

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

Yeming He, Ruifen Jiang, Yangyi Yang, Zhongqi Huang, and Gangfeng Ouyang*

School of Chemistry and Chemical Engineering, Sun Yat-sen University, Guangzhou 510275, China

Densities and surface tensions for binary mixtures of 1,2,4-trimethylbenzene and 1,3,5-trimethylbenzene with 1,1-diethoxyethane and 2,2-dimethoxypropane have been measured over the whole concentration range. Measurements were made under normal atmospheric pressure at (298.15, 308.15, and 313.15) K. The experimental data are used to calculate the excess molar volumes and the surface tension deviations, respectively.

Introduction

The density, surface tension, and excess properties are crucial physical properties since they 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 this work, densities and surface tensions of 1,2,4-trimethylbenzene and 1,3,5-trimethylbenzene with 1,1-diethoxyethane, and 2,2-dimethoxypropane at different temperatures [(298.15, 308.15 and 313.15) K] are determined. The excess molar volumes and the surface tension deviations of these systems have been calculated and fitted to the Redlich–Kister polynomials. There is no detailed report about the excess properties of the studied systems in the open literature.

Experimental Section

All the chemicals 1,2,4-trimethylbenzene (Acros Organics), 1,3,5-trimethylbenzene (Acros Organics), 1,1-diethoxyethane (Acros Organics), and 2,2-dimethoxypropane (Alfa Aesar) are commercially available and used without further purification. The mass fractions of the substances, determined by a PE autosystem XL gas chromatograph, were as follows: 1,2,4-trimethylbenzene (99.20 %), 1,3,5-trimethylbenzene (99.30 %), 1,1-diethoxyethane (99.21 %), and 2,2-dimethoxypropane (99.12 %). All of 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 mole fractions. The uncertainty of the mole 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 estimated uncertainty of the densities is about $5 \times 10^{-5} \text{ g}\cdot\text{cm}^{-3}$. The surface tensions were determined by the pendant drop method, using a Data Physics OCA20 (Germany) contact angle and surface tension measuring device. The uncertainty of the device is $\pm 0.05 \text{ mN}\cdot\text{m}^{-1}$. The experimental densities and surface tensions of the pure substances are tabulated in Table 1 and compared with the literature values.

* Corresponding author. Telephone/fax: +86-20-84110953. E-mail: cesoygf@mail.sysu.edu.cn.

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

substance	$\rho/\text{g}\cdot\text{cm}^{-3}$		$\sigma/\text{mN}\cdot\text{m}^{-1}$	
	exptl.	lit.	exptl.	lit.
<i>T</i> = 298.15 K				
1,2,4-trimethylbenzene	0.87171	0.87164 ³ 0.87178 ⁵ 0.87174 ⁶	29.30	29.25 ¹ 29.29 ³ 29.20 ⁷
1,3,5-trimethylbenzene	0.86112	0.86103 ¹ 0.86104 ² 0.86114 ⁵ 0.86109 ⁸	28.05	27.55 ⁷ 28.09 ³
1,1-diethoxyethane	0.82196		20.88	20.89 ⁷
2,2-dimethoxypropane	0.84509	0.847 ⁷	21.46	
<i>T</i> = 308.15 K				
1,2,4-trimethylbenzene	0.86368	0.86367 ⁵	28.24	28.17 ⁷
1,3,5-trimethylbenzene	0.85294	0.85290 ⁵	27.21	26.65 ⁷
1,1-diethoxyethane	0.81148		19.89	19.86 ⁷
2,2-dimethoxypropane	0.83441		20.43	
<i>T</i> = 313.15 K				
1,2,4-trimethylbenzene	0.85958	0.85954 ²	27.71	27.67 ² 27.66 ⁷
1,3,5-trimethylbenzene	0.84882	0.84874 ²	26.78	26.82 ² 26.20 ⁷
1,1-diethoxyethane	0.80618		19.42	19.34 ⁷
2,2-dimethoxypropane	0.82899		19.91	

Results and Discussion

The excess molar volumes (V^E) are determined by densities and molar masses by the following equation:⁹

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

where V^E is the excess molar volume; x_i and M_i are mole fraction and molar mass of the component i , respectively; ρ and ρ_i are density of the mixture and the i th pure component, respectively; and the subscript i ($i = 1$ or 2) represents component 1 or 2. The experimental excess molar volumes for the four binary mixtures (1,1-diethoxyethane + 1,2,4-trimethylbenzene, or + 1,3,5-trimethylbenzene and 2,2-dimethoxypropane + 1,2,4-trimethylbenzene, or + 1,3,5-trimethylbenzene) at temperatures of (298.15, 308.15, and 313.15) K are listed in Table 2. The curves of the excess molar volumes versus the composition of these binary systems at the experimental temperature are shown in Figure 1.

