Isothermal Vapor−Liquid Equilibrium at 333.15 K and Excess Molar Volumes, Refractive Indices, and Excess Molar Enthalpies at 303.15 K for the Binary and Ternary Mixtures of Di-isopropyl Ether, Ethanol, and 2,2,4-Trimethylpentane

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Isothermal vapor−liquid equilibrium (VLE) data at 333.15 K are measured for the binary systems {di-isopropyl ether (DIPE) + ethanol} and {DIPE + 2,2,4-trimethylpentane} and for the ternary system {DIPE + ethanol + 2,2,4-trimethylpentane} by using headspace gas chromatography. The experimental VLE data were correlated with the G^E model: Margules, van Laar, Wilson, nonrandom two-liquid, and UNIQUAC equations. The excess molar volume and deviations in molar refractivity data are reported for the binary systems {DIPE + ethanol}, {DIPE + 2,2,4-trimethylpentane}, and {ethanol + 2,2,4-trimethylpentane} at 303.15 K. In addition, excess molar enthalpies for two binaries, {DIPE + ethanol} and {DIPE + 2,2,4-trimethylpentane}, at 303.15 K are also reported. These data were correlated with the Redlich−Kister equation. The excess molar volume and deviations in molar refractivity data are also reported for the ternary system {DIPE + ethanol + 2,2,4-trimethylpentane} at 303.15 K. The ternary data were correlated with the Cibulka equation. Also, the isocline of excess molar enthalpies for the same ternary system at 303.15 K was calculated using the Radojkovič equation.

Introduction

Since MTBE (methyl *tert*-butyl ether) was phased out as a fuel additive in gasoline in California in 2004, there has been much interest in new gasoline additives as an octane booster for this related industry. Some primary alcohols and ethers that have low solubilities in water and some alkylates are considered for a new octane booster.

Di-isopropyl ether (DIPE, 2-propan-2-yloxypropane) is one of the most suitable and alternative candidates for a gasoline additive.[1] It is considered as a gasoline octane booster separately or together with alcohol, another gasoline additive. However, very few investigations of mixture properties for gasoline additive mixtures with model compounds of gasoline have been reported in the literature. Therefore, we have reported so far the phase equilibria and mixture properties for binary and ternary systems that involve gasoline additives.[2−4]

As a continuous work on the phase equilibrium and mixture properties for gasoline additives, we report vapor−liquid equilibrium (VLE) data at 333.15 K for the binary systems {DIPE + ethanol} and {DIPE + 2,2,4-trimethylpentane} and also for the ternary system {DIPE + ethanol + 2,2,4-trimethylpentane} using headspace gas chromatography (HSGC). The experimental binary VLE data were correlated with common G^E models (Margules, van Laar, Wilson, nonrandom two-liquid (NRTL), and UNIQUAC), while the experimental ternary VLE data were correlated with Wilson, NRTL, and UNIQUAC models. Additionally, we report the excess molar volumes (V^E), deviations in molar refractivity (ΔR), and excess molar enthalpies (H^E) at 303.15 K for the same binary systems. In the case of V^E and ΔR, we also measured data for the system {ethanol + 2,2,4-trimethylpentane}. These binary data were correlated with the Redlich−Kister polynomial.[5] The ternary V^E and ΔR data at 303.15 K are also reported and shown as isoclines for the system {DIPE + ethanol + 2,2,4-trimethylpentane}. The ternary data were correlated with Cibulka equation.[6] Also, isoclines of H^E for the same ternary system at 303.15 K were also calculated by the Radojkovič equation.[7]

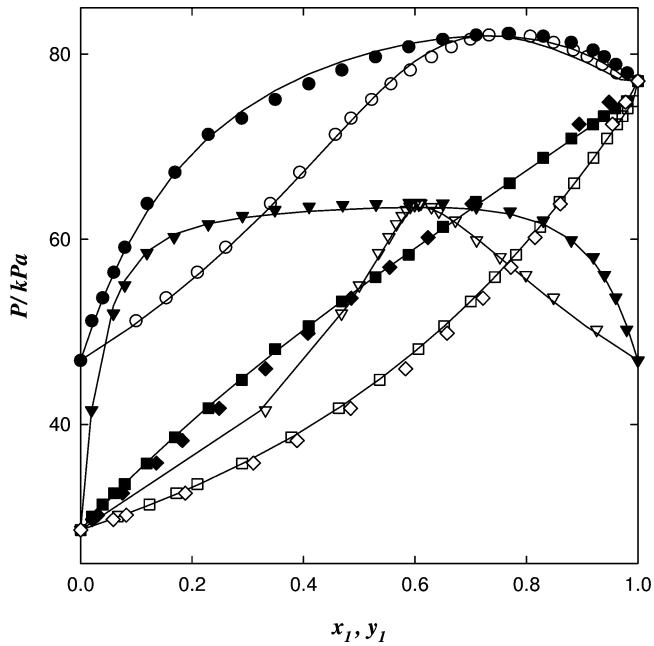

Figure 1. $P-x-y$ for three binary systems at 333.15 K: Filled symbols are liquid phase; open symbols are vapor phase; ●, {DIPE (1) + ethanol (2)}; ■, {DIPE (1) + 2,2,4-trimethylpentane (2)}; ♦, {DIPE (1) + 2,2,4-trimethylpentane (2)} by Wichterle;[16] ▼, {ethanol (1) + 2,2,4-trimethylpentane (2)} from previous work.[15] Solid curves were calculated from the best-fitted G^E model parameters.

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

	ρ at $T = 298.15$ K					critical properties[a]					
	g·cm^{-3}		Antoine constants[a]			T_c	P_c	V_c		UNIQUAC	
chemical	present study	literature value	A	B	C	K	kPa	cm^3·mol^{-1}	Ω	r	q
DIPE	0.71876	0.71870[b]	6.8495	1139.34	218.742	500.00	2877.63	386.00	0.3400	4.7421	4.0880
ethanol	0.78523	0.78517[b]	8.2042	1642.89	230.300	516.20	6383.48	167.00	0.6350	2.1055	1.9720
2,2,4-trimethyl pentane	0.68783	0.68774[b]	6.9660	1339.49	229.033	543.80	2569.60	468.00	0.3170	5.8462	4.9240

[a] Ref 8. [b] Ref 9.

