Measurement and Correlation of Densities and Viscosities of Thiourea in Triglycol + Water at Temperatures from (302.85 to 341.45) K

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The densities and viscosities of thiourea in triglycol + water had been determined at temperatures from (302.85 to 341.45) K. The relative viscosities were correlated using the extended Jones–Dole equation equation. The results showed that the model agreed very well with the experimental data.

Introduction

Isopropyl mercaptan is an important pharmaceutical intermediate and a widely used chemical material. Li et al.¹ developed a new technique for the synthesis of isopropyl mercaptan using thiourea as the raw material and triglycol as solvent.^{1,2} This new technique was characterized by mild reaction conditions and high product purity. The densities and viscosities were basic data in chemical engineering design, process optimization, and molecular thermodynamic study of solution. In the synthesis and purification process of isopropyl mercaptan, it was useful to know the data of the densities and viscosities of thiourea in triglycol + water. In this study, densities and viscosities of thiourea in triglycol + water had been measured at temperatures from (302.85 to 341.45) K according to the reaction conditions of this product. From measurements of the densities and viscosities, the relative viscosities of thiourea in triglycol + water were calculated and correlated using the extended Jones-Dole equation. Results were fit to obtain the adjustable parameters and standard deviations between the measured and the fitted values. These parameters could be used to study the molecular interactions among the components of the mixture and had certain practical value for the synthesis and design of isopropyl mercaptan.

Experimental Section

Materials. Thiourea and triglycol were of analytical reagent grade, obtained from Shanghai Chemical Reagent Co., and have mass fraction purities of 0.995. The double-distilled water used in the experiments was deionized, and its conductivity was less than $1 \cdot 10^{-4} \text{ S} \cdot \text{m}^{-1}$.

Measurements of Densities. The density of the mixtures and the corresponding pure substances were measured with an Anton Paar model DMA 5000 digital vibrating U-tube densimeter, with an automatic viscosity correction and a stated accuracy of \pm 5 · 10⁻⁶ g · cm⁻³. The temperature in the cell was regulated to \pm 0.001 K with a built-in solid-state thermostat. It was measured

Table 1.	Comparison	of Experin	nental Data	and	Literature	Data	for
Densities	of Triglycol,	Water, or	Thiourea				

	Т	ρ	$\rho(\text{lit.})$	
substance	K	$\overline{g \cdot cm^{-3}}$	$g \cdot cm^{-3}$	$100(\rho - \rho(lit.))/\rho$
triglycol	293.35	1.1232	1.1274 ⁵	-0.37
	293.15	1.1245	1.124^{6}	0.044
thiourea	298.15	1.4051	1.405^{5}	0.007

Table 2. Densities and Viscosities for Triglycol (1) + Water (2) Mixtures at Various Temperatures and Mass Fractions w_1

Т	ρ	η	Т	ρ	η
Κ	g·cm ⁻³	mPa•s	Κ	g•cm ⁻³	mPa•s
	$w_1 = 1.00$			$w_1 = 0.91$	
302.85	1.1166	27.101	302.85	1.1117	20.365
307.75	1.1119	19.701	307.75	1.1083	15.356
312.65	1.1084	15.866	312.65	1.1039	12.306
317.45	1.1047	13.023	317.45	1.1005	10.165
322.25	1.1010	10.255	322.25	1.0970	8.100
327.05	1.0979	7.953	327.05	1.0939	6.294
332.15	1.0935	5.316	332.15	1.0896	4.238
341.45	1.0861	1.600	341.45	1.0832	1.270
	$w_1 = 0.82$			$w_1 = 0.72$	
302.85	1.1066	14.855	302.85	1.0969	9.793
307.75	1.1026	11.222	307.75	1.0942	7.514
312.65	1.0986	9.034	312.65	1.0902	6.176
317.45	1.0945	7.516	317.45	1.0863	5.149
322.25	1.0910	6.011	322.25	1.0828	4.121
327.05	1.0876	4.693	327.05	1.0793	3.272
332.15	1.0838	3.161	332.15	1.0753	2.265
341.45	1.0759	0.955	341.45	1.0674	0.693

by means of two integrated Pt 100 platinum thermometers, and its stability was better then \pm 0.002 K. Before each series of measurements, the apparatus was calibrated with double-distilled and degassed water. To minimize the errors in composition, all mixtures were prepared by mass using the cell and the procedure described by Tasic et al.³ and a Mettler AG 204 balance with a precision of $1 \cdot 10^{-4}$ g. The uncertainty of the mole fraction calculation was less than $\pm 1 \cdot 10^{-4}$. All molar quantities were based on the International Union of Pure and Applied Chemistry (IUPAC) relative atomic mass table. The experimental uncertainty in density was about $\pm 1 \cdot 10^{-4}$ g·cm⁻³.

