Density and Viscosity of (2,2-Dichloro-*N*,*N*-di-2-propenylacetamide + Acetone) and (2,2-Dichloro-*N*,*N*-di-2-propenylacetamide + Ethanol) at T = (278.15 to 313.15) K

Li-Ping Yang, Ting-Liang Luo, Hong-Lei Lian, and Guo-Ji Liu*

College of Chemical and Energy Engineering, Zhengzhou University, Zhengzhou, Henan 450001, People's Republic of China

The density and viscosity of (2,2-dichloro-*N*,*N*-di-2-propenylacetamide + acetone) and (2,2-dichloro-*N*,*N*-di-2-propenylacetamide + ethanol) have been determined at temperatures from (278.15 to 313.5) K. The apparent molar volumes were calculated from experimental measurements.

Introduction

The density and viscosity data are essential for engineering designs involving chemical separations and are important from practical and theoretical points of view for understanding liquid theory.[1] 2,2-Dichloro-*N*,*N*-di-2-propenylacetamide is a herbicide antidote. It is mainly used for corn, rice, wheat, sorghum, oats, and so on. It not only can be used for seed dressing but also can be mixed with other herbicides for soil treatment. It can relieve the chemical injury of crops from herbicide such as butachlor, acetochlor, atrazine, metolachlor, alachlor, pretilachlor, and triallate.[2] Acetone and ethanol are necessary solvents in the synthesis and purification process of 2,2-dichloro-*N*,*N*-di-2-propenylacetamide, so it is useful to know the physiochemical properties of (2,2-dichloro-*N*,*N*-di-2-propenylacetamide + acetone) and (2,2-dichloro-*N*,*N*-di-2-propenylacetamide + ethanol) mixtures. However, a survey of the literature shows that very few measurements have been made on the physicochemical properties of (2,2-dichloro-*N*,*N*-di-2-propenylacetamide + acetone) and (2,2-dichloro-*N*,*N*-di-2-propenylacetamide + ethanol). Nevertheless, to our knowledge, no density and viscosity data for these mixtures have been reported previously in the literature. In the study, the densities and viscosities of (2,2-dichloro-*N*,*N*-di-2-propenylacetamide + acetone) and (2,2-dichloro-*N*,*N*-di-2-propenylacetamide + ethanol) have been measured at temperatures from (278.15 to 313.15) K at atmospheric pressure of 0.1 MPa. From measurements of densities, the apparent molar volumes were calculated.

Experimental Section

Materials. Analytical reagent acetone and ethanol obtained from Shuangshuang Yantai Chemical Co., Ltd., Shandong Province, were purified by distillation. The mass fractions were determined by gas chromatography (type GC2010 Shimadzu Co. Ltd.) using a DB-1 capillary column with a FID detector, and they were 0.998 and 0.998, respectively. 2,2-Dichloro-*N*,*N*-di-2-propenylacetamide (CAS # 37764-25-3) was obtained from Mingxing Chem. Co., Ltd., Zouping, Shandong Province, and was further purified by rotary evaporation, and its purity was determined by high-performance liquid chromatography (type HPLC1100 Agilent Co. Ltd.) using a C-18 column with a DAD detector and found to have a mass fraction purity of 0.990. All the chemicals were stored over molecular sieves before use. Water used in the experiments was double distilled; the conductivity was less than $1 \cdot 10^{-4}$ S·m^{-1}.

Apparatus and Procedure. The mixtures were prepared gravimetrically using an electronic balance (type AB204, METTLER TOLEDO) with an uncertainty of ± 0.0001 g and were stored in ground-glass-stoppered bottles of volume of 250 cm^3. It was ensured that the components were adequately mixed before being transferred to the pycnometers. The possible error in the mass fractions is estimated to be ± 0.00005.

The density was measured with five Ostwald−Sprengel-type pycnometers having a bulb volume of about 25 cm^3 and an internal capillary diameter of about 1 mm. The internal volumes of the pycnometers were calibrated with water at each temperature with the densities of water taken from the literature.[3] The cleaned and dried pycnometers were then weighed on an electronic balance (type AB204, METTLER TOLEDO) with an uncertainty of ± 0.0001 g and were then filled with liquid and immersed in a thermostat (type DC-2006, Shanghai Bilon Instrument Co., Ltd.), and the temperature was controlled to ± 0.01 K. After thermal equilibrium had been achieved at the required temperature, the pycnometers were removed from the thermostat and cleaned, dried, and weighed. The density was then determined from the mass of the sample and the volume of each of the pycnometers and the average used to determine the density. Uncertainties in density measurements were estimated to be within ± 0.001 g·cm^{-3} at the 95 % confidence interval. The errors were mainly caused by the weighing process, repeatability of the measurement, and glassware.