Table 2. Isothermal VLE Data for Binary Systems {DIPE (1) + Ethanol (2)} and {DIPE (1) + 2,2,4-Trimethylpentane (2)} at 333.15 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) + Ethanol (2)					DIPE (1) + 2,2,4-Trimethylpentane (2)			
50.46	0.0201	0.0995	3.33	1.00	29.93	0.0202	0.0669	1.32	1.00
53.57	0.0398	0.1534	2.71	1.01	31.17	0.0396	0.1232	1.29	1.00
56.33	0.0596	0.2098	2.60	1.01	32.44	0.0600	0.1718	1.23	1.00
58.81	0.0795	0.2604	2.54	1.01	33.61	0.0793	0.2093	1.17	1.01
63.02	0.1194	0.3404	2.39	1.02	35.93	0.1188	0.2899	1.15	1.01
67.19	0.1694	0.3934	2.05	1.05	38.75	0.1692	0.3780	1.14	1.01
70.97	0.2290	0.4571	1.87	1.07	41.93	0.2292	0.4634	1.12	1.02
73.86	0.2891	0.4849	1.61	1.13	44.96	0.2893	0.5366	1.10	1.02
76.08	0.3492	0.5223	1.47	1.17	47.83	0.3490	0.6058	1.10	1.02
77.83	0.4095	0.5568	1.37	1.23	50.64	0.4093	0.6520	1.07	1.04
79.20	0.4690	0.5918	1.29	1.28	53.34	0.4690	0.7002	1.05	1.05
80.29	0.5292	0.6298	1.24	1.34	55.99	0.5292	0.7434	1.04	1.07
81.10	0.5889	0.6653	1.20	1.40	58.55	0.5887	0.7814	1.02	1.08
81.68	0.6498	0.6994	1.15	1.49	61.15	0.6500	0.8246	1.03	1.07
81.96	0.7099	0.7328	1.11	1.61	63.63	0.7090	0.8596	1.03	1.08
81.91	0.7694	0.7669	1.07	1.77	66.15	0.7697	0.8856	1.00	1.15
81.44	0.8301	0.8072	1.04	1.98	68.63	0.8297	0.9203	1.01	1.13
80.61	0.8804	0.8491	1.03	2.19	70.72	0.8804	0.9445	1.01	1.15
79.62	0.9196	0.8841	1.01	2.47	72.34	0.9197	0.9625	1.00	1.18
78.97	0.9398	0.9090	1.01	2.57	73.14	0.9392	0.9724	1.00	1.16
78.17	0.9606	0.9361	1.01	2.73	73.97	0.9592	0.9817	1.00	1.16
77.26	0.9811	0.9621	1.00	3.32	74.84	0.9802	0.9906	1.00	1.24

Since the ternary H^E data are still very rare, it is therefore of interest to estimate ternary H^E data from binary H^E data.

Experimental Section

Materials. Commercial grade DIPE ($C_6H_{14}O$, $M = 102.18$ g·mol^{-1}, CAS-RN 108-20-3) and 2,2,4-trimethylpentane (C_8H_{18}, $M = 114.23$ g·mol^{-1}, CAS-RN 540-84-1) were obtained from Aldrich. Ethanol (C_2H_6O, $M = 46.07$ g·mol^{-1}, CAS-RN 64-17-5) was supplied from J.T. Baker Chemical Co. All of the chemicals were dried using molecular sieves with a pore diameter of 0.4 nm. After that the purity of the chemicals was examined by gas chromatography and by comparing the density with reported values in the literature.[8,9] It is shown that the mass fraction of all of the chemicals was better than 0.999 by gas chromatographic analysis. The water mass fraction, determined by Karl Fischer titration (Metrohm 684 KF coulometer), was less than $7 \cdot 10^{-5}$. The measured densities of the samples are summarized in Table 1 with reported Antoine constants and critical properties of the pure substances.[8]

Apparatus and Procedure. HSGC was used for the measurement of isothermal VLE data for all of the binary and ternary systems. HSGC consists of a gas chromatograph (HP 6890N) and a headspace sampler (HP 19395A), 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 estimated as ± $1 \cdot 10^{-4}$. The procedure of measurement has been described in detail elsewhere.[10,11]

Densities were measured by a digital vibrating glass tube density meter (Anton Paar, model DMA 5000, Graz, Austria).

Table 3. G^E Model Parameters and Mean Deviations between the Calculated and the Experimental Vapor-Phase Mole Fraction (Δy_1) for the Binary Systems at 333.15 K

model equation	A_{12} / J·mol^{-1}	A_{21} / J·mol^{-1}	α	Δy_1
	DIPE (1) + Ethanol (2)			
Margules	4.566	4.224		0.0083
van Laar	4.591	4.211		0.0083
Wilson	−451.115	3884.641		0.0074
NRTL	1193.374	2006.000	0.3000	0.0081
UNIQUAC	2411.697	−616.459		0.0083
	DIPE (1) + 2,2,4-Trimethylpentane (2)			
Margules	0.936	0.765		0.0026
van Laar	0.954	0.765		0.0025
Wilson	1360.227	−713.300		0.0025
NRTL	−1657.420	2413.823	0.1254	0.0025
UNIQUAC	−694.894	956.043		0.0025
	Ethanol (1) + 2,2,4-Trimethylpentane (2)[a]			
Margules	9.681	8.133		0.0114
van Laar	13.914	8.202		0.0107
Wilson	9101.842	880.552		0.0094
NRTL	4026.583	5510.533	0.4649	0.0087
UNIQUAC	−832.777	4784.076		0.0102

[a] Parameters taken from ref 15.

The uncertainty of the density meter is stated by manufacturer as $5 \cdot 10^{-6}$ g·cm^{-3} in the range of 0 to 3. Temperature is controlled within ± 0.01 K in the range from (273.15 to 363.15) K. The details of operating procedures have been described elsewhere.[11,12] Refractive indices (n_D) of the pure components and mixture samples were measured by a digital precision refractometer (KEM, model RA-520N, Kyoto, Japan). The uncertainty of this refractometer is stated as ± $5 \cdot 10^{-5}$ within the range from 1.32 to 1.40 and ± $1 \cdot 10^{-4}$ within the range

Table 4. Isothermal VLE Data for Ternary System {DIPE (1) + Ethanol (2) + 2,2,4-Trimethylpentane (3)} at 333.15 K

