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Excess Molar Volumes and Surface Tensions of 1,2,4-Trimethylbenzene and 1,3,5-Trimethylbenzene with Isopropyl Acetate and Isobutyl Acetate at (298.15, 308.15, and 313.15) K

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Densities and surface tensions for the binary mixtures of 1,2,4-trimethylbenzene and 1,3,5-trimethylbenzene with isopropyl acetate and isobutyl acetate have been measured over the whole composition range. The measurements were made under normal atmospheric pressure and at the temperatures (298.15, 308.15, and 313.15) K. The excess molar volumes and surface tension deviations are derived from the experimental data. The excess molar volumes for all the binary systems are positive, and the surface tension deviations are negative.

Introduction

The density and surface tension of the liquid mixtures are important physical properties for understanding and interpreting the interaction between unlike molecules of the mixtures. They also play an important role in the process of the mass and heat transfer at an interface, such as in liquid−liquid extraction, gas absorption, and distillation. In the course of separating mixed isomeric xylene and trimethylbenzene, our group has developed a high-performance separation method (called urging rectification).[1] The key point to urging rectification is to add a proper solvent (called urging solvent) to the rectification system, which has the function of urging the separation of different components. The determination of excess properties of the mixtures involved is vital for selecting an efficient urging solvent. For contributing to the project of separating mixed trimethylbenzene, this work measured densities and surface tensions for the binary mixtures of 1,2,4-trimethylbenzene and 1,3,5-trimethylbenzene with isopropyl acetate and isobutyl acetate over the whole concentration range at the temperatures (298.15, 308.15, and 313.15) K. The experimental data were used to calculate the excess molar volumes and surface tension deviations of these systems, and the excess functions were fitted to the Redlich−Kister polynomials.

Experimental Section

All the chemicals, 1,2,4-trimethylbenzene (Acros Organics), 1,3,5-trimethylbenzene (Acros Organics), isopropyl acetate (Acros Organics), and isobutyl acetate (Tokyo Kosei Kogyo Co.), are commercially available and used without further purification. Except isobutyl acetate (chromatographical grade), the other reagents are chemically pure. The mass fractions of the chemically pure substance, determined by a Varian CP-3800 chromatograph, were as follows: 1,2,4-trimethylbenzene (99.20 %), 1,3,5-trimethylbenzene (99.30 %), and isopropyl acetate (99.80 %). All the binary mixtures studied were prepared by mass using an Ohaus E12140 balance with an uncertainty of ± 0.0001 g. The relative atomic masses issued by IUPAC in 2001 were applied for the conversion of the masses to the molar fractions. The uncertainty of the molar fraction is estimated within ± 0.0001 in all cases.

Densities of the pure liquids and their mixtures were measured with an Anton Paar (Austria, DMA 4500) vibrating-tube densimeter where a built-in solid-state thermostat is used to obtain an uncertainty of ± 0.01 K. The densimeter is calibrated with dry air and distilled water before the measurement. The densities of air and water at different temperatures were selected from the instruction manual.[2] The estimated uncertainty of the densities is about $5 \cdot 10^{-5}$ g·cm^{-3}. The surface tensions were determined by the pendant drop method, using a Data Physics OCA20 (Germany) contact angle and surface tension measuring

Table 1. Densities (ρ) and Surface Tensions (σ) of the Pure Components at Experimental Temperatures

	T	ρ/g·cm^{-3}		σ/mN·m^{-1}	
component	K	exptl	lit.	exptl	lit.
1,3,5-trimethylbenzene	298.15	0.86112	0.86114[3]	28.05	28.09[4]
			0.86103[4]		27.55[6]
			0.86104[5]		
	308.15	0.85294	0.85290[3]	27.21	26.65[6]
	313.15	0.84882	0.84874[5]	26.78	26.82[5]
					26.20[6]
1,2,4-trimethylbenzene	298.15	0.87171	0.87178[3]	29.30	29.25[4]
			0.87164[4]		29.29[5]
			0.87174[7]		29.20[6]
	308.15	0.86368	0.86367[3]	28.24	28.17[6]
	313.15	0.85958	0.85954[5]	27.71	27.67[5]
					27.66[6]
isopropyl acetate	298.15	0.87205[a]	0.8718[a,6]	21.89	21.76[6]
		0.86625			
	308.15	0.85454		20.81	20.69[6]
	313.15	0.84861		20.29	20.15[6]
isobutyl acetate	298.15	0.87129[a]	0.8712[a,6]	23.15	23.06[6]
		0.86606			
	308.15	0.85551		22.16	22.04[6]
	313.15	0.85016		21.64	21.54[6]

[a] The data are obtained at 293.15 K.

