.7210	1.042	1.045
19.51	0.5296	0.8774	1.327	1.346	17.57	0.5289	0.7684	1.048	1.039
20.23	0.5902	0.889	1.251	1.452	18.43	0.5883	0.8038	1.034	1.057
20.71	0.6505	0.8974	1.173	1.611	19.19	0.6500	0.8337	1.010	1.097
21.35	0.7101	0.9093	1.123	1.770	20.12	0.7095	0.8687	1.012	1.094
21.92	0.7685	0.9209	1.078	1.984	20.93	0.7696	0.8971	1.002	1.124
22.62	0.8300	0.9372	1.049	2.214	21.88	0.8293	0.9283	1.006	1.105
23.20	0.8803	0.9521	1.030	2.460	22.60	0.8786	0.9499	1.003	1.121
23.59	0.9179	0.9637	1.017	2.764	23.19	0.9194	0.9671	1.002	1.137
23.80	0.9397	0.9709	1.009	3.047	23.50	0.9404	0.9758	1.001	1.148
23.99	0.9581	0.9785	1.006	3.259	23.77	0.9595	0.9836	1.001	1.159
24.19	0.9804	0.9885	1.001	3.750	24.06	0.9797	0.9918	1.000	1.170

systems. The HSGC consists of a gas chromatograph (HP 6890N) and a headspace sampler (HP19395A) in which the precision thermostat, having an accuracy of ± 0.1 K is equipped. The HP-5 (5 % diphenyl−95 % dimethylsiloxane, 30 m × 0.32 mm × 0.25 μm) capillary column and a thermal conductivity detector were used for the analysis. The uncertainty of the measured equilibrium mole fraction is about ± 1·10^{-4}. The procedure of measurement has been described in detail elsewhere.[2,6] The excess volume was calculated directly from measured pure and mixture density using Anton−Paar model 5000 vibrating tube digital density meter. The accuracy of this density meter is ± 5·10^{-6} g·cm^{-3}. The measuring procedure can be found elsewhere.[2]

Results and Discussion

Isothermal VLE. In the HSGC−VLE measurement method, the equilibrium pressure cannot be measured but is calculated from the experimental vapor-phase composition and thermodynamic equations.[6] The true liquid compositions can be calculated from the experimental vapor-phase equilibrium composition using the mass balance. The experimental VLE compositions and calculated pressures for the binary systems of DIPE (1) + 1-propanol (2), and DIPE (1) + 2,2,4-trimethylpentane at 303.15 K are listed and plotted in Table 2 and Figure 1. The binary VLE for the 1-propanol (1) + 2,2,4-trimethylpentane (2) were taken from our previous work[7] and also represented in Figure 1 for comparison.

As shown in Figure 1, the binary systems DIPE + 1-propanol and DIPE + 2,2,4-trimethylpentane are zeotrope systems. The

Table 3. The G^E Model Parameters and Mean Deviation between the Calculated and Experimental Vapor-Phase Mole Fraction (Δy_1) for the Binary Systems at 303.15 K

model equation	A_{12}	A_{21}	α	Δy_1
	DIPE (1) + 1-propanol (2)			
Margules	4.3723	5.3480		0.0026
van Laar	4.4058	5.3932		0.0025
Wilson	−432.9135	4037.1316		0.0030
NRTL	2361.3592	1234.2972	0.4954	0.0029
UNIQUAC	2298.2113	−769.5016		0.0025
	DIPE (1) + 2,2,4-trimethylpentane (2)			
Margules	0.7791	0.6552		0.0021
van Laar	0.7845	0.6590		0.0021
Wilson	1068.9451	−588.2419		0.0021
NRTL	−441.4760	936.8951	0.3000	0.0021
UNIQUAC	−580.0329	779.4537		0.0021
	1-propanol (1) + 2,2,4-trimethylpentane (2)[a]			
Margules	2.4457	1.7514		0.0234
van Laar	2.5459	1.7674		0.0213
Wilson	2001.1213	178.5385		0.0047
NRTL	827.7101	1433.8981	0.5024	0.0083
UNIQUAC	−222.4994	930.5280		0.0209