The viscosity was measured using a commercial Ubbelohde capillary viscometer (type 1836-A, Shanghai Glass Instruments Factory, China) of 0.55 mm diameter calibrated with double-distilled water at temperatures of (278.15, 283.15, 288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K. A cleaned and dried viscometer was filled with liquid and placed vertically in

Table 1. Comparison of Experimental Densities, ρ, and Viscosities, η, of Ethanol with Literature Values

	ρ/kg·m^{-3}		η/mPa·s	
T/K	exptl	lit.	exptl	lit.
298.15	787	7854[5]	1086	1.0820[5]
303.15	783	7834[6]	983	0.9940[7]
308.15	780	7790[6]	895	0.9069[8]
313.15	777	7746[6]	818	0.8248[8]

* Corresponding author. E-mail: guojiliu@zzu.edu.cn. Tel.: +86 371 67781101. Fax: +86 371 67781696.

10.1021/je900535d
Published on Web 09/04/2009

Table 2. Density ρ, Viscosity η, and Apparent Molar Volumes $V_{\phi,m}$ of (2,2-Dichloro-*N*,*N*-di-2-propenylacetamide + Acetone) at T = (278.15 to 313.15) K and Molality *m*

m	ρ	$10^6 V_{\phi,m}$	η	*m*	ρ	$10^6 V_{\phi,m}$	η
mol·kg^{-1}	kg·m^{-3}	m^3·mol^{-1}	mPa·S	mol·kg^{-1}	kg·m^{-3}	m^3·mol^{-1}	mPa·S
			T = 278.15 K				
0.0000	807		0.385	0.6524	842	169	0.453
0.1094	814	159	0.396	0.8046	849	170	0.470
0.2071	820	161	0.408	0.9073	853	170	0.482
0.2997	823	173	0.421	1.001	0.858	169	0.492
0.5018	834	172	0.436				
			T = 283.15 K				
0.0000	803		0.366	0.6524	838	167	0.430
0.1094	809	162	0.380	0.8046	845	168	0.444
0.2071	814	170	0.385	0.9073	850	168	0.455
0.2997	819	170	0.400	1.001	854	169	0.471
0.5018	830	170	0.412				
			T = 288.15 K				
0.0000	797		0.351	0.6524	833	167	0.409
0.1094	805	150	0.363	0.8046	840	168	0.423
0.2071	809	168	0.368	0.9073	845	169	0.432
0.2997	814	170	0.380	1.001	849	169	0.449
0.5018	825	169	0.394				
			T = 293.15 K				
0.0000	792		0.334	0.6524	828	168	0.388
0.1094	799	150	0.343	0.8046	835	168	0.400
0.2071	804	166	0.350	0.9073	840	169	0.408
0.2997	809	170	0.362	1.001	844	169	0.416
0.5018	819	170	0.372				
			T = 298.15 K				
0.0000	787		0.321	0.6524	823	168	0.371
0.1094	794	162	0.334	0.8046	829	171	0.382
0.2071	797	186	0.336	0.9073	834	170	0.391
0.2997	803	172	0.348	1.001	839	169	0.399
0.5018	814	171	0.359				
			T = 303.15 K				
0.0000	781		0.309	0.6524	818	166	0.354
0.1094	789	149	0.319	0.8046	824	169	0.365
0.2071	793	173	0.323	0.9073	829	169	0.372
0.2997	798	170	0.331	1.001	834	169	0.379
0.5018	809	169	0.342				
			T = 308.15 K				
0.0000	776		0.294	0.6524	814	163	0.337
0.1094	785	130	0.304	0.8046	820	168	0.348
0.2071	788	168	0.309	0.9073	824	168	0.355
0.2997	793	169	0.319	1.001	830	167	0.363
0.5018	805	166	0.327				
			T = 313.15 K				
0.0000	771		0.284	0.6524	809	164	0.325
0.1094	780	131	0.294	0.8046	815	169	0.334
0.2071	784	162	0.296	0.9073	821	166	0.342
0.2997	789	162	0.308	1.001	824	168	0.344
0.5018	800	166	0.313				