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

V^E		V^E		V^E		V^E		V^E		V^E		V^E	
x_1	$\text{cm}^3\cdot\text{mol}^{-1}$	x_1	$\text{cm}^3\cdot\text{mol}^{-1}$	x_1	$\text{cm}^3\cdot\text{mol}^{-1}$	x_1	$\text{cm}^3\cdot\text{mol}^{-1}$	x_1	$\text{cm}^3\cdot\text{mol}^{-1}$	x_1	$\text{cm}^3\cdot\text{mol}^{-1}$	x_1	$\text{cm}^3\cdot\text{mol}^{-1}$
$T = 298.15 \text{ K}$													
1,1-Diethoxyethane (1) + 1,2,4-Trimethylbenzene (2)													
0.0500	-0.046	0.2005	-0.167	0.3526	-0.245	0.5034	-0.278	0.6519	-0.270	0.8003	-0.209	0.9399	-0.090
0.1000	-0.090	0.2511	-0.199	0.4010	-0.263	0.5513	-0.281	0.7012	-0.255	0.8491	-0.178		
0.1510	-0.130	0.3005	-0.225	0.4538	-0.275	0.5998	-0.280	0.7499	-0.237	0.9000	-0.138		
1,1-Diethoxyethane (1) + 1,3,5-Trimethylbenzene (2)													
0.0491	-0.004	0.1996	-0.014	0.3501	-0.019	0.4997	-0.023	0.6508	-0.023	0.8014	-0.020	0.9487	-0.008
0.1013	-0.007	0.2501	-0.015	0.4067	-0.021	0.5523	-0.024	0.7006	-0.023	0.8510	-0.017		
0.1538	-0.011	0.3009	-0.018	0.4506	-0.022	0.6010	-0.024	0.7507	-0.023	0.8994	-0.015		
2,2-Dimethoxypropane (1) + 1,2,4-Trimethylbenzene (2)													
0.0523	-0.010	0.1996	-0.030	0.3494	-0.047	0.4994	-0.056	0.6508	-0.058	0.7992	-0.044	0.9489	-0.017
0.0998	-0.016	0.2517	-0.038	0.3987	-0.051	0.5498	-0.056	0.6997	-0.054	0.8508	-0.037		
0.1497	-0.023	0.3009	-0.043	0.4502	-0.053	0.5996	-0.058	0.7498	-0.051	0.8997	-0.029		
2,2-Dimethoxypropane (1) + 1,3,5-Trimethylbenzene (2)													
0.0500	0.026	0.2001	0.086	0.3496	0.125	0.4998	0.141	0.6506	0.137	0.7993	0.095	0.9494	0.022
0.1002	0.047	0.2520	0.102	0.3998	0.134	0.5497	0.145	0.7002	0.127	0.8511	0.073		
0.1494	0.067	0.3001	0.115	0.4525	0.139	0.5996	0.142	0.7503	0.114	0.8986	0.050		
$T = 308.15 \text{ K}$													
1,1-Diethoxyethane (1) + 1,2,4-Trimethylbenzene (2)													
0.0488	-0.049	0.2003	-0.178	0.3499	-0.267	0.5016	-0.312	0.6514	-0.305	0.8007	-0.240	0.9488	-0.109
0.0993	-0.096	0.2497	-0.214	0.4004	-0.286	0.5500	-0.313	0.7003	-0.291	0.8502	-0.208		
0.1486	-0.141	0.3001	-0.244	0.4534	-0.303	0.6017	-0.313	0.7498	-0.270	0.8989	-0.166		
1,1-Diethoxyethane (1) + 1,3,5-Trimethylbenzene (2)													
0.0488	-0.006	0.1991	-0.023	0.3503	-0.033	0.5011	-0.039	0.6511	-0.041	0.7977	-0.034	0.9418	-0.014
0.1009	-0.011	0.2498	-0.026	0.4004	-0.036	0.5503	-0.040	0.6997	-0.039	0.8462	-0.030		
0.1495	-0.017	0.3014	-0.030	0.4508	-0.037	0.5979	-0.041	0.7503	-0.037	0.8993	-0.024		
2,2-Dimethoxypropane (1) + 1,2,4-Trimethylbenzene (2)													
0.0515	-0.011	0.2001	-0.040	0.3512	-0.064	0.4989	-0.079	0.6518	-0.080	0.7962	-0.062	0.9456	-0.023
0.0998	-0.020	0.2475	-0.049	0.3955	-0.069	0.5542	-0.081	0.6987	-0.077	0.8510	-0.051		