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Table 2. Experimental Excess Molar Volumes (V^E) at Temperatures (298.15, 308.15, and 313.15) K

x_1	V^E / cm^3·mol^{-1}	x_1	V^E / cm^3·mol^{-1}	x_1	V^E / cm^3·mol^{-1}	x_1	V^E / cm^3·mol^{-1}	x_1	V^E / cm^3·mol^{-1}
				$T = 298.15$ K					
				Isopropyl Acetate (1) + 1,2,4-Trimethylbenzene (2)					
0.0492	0.006	0.2510	0.020	0.4500	0.024	0.6492	0.019	0.8495	0.009
0.1010	0.010	0.3006	0.022	0.4998	0.024	0.7004	0.017	0.8995	0.006
0.1507	0.014	0.3513	0.023	0.5498	0.023	0.7501	0.014	0.9492	0.003
0.1995	0.017	0.4008	0.024	0.6007	0.021	0.7968	0.012		
				Isopropyl Acetate (1) + 1,3,5-Trimethylbenzene (2)					
0.0495	0.049	0.2514	0.184	0.4502	0.254	0.6502	0.251	0.8498	0.152
0.1008	0.088	0.2996	0.209	0.5002	0.263	0.7003	0.237	0.8998	0.111
0.1504	0.126	0.3510	0.227	0.5497	0.261	0.7496	0.215	0.9505	0.059
0.1990	0.155	0.4009	0.245	0.6001	0.259	0.7987	0.190		
				Isobutyl Acetate (1) + 1,2,4-Trimethylbenzene (2)					
0.0494	0.012	0.2498	0.047	0.4505	0.068	0.6496	0.066	0.8499	0.040
0.0992	0.023	0.2989	0.054	0.4991	0.070	0.7006	0.065	0.9006	0.029
0.1493	0.033	0.3495	0.060	0.5504	0.070	0.7500	0.058	0.9477	0.014
0.2002	0.040	0.3997	0.064	0.6000	0.068	0.8002	0.052		
				Isobutyl Acetate (1) + 1,3,5-Trimethylbenzene (2)					
0.0510	0.047	0.2498	0.179	0.4502	0.247	0.6494	0.243	0.8502	0.146
0.1006	0.085	0.3003	0.204	0.5004	0.254	0.6998	0.227	0.8998	0.104
0.1506	0.121	0.3500	0.223	0.5499	0.256	0.7498	0.208	0.9491	0.057
0.2004	0.151	0.4004	0.238	0.5996	0.252	0.8007	0.181		
				$T = 308.15$ K					
				Isopropyl Acetate (1) + 1,2,4-Trimethylbenzene (2)					
0.0488	0.004	0.2504	0.013	0.4500	0.018	0.6499	0.015	0.8500	0.007
0.0999	0.007	0.3001	0.014	0.4964	0.018	0.7004	0.013	0.8997	0.004
0.1499	0.009	0.3519	0.016	0.5495	0.017	0.7494	0.010	0.9498	0.003
0.2002	0.011	0.4000	0.017	0.6008	0.016	0.7986	0.009		
				Isopropyl Acetate (1) + 1,3,5-Trimethylbenzene (2)					
0.0501	0.052	0.2514	0.180	0.4503	0.246	0.6500	0.241	0.8488	0.149
0.0993	0.089	0.3018	0.202	0.4993	0.251	0.7003	0.227	0.9004	0.106
0.1514	0.124	0.3530	0.222	0.5492	0.254	0.7499	0.206	0.9506	0.059
0.2000	0.152	0.3991	0.234	0.6000	0.249	0.7993	0.182		
				Isobutyl Acetate (1) + 1,2,4-Trimethylbenzene (2)					
0.0495	0.010	0.2500	0.046	0.4501	0.066	0.6500	0.063	0.8497	0.036
0.0992	0.020	0.2995	0.052	0.4995	0.067	0.6987	0.061	0.8999	0.025
0.1490	0.030	0.3497	0.057	0.5505	0.068	0.7505	0.054	0.9491	0.010
0.1998	0.038	0.4004	0.062	0.5994	0.066	0.7986	0.047		
				Isobutyl Acetate (1) + 1,3,5-Trimethylbenzene (2)					
0.0513	0.052	0.2505	0.178	0.4506	0.246	0.6503	0.242	0.8502	0.144
0.0999	0.087	0.3013	0.203	0.5000	0.253	0.6995	0.225	0.8997	0.101
0.1503	0.122	0.3500	0.222	0.5505	0.251	0.7500	0.205	0.9498	0.055
0.2007	0.153	0.4002	0.237	0.5997	0.250	0.8002	0.180		
				$T = 313.15$ K					
				Isopropyl Acetate (1) + 1,2,4-Trimethylbenzene (2)					
0.0494	0.002	0.2506	0.009	0.4493	0.013	0.6493	0.010	0.8504	0.005
0.0983	0.005	0.3004	0.011	0.4992	0.013	0.6995	0.009	0.9004	0.003
0.1504	0.006	0.3508	0.012	0.5492	0.013	0.7501	0.008	0.9478	0.001
0.1999	0.008	0.3995	0.013	0.6000	0.012	0.8000	0.006		
				Isopropyl Acetate (1) + 1,3,5-Trimethylbenzene (2)					
0.0498	0.047	0.2500	0.171	0.4508	0.236	0.6504	0.231	0.8507	0.141
0.1001	0.084	0.3005	0.194	0.4998	0.242	0.7000	0.217	0.9008	0.102
0.1495	0.116	0.3497	0.210	0.5496	0.243	0.7495	0.199	0.9504	0.053
0.2006	0.146	0.3998	0.227	0.6007	0.241	0.7993	0.173		
				Isobutyl Acetate (1) + 1,2,4-Trimethylbenzene (2)					
0.0506	0.009	0.2505	0.042	0.4501	0.059	0.6492	0.057	0.8480	0.031
0.1002	0.017	0.3001	0.047	0.5001	0.059	0.6997	0.052	0.8998	0.018
0.1499	0.027	0.3502	0.052	0.5503	0.060	0.7500	0.046	0.9498	0.007
0.2001	0.034	0.3995	0.055	0.6007	0.059	0.8010	0.040		
				Isobutyl Acetate (1) + 1,3,5-Trimethylbenzene (2)					
0.0494	0.047	0.2499	0.173	0.4492	0.238	0.6503	0.232	0.8499	0.133
0.1000	0.083	0.2990	0.195	0.5003	0.246	0.6995	0.218	0.9002	0.096
0.1493	0.114	0.3492	0.214	0.5518	0.245	0.7512	0.196	0.9504	0.047
0.2002	0.146	0.3988	0.229	0.5992	0.242	0.8005	0.168		