P_{cal}/kPa	x_1	x_2	y_1	y_2	γ_1	γ_2	γ_3	P_{cal}/kPa	x_1	x_2	y_1	y_2	γ_1	γ_2	γ_3
61.27	0.0599	0.5413	0.0831	0.5781	1.08	1.42	1.78	70.06	0.4200	0.3999	0.4628	0.4063	1.03	1.47	1.56
60.28	0.0496	0.4504	0.0480	0.5482	1.00	1.63	1.55	69.72	0.3502	0.5001	0.4215	0.4507	1.12	1.30	1.88
59.06	0.0396	0.3627	0.0606	0.5723	0.92	1.92	1.38	68.78	0.2800	0.5997	0.3713	0.5059	1.24	1.18	2.33
57.63	0.0305	0.2726	0.0351	0.5373	0.85	2.41	1.25	67.07	0.2100	0.6998	0.3298	0.5534	1.40	1.10	2.99
55.94	0.0202	0.1790	0.0230	0.5062	0.79	3.41	1.13	58.92	0.0700	0.8995	0.1810	0.7372	1.87	1.01	5.86
63.48	0.1792	0.4198	0.2075	0.5088	0.98	1.61	1.50	76.55	0.5392	0.4007	0.5859	0.3687	1.10	1.38	1.68
59.87	0.1203	0.2797	0.1355	0.4972	0.87	2.25	1.24	76.33	0.4508	0.4991	0.5272	0.4274	1.19	1.24	2.03
57.85	0.0899	0.2108	0.1035	0.4893	0.83	2.85	1.15	75.31	0.3596	0.5997	0.4650	0.4925	1.32	1.14	2.54
51.47	0.0303	0.0722	0.0396	0.4273	0.80	6.60	1.02	73.65	0.2695	0.7009	0.4087	0.5523	1.48	1.07	3.28
62.37	0.2510	0.2491	0.2746	0.4285	0.87	2.26	1.18	70.22	0.1802	0.7996	0.3948	0.5640	1.68	1.03	4.38
59.90	0.1998	0.2006	0.2238	0.4283	0.84	2.73	1.12	56.09	0.3991	0.0618	0.4790	0.2385	0.86	3.97	0.95
57.22	0.1495	0.1505	0.1750	0.4267	0.82	3.48	1.87	57.64	0.4996	0.0490	0.5888	0.1771	0.88	3.71	0.94
53.94	0.1000	0.0994	0.1255	0.4143	0.81	4.84	1.03	59.88	0.6007	0.0389	0.6810	0.1166	0.89	3.42	0.93
61.37	0.3492	0.1510	0.3825	0.3385	0.85	2.88	1.05	62.53	0.6995	0.0299	0.7695	0.0789	0.91	3.16	0.92
58.13	0.2801	0.1194	0.3208	0.3458	0.84	3.50	1.02	65.43	0.8007	0.0188	0.8527	0.0458	0.94	2.94	0.92
54.61	0.2094	0.0894	0.2560	0.3442	0.83	4.43	1.00	63.87	0.3998	0.1807	0.4254	0.3388	0.87	2.49	1.09
44.00	0.0702	0.0296	0.1131	0.2841	0.86	9.01	0.99	65.13	0.5006	0.1500	0.5228	0.2843	0.89	2.52	1.05
52.41	0.3590	0.0417	0.4600	0.1899	0.86	4.66	0.94	66.41	0.5988	0.1216	0.6129	0.2333	0.90	2.53	1.03
47.85	0.2697	0.0297	0.3826	0.1835	0.87	5.82	0.94	67.68	0.6982	0.0910	0.7082	0.1767	0.92	2.55	1.00
43.96	0.1796	0.0228	0.2828	0.1902	0.87	7.35	0.96	71.21	0.9018	0.0279	0.9033	0.0583	0.97	2.57	0.95
60.92	0.0398	0.5995	0.0582	0.5984	1.14	1.34	1.96	67.32	0.4009	0.2990	0.4266	0.3855	0.94	1.81	1.29
60.58	0.0299	0.6999	0.0501	0.6225	1.26	1.20	2.43	68.78	0.4999	0.2503	0.5162	0.3300	0.93	1.91	1.22
59.39	0.0196	0.8002	0.0358	0.6861	1.42	1.10	3.25	70.07	0.5986	0.2013	0.5979	0.2858	0.94	2.01	1.15
63.54	0.1498	0.5003	0.1861	0.5332	1.05	1.44	1.70	71.20	0.7016	0.1483	0.6854	0.2302	0.95	2.14	1.09
63.33	0.1196	0.6001	0.1621	0.5651	1.16	1.28	2.05	72.40	0.8002	0.1004	0.7757	0.1706	0.96	2.26	1.03
62.53	0.0902	0.6999	0.1387	0.6063	1.29	1.16	2.58	71.59	0.4998	0.3495	0.5278	0.3699	1.02	1.54	1.46
56.88	0.0301	0.8998	0.0773	0.7417	1.75	1.02	5.25	73.24	0.6011	0.2793	0.6051	0.3201	1.00	1.67	1.33
66.49	0.3001	0.4001	0.3394	0.4501	0.99	1.56	1.49	74.65	0.7010	0.2093	0.6809	0.2667	0.98	1.83	1.21
66.43	0.2509	0.4990	0.3057	0.4873	1.08	1.37	1.77	76.77	0.9006	0.0691	0.8654	0.1178	0.99	2.27	1.01
65.84	0.2000	0.6002	0.2699	0.5315	1.19	1.23	2.17	79.67	0.6007	0.3586	0.6280	0.3413	1.08	1.43	1.58
64.54	0.1496	0.7006	0.2261	0.5894	1.33	1.13	2.77	81.79	0.6999	0.2695	0.6894	0.2913	1.04	1.60	1.36
62.14	0.1000	0.7993	0.1838	0.6522	1.52	1.06	3.72	83.36	0.8016	0.1785	0.7630	0.2254	1.01	1.84	1.19

Table 5. Fitted G^E Model Parameters and Standard Deviations for the Ternary System {DIPE (1) + Ethanol (2) + 2,2,4-Trimethylpentane (3)} at 333.15 K

G^E model	A_{ij}/J·mol^{-1}	A_{ji}/J·mol^{-1}	α	Δy	
Wilson	1 + 2	−518.553	3721.157		
	2 + 3	8798.133	278.723		0.0155
	1 + 3	164.886	−192.609		
NRTL	1 + 2	2818.793	−220.056	0.1000	
	2 + 3	4578.878	6039.814	0.5764	0.0146
	1 + 3	880.493	−1038.619	0.1000	
UNIQUAC	1 + 2	2482.263	−752.403		
	2 + 3	−1014.734	4986.466		0.0181
	1 + 3	−180.570	152.366		

from 1.40 to 1.58. The experimental procedure is described in detail elsewhere.[13] The calibration of the density meter and refractometer were carried out periodically by using doubly distilled water and dried air. Mixture samples were prepared simultaneously for density and refractive indices measurements.