Measurements of Viscosities. Viscosity was measured using an Ubbelohde-type glass capillary viscometer of 0.9 mm diameter (type 1836-A, Shanghai Glass Instruments Factory, China), calibrated with double-distilled water at (298.15 and

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Table 3. Densities and Viscosities for Thiourea (3) in Triglycol (1) + Water (2) Mixtures at Various Temperatures and Mass Fractions w_1

С	ρ	η		ρ	η		С	ρ	η		ρ	η	
$mol \cdot L^{-1}$	g·cm ⁻³	mPa•s	100 RD	g·cm ⁻³	mPa•s	100 RD	$\overline{\mathrm{mol} \cdot \mathrm{L}^{-1}}$	g·cm ⁻³	mPa•s	100 RD	g·cm ⁻³	mPa•s	100 RD
			$w_1 = 1.00$							$w_1 = 1.00$			
0.0756	1 1165	r = 302.85	K -2.76	1 1129	r = 307.75 J	C —1 51	1.0575	1 1263	r = 302.85 I	K -1.68	1 1224	T = 307.75 k	-1.87
0.2294	1.1179	25.842	0.59	1.1129	19.105	1.49	1.2361	1.1284	22.088	-0.68	1.1248	16.275	-0.61
0.3869 0.7981	1.1185	24.336 23.929	-2.62 2.25	1.1154	17.985 17.652	-1.98 2.38	1.6076	1.1320	22.009	1.53	1.1284	16.050	0.91
0.7901	1.1257	r = 312.65	2.23 K	1.1205	T = 317.45 K	2.50		7	r = 312.65 I	X	2	T = 317.45 k	<u> </u>
0.0756	1.1091	15.336	-1.67	1.1047	12.821	0.02	1.0575	1.1187	13.152	-1.21	1.1151	10.774	-0.96
0.2294 0.3869	1.1106	15.290 14.421	-1.08	1.1071	12.580	-1.65	1.6076	1.1214 1.1246	12.979	-0.62 0.94	1.11//	10.596	-0.87 0.32
0.7981	1.1165	14.010	1.76	1.1126	11.493	2.18							
0.0756	1 1020 T	$^{2} = 322.25$	K -0.08	7 1 0984	T = 327.05 k 7 844	C 0.22	1.0575	1 1115	r = 322.25 I	K -0.45	1 1085	T = 327.05 k	-0.17
0.2294	1.1031	9.836	0.71	1.1003	7.688	1.54	1.2361	1.1142	8.353	-0.70	1.1110	6.450	-0.96
0.3869 0.7981	1.1054	9.292 9.007	-1.93	1.1011	6.930	-1.25 1.39	1.6076	1.11/8	8.254	0.32	1.1145	6.413	0.08
	7	= 332.15	K	7	r = 341.45 J	K		Т	r = 332.15 I	K	1	T = 341.45 k	<u> </u>
0.0756 0.2294	1.0950 1.0964	5.235 5.108	0.07 0.71	$1.0878 \\ 1.0890$	1.568 1.518	-0.12 0.11	0.7981 1.2361	$1.1019 \\ 1.1071$	4.687 4.306	$1.93 \\ -0.98$	1.0949 1.1005	1.388 1.273	$1.89 \\ -1.07$
0.3869	1.0973	4.801	-2.54	1.0902	1.434	-2.33	1.6076	1.1105	4.229	0.31	1.1033	1.259	0.51
			$w_1 = 0.91$							$w_1 = 0.91$			
0 1235	1 1 1136	$^{\circ} = 302.851$ 21.061	K 1 43	7 1 1109	T = 307.75 F	C 0.80	1 0114	T 1 1257	r = 302.85 I 22.928	X 0.13	1 1232	T = 307.75 k 16 872	0.53
0.3730	1.1168	21.493	0.53	1.1140	15.845	-0.17	1.2730	1.1295	23.455	-0.30	1.1263	17.125	-0.37
0.6258	1.1205	22.081	0.46 v	1.11/3	16.235 r — 317.45 k	0.08		т	- 212 65 I	Z	-	T = 317.45 k	
0.1235	1.1072	12.409	-0.06	1.1032	10.256	0.05	1.0114	1.1195	13.434	0.82	1.1155	11.049	1.35
0.3730	1.1101	12.577 12.883	-0.76 -0.39	1.1058 1.1096	10.416 10.518	-0.23 -1.03	1.2730	1.1225	13.538	-0.33	1.1189	11.014	-0.58
0.0200	11101	r = 322.25	K	7	r = 327.05 H	K		Т	= 322.25 I	K	2	T = 327.05 K	ī.
0.1235	1.0995	8.181	0.45	1.0960	6.362	0.62	1.0114	1.1120	8.653	1.37	1.1086	6.721	1.61
0.6258	1.1022	8.201	-0.68	1.1021	6.398	-0.99	1.2750	1.1155	8.010	0.07	1.1120	0.084	0.81
0.1005	7	= 332.15	K	7	r = 341.45 H	K a ca	1.0114	7	= 332.15 I	X	1 0000	T = 341.45 K	
