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Study of structural effects of binary mixtures of Nitrobenzene and 2-Alcohols

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ABSTRACT

Densities, structural effects and viscosities of binary nonelectrolyte systems including nitrobenzene + 2-propanol, 2-butanol and 2-pentanol at temperatures (293.15 to 323.15) K and normal atmospheric pressure were measured using an Anton-Paar SVM 3000 stabinger viscometer. Excess molar volumes V_m^E and viscosity deviations $\Delta\eta$ were calculated and correlated by the Redlich-Kister equation to estimate the standard uncertainty. These values are negative over the full range of composition for all studied mixtures. Free volume theory coupled with the Peng-Robinson equation of state was used to correlate liquid viscosities of pure compounds and binary mixtures. The agreement between measured viscosity data and values calculated from this model is within experimental uncertainties.

Keywords: Density; Viscosity; Free volume theory; Peng-Robinson equation

Introduction

From the experimental viewpoint, excess and deviation functions are powerful tools for analyzing structural and physicochemical properties of mixtures. Among them, the excess molar volume has been of much interest for the practical purpose of determining composition from the density measurements. Excess molar volumes can also provide information on possible interactions between components of a binary mixture, such as molecular associations and dipole–dipole and induced dipole–dipole interactions [1]. The interest in studying thermodynamic properties of mixtures containing nitrobenzene is because of their inherent toxicity and hazardous effects to human health and also because of widespread industrial use [2]. This study of the density and viscosity of binary mixtures formed by nitrobenzene with selected 2-alkanols continues our recent systematic studies of the thermodynamic and transport properties of binary mixtures [3,4]. A literature survey reveals that some thermodynamic and transport properties of binary mixtures containing nitrobenzene have been studied [5].

Our approach is to correlate the viscosity of the binary mixtures with the free volume theory which relates the viscosity to the probability of occurrence of an empty neighboring site into which a molecule can jump. This probability is exponentially related to the free volume of the liquids. In this study, the free-volume theory (FVT) has been coupled with the Peng–Robinson equation of state to the correlation of viscosities of pure compounds and binary mixtures. Applicability of this model to the mixtures examined in this work has not yet been verified in the literature.

The importance of free-volume theories for the calculation of viscosities owes to the following facts: (i) Their equations are simple and involve only few parameters; (ii) The parameters have, almost always, a physical meaning; (iii) They can be used over wide ranges of temperature and pressure; (iv) The theories are based on statistical mechanics, therefore, giving them a theoretical background and, (v) they may easily be extended to multicomponent systems [6].

Experimental

Materials

All pure materials were obtained from Merck with mass purity >99% and were used as purchased without further purification. Measured densities and viscosities at T= 298.15 K are presented in Table 1 along with the data from the literature [7,8]. The largest percentage deviation of our data from the literature data is 0.04% for density and 1.17% for viscosity.

Methods

Density and viscosity measurements were performed with a fully automated SVM 3000 Anton-Paar Stabinger viscometer. The viscometer is based on a modified Couette principle with a rapidly rotating outer tube and an inner measuring bob which rotates more slowly. The uncertainty is 1×10^{-4} g·cm^{-3} for density measurements and 1% for viscosity measurements. Three to five sets of readings for the flow times were taken for each sample. The mixtures were prepared just before use by mass on an electronic balance (Mettler AE 163, Switzerland) accurate to 0.01 mg and kept in airtight stoppered glass bottles to avoid evaporation. The maximum estimated uncertainty in the mole fractions is 1×10^{-4}.

Results and discussions

Densities and excess molar volumes

From the experimental data, excess molar volumes V_m^E at different temperatures were calculated using

$$V_m^E = \sum_{i=1}^{N} x_i M_i (\rho^{-1} - \rho_i^{-1}) \tag{1}$$

where ρ is the density of the mixture, ρ_i is the density of pure component *i*, x_i is the mole fraction, M_i is the molar mass of component *i*, and *N* stands for the number of components in the mixture. The density data as a function of mole fraction for nitrobenzene + 2-propanol, 2-butanol, and 2-pentanol mixtures at various temperatures are reported in Table 2. The densities of the binary mixtures decrease with increasing temperature and increase with increasing carbon chain length. Excess molar volumes of binary mixtures of nitrobenzene + 2-alkanols as a function of mole fraction at T= 298.15 K are plotted in Fig. 1. The V_m^E values were correlated with a Redlich–Kister type equation [9]

$$V_m^E = x_1(1-x_1)\sum_{k=0}^{N} A_k (1-2x_1)^k \tag{2}$$

where x_1 is the mole fraction of nitrobenzene and A_k is an adjustable coefficient. Standard deviations were obtained by the equation

$$\sigma = \left[\sum (V_{\exp}^E - V_{cal}^E)^2 / (n-p)\right]^{1/2} \tag{3}$$

where $V_{\exp}^E$ and V_{cal}^E are the experimental and calculated data, respectively. Adjustable parameters of the Redlich–Kister equation and standard deviation values are presented in Table 3.