A commercial isothermal flow calorimeter (model 7501, Hart Scientific) was used for the measurement of excess enthalpy for binary systems. The calorimeter consists of two solvent pumps (ISCO, LC 2600, 260 cm^3), a temperature-regulated flow cell equipped with a pulsed heater, a Peltier cooler, and a back-pressure regulator to prevent evaporation. The Peltier cooler operated at constant power, producing constant heat loss from the calorimeter cell. The temperature of the cell was kept constant by adjusting the frequency of the pulsed heater to compensate for the cooling from the Peltier cooler and the heat of mixing effect. The uncertainty of the experimental values was estimated to be less than ± 1 % of the H^E values measured. This apparatus has been described in detail.[14]

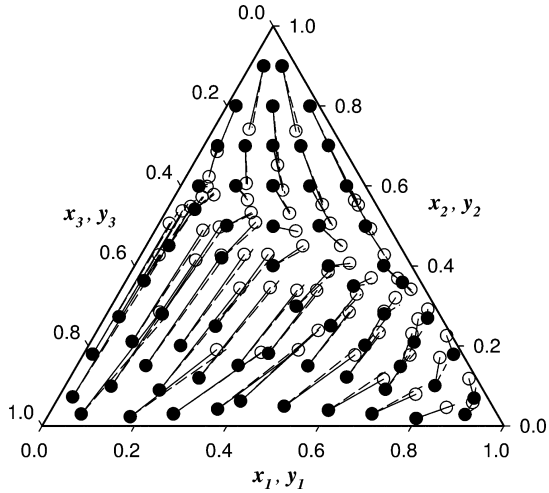

Figure 2. VLE for the ternary system {DIPE (1) + ethanol (2) + 2,2,4-trimethylpentane (3)} at 333.15 K; ●, liquid phase; ○, vapor phase. Dashed lines were calculated from the NRTL equation.

Results and Discussion

Isothermal VLE. In the HSGC method, equilibrium pressure cannot be measured but is calculated from the experimental vapor phase composition and thermodynamic equations.[10] Vapor pressures of each pure component at 333.15 K were calculated using the Antoine constants in Table 1.

$$\ln P^{sat}(\text{kPa}) = A - \frac{B}{C + T(\text{K})} \quad (1)$$

The experimental VLE compositions and pressures for the binary systems {DIPE + ethanol} and {DIPE + 2,2,4-trimethylpentane} at 333.15 K are listed and plotted in Table 2 and Figure 1, respectively. The binary VLE for the system {ethanol + 2,2,4-trimethylpentane} was taken from our previous work[15] and also represented in Figure 1 for completion of sub-binary systems of the {DIPE + ethanol + 2,2,4-trimethylpentane} mixture.

As shown in Figure 1, the binary system {DIPE + 2,2,4-trimethylpentane} is a zeotrope system, while a minimum

Table 6. Densities, Excess Molar Volumes, Refractive Indices, and Deviations in Molar Refractivity for the Binary Systems {DIPE (1) + Ethanol (2)}, {DIPE (1) + 2,2,4-Trimethylpentane (2)}, and {Ethanol (1) + 2,2,4-Trimethylpentane (2)} at 303.15 K

x_1	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}	n_D	ΔR / cm^3·mol^{-1}
		DIPE (1) + Ethanol (2)		
0.0000	0.78199	0.0000	1.35733	0.0000
0.0495	0.77655	−0.1813	1.35854	−1.6472
0.0994	0.77145	−0.3385	1.35989	−2.9239
0.2002	0.76241	−0.6174	1.36147	−4.6696
0.2997	0.75404	−0.7618	1.36232	−5.5309
0.4003	0.74663	−0.8486	1.36325	−5.7491
0.5012	0.74001	−0.8768	1.36309	−5.5432
0.6012	0.73410	−0.8489	1.36285	−4.9740
0.7018	0.72875	−0.7802	1.36225	−4.1387
0.8040	0.72360	−0.6290	1.36246	−2.9733
0.8996	0.71896	−0.4084	1.36213	−1.7337
0.9505	0.71637	−0.2244	1.36303	−0.8982
1.0000	0.71378	0.0000	1.36425	0.0000
		DIPE (1) + 2,2,4-Trimethylpentane (2)		
0.0000	0.68410	0.0000	1.38650	0.0000
0.0614	0.68550	0.0420	1.38505	−0.0938
0.1204	0.68692	0.0705	1.38372	−0.1700
0.2365	0.68982	0.1181	1.38115	−0.2859
0.3486	0.69278	0.1508	1.37862	−0.3658
0.4525	0.69560	0.1829	1.37619	−0.4103
0.5542	0.69854	0.1920	1.37383	−0.4218
0.6497	0.70145	0.1886	1.37172	−0.3912
0.7437	0.70450	0.1635	1.36963	−0.3353
0.8322	0.70761	0.1075	1.36774	−0.2532
0.9187	0.71076	0.0510	1.36596	−0.1360
0.9598	0.71233	0.0149	1.36512	−0.0714
1.0000	0.71378	0.0000	1.36425	0.0000
		Ethanol (1) + 2,2,4-Trimethylpentane (2)		
0.0000	0.68410	0.0000	1.38650	0.0000
0.0610	0.68545	0.1982	1.38633	−1.2465
0.1201	0.68720	0.3136	1.38632	−2.3961
0.2363	0.69181	0.3930	1.38482	−4.6213
0.3467	0.69727	0.4212	1.38404	−6.3421
0.4530	0.70374	0.4178	1.38109	−7.7670
0.5525	0.71114	0.4013	1.37746	−8.6596
0.6502	0.72018	0.3606	1.37322	−8.9483
0.7431	0.73088	0.3166	1.36851	−8.4713
0.8322	0.74405	0.2433	1.36386	−7.0318
0.9176	0.76058	0.1389	1.36145	−4.2809
0.9599	0.77078	0.0697	1.35789	−2.4025
1.0000	0.78199	0.0000	1.35733	0.0000

boiling azeotrope was observed in the {DIPE + ethanol} system. The interpolated azeotropic point for system {DIPE + ethanol} is $x_1^{az} = 0.768$ and $P^{az} = 81.23$ kPa. The measured binary VLE for the system {DIPE + 2,2,4-trimethylpentane} was compared with the reported data of Wichterle.[16] The comparison data agreed well within $\Delta y_1 = 0.0093$. These literature data for the system {DIPE + 2,2,4-trimethylpentane} were measured at 313.15 K. So we converted these data to the data at 333.15 K using their binary model parameters for comparison.