0.1235 0.3730	1.0924	4.249 4.259	0.40 0.54	1.0863	1.274 1.276	0.39	1.0114 1.2730	1.1051 1.1076	4.477 4.442	-1.04	1.0980	1.322	-0.63
0.6258	1.0994	4.187	-1.98	1.0919	1.263	-1.13							
	7	- 202 05 1	$w_1 = 0.82$	7	- 207 75 I	7		7	- 202.95 1	$w_1 = 0.82$	-	E - 207 75 I	-
0.1712	1.1064	= 302.851 14.560	-2.33	1.1039	= 307.75 r 10.965	-2.58	1.3765	1.1266	= 302.851 16.837	0.90	1.1233	I = 307.75 K 12.534	0.69
0.5143	1.1151	15.117	-1.33	1.1099	11.432	-0.86	1.7231	1.1310	17.426	0.63	1.1279	12.931	0.50
0.0504	1.1105	r = 312.65	0.02 K	7	T = 317.45 k	0.19	2.7072	1.1400 T	r = 312.65	2.00 K	1.1425	T = 317.45 k	2.02
0.1712	1.1000	8.845	-2.49	1.0963	7.461	-1.30	1.3765	1.1194	10.091	0.75	1.1160	8.409	1.20
0.8584	1.1062	9.232 9.616	-0.67 0.54	1.1026	7.638 8.011	-1.32 0.76	2.7692	1.1242	10.340 11.657	-0.03	1.1207	8.513 9.589	-0.67
	7	r = 322.25	K	7	r = 327.05 H	K		Т	r = 322.25 I	X	1	T = 327.05 k	2
0.1712 0.5143	1.0934 1.0985	5.899 6.052	-2.03 -1.66	1.0898 1.0948	4.647 4.725	-1.39 -2.06	1.3765 1.7231	1.1126 1.1176	6.635 6.792	0.91 0.44	$1.1096 \\ 1.1140$	5.244 5.265	1.74 - 0.60
0.8584	1.1045	6.336	0.39	1.1012	4.979	0.61	2.7692	1.1317	7.521	2.00	1.1288	5.857	1.72
0 1712	1 0861	r = 332.15	K -1.51	1 0792	T = 341.45 K	C —1 19	1 3765	1 1057	r = 332.15 I	K 1 14	1 0991	T = 341.45 k 1 045	0.20
0.5143	1.0910	3.182	-1.95	1.0834	0.969	-1.47	1.7231	1.1102	3.553	0.33	1.1036	1.063	-0.31
0.8584	1.0975	3.335	0.26	1.0906	1.023	1.59	2.7692	1.1252	3.875	1.81	1.1179	1.151	1.22
	7	7 = 302.851	$w_1 = 0.72$	7	r = 307.75 k	7		Т	r = 302.85 I	$w_1 = 0.72$	2	T = 307.75 k	-
0.2186	1.1011	10.267	1.20	1.0982	7.743	0.03	2.1502	1.1306	12.486	-1.12	1.1279	9.474	-0.29
0.6535 1.0850	1.1093 1.1148	10.857 11.206	1.79 0.17	$1.1054 \\ 1.1110$	8.268 8.515	1.78 0.15	2.7800 3.4029	1.1412 1.1498	13.434 14.295	-1.18 -2.39	1.1378 1.1466	$10.045 \\ 10.685$	-0.92 -1.09
1.7265	1.1238	11.742	-2.41	1.1210	8.935	-1.76							
0.2186	7 1.0945	r = 312.65 1 6.400	K 0.64	7 1.0909	T = 317.45 F 5.369	0.82	2,1502	T 1.1244	r = 312.65 I 7.739	≤ −0.20	1.1206	T = 317.45 k 6.401	-1.61
0.6535	1.1018	6.712	0.67	1.0976	5.669	1.44	2.7800	1.1343	8.222	-0.28	1.1308	6.872	-0.73
1.0850	1.10/4 1.1174	7.283	-2.11	1.1039	5.903 6.091	-2.36	3.4029	1.1429	8.632	-1.38	1.1395	7.202	-2.19
	7	= 322.25	K	Т	r = 327.05 H	κ		Т	= 322.25 I	X	2	T = 327.05 K	
0.2186 0.6535	1.0870 1.0938	4.322 4.535	1.15 1.14	1.0842 1.0907	3.398 3.642	0.23 2.23	2.1502 2.7800	1.1168 1.1273	5.074 5.442	-2.59 -1.66	1.1137 1.1243	4.005 4.332	-2.74 -0.43
1.0850	1.1002	4.749	1.31	1.0970	3.776	1.43	3.4029	1.1361	5.743	-2.27	1.1330	4.482	-2.35
1.7203	1.1105	4.920 = 332.151	-1.55 K	1.1005	ی.2000 ۳ = 341 45 ه	-2.40		т	r = 332.15	<	5	T = 341.45 k	-
0.2186	1.0797	2.330	0.18	1.0731	0.720	0.79	2.1502	1.1099	2.743	-0.90	1.1046	0.846	-0.72
0.6535 1.0850	1.0868 1.0935	2.447 2.550	0.74 0.88	1.0797 1.0872	0.754 0.785	0.99 1.08	2.7800 3.4029	1.1203 1.1294	2.905 3.020	-0.18 -1.04	1.1134 1.1230	0.886 0.930	-1.40 -1.72
1.7265	1.1035	2.636	-1.38	1.0962	0.804	-2.31							