an insulated jacket, in which the temperature was maintained constant to ± 0.01 K by circulating water from a thermostatically controlled water bath at the required temperature. After thermal stability was attained, the flow times of the liquids were recorded with an electronic digital stopwatch with an uncertainty of ± 0.01 s. The measurements were found reproducible to ± 0.05 s and the results averaged to provide the final value. Because the flow times were greater than 200 s and the capillary diameter was 0.55 mm, which is much less than the tube length of 100 m, both kinetic energy and tube end corrections were negligible. The viscosity, η, was calculated from the relationship[4]

$$\frac{\eta}{\eta_w} = \frac{\rho t}{\rho_w t_w} \qquad (1)$$

where η, ρ, and t and η_w, ρ_w, and t_w are the viscosities, densities, and flow times of the mixture and water, respectively. The

Table 3. Density ρ, Viscosity η, and Apparent Molar Volumes $V_{\phi,m}$ of (2,2-Dichloro-*N*,*N*-di-2-propenylacetamide + Ethanol) as a Function of Molality *m* from T = (278.15 to 313.15) K

m	ρ	$10^6 V_{\phi,m}$	η	*m*	ρ	$10^6 V_{\phi,m}$	η
mol·kg^{-1}	kg·m^{-3}	m^3·mol^{-1}	mPa·s	mol·kg^{-1}	kg·m^{-3}	m^3·mol^{-1}	mPa·s
			T = 278.15 K				
0.0000	801		1.61	0.5463	831	169	1.76
0.1039	808	156	1.65	0.7007	839	168	1.81
0.2471	817	159	1.70	0.8398	845	168	1.85
0.3945	823	168	1.73	1.001	852	169	1.90
			T = 283.15 K				
0.0000	799		1.45	0.5463	828	172	1.58
0.1039	805	171	1.48	0.7007	836	170	1.62
0.2471	813	168	1.52	0.8398	843	170	1.65
0.3945	821	169	1.56	1.001	849	171	1.68
			T = 288.15 K				
0.0000	795		1.32	0.5463	824	172	1.43
0.1039	801	173	1.35	0.7007	832	171	1.46
0.2471	809	171	1.37	0.8398	838	171	1.49
0.3945	817	169	1.40	1.001	845	171	1.53
			T = 293.15 K				
0.0000	791		1.19	0.5463	820	174	1.28
0.1039	796	184	1.21	0.7007	827	173	1.31
0.2471	805	173	1.24	0.8398	833	174	1.33
0.3945	813	172	1.26	1.001	841	173	1.37
			T = 298.15 K				
0.0000	787		1.09	0.5463	816	172	1.18
0.1039	793	173	1.11	0.7007	824	172	1.20
0.2471	801	172	1.13	0.8398	830	173	1.22
0.3945	809	169	1.16	1.001	838	172	1.24
			T = 303.15 K				
0.0000	783		0.984	0.5463	812	174	1.06
0.1039	789	172	1.01	0.7007	820	172	1.08
0.2471	797	172	1.02	0.8398	826	173	1.10
0.3945	805	171	1.04	1.001	833	174	1.12
			T = 308.15 K				
0.0000	780		0.895	0.5463	809	175	0.964
0.1039	785	184	0.913	0.7007	817	174	0.985
0.2471	794	175	0.932	0.8398	823	174	1.00
0.3945	802	173	0.945	1.001	830	174	1.02
			T = 313.15 K				
0.0000	777		0.818	0.5463	805	177	0.874
0.1039	782	189	0.832	0.7007	813	175	0.894
0.2471	791	175	0.848	0.8398	819	175	0.914
0.3945	798	175	0.860	1.001	826	176	0.926

values of the viscosity and density of pure water were taken from the literature.[3] The overall uncertainty of the viscosity measurements is dependent on the equilibrium stability of the viscometer, the time of flow, and the change in density, and the uncertainty in the viscosity measurement is estimated to be ± 0.6 %. The density and viscosity of ethanol were measured with these instruments and the results compared with the values form the literature and found to differ within the combined experimental uncertainty.