On the other hand, the measured binary VLE data were correlated with five common G^E models: Margules, van Laar, Wilson, NRTL, and UNIQUAC equations. The adjustable binary parameters of the G^E model correlation are listed in Table 3, along with the mean deviation of vapor-phase equilibrium composition. In most cases, the mean deviations of correlation results were less than 1.0 %. This mean deviation of the vapor-phase mole fraction (Δy_1) was calculated from eq 2.

$$\Delta y_1 = \frac{|\Delta y_{1,exp} - \Delta y_{1,cal}|}{N} \quad (2)$$

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

$$A_{ij} = (\lambda_{ij} - \lambda_{ii}) \quad \text{(Wilson)}$$

$$A_{ij} = (g_{ij} - g_{ii}) \quad \text{(NRTL)}$$

$$A_{ij} = (u_{ij} - u_{ii}) \quad \text{(UNIQUAC)}$$

The measured ternary VLE data of the system {DIPE + ethanol + 2,2,4-trimethylpentane} at 333.15 K are listed in Table 4 and illustrated in Figure 2. The ternary VLE data were correlated with the Wilson, NRTL, and UNIQUAC models. Their correlation result shows about 1.9 % mean deviation of the vapor phase mole fraction. This relatively large deviation may be caused from small amount of data points. The NRTL model gave a slightly better correlation result compare to the Wilson and UNIQUAC models. Dashed lines in Figure 2 represent the recalculated values from the NRTL model. The G^E model parameters and the mean deviation of vapor-phase mole fractions (Δy) are given in Table 5. Δy is then determined by

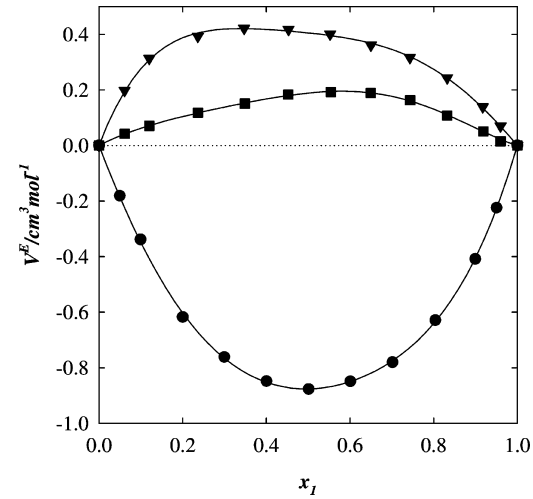

Figure 3. V^E for three binary systems at 303.15 K: ●, {DIPE (1) + ethanol (2)}; ■, {DIPE (1) + 2,2,4-trimethylpentane (2)}; ▼, {ethanol (1) + 2,2,4-trimethylpentane (2)}. Solid curves were calculated from the Redlich−Kister parameters.

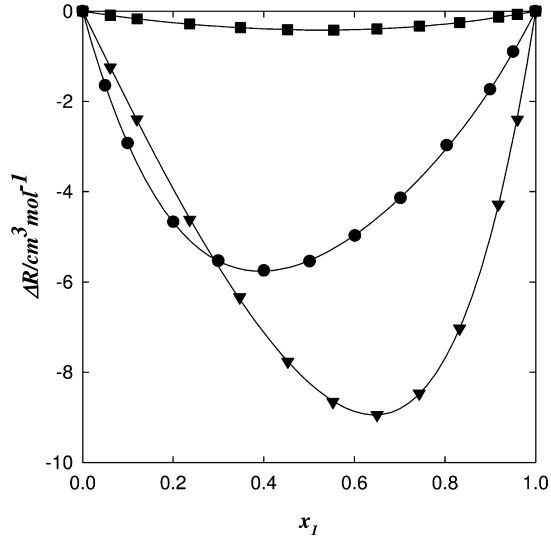

Figure 4. ΔR for three binary systems at 303.15 K: ●, {DIPE (1) + ethanol (2)}; ■, {DIPE (1) + 2,2,4-trimethylpentane (2)}; ▼, {ethanol (1) + 2,2,4-trimethylpentane (2)}. Solid curves were calculated from the Redlich−Kister parameters.

$$\Delta y = \frac{\Delta y_1 + \Delta y_2 + \Delta y_3}{3} \quad (3)$$

Excess Molar Volumes and Refractive Indices. The measured density, refractive indices, and calculated V^E and ΔR at 303.15 K for the binary systems {DIPE + ethanol}, {DIPE + 2,2,4 trimethylpentane}, and {ethanol + 2,2,4 trimethylpentane} are listed in Table 6. The V^E data for ternary mixtures are calculated from the measured densities of pure substances and mixtures with eq 4.

$$V^E = \frac{\sum_i x_i M_i}{\rho_m} - \sum_i \left(\frac{x_i M_i}{\rho_i} \right) \quad (4)$$

where x_i, M_i, ρ_i and ρ_m are the mole fraction, molar mass, densities of pure component i and mixture (m), respectively.

ΔR were calculated from molar refractivity (R_m) of each of the pure and mixture components, which are derived from measured densities and refractive indices using eqs 5 to 8.[17,18]

Table 7. Densities, Excess Molar Volumes, Refractive Indices, and Deviations in Molar Refractivity for the Ternary System {DIPE (1) + Ethanol (2) + 2,2,4-Trimethylpentane (3)} at 303.15 K