Figure 1. Viscosity curves of thiourea in pure triglycol: \blacksquare , 302.85 K; \blacklozenge , 307.75 K; \bigstar , 312.65 K; \blacktriangledown , 317.45 K; \diamondsuit , 322.25 K; \bigcirc , 327.05 K; \square , 332.15 K; \triangle , 341.45 K; solid line, calculated value.

313.15) K. A thoroughly cleaned and dried viscometer, filled with experimental solutions, was placed vertically in an insulated jacket, wherein constant temperature (± 0.02 K) was maintained by circulating water from a thermoelectric controller (type 501, Shanghai Laboratory Instrument Works Co., Ltd.) at the required temperature. After thermal stability was attained, the flow times of the solutions were recorded with an electronic digital stopwatch correct to ± 0.01 s. At least five repetitions of each data point obtained were reproducible to ± 0.06 s, and the results were averaged. Because all flow times were greater than 200 s and the capillary diameter (0.9 mm) was far less than its length (120 mm), the kinetic energy and end corrections, respectively, were found to be negligible. The viscosity was then calculated from the fundamental relationship.⁴

The values of viscosity and density of pure water come from the literature.⁵ The uncertainty in the viscosity measurement is estimated to be ± 0.006 mPa·s.

Experiment Reliability Proof. The measured densities of triglycol, water, or thiourea have been compared with literature values.^{5,6} The results are listed in Table 1. It could be seen that the present experimental values of densities are in good agreement with those reported in the literature.