Results and Discussion

The experimental densities and viscosities at temperatures of (278.15, 283.15, 288.15, 293.15, 298.15, 303.15, 308.15, and 313.15) K are listed in Tables 2 and 3 and shown in Figures 1 and 2. The density and viscosity increase with increasing concentration of 2,2-dichloro-*N*,*N*-di-2-propenylacetamide at constant temperature and decrease with increasing temperature at a fixed concentration of 2,2-dichloro-*N*,*N*-di-2-propenylacetamide. The dependence of density and viscosity on temperature and concentration has been fit with the Vogel−Tamman−Fulcher (VTF) equation[9]

$$F = P_1 \exp\left(\frac{P_2 + P_3 m}{T - P_4}\right) \tag{2}$$

where F can be either density or viscosity; m is the molality of 2,2-dichloro-*N*,*N*-di-2-propenylacetamide; T is the absolute temperature; and P_1, P_2, P_3, and P_4 are parameters obtained by regression analysis and listed in Table 4 along with standard deviations. The standard deviation is defined by

$$\sigma = [\sum_{i=1}^{p} ((Y_i^{\text{exptl}} - Y_i^{\text{calcd}})^2/(p - n))]^{1/2} \tag{3}$$

where p is the number of experimental points and n is the number of parameters. Y_i^{calcd} and Y_i^{exptl} refer to the calculated values from the equation and to the experimental value. On the basis of the obtained standard deviation values, we conclude that eq 2 can be successfully used for the correlation of the investigated physical properties.

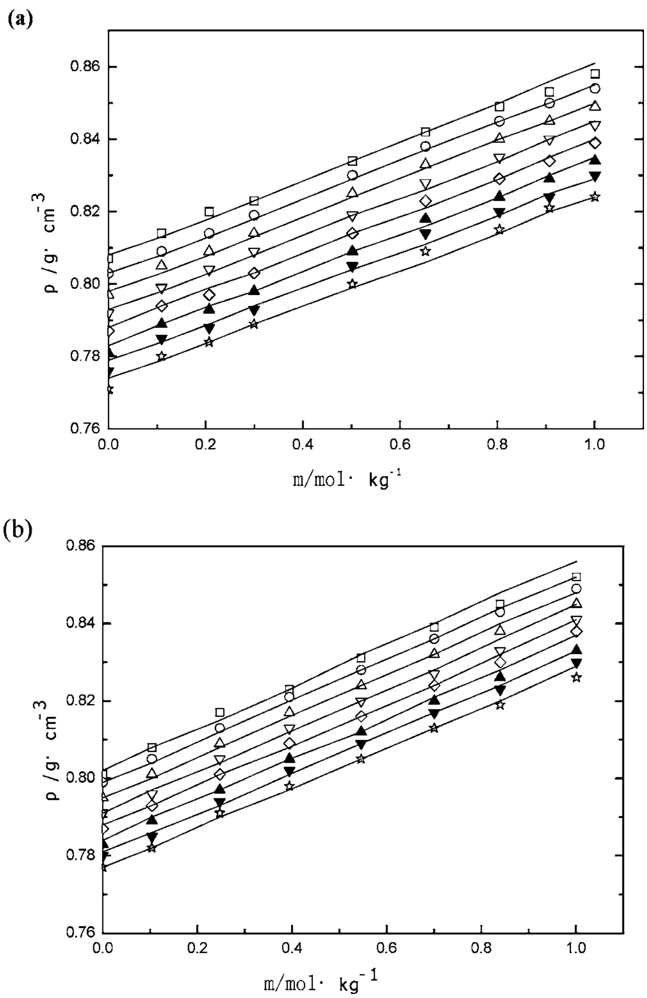

Figure 1. Variation of density with molality at □, 278.15 K; ○, 283.15 K; △, 288.15 K; ▽, 293.15 K; ◇, 298.15 K; ▲, 303.15 K; ▼, 308.15 K; and ☆, 313.15 K for the following mixtures: (a) 2,2-dichloro-*N*,*N*-di-2-propenylacetamide + acetone, (b) 2,2-dichloro-*N*,*N*-di-2-propenylacetamide + ethanol. Solid line, calculated from eq 2.

