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Density and Viscosity of 1-Methoxy-2-Propanol, 2-Methyltetrahydrofuran, α,α,α-Trifluorotoluene, and Their Binary Mixtures with 1,1,1-Trichloroethane at Different Temperatures

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The density and kinematic viscosity at nine temperatures in the range between 288.36 K and 328.30 K were measured at atmospheric pressure for 1-methoxy-2-propanol, 2-methyltetrahydrofuran, and α,α,α-trifluorotoluene. Density and kinematic viscosity were measured for 1,1,1-trichloroethane + 1-methoxy-2-propanol, + 2-methyltetrahydrofuran, and + α,α,α-trifluorotoluene at different temperatures and excess volumes, and deviations of the viscosity from a mole fraction average were determined. The results were used for the estimation of the adjustable parameters of a density Redlich−Kister expansion and of the viscosity UNIMOD model.

Introduction

Among the various methods developed for the prediction of thermodynamic and transport properties in the framework of the group contribution concept, the group contribution thermodynamic viscosity model CG-UNIMOD (Cao et al., 1992, 1993a,b) plays a very important role, since no experimental information is directly used to calculate the viscosity of liquid multicomponent mixtures. CG-UNIMOD is based on the molecular model developed by Cao (UNIMOD), which is not predictive but which gives excellent results in the correlation of viscosity of binary systems and in the calculation of viscosity of multicomponent systems. Both models need some pure component parameters that are obtained by fitting pure component viscosity data as a function of temperature.

The UNIMOD model has been used in a previous characterization of the viscosity and density behavior of a number of binary systems, containing 1,1,1-trichloroethane (De Lorenzi et al., 1994, 1995). It gave excellent results in the correlation of the binary mixture viscosity for a number of systems, but its application could not be extended to the mixtures containing 1-methoxy-2-propanol, 2-methyltetrahydrofuran, and α,α,α-trifluorotoluene, since for these three solvents the pure component parameters were not available.

This work fills the experimental gap for the mentioned pure components. UNIMOD's pure component parameters are evaluated for 1-methoxy-2-propanol, 2-methyltetrahydrofuran, and α,α,α-trifluorotoluene to be used for both UNIMOD and GC-UNIMOD. To this end, data of density and kinematic viscosity had to be determined in a temperature interval, in this instance, between 288.15 K and 328.15 K.

Furthermore, the study of the binary systems of the three mentioned solvents with 1,1,1-trichloroethane, already carried out at 298.15 K (De Lorenzi et al., 1995), was extended to the temperatures of 289.32 K and 313.39 K. Data obtained were regressed and the binary interaction parameters of the UNIMOD model obtained. Excess volumes and excess viscosity deviation functions were derived from the experimental data of mixture viscosity and mixture density.

Experimental Section

Materials. The solvents used were Aldrich, purity >99 mol %, used as received, without further treatment. The purities of nitrogen and water employed for the calibration of the instruments were 99.9999 mol % and 99.9 mol %, respectively.

Apparatus. The same equipment used and described in a previous paper (De Lorenzi et al., 1994) was employed. Densities were measured by a vibrating tube digital densimeter, Anton Paar, model DMA 602H-DMA 60, connected with a Heterofrig (Heto Birkerød) constant-temperature bath circulator, with a precision of ±0.01 K. Calibration of the apparatus and working procedures are described in detail elsewhere (Fermeglia and Lapasin, 1988; Fermeglia et al., 1990). Special care was taken to check that the temperature in the apparatus was the same before and after injecting the samples. Constant readings of Paar period data were a further check of the temperature stability. A series of piezoelectric thermometers (YSI 44031 thermistor) were used in the temperature measurements, each thermometer covering a range of 10 K, and checked against a reference platinum resistance thermometer. Following this procedure, we estimated the density precision to be higher than 3×10^{-5} g·cm^{-3} and the temperature precision to be higher than 0.01 K.