device. The uncertainty of the device is ± 0.05 mN·m^{-1}. The experimental densities and surface tensions of the pure substances are listed in Table 1 and compared with the literature values.

Results and Discussion

The excess molar volumes are determined from the density and molar mass data by the following equation[8]

$$V^{E} = \frac{x_1 M_1 + x_2 M_2}{\rho} - \frac{x_1 M_1}{\rho_1} - \frac{x_2 M_2}{\rho_2} \quad (1)$$

where V^E is the excess molar volumes; x_i and M_i are mole faction and molar mass of the component i, respectively; ρ and ρ_i are the density of the mixture and pure component i, respectively. The experimental excess molar volumes for the four binary mixtures (isopropyl acetate + 1,2,4-trimethylbenzene or + 1,3,5-trimethylbenzene and isobutyl acetate + 1,2,4-trimethylbezene or + 1,3,5-trimethylbenzene) are tabulated in Table 2. The curves of the excess molar volumes versus the composition of the binary mixtures are shown in Figure 1 and Figure 2.

The surface tension deviations of binary mixtures are calculated by the following equation[9]

$$\Delta\sigma = \sigma - x_1\sigma_1 - x_2\sigma_2 \quad (2)$$

where $\Delta\sigma$ is surface tension deviation; σ is surface tension of the binary mixture; σ_1 and σ_2 are surface tensions of the pure components 1 and 2, respectively; and x_1 and x_2 are mole fractions of the component 1 and 2 in the mixture, respectively. The experimental surface tensions and values of surface tension deviations for the four binary mixtures (isopropyl acetate + 1,2,4-trimethylbenzene or + 1,3,5-trimethylbenzene and isobutyl acetate + 1,2,4-trimethylbezene or + 1,3,5-trimethylbenzene) are listed in Table 3. The surface tension deviations are graphically presented in Figure 3 and Figure 4.

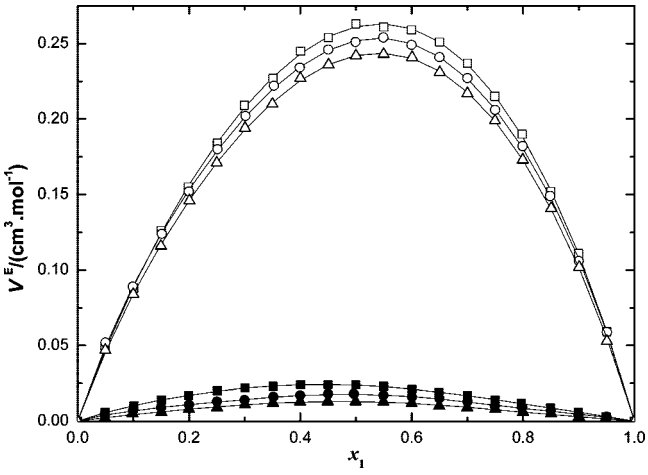

Figure 1. Plots of excess molar volumes (V^E) for isopropyl acetate (1) + 1,2,4-trimethylbenzene (2): at ■, 298.15 K; ●, 308.15 K; ▲, 313.15 K. For isopropyl acetate (1) + 1,3,5-trimethylbenzene (2) at □, 298.15 K; ○, 308.15 K; Δ, 313.15 K. The lines correspond to the calculated values according to the Redlich−Kister equation.

