Densities and Viscosities of Propane-1,2,3-triol + Ethane-1,2-diol at T = (298.15 to 338.15) K

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Experimental data of densities and viscosities of propane-1,2,3-triol + ethane-1,2-diol binary mixtures were measured over the entire mole fraction range from (298.15 to 338.15) K at atmospheric pressure. Excess molar volumes as a function of mole fraction average have been obtained and fitted to the Redlich−Kister equation. Estimated coefficients of the Redlich−Kister equation and standard error calculated from the Redlich−Kister equation to the experimental data were also presented.

Introduction

Both propane-1,2,3-triol and ethane-1,2-diol are important nonaqueous solvents with extensive use. They are completely miscible. Densities and viscosities are needed for the design of new processes on an industrial scale. Further experimental data of density and viscosity of a binary mixture are important from a theoretical viewpoint to understand the liquid theory. The liquid densities and excess molar volume V^E for the binary mixtures propane-1,2,3-triol + 1-propanol, + 2-propanol, + 1,2-propanediol, and + 1,3-propanediol have been presented in the literature.[1] Ethane-1,2-diol is the simplest homologue of the diol series; however, few experimental data concerning the binary mixture of propane-1,2,3-triol and ethane-1,2-diol are available in the literature.

In this work, the densities and viscosities of mixtures consisting of propane-1,2,3-triol and ethane-1,2-diol were measured over the entire range of their compositions from (298.15 to 338.15) K at atmospheric pressure. The excess molar volumes V^E of this binary system have been obtained and fitted to the Redlich−Kister equation.

Experimental Section

Materials. Propane-1,2,3-triol and ethane-1,2-diol were purchased from Beijing Chemical Reagents Company. They were purified by simple vacuum fractionation before use. The absolute pressure ranges used were (1.3 to 2.0) kPa, and the temperature was 170 °C for propane-1,2,3-triol and 70 °C for ethane-1,2-diol. Their purities were greater than 0.997 mass fraction analyzed by gas chromatography (SP-2100) fitted with capillary columns and a FID detector. Nitrogen was used as carrier gas.

Apparatus and Procedure. The mixtures of propane-1,2,3-triol and ethane-1,2-diol were prepared by mass. A TE2101-L electronic digital balance accurate to within ± 0.1 mg was used. The uncertainty in the mole fraction of the mixtures was estimated to less than ± 0.0001. All molar quantities are based on the IUPAC 2005 relative atomic mass table.[2] At atmospheric pressure, densities of pure liquids and their mixtures were determined by using a 10 mL pycnometer, and since its volume varied with temperature it was calibrated with pure water from (298.15 to 338.15) K. The temperature was controlled by a water bath to within an uncertainty of ± 0.05 K. The absolute density of water for calibration was obtained from literature values.[3] For viscosity measurement, the BROOKFIELD DV-II+Pro digital rotational viscometer was used at atmospheric pressure, and the temperature was controlled by a Brookfield TC-02 thermostat water bath with an uncertainty of ± 0.02 K. Relative uncertainty of the viscometer in the measurements was ± 1 % in the full range, and the repeatability was ± 0.2 % declared by the manufacturer.

Experiments were repeated at least four times at each temperature for all mixtures, and the results were averaged. The experimental average uncertainties of density and viscosity were estimated to be about ± 1 %. Accordingly, the relative deviations of V^E were estimated to be about ± 2 %.

Result and Discussion

The density and viscosity values of pure liquids in this work are listed in Table 1. The available literature values[1,4−14] are also given in Table 1. Compared to the literature, the maximum absolute deviation of the density values is about 0.0011 g·cm^{-3} for pure propane-1,2,3-triol and is 0.00095 g·cm^{-3} for pure ethane-1,2-diol, and the maximum absolute deviation of the viscosity values is 16.9 mPa·s for pure propane-1,2,3-triol. For pure ethane-1,2-diol at 298.15 K, the viscosity values are lower (by about 0.477 mPa·s and 1.28 mPa·s) than those reported by Pal et al.[8] and Tsierkezos et al.[10] and notably higher (by about 1.3 mPa·s) than that given by Lide et al.[11] The densities and viscosities of the propane-1,2,3-triol + ethane-1,2-diol mixture, as a function of propane-1,2,3-triol content over the temperature range from (298.15 to 338.15) K, are presented in Tables 2 and 3.