0.1499	-0.031	0.3020	-0.059	0.4485	-0.076	0.5998	-0.082	0.7455	-0.072	0.8973	-0.039		
2,2-Dimethoxypropane (1) + 1,3,5-Trimethylbenzene (2)													
0.0562	0.020	0.2023	0.075	0.3497	0.107	0.4964	0.123	0.6502	0.118	0.7999	0.086	0.9492	0.020
0.0995	0.039	0.2502	0.088	0.3982	0.115	0.5493	0.126	0.7006	0.111	0.8492	0.066		
0.1481	0.057	0.3002	0.099	0.4499	0.120	0.6001	0.124	0.7454	0.101	0.8998	0.044		
$T = 313.15 \text{ K}$													
1,1-Diethoxyethane (1) + 1,2,4-Trimethylbenzene (2)													
0.0498	-0.057	0.2003	-0.205	0.3505	-0.306	0.4990	-0.353	0.6503	-0.352	0.7998	-0.294	0.9497	-0.136
0.0992	-0.110	0.2496	-0.242	0.4000	-0.327	0.5463	-0.356	0.7002	-0.340	0.8507	-0.256		
0.1501	-0.161	0.3027	-0.277	0.4501	-0.343	0.6011	-0.358	0.7491	-0.319	0.8990	-0.209		
1,1-Diethoxyethane (1) + 1,3,5-Trimethylbenzene (2)													
0.0487	-0.009	0.1999	-0.029	0.3501	-0.042	0.5000	-0.049	0.6506	-0.050	0.7996	-0.044	0.9498	-0.021
0.0991	-0.017	0.2468	-0.034	0.4008	-0.044	0.5495	-0.050	0.7005	-0.049	0.8494	-0.040		
0.1507	-0.023	0.3001	-0.039	0.4502	-0.047	0.6005	-0.051	0.7514	-0.047	0.9003	-0.034		
2,2-Dimethoxypropane (1) + 1,2,4-Trimethylbenzene (2)													
0.0506	-0.013	0.1994	-0.049	0.3475	-0.079	0.5000	-0.095	0.6504	-0.096	0.7987	-0.075	0.9487	-0.029
0.0996	-0.025	0.2511	-0.061	0.3981	-0.087	0.5487	-0.099	0.6993	-0.093	0.8417	-0.065		
0.1509	-0.037	0.3032	-0.071	0.4501	-0.092	0.5993	-0.100	0.7486	-0.084	0.8929	-0.048		
2,2-Dimethoxypropane (1) + 1,3,5-Trimethylbenzene (2)													
0.0511	0.019	0.2014	0.065	0.3498	0.097	0.5014	0.110	0.6488	0.106	0.7994	0.075	0.9440	0.019
0.1023	0.035	0.2506	0.079	0.3960	0.104	0.5508	0.112	0.6988	0.099	0.8388	0.061		
0.1503	0.051	0.3013	0.090	0.4486	0.108	0.5931	0.112	0.7499	0.088	0.8976	0.040		

The experimental surface tensions (σ) and values of surface tension deviations ($\delta\sigma$) for the four binary mixtures (1,1-diethoxyethane + 1,2,4-trimethylbenzene, or + 1,3,5-trimethylbenzene and 2,2-dimethoxypropane + 1,2,4-trimethylbenzene, or + 1,3,5-trimethylbenzene) at temperatures of (298.15, 308.15 and 313.15) K are listed in Table 3, respectively. The surface tension deviations are calculated by the following equation:¹⁰

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

where $\delta\sigma$ is surface tension deviation; σ is surface tension of the binary system; x_1 and x_2 are mole fraction of components 1 and 2 in the mixture, respectively; and σ_1 and σ_2 are surface tension of pure components 1 and 2, respectively. The values

of surface tension deviations at the experimental temperature are graphically presented in Figure 2.