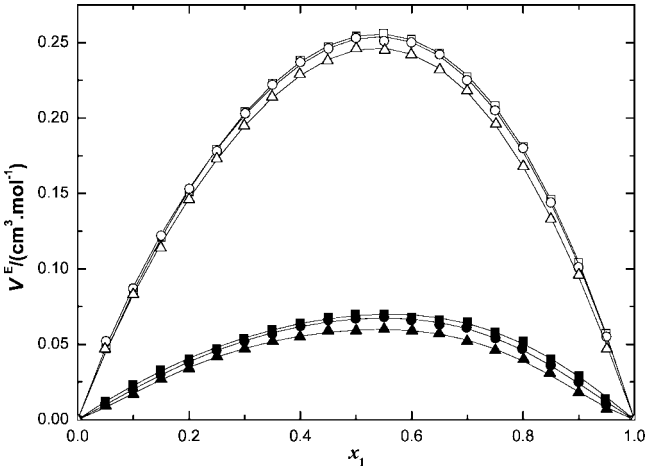

Figure 2. Plots of excess molar volumes (V^E) for isobutyl acetate (1) + 1,2,4-trimethylbenzene (2) at: ■, 298.15 K; ●, 308.15 K; ▲, 313.15 K. For isobutyl acetate (1) + 1,3,5-trimethylbenzene (2) at: □, 298.15 K; ○, 308.15 K; Δ, 313.15 K. The lines correspond to the calculated values according to the Redlich−Kister equation.

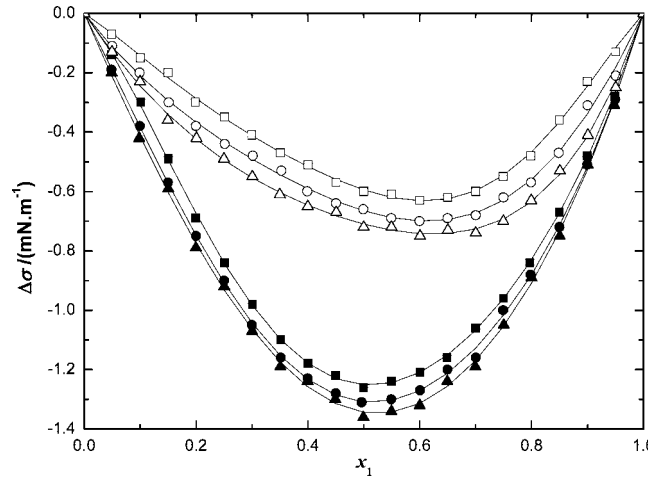

Figure 3. Plots of surface tension deviations ($\Delta\sigma$) for isopropyl acetate (1) + 1,2,4-trimethylbenzene (2) at: ■, 298.15 K; ●, 308.15 K; ▲, 313.15 K. For isopropyl acetate (1) + 1,3,5-trimethylbenzene (2) at: □, 298.15 K; ○, 308.15 K; Δ, 313.15 K. The lines correspond to the calculated values according to the Redlich−Kister equation.

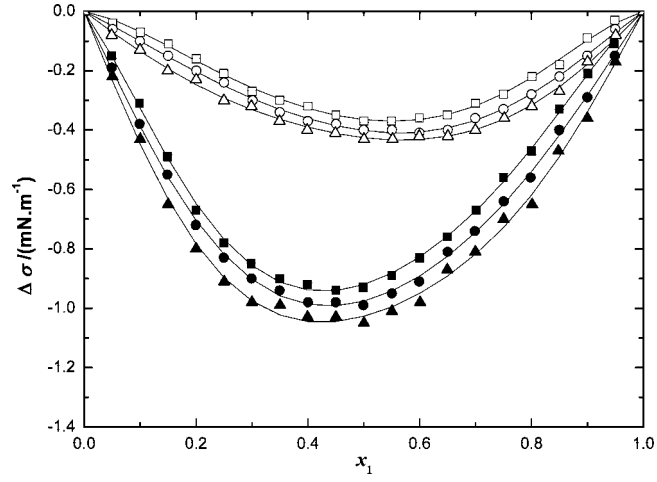

Figure 4. Plots of surface tension deviations ($\Delta\sigma$) for isobutyl acetate (1) + 1,2,4-trimethylbenzene (2) at: ■, 298.15 K; ●, 308.15 K; ▲, 313.15 K. For isobutyl acetate (1) + 1,3,5-trimethylbenzene (2) at: □, 298.15 K; ○, 308.15 K; Δ, 313.15 K. The lines correspond to the calculated values according to the Redlich−Kister equation.

The experimental results of excess molar volumes and surface tension deviations over the whole concentration range are fitted by the Redlich−Kister[10] polynomial equation:

$$f(x) = x(1-x)\sum_{i=0}^{k} A_i(1-2x)^i \quad (3)$$

where $f(x)$ represents the excess properties V^E or $\Delta\sigma$; x is mole fraction; A_i represents the ith parameter used for smoothing the curves of $V^E \sim x$ or $\Delta\sigma \sim x$ according to eq 3. A nonlinear least-squares method is used to estimated the parameters A_i.