The excess molar volumes are negative for all studied mixtures and increase with the number of carbon atoms of the alcohols. This behavior arises from the specific interactions between the nitrobenzene and 2-alkanol molecules through dipole-dipole interactions, forming complexes through hydrogen bonds. With the higher chain length of 2-alkanols, the structural contributions arising from the geometrical fitting of one component into the other are negligible because of steric hindrance of carbon chain length. Therefore, mixtures containing higher 2-alkanols have less negative V_m^E values. On the other hand, in all cases the number of cross-associated hydrogen bonds decreases with temperature which leads to less negative values of V_m^E.

Dynamic Viscosities

The measured viscosities are reported in Table 2. The viscosities for binary mixtures increase with chain length and decrease with temperature. The viscosity deviation can be calculated as

$$\Delta\eta = \eta - x_1\eta_1 - x_2\eta_2 \tag{4}$$

where η is the mixture viscosity and η_1 and η_2 are the viscosities of pure components. Values of viscosity deviations were correlated by the Redlich–Kister equation and adjustable coefficients are reported in Table 3. The viscosity deviations for the mixtures of nitrobenzene with 2-alkanol at *T*= 298.15 K are shown in Fig. 2. This figure indicates that the viscosity deviations are negative for all three binary mixtures and become more negative with increasing chain length of the alcohols. This behaviour indicates that specific interactions between nitrobenzene and 2-alkanols decrease with the carbon chain length.

Free Volume Theory

In the free volume theory [10,11], the viscosity is expressed as the sum of two terms

$$\eta = \eta_0 + \Delta\eta^{res} \tag{5}$$

η_0 is the viscosity in the dilute gas limit, while the residual viscosity $\Delta\eta^{res}$ describes deviations from the dilute gas. For η_0 the form proposed by Chung et al [12]

$$\eta_0 = 40.785\frac{\sqrt{M_W T}}{v_c^{2/3}\Omega^*}F_c \tag{6}$$

was used. M$_W$ is Molecular weight and v_c is critical volume. The reduced collision integral Ω^* is calculated by

$$\Omega^* = \frac{1.16145}{T^*} + \frac{0.52478}{\exp(0.77320\,T^*)} + \frac{2.16178}{\exp(2.43787\,T^*)} \\ -6.435.10^{-4}T^*\sin(18.0323\,T^{*-0.76830} - 7.27371) \tag{7}$$

$$\text{where } T^* = \frac{1.2593T}{T_c} \tag{8}$$

and F_c is given by

$$F_c = 1 - 0.275\omega + 0.059035\mu_r^4 + \chi \tag{9}$$

where ω is the acentric factor and χ is a correction for the influence of hydrogen bonds that can be calculated [13] by

$$\chi = 0.0682 + 0.276659\left(\frac{17N_{OH}}{M_W}\right) \tag{10}$$

where N_{OH} is the number of OH groups in the alcohol. The dimensionless dipole moment term [13] μ_{r} is expressed as

$$\mu_r = 131.3\frac{\mu}{\left(v_c T_c\right)^{1/2}} \tag{11}$$

where μ is the dipole moment in Debye. The residual viscosity is described by a generalized dumbbell model

$$\Delta\eta^{res} = 10^{-14}\rho N_a \zeta L^2 \tag{12}$$

where ρ is the density, ζ is the friction coefficient, N_a is Avogadro's number and L^2 is an average quadratic length related to the size of the molecule. On the other hand, the viscosity depends on free spaces among the molecules defined as a free volume fraction f_V through the exponential relation [14]

$$\Delta\eta^{res} = A\exp\left(\frac{B}{f_V}\right) \tag{13}$$

The combination of eqs 12 and 13 leads to

$$\Delta\eta^{res} = 10^{-14}\rho N_a L^2 \zeta_0 \exp\left(\frac{B}{f_V}\right) \tag{14}$$

in which ζ_0 is a friction coefficient related the mobility of the molecule and B is a parameter related to the free-volume overlap among the molecules [15]. The friction coefficient ζ_0 is related to the energy of dissipation E by the expression