Viscosities were measured by means of an Ubbelohde suspended-level capillary viscometer, coupled with a Schott electronic timer AVS 300, with a precision of ±0.01 s, and a Schott TA 20-T 100 automatic diluting device. The thermostat was a Haake F3 instrument, with a precision of ±0.02 K. The viscometer constant was determined at each working temperature in the interval between 288.15 K and 328.15 K. The calibrating fluid was fresh double distilled water. Great care was taken in checking the temperature stability during the tests. For the 0.001 Schott-Ubbelohde type viscometer the maximum variation among the single data was less than 0.4%, while for the 0.003 Schott-Ubbelohde type viscometer the maximum variation was less than 0.6%. The apparatus working technique is described elsewhere (Fermeglia and Lapasin, 1988; Fermeglia et al., 1990). The estimated precision in kinematic viscosity measurements is approximately 1×10^{-10} m^2·s^{-1}, while the temperature precision is better than 0.02 K over the entire range.

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Table 1. Comparison between Measured and Literature Data for Density ρ and Viscosity ν of pure Components at 298.15 K

	ρ/g·cm^{-3}			ν/10^{-6} m^2·s^{-1}		
solvent	this work	lit.[a]	other lit.	this work	lit.[a]	other lit.
1-methoxy-2-propanol	0.916 92	0.916 50		1.8207	1.8237	1.811[c]
2-methyltetrahydrofuran	0.849 37	0.848 82	0.844 46[b]	0.5586	0.5600	
α,α,α-trifluorotoluene	1.181 56	1.180 98		0.4659	0.4677	

[a] De Lorenzi et al. (1995). [b] Shinsaka et al. (1985). [c] Fermeglia et al. (1990).

Table 2. Experimental Densities and Calculated Deviations (Eq 1)

T/K	ρ/g·cm^{-3} experimental	$\Delta\rho$/g·cm^{-3} exp − calc
	1-Methoxy-2-propanol	
288.36	0.926 37	0.000 15
293.20	0.921 57	−0.000 07
298.04	0.916 90	−0.000 12
303.17	0.912 02	−0.000 07
308.44	0.907 11	0.000 14
313.30	0.902 21	−0.000 01
318.37	0.897 16	−0.000 05
323.14	0.892 49	0.000 04
328.30	0.887 27	0.000 00
	2-Methyltetrahydrofuran	
288.36	0.859 49	0.000 20
293.20	0.854 37	−0.000 04
298.04	0.849 31	−0.000 16
303.17	0.844 07	−0.000 14
308.44	0.838 85	0.000 12
313.30	0.833 56	−0.000 07
318.37	0.828 20	−0.000 05
323.14	0.823 20	0.000 07
328.30	0.817 60	0.000 07
	α,α,α-Trifluorotoluene	
288.36	1.195 47	0.000 22
293.20	1.188 45	−0.000 05
298.04	1.181 54	−0.000 17
303.17	1.174 33	−0.000 14
308.44	1.167 22	0.000 24
313.30	1.159 86	−0.000 15
318.37	1.152 64	−0.000 05
323.14	1.145 71	−0.000 03
328.30	1.138 31	0.000 14

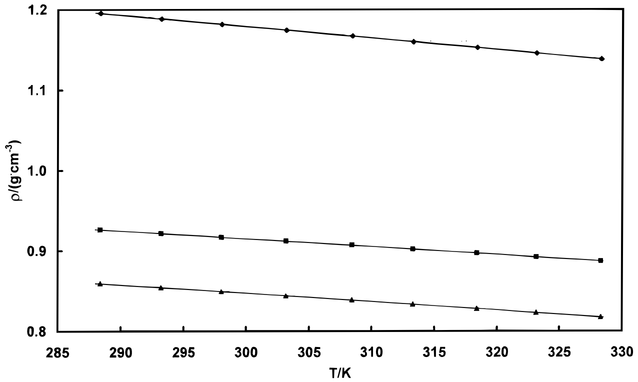

Figure 1. Density vs temperature for (◆) α,α,α-trifluorotoluene, (▲) 2-methyltetrahydrofuran, and (■) 1-methoxy-2-propanol. Lines are calculated values (eq 1).