Table 3. Experimental Surface Tensions (σ) and Surface Tension Deviations ($\Delta\sigma$) at Temperatures of (298.15, 308.15, and 313.15) K

x_1	σ / mN·m^{-1}	$\Delta\sigma$ / mN·m^{-1}	x_1	σ / mN·m^{-1}	$\Delta\sigma$ / mN·m^{-1}	x_1	σ / mN·m^{-1}	$\Delta\sigma$ / mN·m^{-1}	x_1	σ / mN·m^{-1}	$\Delta\sigma$ / mN·m^{-1}	x_1	σ / mN·m^{-1}	$\Delta\sigma$ / mN·m^{-1}
						$T = 298.15$ K								
						Isopropyl Acetate (1) + 1,2,4-Trimethylbenzene (2)								
0.0000	29.30	0.00	0.2510	26.60	−0.84	0.4998	24.34	−1.26	0.7501	22.78	−0.96	1.0000	21.89	0.00
0.0492	28.80	−0.14	0.3006	26.09	−0.98	0.5498	23.99	−1.24	0.7968	22.56	−0.84			
0.1010	28.25	−0.30	0.3513	25.60	−1.10	0.6007	23.64	−1.21	0.8495	22.34	−0.67			
0.1507	27.69	−0.49	0.4008	25.15	−1.18	0.6492	23.33	−1.16	0.8995	22.15	−0.48			
0.1995	27.13	−0.69	0.4500	24.75	−1.22	0.7004	23.05	−1.06	0.9492	21.99	−0.28			
						Isopropyl Acetate (1) + 1,3,5-Trimethylbenzene (2)								
0.0000	28.05	0.00	0.2514	26.15	−0.35	0.5002	24.37	−0.60	0.7496	22.88	−0.55	1.0000	21.89	0.00
0.0495	27.68	−0.07	0.2996	25.79	−0.41	0.5497	24.05	−0.61	0.7987	22.65	−0.48			
0.1008	27.28	−0.15	0.3510	25.42	−0.47	0.6001	23.72	−0.63	0.8498	22.46	−0.36			
0.1504	26.92	−0.20	0.4009	25.07	−0.51	0.6502	23.42	−0.62	0.8998	22.28	−0.23			
0.1990	26.52	−0.30	0.4502	24.71	−0.57	0.7003	23.14	−0.60	0.9505	22.06	−0.13			
						Isobutyl Acetate (1) + 1,2,4-Trimethylbenzene (2)								
0.0000	29.30	0.00	0.2498	26.98	−0.78	0.4991	25.30	−0.93	0.7500	24.13	−0.56	1.0000	23.15	0.00
0.0494	28.85	−0.15	0.2989	26.61	−0.85	0.5504	25.03	−0.89	0.8002	23.91	−0.47			
0.0992	28.38	−0.31	0.3495	26.25	−0.90	0.6000	24.78	−0.83	0.8499	23.74	−0.33			
0.1493	27.89	−0.49	0.3997	25.92	−0.92	0.6496	24.54	−0.76	0.9006	23.55	−0.21			
0.2002	27.40	−0.67	0.4505	25.59	−0.94	0.7006	24.32	−0.67	0.9477	23.36	−0.11			
						Isobutyl Acetate (1) + 1,3,5-Trimethylbenzene (2)								
0.0000	28.05	0.00	0.2498	26.62	−0.21	0.5004	25.23	−0.37	0.7498	24.10	−0.28	1.0000	23.15	0.00
0.0510	27.76	−0.04	0.3003	26.31	−0.27	0.5499	24.99	−0.37	0.8007	23.91	−0.22			
0.1006	27.49	−0.07	0.3500	26.04	−0.30	0.5996	24.75	−0.36	0.8502	23.70	−0.18			
0.1506	27.20	−0.11	0.4004	25.77	−0.32	0.6494	24.52	−0.35	0.8998	23.55	−0.09			
0.2004	26.91	−0.16	0.4502	25.49	−0.35	0.6998	24.31	−0.31	0.9491	23.37	−0.03			
						$T = 308.15$ K								
						Isopropyl Acetate (1) + 1,2,4-Trimethylbenzene (2)								
0.0000	28.24	0.00	0.2504	25.48	−0.90	0.4964	23.24	−1.31	0.7494	21.67	−1.00	1.0000	20.81	0.00
0.0488	27.69	−0.19	0.3001	24.96	−1.05	0.5495	22.86	−1.30	0.7986	21.43	−0.88			
0.0999	27.12	−0.38	0.3519	24.47	−1.16	0.6008	22.51	−1.27	0.8500	21.20	−0.72			
0.1499	26.56	−0.57	0.4000	24.04	−1.23	0.6499	22.21	−1.20	0.8997	21.05	−0.51			