$$\zeta_0 = 10^{10}\frac{E}{N_a b_f}\left(\frac{10^{-3}M_W}{3RT}\right)^{0.5} \tag{15}$$

where b_f is the dissipation length of the energy E. Combination of eqs. 13 to 15 leads to the final expression

$$\Delta\eta^{res} = L_V(0.1P + 10^{-4}\alpha\rho^2 M_W)\sqrt{\frac{10^{-3}M_W}{3RT}}\ \exp\left[B\left(\frac{10^3 P + \alpha\rho^2 M_W}{\rho RT}\right)^{1.5}\right] \tag{16}$$

or, with P =0 to the equivalent condensed free-volume-dependent expression

$$\Delta\eta^{res} = 10^{-4}\rho L_V \sqrt{\frac{10^{-3}RTM_W}{3}}\ f_V^{-2/3}\exp\left[\frac{B}{f_V}\right] \tag{17}$$

This approach includes three adjustable parameters related to the structural and energetic properties of the fluid: L_V, α and B. The theory can be applied to mixtures by employing mixing rules for the three parameters. In the literature, there is no agreement about the best mixing rules to work [16–22]. The appropriateness of mixing rules is assessed by comparing molecular predictions with experimental data. In some cases, L_V, α and B are defined such that the mixing rules contain adjustable parameters. These binary interaction parameters are added to the mixture rules to improve the fit of the FVM to experimental data. We have decided to apply a linear compositional mixing rule of the Lorentz type for the three parameters of the dense fluid term:

$$\alpha_{mix} = \sum_{i=1}^{n} \alpha_i x_i \tag{18}$$

$$B_{mix} = \sum_{i=1}^{n} B_i x_i \tag{19}$$

$$L_{V,mix} = \sum_{i=1}^{n} L_{v,i} x_i \tag{20}$$

Here, it is important to note that no binary adjustable parameters are used for the viscosity of mixtures. Three viscosity parameters were fitted to viscosity data of the pure fluid at several temperatures whereas the densities were obtained from Peng–Robinson (PR) equations of state [23]. The parameters for the PR equation were obtained from the ref. [24]. Adjustable parameters of the free volume theory associated with the PR are presented in Table 4 along with AAD. The Fig. 3 shows the comparison of results of the free volume theory and experimental viscosities of binary mixtures at 298.15 K. The values calculated by free volume theory are in satisfactory agreement with the experimental data over the entire composition range. The maximum AAD is 3.1%.

Conclusions

This paper reports densities and viscosities for binary mixtures of nitrobenzene with 2-alkanols. Excess molar volumes and viscosity deviations were correlated by the Redlich–Kister equation and are negative over the whole composition range. Our analyses suggest the presence of strong intermolecular interaction in all binary mixtures due to the dipole–dipole interactions between polar components and specific interactions between unlike molecules. Free volume theory has been coupled with Peng–Robinson equation of state for modeling the viscosities. The agreement between measured data and theoretical values is within the experimental uncertainties.

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Figure Captions

Fig. 1. Excess molar volumes V_m^E vs. mole fraction of nitrobenzene for binary mixtures of nitrobenzene with (▲) 2-propanol, (●) 2-butanol, (■) 2-pentanol at $T = 298.15$ K. (—) Redlich–Kister equation.

Fig. 2. Viscosity deviations $\Delta\eta$ vs. mole fraction of nitrobenzene for binary mixtures of nitrobenzene with (▲) 2-propanol, (●) 2-butanol, (■) 2-pentanol at $T = 298.15$ K. (—) Redlich–Kister equation.

Fig. 3. Experimental and calculated viscosities of nitrobenzene with (▲) 2-propanol, (●) 2-butanol, (■) 2-pentanol at $T = 298.15$ K. (…..) Free volume theory.

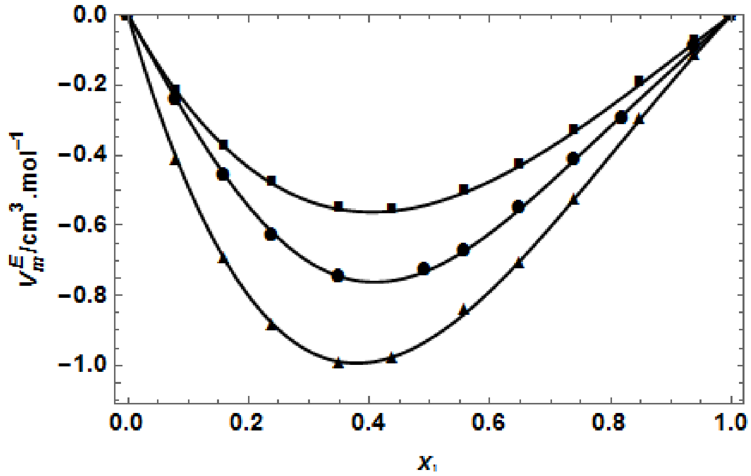

Fig. 1.