The experimental results of excess molar volumes and surface tension deviations over the whole mole fraction range are fitted by the Redlich–Kister¹¹ 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 $\delta\sigma$, and A_i represents the parameters. A nonlinear least-squares method is used to estimate the parameters A_i . The standard deviations (d) between the calculated and the experimental values are defined

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														
1,1-Diethoxyethane (1) + 1,2,4-Trimethylbenzene (2)														
0.0000	29.30	0.00	0.2005	26.29	-1.32	0.4010	24.16	-1.76	0.5998	22.70	-1.55	0.8003	21.58	-0.98
0.0500	28.51	-0.37	0.2511	25.71	-1.48	0.4538	23.73	-1.75	0.6519	22.41	-1.40	0.8491	21.42	-0.73
0.1000	27.76	-0.70	0.3005	25.14	-1.63	0.5034	23.35	-1.71	0.7012	22.08	-1.32	0.9000	21.21	-0.51
0.1510	26.97	-1.06	0.3526	24.60	-1.73	0.5513	23.01	-1.65	0.7499	21.85	-1.14	0.9399	21.09	-0.30
1,1-Diethoxyethane (1) + 1,3,5-Trimethylbenzene (2)														
0.0000	28.05	0.00	0.1996	25.83	-0.79	0.4067	23.83	-1.30	0.6010	22.26	-1.48	0.8014	21.20	-1.10
0.0491	27.45	-0.25	0.2501	25.34	-0.92	0.4506	23.45	-1.37	0.6508	21.92	-1.46	0.8510	21.09	-0.86
0.1013	26.91	-0.41	0.3009	24.81	-1.08	0.4997	23.04	-1.43	0.7006	21.64	-1.39	0.8994	21.02	-0.58
0.1538	26.36	-0.59	0.3501	24.37	-1.17	0.5523	22.62	-1.47	0.7507	21.43	-1.24	0.9487	20.95	-0.30
2,2-Dimethoxypropane (1) + 1,2,4-Trimethylbenzene (2)														
0.0000	29.30	0.00	0.1996	27.12	-0.62	0.3987	25.24	-0.93	0.5996	23.55	-1.05	0.7992	22.24	-0.79
0.0523	28.69	-0.20	0.2517	26.60	-0.73	0.4502	24.79	-0.98	0.6508	23.17	-1.03	0.8508	22.00	-0.63
0.0998	28.17	-0.35	0.3009	26.13	-0.81	0.4994	24.37	-1.01	0.6997	22.82	-0.99	0.8997	21.79	-0.46
0.1497	27.62	-0.51	0.3494	25.68	-0.88	0.5498	23.95	-1.04	0.7498	22.51	-0.91	0.9489	21.62	-0.24
2,2-Dimethoxypropane (1) + 1,3,5-Trimethylbenzene (2)														
0.0000	28.05	0.00	0.2001	26.28	-0.45	0.3998	24.70	-0.72	0.5996	23.26	-0.84	0.7993	22.11	-0.67
0.0500	27.60	-0.12	0.2520	25.88	-0.51	0.4525	24.33	-0.74	0.6506	22.93	-0.83	0.8511	21.89	-0.55
