732 J. Chem. Eng. Data **2004,** *49,* 732−734

Excess Molar Volumes and Surface Tensions of Xylene with Isopropyl Ether or Methyl *tert*-Butyl Ether at 298.15 K

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Densities for binary mixtures of isopropyl ether + *o*-xylene, + *m*-xylene, and + *p*-xylene have been determined at 298.15 K, and excess molar volumes have been derived. Surface tensions for binary mixtures of (isopropyl ether + *o*-xylene, + *m*-xylene, and + *p*-xylene and methyl *tert*-butyl ether + *o*-xylene, + *m*-xylene, and + *p*-xylene) 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

In previous papers, the excess molar volumes and surface tensions at 298.15 K for xylene + alkanol (2-propanol and 2-methyl-2-propanol) and xylene + alkone (acetone and 2-butanone) systems were reported,[1,2] and the excess molar volumes at 298.15 K for xylene + methyl *tert*-butyl ether systems were also reported.[3] In this paper, excess molar volumes at 298.15 K for xylene + ether, including isopropyl ether + *o*-xylene or *m*-xylene or *p*-xylene systems, and surface tensions at 298.15 K for xylene + ether, including isopropyl ether + *o*-xylene, *m*-xylene, or *p*-xylene and methyl *tert*-butyl ether + *o*-xylene, *m*-xylene, or *p*-xylene systems are reported.

Experimental Section

o-Xylene, *m*-xylene, and *p*-xylene (Shanghai Chem., China) were of high grade and were distilled under reduced pressure before use. Isopropyl ether and methyl *tert*-butyl ether (Shanghai Chem., China) were 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%); isopropyl ether (99.5%); methyl *tert*-butyl ether (99.90%); determined by a PE autosystem XL gas chromatograph. All of the mixtures were prepared by mass using an Ohaus E12140 balance with an accuracy of ±0.1 mg. To avoid evaporation, ether must be added in the end, and then the sample bottle must be sealed with a stopper as soon as possible.

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 contact angle and surface tension measuring device. This instrument provides a CCD camera to take pictures and an electronic syringe unit to inject samples, so the surface tension of the sample can be determined very fast. The surface tension was given by[4]

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

Here, g is the gravitational acceleration, $\Delta\rho$ is the density difference between the droplet and the surrounding, and d_e is the largest diameter of the drop. The sharp correction factor H is calculated by the Young−Laplace equation and performed by computer. 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.

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

substance	ρ/g·cm^{-3} exp	ρ/g·cm^{-3} lit	σ/ mN·m^{-1} exp	σ/ mN·m^{-1} lit
o-xylene	0.87592	0.87563[a]	29.35	29.49[a]
m-xylene	0.85978	0.85986[a]	28.36	28.10[a]
p-xylene	0.85685	0.85662[a]	27.89	27.76[a]
isopropyl ether	0.71838	0.71849[b]	17.31	17.27[c]
methyl *tert*-butyl ether	0.73548	0.73536[e]	19.25	19.4[d]

[a] *TRC Databases for Chemistry and Engineering—Thermodynamic Tables*, Version 1998−2s. Thermodynamic Research Center, Taxes A&M University System: College Station, TX, 1998. [b] Reference 7. [c] Reference 8. [d] Reference 9. [e] Reference 10.

Result and Discussion

Excess molar volumes were determined from the density data[5]

$$V^E = \frac{x_1 M_1 + x_2 M_2}{\rho} - x_1 \frac{M_1}{\rho_1} - x_2 \frac{M_2}{\rho_2} \qquad (2)$$

Here M_i is 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.

Experimental excess molar volumes V^E for three binary mixtures (isopropyl ether + *o*-xylene, *m*-xylene, and *p*-xylene) at 298.15 K are listed in Table 2 and are graphically presented in Figure 1. The experimental results were fitted

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10.1021/je034279l CCC: $27.50