[a] Parameters taken from ref 7.

measured binary VLE data for DIPE + 1-propanol, DIPE + 2,2,4-trimethylpentane, and 1-propanol + 2,2,4-trimethylpentane were also compared with the reported data[8−10] as shown in Figure 1, respectively. We compared the calculated data using binary parameters with reference data. The experimental binary VLE data were correlated with Margules, van Laar, Wilson, NRTL, and UNIQUAC equations, and the adjustable binary parameters are listed in Table 3 along with the mean deviations

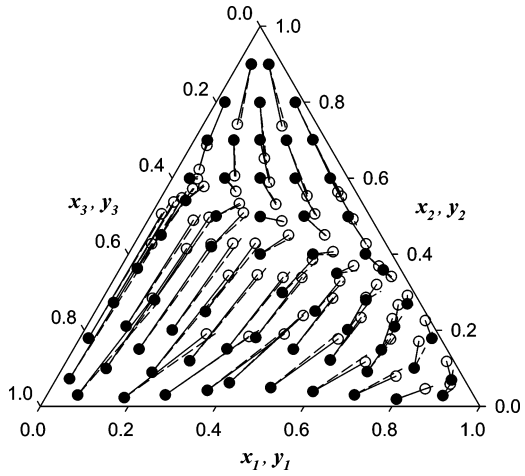

Figure 2. VLE for the ternary system of DIPE (1) + 1-propanol (2) + 2,2,4-trimethylpentane (3) at 303.15 K: ●, liquid phase; ○, vapor phase. Dashed lines were calculated from NRTL equation.

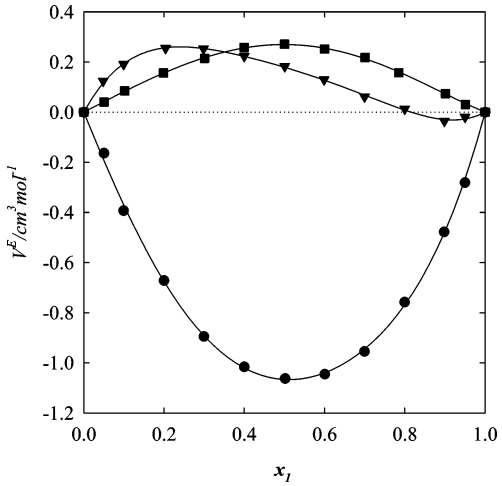

Figure 3. V^E for three binary systems of DIPE, 1-propanol, and 2,2,4-trimethylpentane mixture at 303.15 K: ●, DIPE (1) + 1-propanol (2); ■, DIPE (1) + 2,2,4-trimethylpentane (2); ▼, 1-propanol (1) + 2,2,4-trimethylpentane (2). Solid curves were calculated from Redlich−Kister polynomial.

between experimental and calculated data. The mean deviation of vapor-phase mole fraction (Δy_1) was calculated from eq 1

$$\Delta y_1 = \frac{|\Delta y_{1,\,\mathrm{exp}} - \Delta y_{1,\mathrm{cal}}|}{N} \tag{1}$$

where N is the number of experimental data points. The binary parameters (A_{ij}) for calculation of ln γ(activity coefficient) of Wilson, NRTL, and UNIQUAC models means

$$A_{ij} = (\lambda_{ij} - \lambda_{ii})/\mathrm{J{\cdot}mol^{-1}}\ \text{(Wilson)}$$

$$A_{ij} = (g_{ij} - g_{ii})/\mathrm{J{\cdot}mol^{-1}}\ \text{(NRTL)}$$

$$A_{ij} = (u_{ij} - u_{ii})/\mathrm{J{\cdot}mol^{-1}}\ \text{(UNIQUAC)}$$

The ternary VLE data of DIPE (1) + 1-propanol (2) + 2,2,4-trimethylpentane (3) system at 303.15 K are listed in Table 4 and illustrated in Figure 2. The ternary VLE data were correlated with Wilson, NRTL, and UNIQUAC models. Among them, the NRTL model provided the best correlation result. Dashed lines in Figure 2 represent the calculated values by NRTL equation. We compared the calculated data using binary