Mixture Preparation. The same procedure described in De Lorenzi et al. (1994) was used. A brief description is reported for the sake of completeness. The mixtures for the density measurements were prepared by mass. A Mettler balance with a precision of 3×10^{-5} g and airtight bottles were used. The possible error in the mole fraction is estimated to be lower than 5×10^{-5}.

The mixtures for the kinematic viscosity measurements were prepared by volume. The calibration of the Schott TA 20-T 100 automatic diluting device indicated that the possible error in the mole fraction is approximately 2×10^{-3} (De Lorenzi et al., 1994).

Results and Correlations

Pure Components. Table 1 reports a comparison between density and viscosity data, measured at 298.15 K (or interpolated to that temperature), and literature values. Density and viscosity data differences are lower than 0.6%. These small discrepancies may be explained by taking into account the fact that chemicals of different batches were used in the two subsequent investigations and that a recalibration of the thermometers was meanwhile carried out.

Table 2 reports the experimental density, ρ, as a function of temperature. The DIPPR (Daubert and Danner, 1989) expression for density as a function of temperature has been used for the data regression as follows:

$$\rho = \frac{a}{b^{1+(1-T/c)^d}} \tag{1}$$

where T is the temperature and $a-d$ are adjustable parameters.

A modified Levenberg−Marquardt numerical algorithm was used to estimate the parameters $a-d$ from the experimental data, minimizing the objective function, written in terms of a sum of the squares of the differences between experimental and calculated values, divided by the experimental ones. As can be seen from Table 2, the correlation quality is good. The data for the three solvents are reported in Figure 1, where the experimental results (symbols) are compared with the calculated ones (lines), while the parameters of eq 1 are reported in Table 3 along with the standard deviation, defined as

$$\sigma_\rho = \left[\sum \frac{(\rho_{\rm calc} - \rho_{\rm exp})^2}{N - n}\right]^{1/2} \tag{2}$$

where N is the number of experimental points and n is the number of parameters.

Table 4 reports the experimental kinematic viscosities ν, the deviation between the calculated and experimental viscosities, and the dynamic viscosity η calculated from experimental ν/ρ as a function of temperature. The dynamic viscosity has been calculated using the density data reported in Table 2, interpolated by eq 1. The calculated viscosity values have been obtained by the UNIMOD model for the pure component considered:

$$\nu_i = \frac{r_i^2}{M_i}(2\pi RT)\left(\frac{M_i}{r_i}\right)^{1/2} V_{\rm fi}^{1/3} \exp\left(\frac{zq_in_iU_{ii}}{2r_iRT}\right) \tag{3}$$

where M_i is the molecular weight, r_i is the number of segments in the molecule, U_{ii} is the interaction energy, z is the coordination number, q_i is the external area parameter, $V_{\rm f}$ is the free volume, and n_i is the proportion constant for the component i. U_{ii} is a temperature function which,

Table 3. Values of the Coefficients and Relevant Standard Deviations for Eq 1

	1-methoxy-2-propanol	2-methyltetra-hydrofuran	α,α,α-tri-fluorotoluene
a/g·cm^{-3}	0.192	0.281	0.294
b	0.408	0.504	0.435
c/K	532.41	464.51	511.74
d	0.370	0.477	0.455
σ/g·cm^{-3}	0.000 12	0.000 15	0.000 20

Table 4. Experimental Viscosities and Calculated Deviations (Eq 3)