Table 2. Experimental Excess Molar Volumes V^E at 298.15 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 (CH$_3$)$_2$CHOCH(CH$_3$)$_2$ + (1-x) o-C$_6$H$_4$(CH$_3$)$_2$				
0.0506	−0.177	0.3003	−0.782	0.5505	−0.948	0.7999	−0.631
0.0997	−0.315	0.3500	−0.839	0.6001	−0.910	0.8502	−0.511
0.1501	−0.449	0.4004	−0.883	0.6509	−0.882	0.8997	−0.369
0.2003	−0.574	0.4497	−0.922	0.7000	−0.811	0.9493	−0.210
0.2503	−0.691	0.5050	−0.936	0.7502	−0.747		
			x (CH$_3$)$_2$CHOCH(CH$_3$)$_2$ + (1-x) m-C$_6$H$_4$(CH$_3$)$_2$				
0.0514	−0.135	0.3002	−0.579	0.5509	−0.718	0.8005	−0.477
0.1002	−0.242	0.3498	−0.637	0.6001	−0.692	0.8506	−0.393
0.1526	−0.355	0.4001	−0.670	0.6500	−0.671	0.8998	−0.283
0.1997	−0.441	0.4516	−0.711	0.6944	−0.617	0.9500	−0.164
0.2501	−0.520	0.5012	−0.715	0.7498	−0.558		
			x (CH$_3$)$_2$CHOCH(CH$_3$)$_2$ + (1-x) p-C$_6$H$_4$(CH$_3$)$_2$				
0.0527	−0.136	0.3004	−0.658	0.5507	−0.795	0.7999	−0.537
0.1016	−0.279	0.3509	−0.730	0.6002	−0.787	0.8512	−0.432
0.1500	−0.398	0.4007	−0.761	0.6498	−0.756	0.9000	−0.318
0.2011	−0.510	0.4506	−0.785	0.7007	−0.702	0.9507	−0.178
0.2527	−0.588	0.5044	−0.802	0.7497	−0.625		

Table 3. Least-Squares Parameters and Standard Deviations s

	A_0	A_1	A_2	A_3	A_4	s/cm^3·mol^{-1}
o-xylene + isopropyl ether	−3.7617	0.2483	−0.1027	0.1693	0.0002	0.0082
m-xylene + isopropyl ether	−2.8679	0.7165	0.1590	0.1509	−0.4754	0.0052
p-xylene + isopropyl ether	−3.2101	0.1727	−0.2068	0.1873	0.1754	0.0078

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$_3$)$_2$CHOCH(CH$_3$)$_2$ + (1-x)o-C$_6$H$_4$(CH$_3$)$_2$						x(CH$_3$)$_3$COCH$_3$ + (1-x)o-C$_6$H$_4$(CH$_3$)$_2$				
0.1022	27.21	−0.91	0.5998	21.03	−1.10	0.0997	27.90	−0.44	0.6012	22.17	−1.11
0.2010	25.55	−1.38	0.7013	20.00	−0.91	0.1996	26.62	−0.71	0.7002	21.30	−0.98
0.3018	24.17	−1.55	0.7987	19.15	−0.58	0.3012	25.28	−1.03	0.8000	20.57	−0.70
0.4037	23.01	−1.48	0.8987	18.08	−0.45	0.4008	24.14	−1.16	0.8999	19.78	−0.48
0.4997	22.00	−1.33				0.4997	23.12	−1.18			
	x(CH$_3$)$_2$CHOCH(CH$_3$)$_2$ + (1-x)m-C$_6$H$_4$(CH$_3$)$_2$						x(CH$_3$)$_3$COCH$_3$ + (1-x)m-C$_6$H$_4$(CH$_3$)$_2$				
0.1019	26.38	−0.85	0.6006	20.86	−0.86	0.1019	27.13	−0.30	0.6006	22.08	−0.81
0.2111	24.88	−1.15	0.6994	19.91	−0.72	0.2019	26.05	−0.47	0.7009	21.26	−0.72
0.3002	23.72	−1.32	0.7998	19.02	−0.50	0.3028	24.98	−0.62	0.8001	20.49	−0.58
0.3999	22.67	−1.27	0.8981	18.12	−0.32	0.4014	23.99	−0.71	0.9004	19.76	−0.40
0.4991	21.73	−1.12				0.4996	23.01	−0.80			
	x(CH$_3$)$_2$CHOCH(CH$_3$)$_2$ + (1-x)p-C$_6$H$_4$(CH$_3$)$_2$						x(CH$_3$)$_3$COCH$_3$ + (1-x)p-C$_6$H$_4$(CH$_3$)$_2$				
0.0988	26.30	−0.55	0.6030	20.76	−0.75	0.1008	26.85	−0.17	0.6004	22.08	−0.62
0.2012	24.84	−0.92	0.7000	19.91	−0.57	0.1998	25.81	−0.35	0.6993	21.24	−0.61
0.2991	23.73	−1.00	0.7987	19.02	−0.42	0.3012	24.78	−0.51	0.8000	20.48	−0.50
0.4045	22.68	−0.93	0.8980	18.18	−0.21	0.4026	23.84	−0.57	0.9002	19.78	−0.33
0.5096	21.66	−0.84				0.4997	22.96	−0.61			

by the method of least squares with all points weighted equally to the smoothing equation[6]

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

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 negative for mixtures of o-, m-, and p-xylene with isopropyl ether. The V^E values at $x = 0.5$ for (o-, m-, and p-xylene + isopropyl ether) follow the order m-xylene > p-xylene > o-xylene.