The excess molar volumes V^E were calculated from the measurements according to the following equations[15,16]

$$V^E = \frac{x_1M_1 + x_2M_2}{\rho} - \frac{x_1M_1}{\rho_1} - \frac{x_2M_2}{\rho_2} \quad (1)$$

where ρ is density of mixtures; x_1 and x_2 are mole fractions; M_1 and M_2 are molar masses; and ρ_1 and ρ_2 are densities of

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Table 1. Comparison of Experimental Densities (ρ) and Viscosities (η) of Pure Liquids with Literature Values

	ρ/g·cm^{-3}		η/mPa·s	
T/K	exptl	lit.	exptl	lit.
		Propane-1,2,3-triol		
298.15	1.2578	1.2589,[1] 1.2581[4]	943.8	945[5,a]
303.15	1.2547	1.2556[1]	628.9	624[5,a], 612[6]
308.15	1.2522	1.2527[1]	431.9	
313.15	1.2494	1.2495[1]	295.9	284[6]
318.15	1.2458	1.2462[1]	185.8	
323.15	1.2423	1.2429[1]	151.2	142[6]
328.15	1.2393	1.2396[1]	108.4	
333.15	1.2361	1.2360[1]	84.8	81.3[6]
338.15	1.2328		62.2	
		Ethane-1,2-diol		
298.15	1.1101	1.10986,[7] 1.1098,[8] 1.10988[9]	17.4	17.877,[8] 18.6826[10,a], 16.1[11]
303.15	1.1071	1.10682,[7] 1.1064,[9] 1.106512[12]	13.8	13.8678[10]
308.15	1.1035	1.10320,[7] 1.10289,[9] 1.10294,[13] 1.103089[12]	11.5	11.6956[10,a], 10.591[13]
313.15	1.1003	1.09980,[7] 1.09935,[9] 1.099747[12]	9.42	9.5348[10]
318.15	1.0965	1.09623,[7] 1.096301,[14] 1.096312[12]	8.1	
323.15	1.0935	1.09259,[7] 1.092946[12]	6.95	
328.15	1.0892	1.08866,[7] 1.088314,[14] 1.089471[12]	5.96	
333.15	1.0856	1.086011[12]	5.22	
338.15	1.0821	1.082634[12]	4.53	

[a] Interpolated value.

Table 2. Experimental Densities ρ for the Binary Mixture of Propane-1,2,3-triol (1) + Ethane-1,2-diol (2)

	T/K								
x_1	298.15	303.15	308.15	313.15	318.15	323.15	328.15	333.15	338.15
	ρ/g·cm^{-3}								
0.0000	1.1101	1.1071	1.1035	1.1003	1.0965	1.0935	1.0892	1.0856	1.0821
0.1001	1.1292	1.1263	1.1229	1.1199	1.1163	1.1134	1.1094	1.1060	1.1028
0.2002	1.1472	1.1444	1.1412	1.1382	1.1347	1.1318	1.1280	1.1246	1.1214
0.3001	1.1640	1.1612	1.1582	1.1552	1.1518	1.1487	1.1451	1.1418	1.1386
0.4002	1.1802	1.1773	1.1745	1.1716	1.1682	1.1652	1.1617	1.1584	1.1551
0.4991	1.1950	1.1922	1.1895	1.1867	1.1833	1.1801	1.1767	1.1735	1.1702
0.6011	1.2094	1.2067	1.2040	1.2013	1.1978	1.1946	1.1914	1.1882	1.1850
0.7015	1.2226	1.2197	1.2170	1.2143	1.2109	1.2079	1.2047	1.2015	1.1983
0.7981	1.2345	1.2315	1.2291	1.2265	1.2231	1.2199	1.2169	1.2138	1.2106
0.8961	1.2461	1.2432	1.2407	1.2380	1.2347	1.2312	1.2283	1.2253	1.2222
1.0000	1.2578	1.2547	1.2522	1.2494	1.2458	1.2423	1.2393	1.2361	1.2328