T/K	ν_{exp}/10^{-6} m^2·s^{-1}	$\nu_{(exp-calc)}$/10^{-6} m^2·s^{-1}	η_{exp}/mPa·s
	1-Methoxy-2-propanol		
288.25	2.3258	−0.0038	2.1545
289.32	2.2692	0.0042	2.0998
293.32	2.0439	−0.0011	1.8835
298.15	1.8207	0.0023	1.6694
298.26	1.8122	−0.0014	1.6614
303.50	1.6094	0.0013	1.4674
308.44	1.4428	−0.0019	1.3086
313.39	1.3060	0.0010	1.1782
313.40	1.3031	0.0017	1.1756
318.33	1.1858	0.0005	1.0639
323.36	1.0812	0.0012	0.9647
328.35	0.9885	−0.0006	0.8770
	2-Methyltetrahydrofuran		
289.32	0.6078	0.0000	0.5216
293.06	0.5863	0.0000	0.5010
298.10	0.5589	0.0001	0.4747
298.15	0.5586	0.0001	0.4745
298.15	0.5585	0.0000	0.4744
303.25	0.5324	−0.0002	0.4494
308.25	0.5088	−0.0001	0.4269
313.39	0.4862	−0.0001	0.4053
318.30	0.4667	0.0004	0.3865
323.34	0.4475	0.0001	0.3683
323.34	0.4471	−0.0003	0.3679
328.32	0.4303	0.0000	0.3518
	α,α,α-Trifluorotoluene		
289.32	0.5093	−0.0001	0.6081
293.12	0.4894	−0.0004	0.5818
298.15	0.4659	0.0005	0.5505
303.15	0.4436	0.0006	0.5210
308.20	0.4212	−0.0010	0.4917
313.39	0.4021	−0.0006	0.4664
318.23	0.3867	0.0005	0.4458
323.27	0.3712	0.0005	0.4252
328.27	0.3567	−0.0004	0.4061

according to the original model, can be expressed as

$$\left(\frac{zq_i}{2}\right)U_{ii} = RT - \Delta_{vap}H_{m(i)} \tag{4}$$

$$\Delta_{vap}H_{m(i)} = A_{H1}[1 - T/T_c]^{(A_{H2}+A_{H3}T/T_c+A_{H4}(T/T_c)^2)} \tag{5}$$

where the last term on the right hand side is the molar enthalpy of vaporization of the pure liquid, obtained from DIPPR (Daubert and Danner, 1989).

Consequently, all terms in eq 3 are known, except the n_i parameter, which is fitted to the experimental data. A numerical procedure similar to that mentioned in the case of the density data has been used to estimate the coefficient A_j of the following polynomial expression:

$$\ln(n_i) = \sum_{j=0,3} A_j T^j \tag{6}$$

From the deviations reported in Table 4, the correlation of the results is excellent. Experimental and calculated kinematic viscosity data are presented in Figure 2, where the lines represent the values calculated with eqs 3−6. The estimated parameters of eq 6 are reported in Table 5, along with the standard deviation of the fitting. For the sake of completeness, Table 5 includes all the numerical quantities necessary for the calculation of the viscosity as a function of temperature.

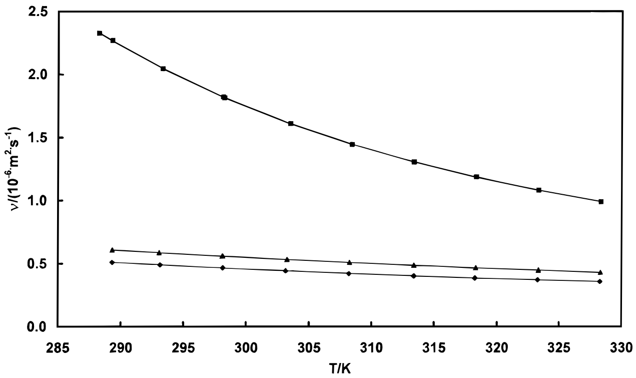

Figure 2. Kinematic viscosity vs temperature for (◆) α,α,α-trifluorotoluene, (▲) 2-methyltetrahydrofuran, and (■) 1-methoxy-2-propanol. Lines are calculated values (eq 5).