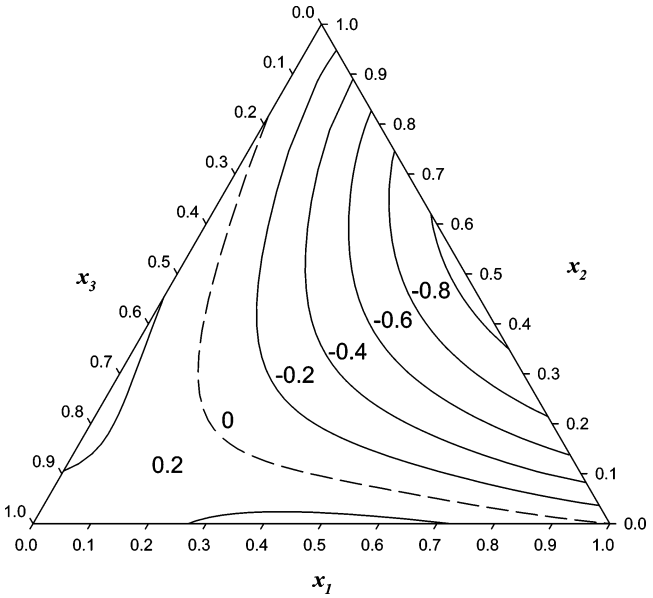

Figure 4. Isoclines of constant V^E ($cm^3{\cdot}mol^{-1}$) for ternary system of DIPE (1) + 1-propanol (2) + 2,2,4-trimethylpentane (3) at 303.15 K.

parameters with ternary correlation data. The mean deviation of comparing result was $\Delta y = 0.0214$. The each G^E model parameters and the mean deviation of vapor-phase mole fraction (Δy_{mean}) are given in the Table 5. Δy_{mean} can be determined by following eq 2

$$\Delta y_{\mathrm{mean}} = \frac{\Delta y_1 + \Delta y_2 + \Delta y_3}{3} \tag{2}$$

Excess Molar Volumes. The measured density and V^E at 303.15 K for the same binary systems are listed in Table 6. V^E for multicomponent mixtures are calculated from the measured densities of pure substances and mixtures by using eq 3

$$V^E = \frac{\sum_i x_i M_i}{\rho_m} - \sum_i \left(\frac{x_i M_i}{\rho_i}\right) \tag{3}$$

where x_i, M_i, ρ_i and ρ_m are the mole fraction, molar mass, pure component density, and mixture density, respectively. The measured binary V^E data were correlated with Redlich−Kister polynomial of eq 4.[11] The solid lines in Figure 3 indicate calculated values using correlated parameters

$$V^E_{12}\,\mathrm{cm^3{\cdot}mol^{-1}} = x_1 x_2 \sum_{i=1}^{4} A_i (x_1 - x_2)^{i-1} \tag{4}$$

The standard deviation of the fits, σ_{st}, is then defined as

$$\sigma_{\mathrm{st}}/\mathrm{cm^3{\cdot}mol^{-1}} = \left[\frac{\sum_i ((V^E)_{\mathrm{cal}} - (V^E)_{\mathrm{exp}})_i^2}{(N-n)}\right]^{1/2} \tag{5}$$

where N is the number of experimental data points, and n is the number of fitted parameters. The experimental densities and excess molar volumes for the binary systems of DIPE (1) + 1-propanol (2), DIPE (1) + 2,2,4-trimethylpentane (2), and 1-propanol (1) + 2,2,4-trimethylpentane (2) at 303.15 K are listed in Table 6 and depicted in Figure 3. V^E of DIPE + 1-propanol show negative deviations and an almost parabolic