		ρ	V^E		ΔR
x_1	x_2	g·cm^{-3}	cm^3·mol^{-1}	n_D	cm^3·mol^{-1}
0.0598	0.5395	0.71397	0.2271	1.37512	−8.3672
0.0509	0.4490	0.70626	0.2932	1.37875	−7.6500
0.0395	0.3607	0.69997	0.3315	1.38170	−6.5711
0.0295	0.2702	0.69455	0.3607	1.38447	−5.1157
0.0193	0.1798	0.69007	0.3481	1.38590	−3.5063
0.1799	0.4196	0.71113	0.0177	1.37620	−6.9149
0.1497	0.3500	0.70447	0.1361	1.37881	−6.2237
0.1197	0.2817	0.69903	0.1959	1.38066	−5.3477
0.0895	0.2112	0.69411	0.2548	1.38267	−4.1958
0.0300	0.0689	0.68658	0.1921	1.38539	−1.4697
0.3015	0.2989	0.70793	−0.0469	1.37502	−5.3100
0.2499	0.2499	0.70251	0.0498	1.37733	−4.7507
0.2002	0.2009	0.69759	0.1637	1.37940	−4.0274
0.1499	0.1509	0.69344	0.1926	1.38153	−3.1567
0.1001	0.0995	0.68964	0.2136	1.38398	−2.0934
0.3501	0.1490	0.70038	0.0388	1.37684	−3.0510
0.2799	0.1194	0.69633	0.1080	1.37889	−2.5803
0.2095	0.0897	0.69264	0.1548	1.38098	−2.0176
0.0702	0.0310	0.68644	0.1425	1.38477	−0.7294
0.3597	0.0409	0.69501	0.1209	1.37789	−1.1599
0.2698	0.0302	0.69196	0.1215	1.38033	−0.8928
0.1793	0.0207	0.68910	0.1151	1.38257	−0.6220
0.0402	0.6003	0.71813	0.2652	1.37373	−8.6714
0.0302	0.6997	0.72812	0.2383	1.36991	−8.5203
0.0198	0.8000	0.74094	0.1991	1.36579	−7.3766
0.1499	0.5003	0.71610	0.0336	1.37375	−7.7063
0.1200	0.6004	0.72378	0.0492	1.37129	−8.1284
0.0902	0.6998	0.73325	0.0472	1.36785	−7.9450
0.0303	0.9000	0.76098	0.0185	1.36141	−4.3750
0.2998	0.4001	0.71578	−0.1568	1.37277	−6.3333
0.2498	0.4998	0.72218	−0.1818	1.37120	−7.1443
0.1999	0.6005	0.72981	−0.1868	1.36928	−7.5033
0.1501	0.6998	0.73900	−0.1963	1.36657	−7.3002
0.1001	0.7999	0.74998	−0.1477	1.36381	−6.2345
0.4202	0.3998	0.72264	−0.4071	1.36966	−5.7960
0.3501	0.4997	0.72895	−0.4432	1.36843	−6.5317
0.2801	0.6002	0.73631	−0.4501	1.36692	−6.8466
0.2103	0.6996	0.74475	−0.4154	1.36513	−6.6121
0.0699	0.9002	0.76689	−0.1873	1.36040	−3.5687
0.5407	0.3996	0.73017	−0.6954	1.36561	−5.2383
0.4501	0.4998	0.73620	−0.7226	1.36521	−5.8726
0.3601	0.5998	0.74300	−0.7036	1.36456	−6.1257
0.2698	0.6999	0.75064	−0.6229	1.36347	−5.8897
0.1798	0.7999	0.75965	−0.5045	1.36195	−4.9928
0.3998	0.0611	0.69712	0.1247	1.37669	−1.5296
0.4993	0.0496	0.69957	0.1307	1.37461	−1.2914
0.6003	0.0397	0.70226	0.1223	1.37228	−1.0881
0.7004	0.0294	0.70498	0.1061	1.37018	−0.8430
0.8005	0.0188	0.70780	0.0743	1.36734	−0.6527
0.4001	0.1795	0.70400	−0.0163	1.37488	−3.4949
0.5008	0.1491	0.70587	−0.0526	1.37314	−2.8922
0.6015	0.1182	0.70775	−0.0993	1.37071	−2.3585
0.6999	0.0892	0.70927	−0.0734	1.36891	−1.7858
0.9011	0.0282	0.71242	−0.0605	1.36484	−0.6677
0.4002	0.2994	0.71266	−0.2038	1.37254	−5.0534
0.5008	0.2491	0.71327	−0.2428	1.37114	−4.2091
0.5994	0.2003	0.71393	−0.2891	1.36910	−3.4542
0.6996	0.1500	0.71411	−0.2609	1.36754	−2.6229
0.7979	0.1023	0.71443	−0.2408	1.36583	−1.8492
0.4999	0.3501	0.72237	−0.4756	1.36851	−5.1594
0.6000	0.2803	0.72109	−0.5016	1.36717	−4.2757
0.7001	0.2094	0.71938	−0.4458	1.36596	−3.3120
0.9009	0.0691	0.71611	−0.2688	1.36356	−1.2743
0.6006	0.3598	0.72931	−0.7101	1.36501	−4.7811
0.6993	0.2708	0.72560	−0.6763	1.36406	−3.8899
0.7993	0.1806	0.72176	−0.5515	1.36295	−2.8401

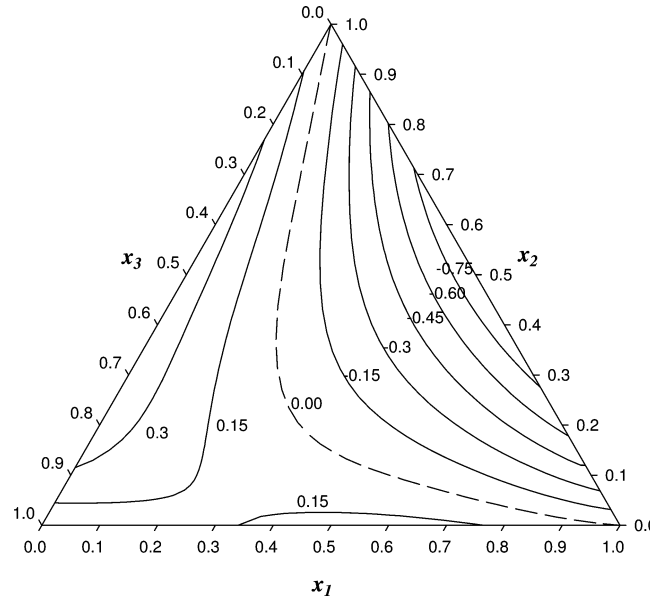

Figure 5. Isoclines of V^E/cm^3·mol^{-1} for the ternary system {DIPE (1) + ethanol (2) + 2,2,4-trimethylpentane (3)} at 303.15 K.

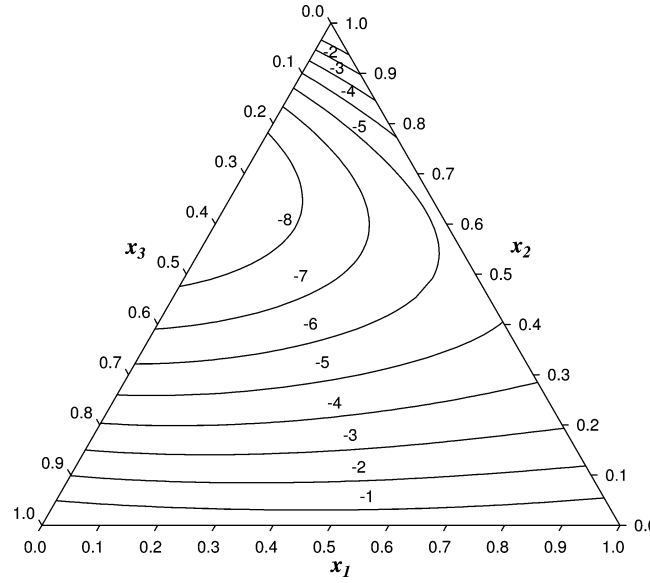

Figure 6. Isoclines of ΔR/cm^3·mol^{-1} for the ternary system {DIPE (1) + ethanol (2) + 2,2,4-trimethylpentane (3)} at 303.15 K.

$$\Delta R/\mathrm{cm}^3\cdot\mathrm{mol}^{-1} = R_m - \sum_i \phi_i R_i \quad (5)$$

$$R_m = \left(\frac{{n_D}^2 - 1}{{n_D}^2 + 1}\right)\left(\frac{\sum_i x_i M_i}{\rho_m}\right) \quad (6)$$

$$R_i = \left(\frac{{n_{D,i}}^2 - 1}{{n_{D,i}}^2 + 1}\right)\left(\frac{M_i}{\rho_i}\right) \quad (7)$$

$$\phi_i = \frac{x_i V_i}{\sum_j x_j V_j} \quad (8)$$

where ϕ_i, n_D, $n_{D,i}$, and V_i are the volume fraction of pure component in mixture, refractive index of mixture, and the refractive index and molar volume of pure component, respectively.