Table 3. Experimental Viscosities η for the Binary Mixture of Propane-1,2,3-triol (1) + Ethane-1,2-diol (2)

	T/K								
x_1	298.15	303.15	308.15	313.15	318.15	323.15	328.15	333.15	338.15
	η/mPa·s								
0.0000	17.4	13.8	11.5	9.42	8.10	6.95	5.96	5.22	4.53
0.1001	25.1	20.7	17.0	14.0	11.7	9.65	8.31	7.06	6.10
0.2002	37.4	30.3	24.1	19.6	16.1	13.1	11.0	9.17	7.81
0.3001	55.0	43.1	33.9	27.0	21.7	17.9	14.6	12.4	10.5
0.4002	82.8	64.2	48.5	38.2	30.6	24.4	20.1	16.4	13.8
0.4991	121.4	91.4	69.4	52.6	41.1	33.6	26.5	21.5	18.1
0.6011	184.2	134.0	100.2	75.2	57.3	45.3	36.0	28.4	23.5
0.7015	272.9	195.0	142.4	107.0	81.0	62.0	48.1	37.6	30.7
0.7981	405.9	285.9	206.2	145.2	108.2	82.4	64.4	49.4	39.5
0.8961	611.8	422.7	299.9	204.6	148.4	111.0	84.6	66.2	50.9
1.0000	943.8	628.9	431.9	295.9	185.8	151.2	108.4	84.8	62.2

propane-1,2,3-triol (1) and ethane-1,2-diol (2), respectively.

All values of V^E for the mixtures of propane-1,2,3-triol (1) + ethane-1,2-diol (2) were fitted to the Redlich−Kister polynominal equation[17]

$$V^E = x_1(1 - x_1)\sum_{i=0}^{m-1} A_i(2x_1 - 1)^i \qquad (2)$$

where A_i are adjustable parameters; x_1 is the mole fraction of propane-1,2,3-triol (1); and m is the number of coefficients of the Redlich−Kister equation. A third-order polynomial was found to be the optimum for the property. The polynomial coefficients A_i were obtained by fitting the equation to the experimental results with the least-squares regression method. The standard deviations are defined as

$$\sigma = \left[\frac{\sum (V^E_{calcd} - V^E_{exptl})^2}{n - m}\right]^{1/2} \qquad (3)$$

n is the number of experimental data.

Table 4. Excess Molar Volume V^E for the Binary Mixture of Propane-1,2,3-triol (1) + Ethane-1,2-diol (2)

	T/K								
x_1	298.15	303.15	308.15	313.15	318.15	323.15	328.15	333.15	338.15
	V^E/cm^3·mol^{-1}								
0.1001	−0.017	−0.022	−0.028	−0.035	−0.045	−0.054	−0.063	−0.073	−0.087
0.2002	−0.032	−0.048	−0.057	−0.062	−0.077	−0.087	−0.100	−0.107	−0.119
0.3001	−0.043	−0.057	−0.067	−0.076	−0.089	−0.101	−0.111	−0.124	−0.138
0.4002	−0.068	−0.077	−0.090	−0.104	−0.118	−0.131	−0.148	−0.153	−0.161
0.4991	−0.071	−0.085	−0.105	−0.115	−0.127	−0.139	−0.149	−0.159	−0.168
0.6011	−0.073	−0.093	−0.104	−0.117	−0.129	−0.140	−0.152	−0.164	−0.173
0.7015	−0.058	−0.069	−0.076	−0.086	−0.102	−0.122	−0.133	−0.141	−0.152
0.7981	−0.037	−0.043	−0.057	−0.074	−0.088	−0.101	−0.113	−0.124	−0.137
0.8961	−0.020	−0.028	−0.035	−0.044	−0.060	−0.062	−0.073	−0.087	−0.098

n is the number of experimental data.

