Excess Molar Volumes and Surface Tensions of Xylene with 2-Propanol or 2-Methyl-2-propanol at 298.15 K

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Densities for binary mixtures of (2-propanol + *o*-xylene, + *m*-xylene, + *p*-xylene, 2-methyl-2-propanol + *o*-xylene, + *m*-xylene, and + *p*-xylene) have been determined at 298.15 K, and excess molar volumes have been derived. Surface tension of these binary mixtures have been measured at 298.15 K by the pendant drop method, and the values of the surface tension deviation for these mixtures were also calculated.

Introduction

The surface tension and density of liquids and liquid mixtures are important properties because they play an important role in the mass and heat transfer at an interface. One of our research directions is xylene separation. We have determined surface tensions and densities at 298.15 K over the entire range of composition for 2-propanol + *o*-xylene, *m*-xylene, or *p*-xylene and 2-methyl-2-propanol + *o*-xylene, *m*-xylene, or *p*-xylene.

Experimental Section

o-Xylene, *m*-xylene, and *p*-xylene were of high grade and were distilled under reduced pressure before use. 2-Methyl-2-propanol and 2-propanol were analytical grade and purified by distillation and then drying. The mass fraction purities of the substances were *o*-xylene (99.99%), *m*-xylene (99.56%), *p*-xylene (99.99%), 2-propanol (99.99%), and 2-methyl-2-propanol (99.99%), determined by PE auto system XL gas chromatograph. All of the mixtures were prepared by mass using an Ohaus E12140 balance with an accuracy of ±0.1 mg.

Densities of the pure liquids and their mixtures were measured with an Anton Paar DMA 4500 vibrating tube densimeter, thermostated at (298.15 ± 0.01) K. The densimeter precision was $\pm 5 \times 10^{-5}$ g·cm^{-3}. The surface tensions of the pure liquids and their mixtures were determined by the pendant drop method, using a Dataphysics OCA20 with a CCD camera. The surface tension was given by[1]

$$\sigma = \frac{g\Delta\rho d_e^{\,2}}{H} \qquad (1)$$

There, g is the gravitational acceleration, $\Delta\rho$ is the density difference between the droplet and the surrounding, d_e is the largest diameter of the drop, and H is a correction factor, which depends on the sharp of the drop. The accuracy of the instrument is ±0.05 mN·m^{-1} (±0.1 K). The densities and surface tensions of the pure compounds are given in Table 1 and compared with the literature values.

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Table 1. Physical Properties of the Pure Components at 298.15 K

	ρ/g·cm^{-3}		σ/mN·m^{-1}	
substance	expt	lit.[a]	expt	lit.[a]
o-xylene	0.87592	0.87563	29.60	29.49
m-xylene	0.85979	0.85986	28.36	28.10
p-xylene	0.85685	0.85662	27.89	27.76
2-propanol	0.78085	0.78126	20.93	20.93
2-methyl-2-propanol	0.78027	0.7812	19.97	20.1

[a] TRC Databases for Chemistry and Engineering—Thermodynamic Tables, Version 1998−2s; Thermodynamic Research Center, Texas A&M University System: College Station, TX, 1998.

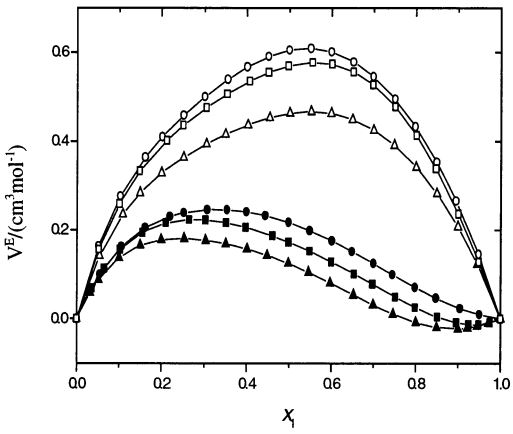

Figure 1. Excess molar volumes V^E for x2-propanol + (1 − x)-*o*-xylene (▲), + (1 − x)*m*-xylene (●), and + (1 − x)*p*-xylene (■) and x2-methyl-2-propanol + (1 − x)*o*-xylene (△), + (1 − x)*m*-xylene (○), and + (1 − x)*p*-xylene (□) at 298.15 K.

Result and Discussion

Excess molar volumes were determined from the density data[2]

$$V^E/(\mathrm{cm}^3\cdot\mathrm{mol}^{-1}) = \frac{x_1M_1 + x_2M_2}{\rho} - x_1\frac{M_1}{\rho_1} - x_2\frac{M_2}{\rho_2} \qquad (2)$$

There, M_i are the molar mass of component i, ρ and ρ_i are the densities of the mixture and component i, and x_i is the molar fraction of component i.