The measured binary V^E and ΔR at 303.15 K were plotted in Figures 3 and 4, respectively. The mean deviations of V^E are (0.0073, 0.0027, and 0.0071) $\mathrm{cm}^3\cdot\mathrm{mol}^{-1}$ for the systems {DIPE + ethanol}, {DIPE + 2,2,4 trimethylpentane}, and {ethanol + 2,2,4 trimethylpentane}, respectively. Among the systems studied, V^E of the system {DIPE + ethanol} show negative deviations from ideal behavior over the whole composition range, while the other two systems show positive deviation. Negative deviation should be caused by the strong polarity of ethanol, and positive deviation may be caused from the mixing of nonpolar hydrocarbon or hydrogen bond rupture or dispersive interaction forces between unlike two molecules as mentioned as explanation by Chen and Tu.[19]

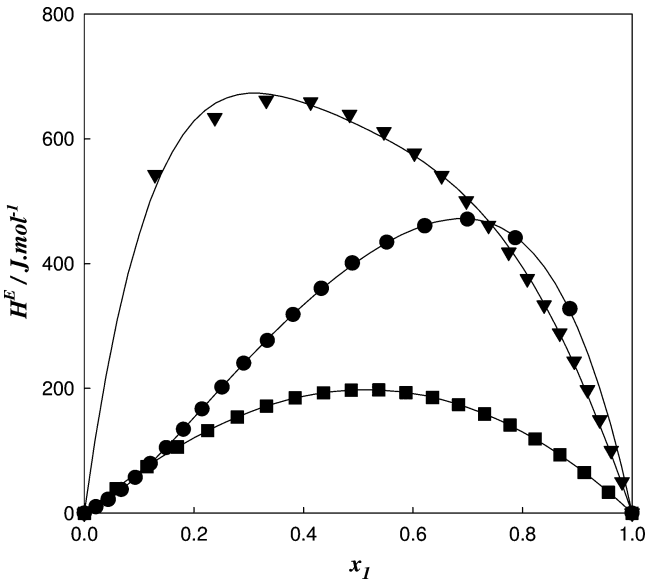

Figure 7. H^E for three binary systems at 303.15 K: ●, {DIPE (1) + ethanol (2)}; ■, {DIPE (1) + 2,2,4-trimethylpentane (2)}; ▼, {ethanol (1) + 2,2,4-trimethylpentane (2)} from previous work.[20] Solid curves were calculated from the Redlich−Kister parameters.

Table 8. Fitted Parameters for the Redlich−Kister or Cibulka Equation and Standard Deviations for V^E and ΔR for the Mixtures of DIPE (1), Ethanol (2), and 2,2,4-Trimethylpentane (3) at 303.15 K

	system	A_1	A_2	A_3	A_4	σ_{st}
V^E	(1) + (2)	−3.5047	0.0507	−1.0614	−0.6869	0.0073
	(2) + (3)	1.6203	−0.3145	1.2468	−0.7651	0.0071
	(1) + (3)	0.7545	0.3060	−0.0094	−0.4648	0.0027
	(1) + (2) + (3)	−3.7207	4.6894	5.3865		0.0127
ΔR	(1) + (2)	−22.1129	8.2950	−5.9334	0.0760	0.0282
	(2) + (3)	−32.9394	−18.0732	−9.4778	−4.1649	0.0346
	(1) + (3)	−1.6694	−0.2012	−0.0594	0.1001	0.0025
	(1) + (2) + (3)	0.9350	16.4338	42.5285		0.0440

The measured binary V^E and ΔR data were correlated with the four-parameter Redlich−Kister polynomial.[5]

$$V^E \text{ or } \Delta R/\mathrm{cm}^3\cdot\mathrm{mol}^{-1} = x_1 x_2 \sum_{i=1}^{4} A_i (x_1 - x_2)^{i-1} \quad (9)$$

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

$$\sigma_{st}/\mathrm{cm}^3\cdot\mathrm{mol}^{-1} = \left[\frac{\sum_i ((V^E \text{ or } \Delta R)_{cal} - (V^E \text{ or } \Delta R)_{exp})_i^2}{(N - n)}\right]^{1/2} \quad (10)$$

where N is the number of experimental data points and n is the number of fitted parameters.

The ternary V^E and ΔR were correlated with Cibulka equation (eq 11)[6] as a modification of Radojkovič equation (eq 12).[7]

$$V^E_{123} = V^E_{12} + V^E_{23} + V^E_{13} + x_1 x_2 x_3 (A_1 + A_2 x_1 + A_3 x_2) \quad (11\text{-}1)$$

$$\Delta R_{123} = \Delta R_{12} + \Delta R_{23} + \Delta R_{13} + x_1 x_2 x_3 (A_1 + A_2 x_1 + A_3 x_2) \quad (11\text{-}2)$$

$$V^E_{123} = V^E_{12^*} + V^E_{23^*} + V^E_{13^*} \quad (12\text{-}1)$$

$$\Delta R_{123} = \Delta R_{12^*} + \Delta R_{23^*} + \Delta R_{13^*} \quad (12\text{-}2)$$

where V^E_{12}, V^E_{23}, V^E_{13}, ΔR_{12}, ΔR_{23}, and ΔR^{13} represent the excess molar volumes or refractive indices of each binary mixture and x_1, x_2, and x_3 are the mole fractions of component 1, 2, and 3. The correlated values are in good agreement with the experimental data with standard deviations of 0.0127 and 0.0440 for the ternary V^E and ΔR, respectively. The correlated parameters