The data of excess molar volume V^E are given in Table 4. The V^E versus the mole fraction of propane-1,2,3-triol is shown in Figure 1. Table 5 lists the values of the parameters A_i together with the standard deviations.

Excess molar volume, which depends on the composition and/or temperature, is of great importance in understanding the nature of molecular interaction that exists in the binary mixtures. As shown in Figure 1, the values of V^E are negative for propane-1,2,3-triol + ethane-1,2-diol mixtures from (298.15 to 338.15) K over the entire range of compositions. The negative V^E values

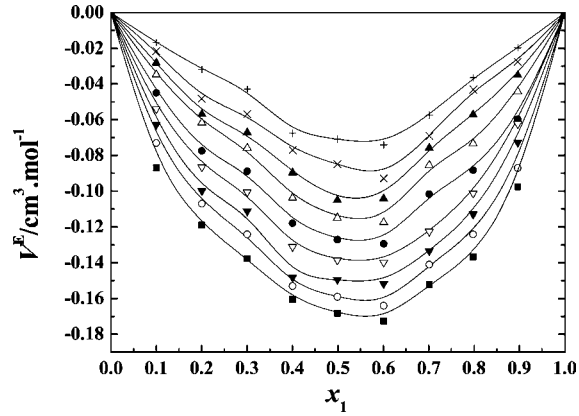

Figure 1. Excess molar volume V^E vs molar fraction of water for propane-1,2,3-triol (1) + ethane-1,2-diol (2). +, 298.15 K; ×, 303.15 K; ▲, 308.15 K; Δ, 313.15 K; ●, 318.15 K; ▽, 323.15 K; ▼, 328.15 K; ○, 333.15 K; ■, 338.15 K. The symbols represent experimental values; the solid curves are calculated with the Redlich−Kister equation.

Table 5. Coefficients of the Redlich−Kister Equation for V^E of the Propane-1,2,3-triol (1) + Ethane-1,2-diol (2) System

property	*T*/K	A_0	A_1	A_2	A_3	σ
V^E/cm^3·mol^{-1}	298.15	−0.2879	−0.0898	0.1896	0.1361	0.0032
	303.15	−0.3453	−0.0908	0.1608	0.1690	0.0055
	308.15	−0.4007	−0.0767	0.1433	0.1142	0.0055
	313.15	−0.4458	−0.0898	0.0890	0.0714	0.0045
	318.15	−0.4934	−0.0810	−0.0489	0.0158	0.0063
	323.15	−0.5468	−0.1337	−0.0934	0.1425	0.0045
	328.15	−0.5955	−0.1108	−0.1713	0.0922	0.0063
	333.15	−0.6265	−0.1173	−0.2851	0.0702	0.0063
	338.15	−0.6583	−0.1137	−0.4328	0.0850	0.0063

for binary mixtures indicate a decrease in the overall volume of the mixture. The contraction of the volume could be attributed to the stronger hydrogen bond that arises from the dipole−dipole interactions between propane-1,2,3-triol and ethane-1,2-diol molecules. The increase of the absolute values of V^E with the increase of the temperature may be attributed to the increasing importance of hydrogen bond with increasing temperature.

Conclusions

The densities and viscosities of mixtures consisting of propane-1,2,3-triol and ethane-1,2-diol have been measured at different temperatures over the entire range of their compositions. The excess molar volumes V^E of this binary system have been obtained and fitted to the Redlich−Kister equation.

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