Table 4. Coefficient of Equation 2 and Standard Deviation, σ, for ρ and η for Different Systems

system		P_1	P_2	P_3	P_4	$10^2\sigma$
2,2-dichloro-*N*,*N*-di-2-propenylacetamide + acetone	ρ	5.2665	20609.0000	260.5200	−3816.8000	0.121
	η	0.0569	351.2800	43.4220	95.4320	0.246
2,2-dichloro-*N*,*N*-di-2-propenylacetamide + ethanol	ρ	20.4620	14549.0000	258.1000	−3687.1000	0.150
	η	0.0002	3943.1000	61.2500	−150.2600	0.645

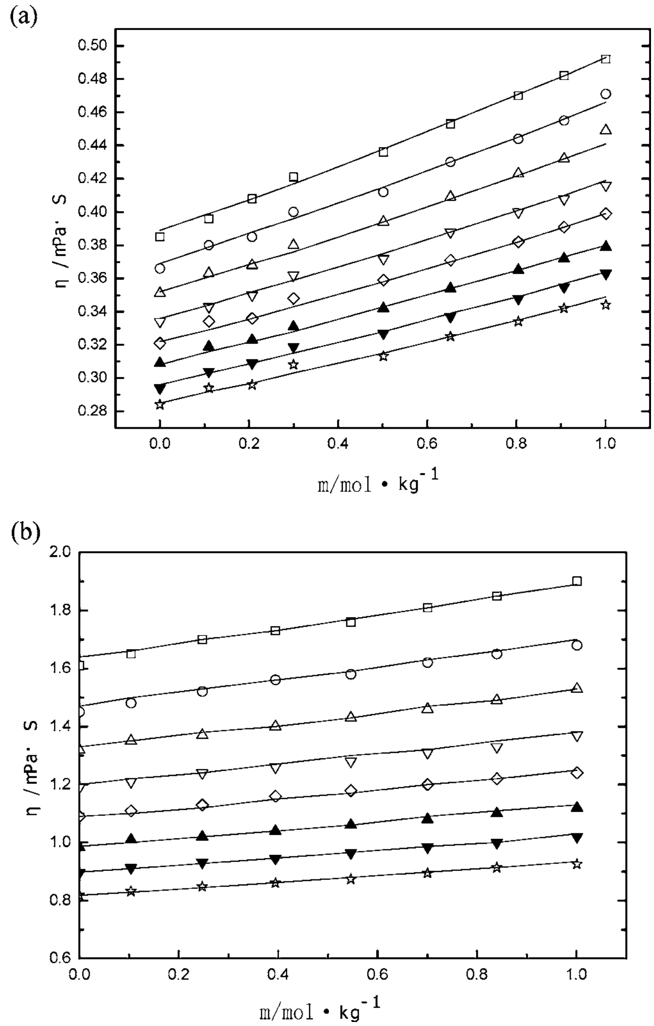

Figure 2. Variation of viscosity with molality at □, 278.15 K; ○, 283.15 K; △, 288.15 K; ▽, 293.15 K; ◇, 298.15 K; ▲, 303.15 K; ▼, 308.15 K; and ☆, 313.15 K for the following mixtures: (a) 2,2-dichloro-*N*,*N*-di-2-propenylacetamide + acetone, (b) 2,2-dichloro-*N*,*N*-di-2-propenylacetamide + ethanol. Solid line, calculated from eq 2.

The apparent molar volume of 2,2-dichloro-*N*,*N*-di-2-propenylacetamide, $V_{\phi,\text{m}}$, is given by

$$V_{\phi,\text{m}} = [M/\rho] - [(\rho - \rho_0)/(m\rho\rho_0)] \tag{4}$$

where M is the molar mass of 2,2-dichloro-*N*,*N*-di-2-propenylacetamide; ρ is the density of the solution; and ρ_0 is the density of pure solvent. The values of the apparent molar volume of 2,2-dichloro-*N*,*N*-di-2-propenylacetamide in the mixtures are also given in Tables 2 and 3. The apparent molar volume increases as temperature increases at fixed concentration of 2,2-dichloro-*N*,*N*-di-2-propenylacetamide and decreases with concentration at the same temperature.

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Received for review June 26, 2009. Accepted August 25, 2009.

JE900535D