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Table 2. Experimental Excess Molar Volumes V^E at 298.15 K

x_1	V^E / cm³·mol⁻¹	x_1	V^E / cm³·mol⁻¹	x_1	V^E / cm³·mol⁻¹	x_1	V^E / cm³·mol⁻¹	x_1	V^E / cm³·mol⁻¹	x_1	V^E / cm³·mol⁻¹
$x(CH_3)_2CHOH + (1-x)o\text{-}C_6H_4(CH_3)_2$						$x(CH_3)_3COH + (1-x)o\text{-}C_6H_4(CH_3)_2$					
0.0310	0.065	0.4004	0.156	0.7457	0.012	0.0536	0.144	0.4020	0.436	0.6992	0.427
0.0506	0.092	0.4474	0.144	0.8000	−0.005	0.1083	0.239	0.4532	0.453	0.7479	0.391
0.0992	0.136	0.4979	0.127	0.8493	−0.018	0.1489	0.283	0.5007	0.464	0.8000	0.344
0.1493	0.161	0.5457	0.104	0.8996	−0.021	0.1992	0.320	0.5513	0.465	0.8494	0.282
0.1988	0.176	0.5971	0.078	0.9223	−0.022	0.2507	0.364	0.5988	0.461	0.8991	0.208
0.2523	0.182	0.6525	0.054	0.9448	−0.017	0.3042	0.398	0.6490	0.448	0.9452	0.121
0.3025	0.180	0.6988	0.029	0.9715	−0.014	0.3490	0.418				
0.3504	0.170										
$x(CH_3)_2CHOH + (1-x)m\text{-}C_6H_4(CH_3)_2$						$x(CH_3)_3COH + (1-x)m\text{-}C_6H_4(CH_3)_2$					
0.0304	0.057	0.3530	0.247	0.6990	0.126	0.0509	0.167	0.4009	0.568	0.6984	0.550
0.0535	0.105	0.3990	0.239	0.7446	0.100	0.1028	0.277	0.4511	0.590	0.7496	0.488
0.1053	0.166	0.4437	0.232	0.7977	0.069	0.1612	0.361	0.4999	0.603	0.7981	0.438
0.1610	0.200	0.4990	0.218	0.8475	0.049	0.2010	0.408	0.5509	0.608	0.8490	0.356
0.2191	0.229	0.5490	0.198	0.9044	0.022	0.2510	0.457	0.5994	0.599	0.8950	0.260
0.2512	0.241	0.6011	0.176	0.9500	0.010	0.3006	0.501	0.6515	0.577	0.9479	0.146
0.3067	0.248	0.6492	0.151			0.3547	0.542				
$x(CH_3)_2CHOH + (1-x)p\text{-}C_6H_4(CH_3)_2$						$x(CH_3)_3COH + (1-x)p\text{-}C_6H_4(CH_3)_2$					
0.0349	0.060	0.3975	0.207	0.7510	0.050	0.0518	0.159	0.4065	0.539	0.6980	0.526
0.0642	0.118	0.4608	0.190	0.7987	0.028	0.1004	0.263	0.4507	0.554	0.7504	0.485
0.1019	0.159	0.4990	0.174	0.8509	0.007	0.1484	0.327	0.4980	0.565	0.8007	0.408
0.1542	0.197	0.5488	0.150	0.8962	−0.010	0.2113	0.400	0.5546	0.577	0.8473	0.339
0.2090	0.212	0.6000	0.129	0.9249	−0.013	0.2501	0.437	0.6012	0.573	0.9002	0.239
0.2638	0.222	0.6536	0.100	0.9485	−0.015	0.3049	0.475	0.6518	0.554	0.9485	0.124
0.3025	0.221	0.6970	0.074	0.9751	−0.010	0.3532	0.508				
0.3511	0.217										

Table 3. Least-Squares Parameters and Standard Deviations *s*

	A_0	A_1	A_2	A_3	A_4	s / cm³·mol⁻¹
o-xylene+2-propanol	0.4964	0.7899	-0.0841	0.5052	0.4994	0.0030
m-xylene+2-propanol	0.8677	0.6540	0.0235	0.4173	0.3253	0.0029
p-xylene+2-propanol	0.6904	0.7804	0.1168	0.5611	0.0959	0.0033
o-xylene+2-methyl-2-propanol	1.8523	−0.3038	0.4772	0.6623	0.5629	0.0032
m-xylene+2-methyl-2-propanol	2.4196	−0.3898	0.2629	0.7797	0.8252	0.0036
p-xylene+2-methyl-2-propanol	2.2787	−0.4699	0.5617	0.9755	0.2734	0.0038