Table 4. Isothermal VLE for the Ternary System of DIPE (1) + 1-Propanol (2) + 2,2,4-Trimethylpentane (3) at 303.15 K

P_{cal}/kPa	x_1	x_2	y_1	y_2	y_1	y_2	P_{cal}/kPa	x_1	x_2	y_1	y_2	y_1	y_2
61.24	0.0685	0.4750	0.0927	0.5324	1.05	1.56	69.97	0.3965	0.4340	0.4987	0.3613	1.09	1.39
59.88	0.0554	0.3858	0.0533	0.5022	0.99	1.86	69.49	0.3256	0.5345	0.4581	0.4042	1.19	1.24
58.41	0.0433	0.3038	0.0676	0.5265	0.93	2.28	68.19	0.2511	0.6412	0.4078	0.4585	1.32	1.13
62.42	0.1987	0.3568	0.2283	0.4620	0.97	1.81	59.95	0.0886	0.8728	0.3655	0.5061	1.75	1.02
58.30	0.1287	0.2293	0.1489	0.4508	0.90	2.71	75.67	0.5949	0.3389	0.2079	0.6989	1.08	1.48
56.16	0.0946	0.1699	0.1136	0.4431	0.88	3.55	74.95	0.5103	0.4330	0.6265	0.3254	1.16	1.31
48.59	0.0308	0.0563	0.0430	0.3829	0.92	8.28	73.50	0.4181	0.5345	0.5700	0.3813	1.26	1.19
59.92	0.2665	0.2028	0.2976	0.3833	0.90	2.65	71.15	0.3222	0.6424	0.5090	0.4449	1.40	1.10
57.29	0.2096	0.1613	0.2426	0.3832	0.89	3.29	67.17	0.2216	0.7536	0.4525	0.5046	1.58	1.04
54.49	0.1550	0.1195	0.1898	0.3818	0.88	4.29	52.44	0.4049	0.0480	0.4382	0.5165	0.91	4.56
50.98	0.1024	0.0780	0.1358	0.3701	0.90	6.04	54.49	0.5054	0.0380	0.5010	0.2059	0.92	4.17
57.93	0.3620	0.1199	0.4076	0.2977	0.90	3.36	57.55	0.6062	0.0301	0.6088	0.1511	0.92	3.79
54.50	0.2881	0.0942	0.3424	0.3046	0.89	4.16	61.31	0.7044	0.0231	0.6964	0.0984	0.94	3.46
50.99	0.2139	0.0700	0.2733	0.3033	0.90	5.33	65.71	0.8042	0.0144	0.7813	0.0661	0.95	3.19
40.96	0.0706	0.0229	0.1196	0.2480	0.96	10.6	60.81	0.4174	0.1447	0.8603	0.0381	0.90	2.86
48.97	0.3626	0.0323	0.4773	0.1626	0.92	5.36	62.32	0.5188	0.1191	0.4531	0.2978	0.91	2.85
44.72	0.2715	0.0229	0.3967	0.1570	0.94	6.72	64.28	0.6163	0.0959	0.5510	0.2473	0.92	2.82
41.18	0.1805	0.0176	0.2938	0.1631	0.96	8.51	66.61	0.7134	0.0713	0.6398	0.2010	0.94	2.81
61.26	0.0463	0.5343	0.0651	0.5532	1.10	1.45	72.93	0.9077	0.0215	0.7315	0.1507	0.98	2.77
61.46	0.0357	0.6412	0.0564	0.5782	1.20	1.27	65.64	0.4310	0.2464	0.9129	0.0486	0.94	2.03
60.88	0.0241	0.7543	0.0407	0.6450	1.34	1.14	67.31	0.5309	0.2038	0.4581	0.3416	0.94	2.12
63.05	0.1696	0.4342	0.2058	0.4864	1.03	1.58	69.05	0.6281	0.1619	0.5485	0.2893	0.95	2.23
63.55	0.1391	0.5350	0.1803	0.5188	1.11	1.37	70.86	0.7267	0.1178	0.6299	0.2485	0.96	2.35
63.43	0.1078	0.6413	0.1555	0.5609	1.23	1.22	72.88	0.8194	0.0788	0.7147	0.1981	0.97	2.46
59.16	0.0380	0.8731	0.0890	0.7045	1.63	1.03	71.44	0.5443	0.2917	0.7999	0.1452	1.01	1.68
65.40	0.3310	0.3383	0.3691	0.4039	0.98	1.73	73.19	0.6430	0.2291	0.5648	0.3266	0.99	1.82
66.10	0.2839	0.4329	0.3348	0.4404	1.05	1.48	74.67	0.7370	0.1687	0.6413	0.2800	0.99	2.00
66.24	0.2326	0.5350	0.2980	0.4844	1.14	1.30	76.67	0.9154	0.0539	0.7145	0.2309	0.99	2.45
65.63	0.1788	0.6420	0.2525	0.5432	1.27	1.17	77.17	0.6556	0.3000	0.8837	0.0992	1.07	1.54
63.85	0.1229	0.7533	0.2077	0.6084	1.43	1.08	78.23	0.7469	0.2205	0.6680	0.2996	1.03	1.74
69.79	0.4632	0.3381	0.4987	0.3613	1.02	1.60	78.74	0.8364	0.1427	0.7265	0.2534	1.01	1.99