Table 5. Values of the Coefficients and Relevant Standard Deviations for Eq 6 and Values for Calculating Viscosities Using Eqs 3−6

	1-methoxy-2-propanol	2-methyltetra-hydrofuran	α,α,α-tri-fluorotoluene
10A_0	−23.972	−4.224	−1.2702
10$^3A_1$/K^{-1}	25.288	10.471	9.9021
10$^5A_2$/K^{-2}	−5.4951	−1.332	−1.2050
10$^9A_3$/K^{-3}	49.927	10.979	9.4847
σ/mPa·s	0.002 07	0.000 17	0.000 56
q	3.904	3.256	3.500
r	4.1674	3.6151	4.4277
M/mol	90.120	86.133	146.112
T_c/K	569.0	540.1	565.0
A_{H1}/J·mol^{-1}	60049	45700	48610
A_{H2}	0.310 14	0.330 92	0.635 71
A_{H3}			−0.8523
A_{H4}			0.6540

[a] Z is calculated according to $Z = 35.2 - 0.1272T + 0.00014T^2$ and $V_f = 1$.

Binary Mixtures. Table 6 reports the binary density and viscosity values, measured for the systems containing 1,1,1-trichloroethane + 1-methoxy-2-propanol, 2-methyltetrahydrofuran, and α,α,α-trifluorotoluene. The measurements have been performed at two different temperatures for each binary system considered, namely 289.32 K and 313.29 K. The data at 298.15 K for the same systems had been reported in a previous paper (De Lorenzi et al., 1995).

Excess volumes were obtained with the following equation:

$$V^E = \frac{x_1M_1 + x_2M_2}{\rho} - \frac{x_1M_1}{\rho_1} - \frac{x_2M_2}{\rho_2} \tag{7}$$

Viscosity deviation functions were obtained with the following equations:

$$\Delta\nu = \nu - \nu^m \tag{8}$$

$$\ln(\nu^m M) = \sum x_j \ln(\nu_j M_j)$$

where x_j is the mole fraction of component j, M_j is the molecular weight of component j, M is the molecular weight of the mixture, ρ_j is the density of component j, ρ is the density of the mixture, ν_j is the kinematic viscosity of component j, and ν^m is the viscosity as defined in eq 8.