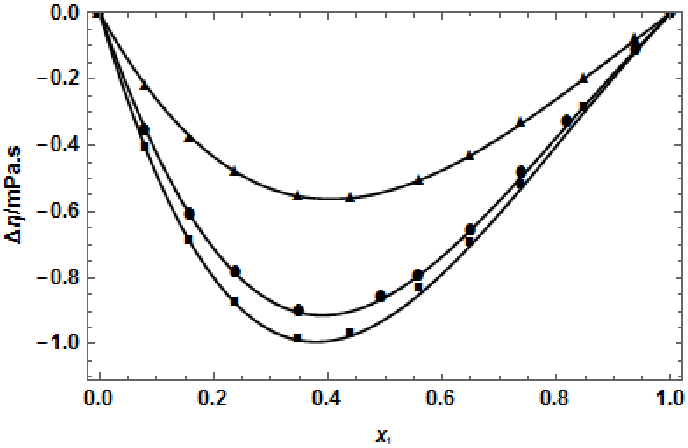

Fig. 2.

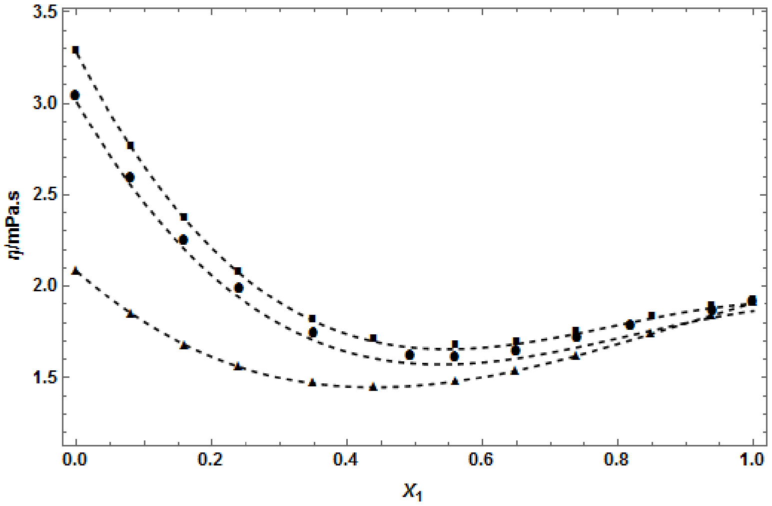

Fig. 3.

Table 1

Densities ρ , and viscosities η, of pure components at T = 298.15 K and P = 0.1 MPa.

Chemical Name	ρ /(g·cm^{-3})		η /(mPa·s)	
	exptl.	Lit.	exptl.	Lit.
Nitrobenzene	1.1978	1.1973 [a]	1.9092	1.9118 [b]
2-Propanol	0.7811	0.7810 [a]	2.0827	2.105 [b]
2-Butannol	0.8027	0.80270 [a]	3.0417	3.114 [b]
2-Pentanol	0.8053	0.80524 [a]	3.2776	3.316 [b]

[a] Ref [7].

[b] Ref [8].

Table 2
Densities, ρ and viscosities, η for the binary mixtures as a function of the mole fraction x_1 of nitrobenzene at pressure P = 0.1 MPa[a].