Table 5. Fitted G^E Model Parameters and Standard Deviations for the Ternary System of DIPE (1) + 1-Propanol (2) + 2,2,4-Trimethylpentane (3) at 303.15 K

G^E model	A_{ij}	A_{ji}	α	Δy
		Wilson		
1 + 2	−1403.1488	4399.2404		
2 + 3	9342.7574	−359.2646		0.0186
1 + 3	389.5559	−266.5681		
		NRTL		
1 + 2	2907.9796	−142.6840	0.2321	
2 + 3	4254.7673	6098.2478	0.5381	0.0183
1 + 3	1050.6756	−821.2188	0.1000	
		UNIQUAC		
1 + 2	2709.4421	−975.3887		
2 + 3	−1199.6415	5484.2767		0.0196
1 + 3	−197.1848	226.7565		

shape. On the other side, V^E of DIPE + 1-propanol show positive deviations. This may be caused according to the hydrogen bond rupture or dispersive interaction force between unlike two molecules as mentioned as explanation of Chen and Tu.[12] The system 1-propanol + 2,2,4-trimethylpentane at 303.15 K shows negative deviation in the 1-propanol rich region resulting from the strong polarity of 1-propanol, while it shows positive deviation in the 2,2,4-trimethylpentane rich region. The binary V^E data were correlated with the Redlich−Kister polynomial, and the calculated values (solid line) with each correlated parameters are in good agreement in experimental values as shown in Figure 3. The V^E data for the ternary system of DIPE + 1-propanol + 2,2,4-trimethylpentane were also derived from measured ternary densities similar to the binary systems. The densities and V^E for the ternary system of DIPE + 1-propanol + 2,2,4-trimethylpentane at 303.15 K are listed in Table 7. The ternary V^E are correlated with Cibulka equation[13]

$$V^E_{123} = V^E_{12*} + V^E_{23*} + V^E_{13*} + x_1x_2x_3(A_1 + A_2x_1 + A_3x_2) \quad (6)$$