Table 9. Experimental H^E Data for the Binary Systems {DIPE (1) + Ethanol (2)} and {DIPE (1) + 2,2,4-Trimethylpentane (2)} at 303.15 K

x_1	H^E / J·mol^{-1}	x_1	H^E / J·mol^{-1}	x_1	H^E / J·mol^{-1}
DIPE (1) + Ethanol (2)					
0.0212	10.048	0.2150	166.780	0.4894	400.777
0.0437	21.906	0.2516	201.984	0.5521	434.130
0.0676	37.741	0.2912	240.109	0.6217	460.345
0.0931	57.098	0.3343	276.573	0.6995	470.996
0.1204	79.274	0.3813	318.279	0.7871	441.139
0.1497	105.006	0.4328	359.941	0.8864	327.487
0.1811	134.259				
DIPE (1) + 2,2,4-Trimethylpentane (2)					
0.0577	38.985	0.4367	192.864	0.7307	158.983
0.1144	74.367	0.4875	197.047	0.7772	141.119
0.1702	105.905	0.5376	197.589	0.8230	118.744
0.2252	132.161	0.5870	193.209	0.8682	93.364
0.2793	154.011	0.6356	185.485	0.9128	65.084
0.3326	171.411	0.6835	173.749	0.9567	33.243
0.3850	184.701				

Table 10. Fitted Parameters for the Redlich−Kister Equation, Standard Deviations, and Partial Molar Excess Enthalpy at Infinite Dilution for Each Binary System at 303.15 K

system	A_1	A_2	A_3	A_4	A_5	σ_{st} / J·mol^{-1}	$\bar{H}_1^{E,\infty}$ / J·mol^{-1}	$\bar{H}_2^{E,\infty}$ / J·mol^{-1}
DIPE (1) + ethanol (2)	1617.79	1231.00	600.10	640.58		1.51	342.32	4093.48
DIPE (1) + 2,2,4-trimethylpentane (2)	790.66	45.05	−23.05	12.71		0.37	709.86	825.38
ethanol (1) + 2,2,4-trimethylpentane (2)[a]	2532.20	−705.90	1130.61	−1481.18	1613.92	4.12	7463.81	3089.65

[a] Parameters taken from ref 20.

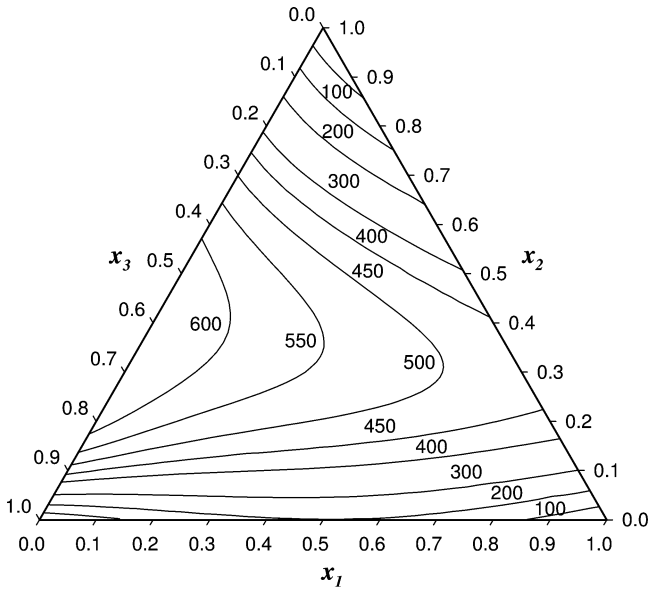

Figure 8. Isoclines of H^E at 303.15 K for the ternary system {DIPE (1) + ethanol (2) + 2,2,4-trimethylpentane (3)}.

for binary and ternary V^E and ΔR data are listed in Table 8 with the standard deviation.

The solid lines in Figures 5 to 6 represent the isocline of ternary V^E and ΔR, calculated by Cibulka equation, respectively.

Excess Molar Enthalpies. The experimental molar excess enthalpies for the binary systems {DIPE + ethanol} and {DIPE + 2,2,4-trimethylpentane} determined at 303.15 K using an isothermal flow calorimeter are listed and plotted in Table 9 and Figure 7. The binary H^E for the system {ethanol + 2,2,4-trimethylpentane} in Figure 7 was taken from our previous work[20] for better comparison. The H^E values of all measured binary systems indicate endothermic mixing of these systems. The binary H^E data were correlated with the Redlich−Kister polynomial,[5] and the values calculated (solid lines) using the correlated parameters are in good agreement with the experimental values, as shown in Figure 7. The adjusted parameters of the Redlich−Kister polynomial are given in Table 10, along with standard deviations between calculated and experimental data. The number of the parameters used to represent the experimental data depends on the molecular complexity of the H^E behavior, the quality of the data, and the number of data points available. The reliable and extensive data justify the use of four and five parameters. For all systems studied, the obtained standard deviations are within the estimated experimental error of 1 %. The partial excess molar enthalpy at infinite dilution, which can be calculated with fitted Redlich−Kister parameters using eq 13, are also reported in Table 10.

$$\bar{H}_1^{E,\infty}/\mathrm{J\cdot mol^{-1}} = A_1 - A_2 + A_3 - A_4 + A_5$$

$$\bar{H}_2^{E,\infty}/\mathrm{J\cdot mol^{-1}} = A_1 + A_2 + A_3 + A_4 + A_5 \qquad (13)$$

Also, the ternary H^E data can be predicted by the Radojkovič equation,[7] and we calculate ternary H^E data for the system {DIPE + ethanol + 2,2,4-trimethylpentane} at 303.15 K. The Radojkovič equation is used only with the constituent binary Redlich−Kister parameters from Table 10. The predicted isoclines are plotted in Figure 8. As shown in the figure, this ternary system shows positive values of H^E at all of the composition ranges as we expected from each constituent binary H^E data.

Conclusion

Isothermal VLE data at 333.15 K were experimentally determined for the binary systems {DIPE + ethanol} and {DIPE + 2,2,4-trimethylpentane} and the ternary system {DIPE + ethanol + 2,2,4-trimethylpentane}. The system {DIPE + ethanol} shows a minimum boiling azeotrope. The excess molar volume (V^E) and deviations in molar refractivity (ΔR) were measured at 303.15 K for the binary systems {DIPE + ethanol}, {DIPE + 2,2,4-trimethylpentane}, and {ethanol + 2,2,4-trimethylpentane} and the ternary system {DIPE + ethanol + 2,2,4-trimethylpentane}. The V^E for the system {DIPE + ethanol} shows negative deviations from ideal behavior, while the other two binary systems show positive deviations. The ΔR at 303.15 K of all of the binary systems show negative values. While the ternary V^E data show negative and positive values, ΔR of the ternary system shows only negative values as we expected from the constituent binary data. In addition, molar excess enthalpies (H^E) were determined at 303.15 K, for two binary systems, {DIPE + ethanol} and {DIPE + 2,2,4-trimethylpentane}. The experimental H^E values show positive deviations (endothermic mixing) from the ideality. The measured VLE, V^E, ΔR, and H^E data were correlated well with the common activity coefficient models and the Redlich−Kister polynomial or Cibulka equation.

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