0.2002	26.00	−0.75	0.4500	23.62	−1.28	0.7004	21.88	−1.16	0.9498	20.89	−0.29			
						Isopropyl Acetate (1) + 1,3,5-Trimethylbenzene (2)								
0.0000	27.21	0.00	0.2514	25.16	−0.44	0.4993	23.35	−0.66	0.7499	21.79	−0.62	1.0000	20.81	0.00
0.0501	26.78	−0.11	0.3018	24.80	−0.48	0.5492	23.01	−0.69	0.7993	21.52	−0.57			
0.0993	26.37	−0.20	0.3530	24.42	−0.53	0.6000	22.67	−0.70	0.8488	21.31	−0.47			
0.1514	25.94	−0.30	0.3991	24.06	−0.60	0.6500	22.36	−0.69	0.9004	21.14	−0.31			
0.2000	25.55	−0.38	0.4503	23.69	−0.64	0.7003	22.05	−0.68	0.9506	20.92	−0.21			
						Isobutyl Acetate (1) + 1,2,4-Trimethylbenzene (2)								
0.0000	28.24	0.00	0.2500	25.89	−0.83	0.4995	24.21	−0.99	0.7505	23.04	−0.64	1.0000	22.16	0.00
0.0495	27.75	−0.19	0.2995	25.52	−0.90	0.5505	23.94	−0.95	0.7986	22.82	−0.56			
0.0992	27.26	−0.38	0.3497	25.17	−0.94	0.5994	23.69	−0.91	0.8497	22.67	−0.40			
0.1490	26.78	−0.55	0.4004	24.83	−0.98	0.6500	23.48	−0.81	0.8999	22.48	−0.29			
0.1998	26.31	−0.72	0.4501	24.52	−0.98	0.6987	23.25	−0.74	0.9491	22.32	−0.15			
						Isobutyl Acetate (1) + 1,3,5-Trimethylbenzene (2)								
0.0000	27.21	0.00	0.2505	25.70	−0.24	0.5000	24.29	−0.40	0.7500	23.09	−0.33	1.0000	22.16	0.00
0.0513	26.89	−0.06	0.3013	25.39	−0.30	0.5505	24.03	−0.40	0.8002	22.89	−0.28			
0.0999	26.61	−0.10	0.3500	25.10	−0.34	0.5997	23.77	−0.41	0.8502	22.70	−0.22			
0.1503	26.30	−0.15	0.4002	24.82	−0.37	0.6503	23.53	−0.40	0.8997	22.52	−0.15			
0.2007	26.00	−0.20	0.4506	24.55	−0.38	0.6995	23.32	−0.36	0.9498	22.35	−0.06			
						$T = 313.15$ K								
						Isopropyl Acetate (1) + 1,2,4-Trimethylbenzene (2)								
0.0000	27.71	0.00	0.2506	24.93	−0.92	0.4992	22.65	−1.36	0.7501	21.09	−1.05	1.0000	20.29	0.00
0.0494	27.14	−0.20	0.3004	24.41	−1.07	0.5492	22.29	−1.34	0.8000	20.88	−0.89			
0.0983	26.56	−0.42	0.3508	23.92	−1.19	0.6000	21.94	−1.32	0.8504	20.65	−0.75			
0.1504	26.00	−0.59	0.3995	23.51	−1.24	0.6493	21.65	−1.24	0.9004	20.52	−0.51			
0.1999	25.44	−0.79	0.4493	23.08	−1.30	0.6995	21.33	−1.19	0.9478	20.37	−0.31			
						Isopropyl Acetate (1) + 1,3,5-Trimethylbenzene (2)								
0.0000	26.78	0.00	0.2500	24.67	−0.49	0.4998	22.82	−0.72	0.7495	21.22	−0.70	1.0000	20.29	0.00
0.0498	26.33	−0.13	0.3005	24.28	−0.55	0.5496	22.49	−0.72	0.7993	20.96	−0.63			
0.1001	25.90	−0.23	0.3497	23.90	−0.61	0.6007	22.13	−0.75	0.8507	20.73	−0.53			
0.1495	25.45	−0.36	0.3998	23.54	−0.65	0.6504	21.83	−0.73	0.9008	20.52	−0.41			
0.2006	25.06	−0.42	0.4508	23.18	−0.67	0.7000	21.50	−0.74	0.9504	20.36	−0.25			
						Isobutyl Acetate (1) + 1,2,4-Trimethylbenzene (2)								
0.0000	27.71	0.00	0.2505	25.28	−0.91	0.5001	23.62	−1.05	0.7500	22.46	−0.70	1.0000	21.64	0.00
0.0506	27.18	−0.22	0.3001	24.91	−0.98	0.5503	23.36	−1.01	0.8010	22.20	−0.65			
0.1002	26.67	−0.43	0.3502	24.59	−0.99	0.6007	23.08	−0.98	0.8480	22.09	−0.47			