Results and Discussion

The measured densities and viscosities for triglycol (1) + water (2) containing mass fractions of triglycol, $w_1 = (0.72, 0.82, 0.91, \text{ or } 1.00)$, were reported in Table 2 for temperatures from (302.85 to 341.45) K. It could be seen that the densities and viscosities for triglycol + water mixtures decreased with increasing temperature at a fixed w_1 in triglycol + water binary mixtures and increased with an increase in w_1 at a fixed temperature in triglycol + water binary mixtures, and the density and temperature had been found to be linear over the whole concentration range studied.

The measured densities and viscosities for thiourea in triglycol + water at various temperatures and mass fractions w_1 are listed in Table 3. It shows that the densities and viscosities for ternary mixtures decreased with increasing temperature under the same mass fraction w_1 of thiourea and increased with an increase of mass fraction w_1 under the same temperature and the density and temperature also had a good linear relationship. The plot of viscosities for thiourea in triglycol + water at various temperatures and mass fractions w_1 are illustrated in Figures 1 to 4. From Figure 1, it could be found that the viscosities



Figure 2. Viscosity curves of thiourea in triglycol + water mixtures ($w_1 = 0.91$): \blacksquare , 302.85 K; \blacklozenge , 307.75 K; \blacktriangle , 312.65 K; \blacktriangledown , 317.45 K; \diamondsuit , 322.25 K; \bigcirc , 327.05 K; \Box , 332.15 K; \triangle , 341.45 K; solid line, calculated value.



Figure 3. Viscosity curves of thiourea in triglycol + water mixtures ($w_1 = 0.82$): **I**, 302.85 K; **O**, 307.75 K; **A**, 312.65 K; **V**, 317.45 K; **O**, 322.25 K; **O**, 327.05 K; **D**, 332.15 K; \triangle , 341.45 K; solid line, calculated value.



Figure 4. Viscosity curves of thiourea in triglycol + water mixtures ($w_1 = 0.72$): \blacksquare , 302.85 K; \blacklozenge , 307.75 K; \blacktriangle , 312.65 K; \blacktriangledown , 317.45 K; \diamondsuit , 322.25 K; \bigcirc , 327.05 K; \square , 332.15 K; \triangle , 341.45 K; solid line, calculated value.

decreased with increasing concentration of thiourea at constant temperature and decreased with increasing temperature under the same concentration of thiourea in pure triglycol. Figures 2 to 4 show that the viscosities increase with increasing concentration of thiourea at constant temperature and decrease with increasing temperature under the same concentration of thiourea for ternary mixtures.

The relative viscosities for thiourea in triglycol + water mixed solvents were calculated from the extended Jones–Dole equation. 7

$$\eta_{\rm r} = \frac{\eta}{\eta_0} = 1 + A(c/c_0^{\phi})^{1/2} + B(c/c_0^{\phi}) + D(c/c_0^{\phi})^2 \quad (1)$$

In this equation, η_r is relative viscosity; η and η_0 are the viscosities of the solution and the pure solvents or solvent mixtures respectively; *c* is the volume mole concentration of thiourea in the solution; c_0° is 1 mol·L⁻¹; and *A*, *B*, and *D* are the constants at a given temperature and characteristic of the solvent and the solute. The *A* coefficient accounts for solute–solute interactions, and the *B* parameter is a measure of the solute–solvent interactions. It reflects the size and shape effect of a solute, structure effect, and salvation effect caused by solute–solvent interaction, and it is a main contributor to η_r . The precise physical meaning of the *D* coefficient is still not clear so far; it seems to account for solute–solute interactions.

Viscosity coefficients obtained by a computerized leastsquares procedure from the experimental data were listed in Table 4 along with the root-mean-square deviation (rmsd) and relative average deviation (RAD).

The rmsd was defined by⁸

rmsd =
$$\left[\frac{1}{N-1}\sum_{i=1}^{N} (\eta_{ci} - \eta_i)^2\right]^{1/2}$$
 (2)

where *N* is the number of experimental points, η_{ci} represents the viscosities calculated from equations, and η_i represents the experimental viscosity values.