Table 6. Experimental Results at 289.32 and 313.39 K

x	ρ/ g·cm^{-3}	V^E/ cm^3·mol^{-1}	x	$\nu/10^{-6}$ m^2·s^{-1}	$\Delta\nu/10^{-6}$ m^2·s^{-1}	η/ mPa·s	x	ρ/ g·cm^{-3}	V^E/ cm^3·mol^{-1}	x	$\nu/10^{-6}$ m^2·s^{-1}	$\Delta\nu/10^{-6}$ m^2·s^{-1}	η/ mPa·s
x 1,1,1-Trichloroethane + (1 − x) 1-Methoxy-2-propanol at 289.32 K							x 1,1,1-Trichloroethane + (1 − x) 1-Methoxy-2-propanol at 313..39 K						
1.0000	1.344 92	0.000	1.000	0.6683	0.0000	0.8988	1.0000	1.304 03	0.000	1.000	0.4916	0.0000	0.6410
0.9079	1.303 95	0.226	0.826	0.7312	−0.0868	0.9283	0.9145	1.267 10	0.266	0.826	0.5243	−0.0526	0.6454
0.7998	1.258 03	0.325	0.700	0.8321	−0.1179	1.0124	0.8047	1.222 09	0.410	0.701	0.5796	−0.0689	0.6845
0.6935	1.213 71	0.346	0.599	0.9420	−0.1297	1.1066	0.7068	1.182 89	0.453	0.601	0.6365	−0.0764	0.7264
0.5736	1.164 07	0.327	0.498	1.0724	−0.1394	1.2145	0.6109	1.144 89	0.444	0.503	0.7018	−0.0821	0.7735
0.4800	1.125 30	0.295	0.397	1.2358	−0.1357	1.3477	0.4994	1.100 74	0.410	0.403	0.7880	−0.0767	0.8371
0.3900	1.088 06	0.251	0.297	1.4299	−0.1216	1.5005	0.4043	1.063 31	0.340	0.303	0.8867	−0.0682	0.9070
0.2773	1.041 19	0.193	0.196	1.6687	−0.0950	1.6806	0.2912	1.018 42	0.268	0.205	1.0005	−0.0545	0.9844
0.1883	1.004 30	0.121	0.098	1.9468	−0.0524	1.8817	0.2019	0.982 97	0.185	0.103	1.1376	−0.0336	1.0738
0.0928	0.964 43	0.055	0.000	2.2692	0.0000	2.0999	0.1004	0.942 47	0.091	0.000	1.3060	0.0000	1.1781
0.0000	0.925 37	0.000					0.0000	0.902 09	0.000				
x 1,1,1-Trichloroethane + (1 − x) 2-Methyltetrahydrofuran at 289.32 K							x 1,1,1-Trichloroethane + (1 − x) 2-Methyltetrahydrofuran at 313.39 K						
1.0000	1.344 91	0.000	1.000	0.6683	0.0000	0.8988	1.0000	1.303 45	0.000	1.000	0.4916	0.0000	0.6407
0.8856	1.290 14	−0.109	0.861	0.6554	0.0026	0.8375	0.9027	1.258 56	−0.097	0.836	0.4880	0.0032	0.5991
0.8015	1.249 72	−0.178	0.701	0.6431	0.0056	0.7732	0.8121	1.216 65	−0.178	0.699	0.4862	0.0054	0.5660
0.6989	1.200 21	−0.240	0.602	0.6360	0.0065	0.7338	0.7032	1.166 07	−0.260	0.598	0.4852	0.0065	0.5419
0.5885	1.146 55	−0.274	0.502	0.6300	0.0074	0.6960	0.6089	1.121 93	−0.296	0.498	0.4845	0.0071	0.5183
0.4862	1.096 83	−0.292	0.402	0.6243	0.0076	0.6589	0.5038	1.072 50	−0.310	0.398	0.4840	0.0070	0.4951
0.3808	1.045 39	−0.284	0.302	0.6192	0.0069	0.6228	0.3971	1.022 23	−0.301	0.297	0.4838	0.0062	0.4717
0.2794	0.995 72	−0.246	0.200	0.6145	0.0054	0.5876	0.3036	0.978 01	−0.271	0.181	0.4840	0.0043	0.4452
0.1853	0.949 59	−0.187	0.104	0.6109	0.0032	0.5560	0.1959	0.926 91	−0.205	0.099	0.4847	0.0027	0.4270
0.0923	0.903 93	−0.111	0.000	0.6078	0.0000	0.5218	0.0994	0.881 05	−0.119	0.000	0.4862	0.0000	0.4054
0.0000	0.858 50	0.000					0.0000	0.833 74	0.000				
x 1,1,1-Trichloroethane + (1 − x) α,α,α-Trifluorotoluene at 289.32 K							x 1,1,1-Trichloroethane + (1 − x) α,α,α-Trifluorotoluene at 313.39 K						
1.0000	1.344 90	0.000	1.000	0.6683	0.0000	0.8988	1.0000	1.304 04	0.000	1.000	0.4887	0.0000	0.6373
0.8902	1.322 65	0.180	0.850	0.6146	−0.0267	0.8081	0.9022	1.284 94	0.172	0.864	0.4665	−0.0092	0.5961
0.7952	1.304 87	0.292	0.699	0.5778	−0.0376	0.7444	0.8135	1.268 90	0.285	0.700	0.4438	−0.0167	0.5548
0.6752	1.284 08	0.387	0.599	0.5597	−0.0390	0.7119	0.7049	1.250 52	0.388	0.601	0.4331	−0.0186	0.5346
0.5969	1.271 42	0.422	0.498	0.5455	−0.0369	0.6854	0.6056	1.235 00	0.436	0.503	0.4263	−0.0168	0.5201
0.4907	1.255 37	0.429	0.396	0.5342	−0.0325	0.6634	0.5030	1.220 06	0.447	0.405	0.4197	−0.0150	0.5064
0.3919	1.241 44	0.401	0.297	0.5254	−0.0263	0.6456	0.3963	1.205 57	0.421	0.304	0.4138	−0.0125	0.4939
0.2843	1.227 17	0.342	0.197	0.5185	−0.0184	0.6306	0.3006	1.193 41	0.365	0.202	0.4075	−0.0105	0.4815
0.1774	1.214 06	0.239	0.100	0.5134	−0.0098	0.6187	0.1922	1.180 60	0.260	0.103	0.4045	−0.0056	0.4735
0.0881	1.203 73	0.130	0.000	0.5093	0.0000	0.6082	0.0885	1.168 99	0.138	0.000	0.4021	0.0000	0.4663
0.0000	1.194 07	0.000					0.0000	1.159 76	0.000				