Table 3. Continued

x_1	σ / mN·m^{-1}	$\Delta\sigma$ / mN·m^{-1}	x_1	σ / mN·m^{-1}	$\Delta\sigma$ / mN·m^{-1}	x_1	σ / mN·m^{-1}	$\Delta\sigma$ / mN·m^{-1}	x_1	σ / mN·m^{-1}	$\Delta\sigma$ / mN·m^{-1}	x_1	σ / mN·m^{-1}	$\Delta\sigma$ / mN·m^{-1}
0.1499	26.15	−0.65	0.3995	24.26	−1.03	0.6492	22.90	−0.87	0.8998	21.89	−0.36			
0.2001	25.70	−0.80	0.4501	23.95	−1.03	0.6997	22.65	−0.81	0.9498	21.77	−0.17			
Isobutyl Acetate (1) + 1,3,5-Trimethylbenzene (2)														
0.0000	26.78	0.00	0.2499	25.20	−0.30	0.5003	23.78	−0.43	0.7512	22.56	−0.36	1.0000	21.64	0.00
0.0494	26.45	−0.08	0.2990	24.92	−0.32	0.5518	23.51	−0.43	0.8005	22.35	−0.32			
0.1000	26.14	−0.13	0.3492	24.62	−0.37	0.5992	23.28	−0.42	0.8499	22.14	−0.27			
0.1493	25.81	−0.20	0.3988	24.33	−0.40	0.6503	23.02	−0.42	0.9002	21.98	−0.17			
0.2002	25.52	−0.23	0.4492	24.06	−0.41	0.6995	22.78	−0.40	0.9504	21.81	−0.08			

Table 4. Least-Squares Parameters (A_i) and Standard Deviations (d) of Excess Molar Volumes (V^E) and Surface Tension Deviations ($\Delta\sigma$) at Various Temperatures

	T/K	A_0	A_1	A_2	A_3	A_4	d
		V^E/(cm^3·mol^{-1})					
isopropyl acetate (1) + 1,2,4-trimethylbenzene (2)	298.15	0.0951	−0.0292	−0.0237	−0.0002	−0.0252	0.0003
	308.15	0.0713	−0.0080	−0.0516	−0.0122	−0.0639	0.0004
	313.15	0.0524	−0.0095	−0.0322	−0.0006	−0.0228	0.0004
isopropyl acetate (1) + 1,3,5-trimethylbenzene (2)	298.15	1.0451	−0.1748	−0.0680	−0.0361	−0.0471	0.0014
	308.15	1.0080	−0.1626	−0.0357	−0.0606	−0.1672	0.0011
	313.15	0.9687	−0.1563	−0.0415	−0.0504	−0.0932	0.0011
isobutyl acetate (1) + 1,2,4-trimethylbenzene (2)	298.15	0.2766	−0.0623	−0.0345	−0.0344	−0.0320	0.0011
	308.15	0.2671	−0.0542	−0.0216	−0.0420	−0.0865	0.0009
	313.15	0.2375	−0.0413	−0.0280	−0.0529	−0.1354	0.0008
isobutyl acetate (1) + 1,3,5-trimethylbenzene (2)	298.15	1.0168	−0.1545	−0.0614	−0.0248	−0.0063	0.0009
	308.15	1.0096	−0.1582	−0.0504	−0.0861	−0.0441	0.0018
	313.15	0.9805	−0.1512	−0.0033	−0.1125	−0.0081	0.0015
		$\delta\sigma$/(mN·m^{-1})					
isopropyl acetate (1) + 1,2,4-trimethylbenzene (2)	298.15	−5.0061	−0.2586	−0.7523	−1.5241	−0.2945	0.0088
	308.15	−5.2331	−0.3697	−0.4509	−0.8717	−0.1302	0.0120
	313.15	−5.3719	−0.5673	−0.4092	−0.3480	−0.2956	0.0162
isopropyl acetate (1) + 1,3,5-trimethylbenzene (2)	298.15	−2.3791	−1.2356	−0.3255	−0.8237	−1.0645	0.0103
	308.15	−2.6593	−1.1450	−0.7134	−0.3901	−0.1586	0.0140
	313.15	−2.8392	−0.9810	−1.3161	−0.3202	−0.0620	0.0116
isobutyl acetate (1) + 1,2,4-trimethylbenzene (2)	298.15	−5.0061	−0.2586	−0.7523	−1.5241	−0.2945	0.0121
	308.15	−5.2331	−0.3697	−0.4509	−0.8717	−0.1302	0.0137
	313.15	−5.3719	−0.5673	−0.4092	−0.3480	−0.2956	0.0239
isobutyl acetate (1) + 1,3,5-trimethylbenzene (2)	298.15	−1.4597	−0.4160	−0.4582	−0.3370	−0.5975	0.0090
	308.15	−1.6082	−0.4839	−0.1707	−0.2620	−0.3230	0.0079
	313.15	−1.7014	−0.4351	−0.2865	−0.2050	−0.3577	0.0102