0.1002	27.14	-0.25	0.3001	25.47	-0.60	0.4998	23.98	-0.78	0.7002	22.64	-0.80	0.8986	21.70	-0.43
0.1494	26.72	-0.35	0.3496	25.10	-0.65	0.5497	23.62	-0.81	0.7503	22.37	-0.74	0.9494	21.57	-0.22
$T = 308.15$ K														
1,1-Diethoxyethane (1) + 1,2,4-Trimethylbenzene (2)														
0.0000	28.24	0.00	0.2003	25.09	-1.48	0.4004	23.02	-1.88	0.6017	21.54	-1.68	0.8007	20.46	-1.09
0.0488	27.35	-0.48	0.2497	24.51	-1.65	0.4534	22.60	-1.85	0.6514	21.24	-1.56	0.8502	20.28	-0.86
0.0993	26.53	-0.88	0.3001	23.95	-1.78	0.5016	22.23	-1.82	0.7003	20.96	-1.43	0.8989	20.09	-0.64
0.1486	25.79	-1.21	0.3499	23.47	-1.85	0.5500	21.90	-1.75	0.7498	20.72	-1.26	0.9488	19.95	-0.37
1,1-Diethoxyethane (1) + 1,3,5-Trimethylbenzene (2)														
0.0000	27.21	0.00	0.1991	24.86	-0.89	0.4004	22.89	-1.39	0.5979	21.25	-1.58	0.7977	20.15	-1.22
0.0488	26.55	-0.30	0.2498	24.32	-1.06	0.4508	22.44	-1.47	0.6511	20.90	-1.54	0.8462	20.04	-0.98
0.1009	25.97	-0.50	0.3014	23.84	-1.16	0.5011	22.03	-1.51	0.6997	20.62	-1.47	0.8993	19.95	-0.68
0.1495	25.40	-0.72	0.3503	23.35	-1.30	0.5503	21.61	-1.57	0.7503	20.33	-1.39	0.9418	19.93	-0.39
2,2-Dimethoxypropane (1) + 1,2,4-Trimethylbenzene (2)														
0.0000	28.24	0.00	0.2001	25.95	-0.73	0.3995	24.12	-1.03	0.5998	22.40	-1.16	0.7962	21.11	-0.91
0.0515	27.59	-0.25	0.2475	25.50	-0.81	0.4485	23.66	-1.08	0.6518	22.02	-1.13	0.8510	20.86	-0.73
0.0998	27.02	-0.44	0.3020	24.97	-0.91	0.4989	23.23	-1.11	0.6987	21.69	-1.09	0.8973	20.71	-0.52
0.1499	26.47	-0.60	0.3512	24.53	-0.97	0.5542	22.77	-1.14	0.7455	21.44	-0.98	0.9456	20.55	-0.30
2,2-Dimethoxypropane (1) + 1,3,5-Trimethylbenzene (2)														
0.0000	27.21	0.00	0.2023	25.29	-0.55	0.3982	23.71	-0.80	0.6001	22.17	-0.97	0.7999	20.99	-0.80
0.0562	26.65	-0.18	0.2502	24.87	-0.64	0.4499	23.31	-0.85	0.6502	21.85	-0.95	0.8492	20.74	-0.71
0.0995	26.21	-0.33	0.3002	24.49	-0.68	0.4964	22.95	-0.89	0.7006	21.52	-0.94	0.8998	20.57	-0.54
0.1481	25.77	-0.44	0.3497	24.06	-0.78	0.5493	22.54	-0.95	0.7454	21.27	-0.89	0.9492	20.48	-0.29