 Table 4. Regression Coefficients and Standard Deviation of

 Thiourea in Triglycol (1) + Water (2) Mixtures

Α	В	D	100 rmsd	100 RAD						
$w_1 = 1.00$										
-0.02368	-0.1835	0.04825	1.85	1.73						
-0.00763	-0.1826	0.04272	1.59	1.54						
-0.01134	-0.1906	0.04668	1.35	1.31						
0.00338	-0.2242	0.06156	1.21	1.04						
-0.00198	-0.2176	0.05982	1.04	0.85						
0.00688	-0.2409	0.07126	0.97	0.80						
-0.00291	-0.2054	0.04909	1.36	1.09						
-0.00676	-0.2278	0.06087	1.26	1.01						
	w1 =	= 0.91								
0.02083	0.09740	0.00482	0.85	0.57						
0.00795	0.07341	0.01043	0.55	0.39						
-0.00650	0.09204	-0.00369	0.65	0.47						
-0.00376	0.08051	-0.00516	0.97	0.65						
0.00012	0.04246	0.01033	0.95	0.73						
0.00374	0.02398	0.02209	1.13	0.82						
0.00244	-0.02533	0.05467	1.66	1.24						
0.00450	-0.02747	0.04946	1.00	0.80						
$w_1 = 0.82$										
-0.03904	0.1104	0.00902	1.78	1.20						
-0.03727	0.1018	0.00677	1.73	1.14						
-0.03261	0.0979	0.00641	1.63	1.06						
-0.02163	0.0836	0.00828	1.37	1.10						
-0.03598	0.0944	0.00322	1.70	1.24						
-0.02904	0.0926	0.00239	1.76	1.35						
-0.03244	0.0970	-0.00145	1.60	1.17						
-0.01856	0.0855	-0.00192	1.33	1.00						
$w_1 = 0.72$										
0.03727	0.08158	0.01281	2.26	1.46						
0.01917	0.09563	0.00664	1.43	0.86						
0.01813	0.09580	0.00497	1.39	0.84						
0.03253	0.08596	0.00663	2.11	1.45						
0.03969	0.08155	0.00644	2.37	1.66						
0.03486	0.09068	0.00253	2.55	1.69						
0.01460	0.09180	0.00066	1.11	0.76						
0.02819	0.08054	0.00326	1.81	1.29						
	$\begin{array}{c} A \\ \hline -0.02368 \\ -0.00763 \\ -0.01134 \\ 0.00338 \\ -0.00198 \\ 0.00688 \\ -0.00291 \\ -0.00676 \\ \hline 0.02083 \\ 0.00795 \\ -0.00650 \\ -0.00376 \\ 0.00012 \\ 0.00374 \\ 0.00244 \\ 0.00450 \\ \hline -0.03904 \\ -0.03727 \\ -0.03261 \\ -0.02163 \\ -0.02904 \\ -0.03224 \\ -0.03598 \\ -0.02904 \\ -0.03244 \\ -0.01856 \\ \hline 0.03727 \\ 0.01917 \\ 0.01813 \\ 0.03253 \\ 0.03969 \\ 0.03486 \\ 0.01460 \\ 0.02819 \\ \hline \end{array}$	A B -0.02368 -0.1835 -0.00763 -0.1826 -0.01134 -0.1906 0.00338 -0.2242 -0.00198 -0.2176 0.00688 -0.2409 -0.00291 -0.2054 -0.00676 -0.278 w_1 = 0.02083 0.00795 0.07341 -0.00650 0.09204 -0.00376 0.08051 0.00012 0.04246 0.00374 0.02398 0.00244 -0.02747 w_1 = w_1 = -0.03904 0.1104 -0.03727 0.1018 -0.03261 0.0979 -0.02163 0.0346 -0.03264 0.0970 -0.02163 0.0856 -0.03244 0.0970 -0.01856 0.08555 w_1 = 0.03277 0.08158 0.01917 0.09563 0.01813 0.09580 <td>A B D $w_1 = 1.00$ $w_1 = 1.00$ -0.02368 -0.1835 0.04825 -0.00763 -0.1826 0.04272 -0.01134 -0.1906 0.04668 0.00338 -0.2242 0.06156 -0.00198 -0.2176 0.05982 0.00688 -0.2409 0.07126 -0.00291 -0.2054 0.04909 -0.00676 -0.2278 0.06087 $w_1 = 0.91$ 0.02083 0.09740 0.00482 0.00795 0.07341 0.01043 -0.00650 0.9204 -0.00369 -0.00376 0.08051 -0.00516 0.00012 0.04246 0.01033 0.00374 0.02398 0.02209 0.00244 -0.02533 0.05467 0.00450 -0.02747 0.04946 $w_1 = 0.82$ -0.03727 0.1104 0.00902 -0.03727 0.1018 0.006671</td> <td>A B D 100 rmsd $w_1 = 1.00$ -0.02368 -0.1835 0.04825 1.85 -0.00763 -0.1826 0.04272 1.59 -0.01134 -0.1906 0.04668 1.35 0.00338 -0.2242 0.06156 1.21 -0.00198 -0.2176 0.05982 1.04 0.00688 -0.2409 0.07126 0.97 -0.00291 -0.2054 0.04909 1.36 -0.00676 -0.2278 0.06087 1.26 $w_1 = 0.91$ 0.02083 0.09740 0.00482 0.85 0.00795 0.07341 0.01043 0.55 -0.00650 0.9204 -0.00369 0.65 -0.00376 0.08051 -0.00516 0.97 0.00012 0.04246 0.01033 0.95 0.00374 0.02398 0.02209 1.13 0.00244 -0.02533 0.05467 1.66 0.00450 -0.02747 0.04946 1.00</td>	A B D $w_1 = 1.00$ $w_1 = 1.00$ -0.02368 -0.1835 0.04825 -0.00763 -0.1826 0.04272 -0.01134 -0.1906 0.04668 0.00338 -0.2242 0.06156 -0.00198 -0.2176 0.05982 0.00688 -0.2409 0.07126 -0.00291 -0.2054 0.04909 -0.00676 -0.2278 0.06087 $w_1 = 0.91$ 0.02083 0.09740 0.00482 0.00795 0.07341 0.01043 -0.00650 0.9204 -0.00369 -0.00376 0.08051 -0.00516 0.00012 0.04246 0.01033 0.00374 0.02398 0.02209 0.00244 -0.02533 0.05467 0.00450 -0.02747 0.04946 $w_1 = 0.82$ -0.03727 0.1104 0.00902 -0.03727 0.1018 0.006671	A B D 100 rmsd $w_1 = 1.00$ -0.02368 -0.1835 0.04825 1.85 -0.00763 -0.1826 0.04272 1.59 -0.01134 -0.1906 0.04668 1.35 0.00338 -0.2242 0.06156 1.21 -0.00198 -0.2176 0.05982 1.04 0.00688 -0.2409 0.07126 0.97 -0.00291 -0.2054 0.04909 1.36 -0.00676 -0.2278 0.06087 1.26 $w_1 = 0.91$ 0.02083 0.09740 0.00482 0.85 0.00795 0.07341 0.01043 0.55 -0.00650 0.9204 -0.00369 0.65 -0.00376 0.08051 -0.00516 0.97 0.00012 0.04246 0.01033 0.95 0.00374 0.02398 0.02209 1.13 0.00244 -0.02533 0.05467 1.66 0.00450 -0.02747 0.04946 1.00						