The standard deviations (d) between the calculated and the experimental values are defined by the equation[11]

$$d = \sqrt{\frac{\sum [f(x)_{\text{calcd}} - f(x)_{\text{exptl}}]^2}{(p-m)}} \quad (4)$$

where p represents the number of the experimental data, and m represents the number of the coefficients A_i. The optimum mumber m of the A_i parameters ($m = k + 1$) was obtained through examination of the standard deviation d. Using five parameters can produce the best standard deviations between the calculated and the experimental values. The coefficients A_i along with the corresponding root-mean-square deviations d are summarized in the Table 4.

Figures 1 and 2 show that the excess molar volumes are positive for all the binary systems at (298.15, 308.15, and 313.15) K. The values of V^E in the entire concentration range follow the order: 1,3,5-trimethylbenzene + isopropyl acetate (or isobutyl acetate) > 1,2,4-trimethylbenzene + isopropyl acetate (or isobutyl acetate). An increase of the temperature has a slight effect on the excess molar volumes for the four binary systems. A sharp difference of the V^E values between 1,2,4-trimethylbenzene's and 1,3,5-trimethylbenzene's system indicates that the molecular structure has an important effect on the excess properties.

Figures 3 and 4 illustrate that the surface tension deviations are negative for all the binary systems at experimental temperatures. The values of $\Delta\sigma$ in the whole composition range are as follows: 1,3,5-trimethylbenzene + isopropyl acetate (or isobutyl acetate) > 1,2,4-trimethylbenzene + isopropyl acetate (or isobutyl acetate). The $\Delta\sigma$ values become slightly negative with the temperature increases for all the systems, which is identical with that observed for the excess molar volumes.

Supporting Information Available:

Density data of the binary mixtures of 1,2,4-trimethylbenzene and 1,3,5-trimethylbenzene with isopropyl acetate and isobutyl acetate at (298.15, 308.15, and 313.15) K. This material is available free of charge via the Internet at http://pubs.acs.org.

Literature Cited

(1) Zou, Y.; Li, Y.; Feng, M.; Che, G. *Separating mixed xylene by urging rectification. Chinese Patent 1105898-A, CN1053386-C*, 1997.

(2) Paar, A. *Instruction Manual*; Graz: Austria.

(3) Morávková, L.; Linek, J. Excess molar volumes of (benzene + isopropylbenzene, or 1,3,5-trimethylbenzene, or 1,2,4-trimethylbenzene) at temperatures between 298.15 and 328.15 K. *J. Chem. Thermodyn.* **2001**, *35*, 1139–1149.

(4) Pan, C.; Ouyang, G.; Lin, J., et al. Excess molar volumes and surface tensions of 1,2,4-trimethylbenzene and 1,3,5-trimethylbenzene with 1-butanol, 2-methyl-1-propanol, 2-butanol, and 2-methyl-2-propanol at 298.15 K. *J. Chem. Eng. Data* **2004**, *49*, 1744–1747.

(5) Deng, J.; Yang, Y.; Wang, P., et al. Excess molar volumes and surface tensions of trimethylbenzene + ethylene glycol ester at 298.15 and 313.15 K. *J. Chem. Eng. Data* **2006**, *51*, 725–729.

(6) Dean, J. A. *Lange's Handbook of Chemistry*, 15th ed., McGraw Hill: New York, 1999.

(7) Anderko, A. Excess volumes of (phenol + butylbenzene or propylbenzene or isopropylbenzene or 1,2,4-trimethylbenzene or ethylbenzene) at 318.15 and 348.15 K. *J. Chem. Thermodyn.* **1990**, *22*, 55–60.
(8) Jiménez, E.; Casas, H.; Segade, L.; Franjo, C. Surface tensions, refractive indexes and excess molar volumes of hexane + 1-alkanol mixtures at 298.15 K. *J. Chem. Eng. Data* **2000**, *45*, 862–866.
(9) Kumar, A.; Mohandas, V. P.; Ghosh, P. K. Experimental surface tensions and derived surface properties of binary mixtures of water + alkoxyethanols (C_1E_m, $m = 1, 2, 3$) and water + ethylene glycol dimethyl ether ($C_1E_1C_1$) at (298.15, 308.15, and 318.15) K. *J. Chem. Eng. Data* **2003**, *48*, 1318–1322.
(10) Redlich, O.; Kister, A. Algebraic representation of thermodynamic properties and the classification of solutions. *Ind. Eng. Chem.* **1848**, *40*, 345–348.
(11) Tsierkezos, N. G.; Filippou, A. C. Thermodynamic investigation of *N,N*-dimethylformamide/toluene binary mixtures in the temperature range from 278.15 to 293.15 K. *J. Chem. Thermodyn.* **2006**, *38*, 952–961.

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