Table 3. (Continued)

x_1	σ mN·m ⁻¹	$\frac{\delta\sigma}{\sigma}$ mN·m ⁻¹	x_1	σ mN·m ⁻¹	$\frac{\delta\sigma}{\sigma}$ mN·m ⁻¹	x_1	σ mN·m ⁻¹	$\frac{\delta\sigma}{\sigma}$ mN·m ⁻¹	x_1	σ mN·m ⁻¹	$\frac{\delta\sigma}{\sigma}$ mN·m ⁻¹	x_1	σ mN·m ⁻¹	$\frac{\delta\sigma}{\sigma}$ mN·m ⁻¹
$T = 313.15 \text{ K}$														
1,1-Diethoxyethane (1) + 1,2,4-Trimethylbenzene (2)														
0.0000	27.71	0.00	0.2003	24.46	-1.59	0.4000	22.43	-1.96	0.6011	20.95	-1.78	0.7998	19.91	-1.17
0.0498	26.73	-0.57	0.2496	23.86	-1.78	0.4501	22.05	-1.93	0.6503	20.68	-1.64	0.8507	19.72	-0.94
0.0992	25.91	-0.98	0.3027	23.34	-1.86	0.4990	21.67	-1.90	0.7002	20.40	-1.51	0.8990	19.53	-0.73
0.1501	25.09	-1.38	0.3505	22.89	-1.91	0.5463	21.37	-1.81	0.7491	20.14	-1.36	0.9497	19.45	-0.39
1,1-Diethoxyethane (1) + 1,3,5-Trimethylbenzene (2)														
0.0000	26.78	0.00	0.1999	24.37	-0.94	0.4008	22.38	-1.45	0.6005	20.73	-1.63	0.7996	19.63	-1.26
0.0487	26.09	-0.33	0.2468	23.86	-1.10	0.4502	21.95	-1.52	0.6506	20.40	-1.59	0.8494	19.52	-1.01
0.0991	25.49	-0.56	0.3001	23.34	-1.23	0.5000	21.54	-1.56	0.7005	20.11	-1.51	0.9003	19.48	-0.67
0.1507	24.91	-0.76	0.3501	22.83	-1.37	0.5495	21.12	-1.62	0.7514	19.80	-1.45	0.9498	19.44	-0.35
2,2-Dimethoxypropane (1) + 1,2,4-Trimethylbenzene (2)														
0.0000	27.71	0.00	0.1994	25.36	-0.79	0.3981	23.52	-1.08	0.5993	21.84	-1.20	0.7987	20.51	-0.97
0.0506	27.03	-0.29	0.2511	24.87	-0.88	0.4501	23.07	-1.13	0.6504	21.45	-1.19	0.8417	20.31	-0.83
0.0996	26.42	-0.51	0.3032	24.38	-0.97	0.5000	22.66	-1.15	0.6993	21.12	-1.14	0.8929	20.12	-0.63
0.1509	25.86	-0.67	0.3475	23.95	-1.05	0.5487	22.25	-1.18	0.7486	20.80	-1.07	0.9487	19.97	-0.34
2,2-Dimethoxypropane (1) + 1,3,5-Trimethylbenzene (2)														
0.0000	26.78	0.00	0.2014	24.79	-0.61	0.3960	23.19	-0.87	0.5931	21.68	-1.03	0.7994	20.40	-0.89
0.0511	26.21	-0.22	0.2506	24.39	-0.67	0.4486	22.77	-0.93	0.6488	21.31	-1.01	0.8388	20.24	-0.78
0.1023	25.71	-0.37	0.3013	23.95	-0.76	0.5014	22.36	-0.98	0.6988	20.99	-0.99	0.8976	20.00	-0.61
0.1503	25.26	-0.49	0.3498	23.56	-0.82	0.5508	21.99	-1.01	0.7499	20.66	-0.97	0.9440	19.95	-0.34

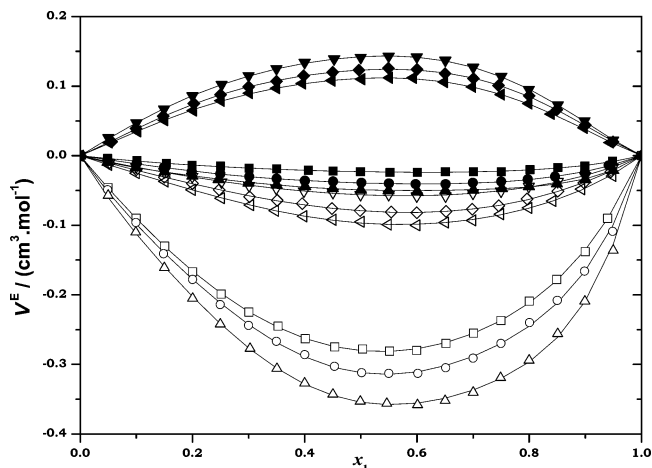


Figure 1. Plots of excess molar volumes (V^E) for 1,1-diethoxyethane (1) + 1,3,5-trimethylbenzene (2) at \blacksquare , 298.15 K; \bullet , 308.15 K; and \blacktriangle , 313.15 K; 1,1-diethoxyethane (1) + 1,2,4-trimethylbenzene (2) at \square , 298.15 K; \circ , 308.15 K; and \triangle , 313.15 K; 2,2-dimethoxypropane (1) + 1,3,5-trimethylbenzene (2) at \blacktriangledown , 298.15 K; \blacklozenge , 308.15 K; and left-facing solid triangle, 313.15 K; and 2,2-dimethoxypropane (1) + 1,2,4-trimethylbenzene (2) at ∇ , 298.15 K; \diamond , 308.15 K; and left-facing open triangle, 313.15 K.