Table 7. Values of the Coefficients and Relevant Standard Deviation for Eq 9

	1-methoxy-2-propanol	2-methyltetrahydrofuran	α,α,α-trifluorotoluene
	289.32 K		
a_0/cm^3·mol^{-3}	1.214 20	−1.165 59	1.720 24
a_1/cm^3·mol^{-4}	0.717 91	0.126 38	0.132 07
a_2/cm^3·mol^{-5}	0.482 00	−0.048 20	0.012 33
a_3/cm^3·mol^{-6}	0.805 46		
a_4/cm^3·mol^{-7}	0.321 80		
σ/cm^3·mol^{-1}	0.004 24	0.003 15	0.002 08
	313.29 K		
a_0/cm^3·mol^{-3}	1.613 21	−1.257 64	1.784 46
a_1/cm^3·mol^{-4}	0.967 12	0.116 96	0.153 07
a_2/cm^3·mol^{-5}	0.622 87	0.061 54	0.046 83
a_3/cm^3·mol^{-6}	0.697 30		
a_4/cm^3·mol^{-7}	0.316 35		
σ/cm^3·mol^{-1}	0.006 14	0.005 16	0.003 15

The composition dependence of the excess volume was fitted to the following Redlich−Kister expansion:

$$V^{E}_{calc}/\mathrm{cm^3{\cdot}mol^{-1}} = x_1x_2\sum_{j=0}^{n-1}a_j(x_1 - x_2)^j \qquad (9)$$

where a_j are parameters and n is the number of polynomial coefficients, which was determined on the basis of a 95% F test. Table 7 reports the parameters of eq 9, obtained in the regression along with the standard deviation of the fit. Excess volumes at 289.32 and 313.39 for all the systems measured are reported in Figure 3, in which continuous lines represent calculated values (eq 9).

The binary viscosity data have been regressed by using the UNIMOD model, written in terms of binary mixtures, making use of the pure component parameters reported in Table 5:

$$\ln(\eta V) = \sum_{i=1}^{n}x_i \ln(\eta_i V_i) - \sum_{i=1}^{n}q_i n_i x_i \sum_{j=1}^{n}\vartheta_{ji} \ln \tau_{ji} \qquad (10)$$

$$\tau_{ij} = \exp\left\{-\frac{z}{2}\left[\frac{U_{ji} - U_{ii}}{RT}\right]\right\} \qquad (11)$$

An explanation of all the terms in eqs 10 and 11 is beyond the scope of this work; consequently, reference is made to Cao et al. (1993). V is the molar volume of the mixture, V_j, the molar volume of component j. The binary parameters $\Delta U_{12} = (U_{12} - U_{22})/R$ and $\Delta U_{21} = (U_{21} - U_{11})/R$ are the interaction potential energy parameters.