The RAD was defined as⁸

$$RAD = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{\eta_i - \eta_{ci}}{\eta_i} \right|$$
(3)

The relative deviations between the experimental value and the calculated value are listed in Table 3. Relative deviations (RDs) were calculated according to:

$$RD = \frac{\eta - \eta_c}{\eta}$$
(4)

where η_c represents the viscosities calculated from equations and η represents the experimental viscosity values.

The *A* coefficients and *B*-coefficient values obtained at various temperatures are listed in Table 4.

From Table 3, it could be found that the calculated viscosities show good agreement with the experimental data and the relative deviations by eq 4 among all of these values did not exceed 2.8 %. From Table 4, it could be found that the relative average deviation was 1.1 % and the rmsd was 1.4 %, which indicated that the Jones-Dole equation was suited to correlate the viscosity data of thiourea in triglycol + water mixtures.

Conclusion

The densities and viscosities of thiourea in triglycol + water had been determined at temperatures from (302.85 to 341.45) K. The relative viscosities were correlated using the extended Jones-Dole equation. It appeared that the relative deviation among all of these values did not exceed 2.8 % and the average relative deviation of 199 data points was 1.1 %; the viscosities calculated by the model showed good agreement with the experimental data.

The experimental viscosities and correlation equation in this work could be used as essential data and as a model for the synthesis of isopropyl mercaptan.

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