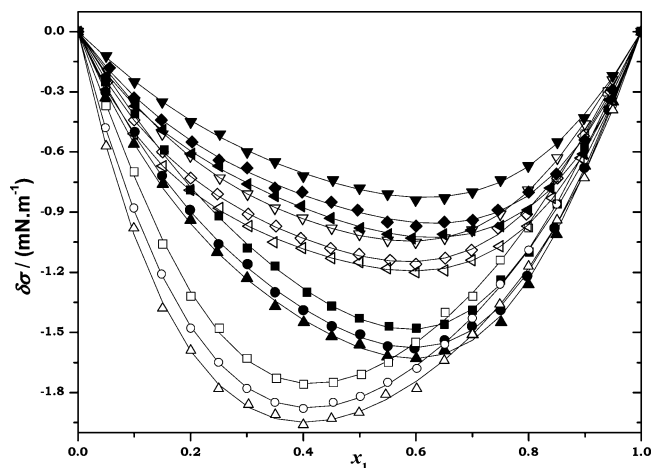


Figure 2. Plots of surface tension deviations ($\delta\sigma$) for 1,1-diethoxyethane (1) + 1,3,5-trimethylbenzene (2) at \blacksquare , 298.15 K; \bullet , 308.15 K; and \blacktriangle , 313.15 K; 1,1-diethoxyethane (1) + 1,2,4-trimethylbenzene (2) at \square , 298.15 K; \circ , 308.15 K; and \triangle , 313.15 K; 2,2-dimethoxypropane (1) + 1,3,5-trimethylbenzene (2) at \blacktriangledown , 298.15 K; \blacklozenge , 308.15 K; and left-facing solid triangle, 313.15 K; and 2,2-dimethoxypropane (1) + 1,2,4-trimethylbenzene (2) at ∇ , 298.15 K; \diamond , 308.15 K; and left-facing open triangle, 313.15 K.

by the equation:¹²

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

where p represents the number of the experimental data, and m represents the number of the coefficients A_i used for fitting the experimental data in eq 3. The optimum number 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 excess properties. The coefficients A_0 , A_1 , A_2 , A_3 , and A_4 along with the corresponding root-mean-square deviations d are summarized in the Table 4.

Figure 1 shows that the excess molar volumes are negative for all the mixtures except for 2,2-dimethoxypropane + 1,3,5-trimethylbenzene at (298.15, 308.15, and 313.15) K. The values of V^E at the whole composition range follow the order 1,1-

Table 4. Least-Squares Parameters (A_i) and Standard Deviations (d) of Excess Molar Volumes and Surface Tension Deviations at Various Temperatures