Table 4 lists the surface tensions and surface tension deviations for (isopropyl ether + o-, m-, and p-xylene and methyl *tert*-butyl ether + o-, m-, and p-xylene) at 298.15 K. The surface tension deviations $\delta\sigma$ are defined by[5]

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

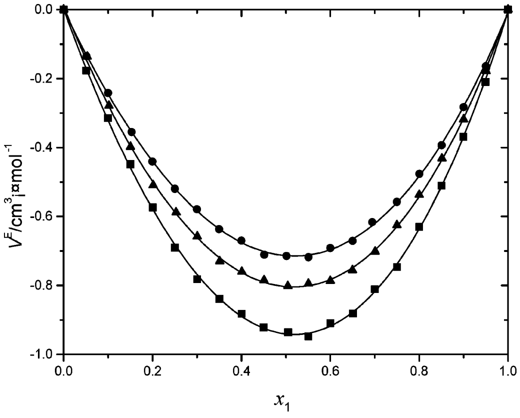

Figure 1. Excess molar volumes V^E for x isopropyl ether: ■, + (1 − x) o-xylene; ●, + (1 − x) m-xylene; ▲, + (1 − x) p-xylene at 298.15 K.

Figures 2 and 3 shows that the surface tension deviations $\delta\sigma$ are negative for mixtures of o-, m-, and p-xylene with isopropyl ether or methyl *tert*-butyl ether. The minimum values of $\delta\sigma$ for isopropyl ether + xylene and methyl *tert*-

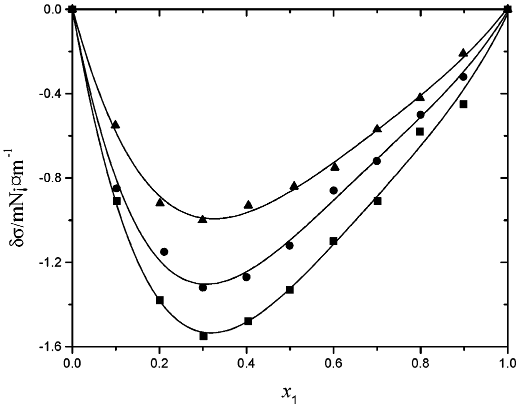

Figure 2. Surface tensions deviation $\delta\sigma$ for x isopropyl ether: ■, + (1 − x) *o*-xylene; ●, + (1 − x) *m*-xylene; ▲, + (1 − x) *p*-xylene at 298.15 K.

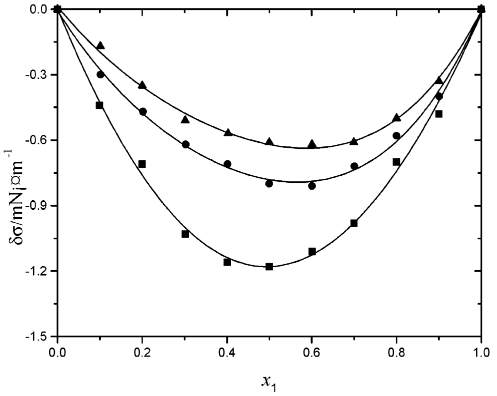

Figure 3. Surface tensions deviation $\delta\sigma$ for x methyl *tert*-butyl ether: ■, + (1 − x) *o*-xylene; ●, + (1 − x) *m*-xylene; ▲, + (1 − x) *p*-xylene at 298.15 K.

butyl ether + xylene follow the order *o*-xylene < *m*-xylene < *p*-xylene.

The result of V^E values and surface-tension deviations for the binary mixtures of xylene + alkanol, alkanone, and ether at 298.15 K shows that the V^E values follow the order 2-mehtyl-2-propanol > 2-propanol > acetone > 2-butanone > methyl *tert*-butyl ether > isopropyl ether and that the surface tension deviations follow the order acetone > 2-butanone > 2-propanol > methyl *tert*-butyl ether > 2-mehtyl-2-propanol > isopropyl ether.

Supporting Information Available:

Density data of xylene with isopropyl ether at 298.15 K. This material is available free of charge via the Internet at http://pubs.acs.org.

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Received for review December 22, 2003. Accepted March 25, 2004. This project was supported by the National Key Basic Research and Development Program of China (No. G 2000026302).

JE034279L