where V^E_{12*}, V^E_{23*}, and V^E_{13*} represent the excess molar volumes

Table 6. Densities, Excess Molar Volumes for the Binary Systems of DIPE (1) + 1-Propanol (2), DIPE (1) + 2,2,4-Trimethylpentane (2) and 1-Propanol (1) + 2,2,4-Trimethylpentane (2) at 303.15 K

x_1	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}	x_1	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}
		DIPE + 1-propanol			
0.0000	0.79655	0.0000	0.6006	0.74173	−1.0450
0.0504	0.79059	−0.1635	0.6995	0.73454	−0.9542
0.0991	0.78596	−0.3926	0.7994	0.72746	−0.7577
0.2001	0.77566	−0.6714	0.8981	0.72072	−0.4776
0.2994	0.76652	−0.8945	0.9498	0.71720	−0.2810
0.4000	0.75767	−1.0156	1.0000	0.71351	0.0000
0.5018	0.74930	−1.0622			
		DIPE + 2,2,4-trimethylpentane			
0.0000	0.68374	0.0000	0.6002	0.69934	0.2515
0.0504	0.68487	0.0401	0.7009	0.70260	0.2176
0.1020	0.68603	0.0846	0.7849	0.70555	0.1572
0.1985	0.68829	0.1563	0.9013	0.70978	0.0737
0.3010	0.69084	0.2146	0.9512	0.71168	0.0302
0.3996	0.69342	0.2576	1.0000	0.71351	0.0000
0.5002	0.69627	0.2714			
		1-propanol + 2,2,4-trimethylpentane			
0.0000	0.68374	0.0000	0.5989	0.72833	0.1295
0.0484	0.68575	0.1242	0.6995	0.74112	0.0611
0.0993	0.68826	0.1911	0.7998	0.75621	0.0129
0.2038	0.69424	0.2548	0.8984	0.77429	−0.0353
0.2983	0.70064	0.2526	0.9502	0.78501	−0.0196
0.4000	0.70863	0.2231	1.0000	0.79655	0.0000
0.5007	0.71782	0.1824			

Table 7. Densities and Excess Molar Volumes for Ternary System of DIPE (1) + 1-Propanol (2) + 2,2,4-Trimethylpentane (3) at 303.15 K

x_1	x_2	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}	x_1	x_2	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}
0.0595	0.5406	0.72568	−0.0204	0.1010	0.7980	0.76555	−0.3487
0.0495	0.4491	0.71567	0.0708	0.4198	0.3987	0.73069	−0.6508
0.0405	0.3605	0.70736	0.1382	0.3488	0.5016	0.73919	−0.6742
0.0293	0.2686	0.69977	0.1987	0.2812	0.5977	0.74819	−0.6945
0.0201	0.1791	0.69355	0.1977	0.2095	0.7004	0.75859	−0.6248
0.1780	0.4230	0.72005	−0.2027	0.0696	0.9007	0.78243	−0.2778
0.1487	0.3511	0.71166	−0.0633	0.5416	0.3995	0.73811	−0.9247
0.1201	0.2827	0.70465	0.0374	0.4497	0.5008	0.74625	−0.9710
0.0912	0.2102	0.69809	0.1261	0.3609	0.5986	0.75454	−0.9304
0.0313	0.0717	0.68769	0.1644	0.2707	0.6998	0.76405	−0.8374
0.3006	0.2973	0.71380	−0.2468	0.1796	0.8000	0.77441	−0.6970
0.2527	0.2469	0.70714	−0.0843	0.4017	0.0556	0.69768	0.0886
0.2000	0.1999	0.70136	0.0253	0.5009	0.0480	0.70019	0.0928
0.1532	0.1499	0.69618	0.0960	0.6012	0.0382	0.70272	0.0798
0.1003	0.1016	0.69155	0.1151	0.7007	0.0307	0.70546	0.0633
0.3488	0.1529	0.70337	−0.0751	0.8005	0.0194	0.70807	0.0292
0.2789	0.1215	0.69847	0.0351	0.4013	0.1781	0.70744	−0.1681
0.2081	0.0922	0.69416	0.1015	0.4961	0.1567	0.70931	−0.2161
0.0692	0.0291	0.68663	0.1056	0.6019	0.1176	0.70993	−0.2121
0.3611	0.0378	0.69507	0.1522	0.6997	0.0908	0.71110	−0.1840
0.2690	0.0312	0.69197	0.1641	0.8967	0.0327	0.71314	−0.1305
0.1806	0.0205	0.68895	0.1543	0.3996	0.3008	0.71891	−0.4271
0.0418	0.5973	0.73114	−0.0214	0.4973	0.2512	0.71843	−0.4566
0.0302	0.6984	0.74349	−0.0580	0.6006	0.2005	0.71794	−0.4571
0.0188	0.7999	0.75791	−0.0450	0.6997	0.1496	0.71715	−0.4328
0.1490	0.5029	0.72693	−0.2158	0.7946	0.1029	0.71634	−0.3599
0.1186	0.6009	0.73686	−0.2433	0.5030	0.3487	0.72946	−0.7081
0.0915	0.6991	0.74841	−0.2407	0.6011	0.2798	0.72672	−0.7141
0.0290	0.9014	0.77787	−0.1175	0.7015	0.2074	0.72355	−0.6539
0.2984	0.4024	0.72428	−0.4043	0.8989	0.0725	0.71757	−0.3510
0.2486	0.5020	0.73304	−0.4697	0.6014	0.3578	0.73644	−0.9661
0.2006	0.5986	0.74248	−0.4859	0.7033	0.2677	0.73082	−0.8821
0.1491	0.7005	0.75350	−0.4402	0.7977	0.1837	0.72569	−0.7437