	A_0	A_1	A_2	A_3	A_4	d
$T = 298.15\text{ K}$						
1,1-Diethoxyethane (1) + 1,2,4-Trimethylbenzene (2)						
$V^E/\text{cm}^3\cdot\text{mol}^{-1}$	-1.120	0.146	-0.114	0.259	-0.139	0.002
$\delta\sigma/\text{mN}\cdot\text{m}^{-1}$	-6.84	-2.16	-1.42	1.05	2.29	0.02
1,1-Diethoxyethane (1) + 1,3,5-Trimethylbenzene (2)						
$V^E/\text{cm}^3\cdot\text{mol}^{-1}$	-0.091	0.029	-0.031	0.025	-0.017	0.001
$\delta\sigma/\text{mN}\cdot\text{m}^{-1}$	-5.73	2.18	-0.76	-1.57	1.50	0.02
2,2-Dimethoxypropane (1) + 1,2,4-Trimethylbenzene (2)						
$V^E/\text{cm}^3\cdot\text{mol}^{-1}$	-0.224	0.067	-0.030	0.025	-0.014	0.001
$\delta\sigma/\text{mN}\cdot\text{m}^{-1}$	-4.07	1.19	-1.47	-0.86	1.24	0.01
2,2-Dimethoxypropane (1) + 1,3,5-Trimethylbenzene (2)						
$V^E/\text{cm}^3\cdot\text{mol}^{-1}$	0.570	-0.099	0.066	0.142	-0.196	0.001
$\delta\sigma/\text{mN}\cdot\text{m}^{-1}$	-3.15	1.26	-1.10	-0.19	0.52	0.01
$T = 308.15\text{ K}$						
1,1-Diethoxyethane (1) + 1,2,4-Trimethylbenzene (2)						
$V^E/\text{cm}^3\cdot\text{mol}^{-1}$	-1.248	0.210	-0.022	0.398	-0.502	0.004
$\delta\sigma/\text{mN}\cdot\text{m}^{-1}$	-7.30	-2.20	-2.05	0.61	0.32	0.01
1,1-Diethoxyethane (1) + 1,3,5-Trimethylbenzene (2)						
$V^E/\text{cm}^3\cdot\text{mol}^{-1}$	-0.156	0.049	-0.057	0.043	0.005	0.001
$\delta\sigma/\text{mN}\cdot\text{m}^{-1}$	-6.09	2.11	-1.83	-1.55	1.57	0.017
2,2-Dimethoxypropane (1) + 1,2,4-Trimethylbenzene (2)						
$V^E/\text{cm}^3\cdot\text{mol}^{-1}$	-0.317	0.113	-0.013	0.010	-0.001	0.001
$\delta\sigma/\text{mN}\cdot\text{m}^{-1}$	-4.47	1.24	-1.72	-1.12	0.57	0.01
2,2-Dimethoxypropane (1) + 1,3,5-Trimethylbenzene (2)						
$V^E/\text{cm}^3\cdot\text{mol}^{-1}$	0.493	-0.089	0.094	0.087	-0.237	0.001
$\delta\sigma/\text{mN}\cdot\text{m}^{-1}$	-3.61	1.44	-1.86	-0.05	0.21	0.01
$T = 313.15\text{ K}$						
1,1-Diethoxyethane (1) + 1,2,4-Trimethylbenzene (2)						
$V^E/\text{cm}^3\cdot\text{mol}^{-1}$	-1.417	0.259	-0.163	0.640	-0.637	0.003
$\delta\sigma/\text{mN}\cdot\text{m}^{-1}$	-7.58	-2.11	-2.93	-0.12	-0.20	0.02
1,1-Diethoxyethane (1) + 1,3,5-Trimethylbenzene (2)						
$V^E/\text{cm}^3\cdot\text{mol}^{-1}$	-0.196	0.047	-0.050	0.101	-0.123	0.001
$\delta\sigma/\text{mN}\cdot\text{m}^{-1}$	-6.31	2.10	-2.17	-1.79	1.73	0.02
2,2-Dimethoxypropane (1) + 1,2,4-Trimethylbenzene (2)						
$V^E/\text{cm}^3\cdot\text{mol}^{-1}$	-0.387	0.119	0.018	-0.047	-0.059	0.001
$\delta\sigma/\text{mN}\cdot\text{m}^{-1}$	-4.65	1.18	-2.31	-0.84	0.02	0.01
2,2-Dimethoxypropane (1) + 1,3,5-Trimethylbenzene (2)						
$V^E/\text{cm}^3\cdot\text{mol}^{-1}$	0.445	-0.073	0.037	0.082	-0.016	0.001
$\delta\sigma/\text{mN}\cdot\text{m}^{-1}$	-3.90	1.50	-1.78	-0.08	-0.56	0.01

diethoxyethane + 1,2,4-trimethylbenzene < 2,2-dimethoxypropane + 1,2,4-trimethylbenzene < 1,1-diethoxyethane + 1,3,5-trimethylbenzene < 2,2-dimethoxypropane + 1,3,5-trimethylbenzene. The minimum (or maximum) values of V^E for them are at about $x_1 \approx 0.55$. The V^E values are more negative with increasing temperature for all the binary mixtures.

Figure 2 illustrates that the surface tension deviations $\delta\sigma$ of all the binary systems investigated are negative at temperatures of (298.15, 308.15, and 313.15) K. The minimum values (at $x \approx 0.4$ or 0.55) of $\delta\sigma$ at the same temperature follow the

sequence 1,1-diethoxyethane + 1,2,4-trimethylbenzene < 1,1-diethoxyethane + 1,3,5-trimethylbenzene < 2,2-dimethoxypropane + 1,2,4-trimethylbenzene < 2,2-dimethoxypropane + 1,3,5-trimethylbenzene.

Supporting Information Available:

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

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