A numerical algorithm similar to that used for the estimation of the pure component parameters has been used to estimate the parameters of the model. UNIMOD parameters at 289.32 K and 313.39 K are reported in Table 8, together with UNIMOD parameters at 298.15 K. Parameters at 298.15 K are obtained from experimental data measured in a previous investigation, but not fitted at that time, since the pure component parameters were not available. Table 8 reports the parameters estimated by fitting each individual data set at each temperature and also the parameters obtained with a global fitting of all the data in the temperature interval considered. The

Table 8. UNIMOD Parameters for the Binary Systems: Specific Parameters at 289.32, 298.15, and 313.39 K and Global Parameters for the Temperature Range 289.32−313.39 K

binary system 1,1,1-trichloroethane (1) +	T/K	ΔU_{12}/K	ΔU_{21}/K	$\sigma/10^{-6}$ $m^2 \cdot s^{-1}$
1-methoxy-2-propanol (2)	289.32	398.64	−300.56	0.009 98
	298.15	416.20	−315.12	0.008 93
	313.39	418.82	−333.00	0.005 32
	289.32−313.39	−112.52	110.90	0.008 39
2-methyltetrahydrofuran (2)	289.32	85.54	−71.43	0.000 17
	298.15	393.95	−189.91	0.013 85
	313.39	−106.71	150.70	0.001 16
	289.32−313.39	145.39	−103.85	0.027 09
α,α,α-trifluorotoluene (2)	289.32	153.97	−112.92	0.000 44
	298.15	158.25	−115.77	0.000 86
	313.39	80.07	−68.82	0.000 87
	289.32−313.39	143.48	−107.99	0.001 00

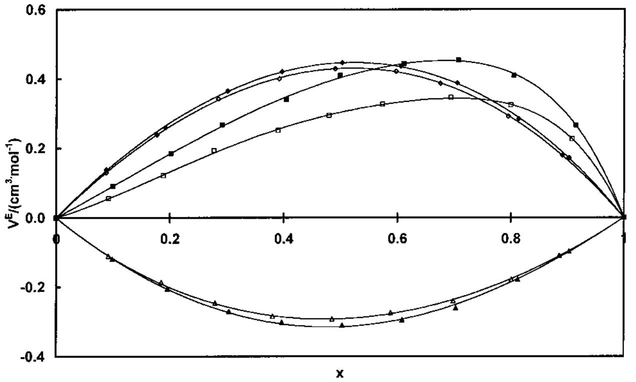

Figure 3. Excess volume for x 1,1,1-trichloroethane + (1 − x) (◇) α,α,α-trifluorotoluene at 289.32 K, (◆) α,α,α-trifluorotoluene at 313.39 K, (△) 2-methyltetrahydrofuran at 289.32 K, (▲) 2-methyltetrahydrofuran at 313.39 K, (□) 1-methoxy-2-propanol at 289.32 K, and (■) 1- methoxy-2-propanol at 313.39 K. Lines are calculated values (eq 7).

results obtained in the case of the global fitting are generally worse than those obtained in the individual fitting but are useful in the case of interpolations with respect to temperature.

Excess volumes are positive for the systems containing α,α,α-trifluorotoluene and 1-methoxy-2-propanol; for the former the behavior is symmetrical and the temperature effect is small, and for the latter the behavior is asymmetrical with the excess shifted toward the α,α,α-trifluorotoluene and the temperature effect is larger. Excess volumes are negative and symmetrical with a small temperature effect for the system containing 2-methyltethahydrofuran.

The deviation of the viscosity from a mole fraction average is positive and very small for 2-methyltetrahydrofuran, negative and small for α,α,α-trifluorotoluene, and negative and larger for 1-methoxy-2-propanol. They are all symmetrical.

Conclusions

The experimental data reported in this work fill a gap in the availability of data for α,α,α-trifluorotoluene, 1-methoxy-2-propanol, and 2-methyltethahydrofuran, considered as a function of temperature, and allows the determination of UNIMOD interaction parameters to be carried out, thus extending the prediction capability of the model to a wider number of multicomponent systems. The reported data have been correlated by using engineering-oriented models, normally built in process simulators, in order to facilitate engineers in their calculations. The fit of the equations selected in this paper to the data was excellent for both the pure component densities and kinematic viscosities. The results reported for binary systems are good. A confident use of the models discussed in this paper is reasonable for the calculation of viscosity and density mixture data.

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