Table 8. Fitted Parameters for the Redlich−Kister or Cibulka Equation and Standard Deviations for Ternary System of DIPE (1) + 1-Propanol (2) + 2,2,4-Trimethylpentane (3) at 303.15 K

system	A_1	A_2	A_3	A_4	σ_{st}
(1) + (2)	−4.2651	−0.1726	−0.6828	−0.8619	0.0170
(1) + (3)	1.0791	−0.0064	−0.3391	−0.0791	0.0030
(2) + (3)	0.7163	−0.9564	0.3070	−0.9350	0.0061
(1) + (2) + (3)	−5.0363	1.0435	5.3948		0.0178

and x_1, x_2, and x_3 are mole fractions of component DIPE (1), 1-propanol (2), and 2,2,4-trimethylpentane (3). The correlated values are in good agreement with the experimental data with standard deviations of 0.0178 cm^3·mol^{-1} for the DIPE + 1-propanol + 2,2,4-trimethylpentane. The correlation results are represented in Figure 4. The solid lines in Figure 4 represent constant excess molar volumes of the ternary systems calculated by Cibulka equation. In Table 8, the parameters of Redlich−Kister and Cibulka equation were listed together with standard deviations of the binary and ternary systems studied in this work.

Conclusion

Isothermal vapor−liquid equilibrium (VLE) and excess molar volumes (V^E) data at 303.15 K were experimentally determined for each binary and ternary mixture of DIPE, 1-propanol, and 2,2,4-trimethylpentane. The binary systems DIPE + 1-propanol and DIPE + 2,2,4-trimethylpentane are zeotrope systems. The binary VLE data were correlated well with common G^E model equations. The ternary data were correlated with the Wilson, NRTL, and UNIQUAC models, and the NRTL model provided better results than the models.

The binary V^E data of DIPE + 1-propanol show negative deviations, while those of DIPE + 2,2,4-trimethylpentane show positive values in the whole composition range. The system 1-propanol + 2,2,4-trimethylpentane shows an S-shaped V^E curve. The V^E were correlated with the Redlich−Kister equation for binary systems and Cibulka equation for ternary systems, respectively.

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