Table 4. Surface Tensions σ at 298.15 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
$x(CH_3)_2CHOH + (1-x)o\text{-}C_6H_4(CH_3)_2$						$x(CH_3)_3COH + (1-x)o\text{-}C_6H_4(CH_3)_2$					
0.0992	28.21	−0.531	0.5971	23.98	−0.529	0.1083	27.80	−0.757	0.5988	22.82	−1.014
0.1988	27.11	−0.768	0.6988	23.15	−0.398	0.1992	26.43	−1.252	0.6992	22.05	−0.817
0.3024	26.07	−0.911	0.8000	22.40	−0.272	0.3042	25.27	−1.401	0.8000	21.38	−0.516
0.4004	25.30	−0.833	0.8896	21.72	−0.176	0.4020	24.32	−1.409	0.8991	20.71	−0.232
0.4979	24.54	−0.748				0.5007	23.60	−1.178			
$x(CH_3)_2CHOH + (1-x)m\text{-}C_6H_4(CH_3)_2$						$x(CH_3)_3COH + (1-x)m\text{-}C_6H_4(CH_3)_2$					
0.1019	27.15	−0.454	0.5957	23.56	−0.380	0.1028	26.83	−0.668	0.5994	22.52	−0.811
0.1933	26.23	−0.696	0.7013	22.87	−0.286	0.2010	25.76	−0.914	0.6984	21.84	−0.660
0.2999	25.40	−0.735	0.7952	22.26	−0.200	0.3006	24.84	−0.998	0.7981	21.22	−0.444
0.4024	24.76	−0.614	0.8987	21.58	−0.112	0.4009	23.98	−1.016	0.8950	20.64	−0.211
0.4983	24.18	−0.483				0.4999	23.21	−0.956			
$x(CH_3)_2CHOH + (1-x)p\text{-}C_6H_4(CH_3)_2$						$x(CH_3)_3COH + (1-x)p\text{-}C_6H_4(CH_3)_2$					
0.1029	26.82	−0.355	0.5985	23.45	−0.280	0.1004	26.69	−0.405	0.6012	22.50	−0.628
0.2014	26.03	−0.460	0.6991	22.86	−0.171	0.2113	25.63	−0.587	0.6980	21.82	−0.542
0.2993	25.32	−0.490	0.7982	22.22	−0.123	0.3049	24.73	−0.745	0.8007	21.15	−0.398
0.4030	24.63	−0.460	0.9047	21.52	−0.082	0.4065	23.90	−0.771	0.9002	20.58	−0.180
0.4979	24.06	−0.370				0.4980	23.25	−0.696			

Experimental excess molar volumes V^E for six binary mixtures at 298.15 K are listed in Table 2 and graphically presented in Figure 1. The experimental results were fitted by the method of least squares with all points weighted equally to the smoothing equation[3]

$$V^E/(\mathrm{cm^3\cdot mol^{-1}}) = x(1-x)\sum_{i=0}^{k} A_i(1-2x)^i \qquad (3)$$

The continuous lines in Figure 1 represent values calculated from the smoothing equation. The parameters A_0, A_1, A_2, A_3, and A_4 and the standard deviation s are given in Table 3.

Figure 1 shows that the excess molar volumes V^E are positive for mixtures of 2-methyl-2-propanol with the xylenes. The V^E values at $x = 0.5$ for (2-methyl-2-propanol + xylenes) follow the order *m*-xylene > *p*-xylene > *o*-xylene. Umesh et al. determined the excess molar volumes of 2-methyl-2-propanol + xylenes at 308.15 K.[4] The V^E values follow the same order. Excess molar volumes V^E are positive for mixtures of 2-propanol with *m*-xylene, and the

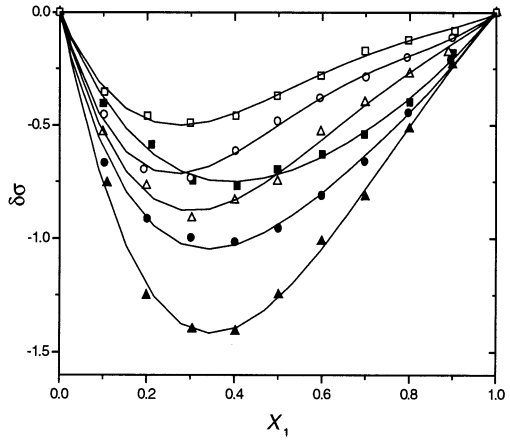

Figure 2. Excess surface tensions $\delta\sigma$ for x2-propanol + (1 − x)-*o*-xylene (△), + (1 − x)*m*-xylene (○), and + (1 − x)*p*-xylene (□) and x2-methyl-2-propanol + (1 − x)*o*-xylene (●), + (1 − x)*m*-xylene (l), and + (1 − x)*p*-xylene (■) at 298.15 K

signs of V^E for 2-propanol + *o*-xylene and 2-propanol + *p*-xylene are S shaped. The V^E values at $x = 0.5$ for (2-propanol + xylenes) follow the order *m*-xylene > *p*-xylene > *o*-xylene.

Table 4 lists the surface tensions and surface tension deviations for {x 2-propanol + *o*-xylene, + *m*-xylene, and + *p*-xylene and x 2-methyl-2-propanol + *o*-xylene, + *m*-xylene, and + *p*-xylene} at 298.15 K. The surface tension deviations $\delta\sigma$ are defined by[2]

$$\delta\sigma = \sigma - x_1\sigma_1 - x_2\sigma_2 \quad (4)$$

Figure 2 shows the surface tension deviations $\delta\sigma$. The minimum values of $\delta\sigma$ for 2-propanol + xylene and 2-methyl-2-propanol + xylene follow the order *o*-xylene < *m*-xylene < *p*-xylene.

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