Nitrobenzene + 2-Propanol							
ρ /(g·cm^{-3})							
x_1	T/K=293.15	T/K=298.15	T/K=303.15	T/K=308.15	T/K=313.15	T/K=318.15	T/K=323.15
0.0000	0.7854	0.7811	0.7768	0.7724	0.7680	0.7634	0.7588
0.0810	0.8321	0.8242	0.8234	0.8192	0.8146	0.8101	0.8054
0.1600	0.8748	0.8640	0.8666	0.8624	0.8580	0.8535	0.8490
0.2401	0.9158	0.9023	0.9078	0.9037	0.8993	0.8949	0.8904
0.3501	0.9684	0.9517	0.9606	0.9565	0.9521	0.9478	0.9434
0.4400	1.0080	0.9897	1.0010	0.9965	0.9921	0.9877	0.9835
0.5600	1.0570	1.0370	1.0500	1.0460	1.0410	1.0370	1.0330
0.6499	1.0910	1.0710	1.0840	1.0790	1.0750	1.0700	1.0660
0.7399	1.1230	1.1030	1.1150	1.1110	1.1060	1.1010	1.0970
0.8500	1.1590	1.1390	1.1500	1.1460	1.1410	1.1360	1.1320
0.9399	1.1860	1.1680	1.1770	1.1720	1.1670	1.1620	1.1570
1.0000	1.2028	1.1978	1.1928	1.1879	1.1829	1.1779	1.1730
η /(mPa·s)							
0.0000	2.4169	2.0827	1.8000	1.5608	1.3591	1.1893	1.0468
0.0810	2.1122	1.8486	1.6253	1.4276	1.2466	1.1011	0.9776
0.1600	1.8921	1.6789	1.4938	1.3332	1.1659	1.0395	0.9339
0.2401	1.7417	1.5600	1.4022	1.2640	1.1112	1.0031	0.9084
0.3501	1.6244	1.4680	1.3322	1.2125	1.0819	0.9879	0.9036
0.4400	1.5967	1.4464	1.3182	1.2028	1.0877	1.0015	0.9207
0.5600	1.6372	1.4815	1.3467	1.2318	1.1337	1.0504	0.9715
0.6499	1.7035	1.5399	1.4007	1.2811	1.1875	1.1050	1.0236
0.7399	1.7948	1.6223	1.4746	1.3495	1.2563	1.1707	1.0867
0.8500	1.9195	1.7392	1.5857	1.4540	1.3550	1.2615	1.1739
0.9399	2.0218	1.8416	1.6846	1.5503	1.4418	1.3421	1.2500
1.0000	2.087	1.9092	1.7549	1.6198	1.5013	1.3966	1.3034

Table 2 Continued

Nitrobenzene + 2-Butanol							
ρ /(g·cm^{-3})							
x_1	T/K=293.15	T/K=298.15	T/K=303.15	T/K=308.15	T/K=313.15	T/K=318.15	T/K=323.15
0.0000	0.8067	0.8027	0.7984	0.7941	0.7898	0.7852	0.7806
0.0810	0.8436	0.8395	0.8379	0.8310	0.8266	0.8220	0.8176
0.1600	0.8786	0.8747	0.8729	0.8662	0.8619	0.8573	0.8528
0.2400	0.9134	0.9095	0.9076	0.9010	0.8968	0.8922	0.8877
0.3500	0.9600	0.9560	0.9538	0.9476	0.9433	0.9388	0.9343
0.4949	1.0190	1.0150	1.0120	1.0060	1.0020	0.9975	0.9931
0.5600	1.0440	1.0400	1.0380	1.0320	1.0270	1.0230	1.0180
0.6500	1.0790	1.0750	1.0720	1.0660	1.0620	1.0570	1.0520
0.7400	1.1120	1.1080	1.1040	1.0990	1.0950	1.0900	1.0850
0.8205	1.1410	1.1370	1.1330	1.1280	1.1230	1.1180	1.1140
0.9399	1.1830	1.1780	1.1730	1.1680	1.1630	1.1580	1.1540
1.0000	2.2028	1.1978	1.1928	1.1879	1.1829	1.1779	1.1730
η /(mPa·s)							
0.0000	3.6693	3.0417	2.5360	2.1285	1.8047	1.5385	1.3255
0.0810	3.1381	2.5910	2.2317	1.9053	1.6271	1.4110	1.2327
0.1600	2.6941	2.2465	1.9890	1.7311	1.4892	1.3088	1.1590
0.2400	2.3495	1.9829	1.8005	1.5984	1.3839	1.2334	1.1042
0.3500	2.0415	1.7403	1.6316	1.4755	1.2885	1.1688	1.0578
0.4949	1.8542	1.6192	1.5284	1.4077	1.2485	1.1473	1.0436
0.5600	1.8382	1.6125	1.5206	1.4046	1.2518	1.1550	1.0551
0.6500	1.8588	1.6466	1.5393	1.4218	1.2755	1.1803	1.0811
0.7400	1.9154	1.7187	1.5800	1.4591	1.3202	1.2235	1.1221
0.8205	1.9750	1.7805	1.6381	1.4981	1.3788	1.2741	1.1684
0.9399	2.0781	1.8613	1.7078	1.5774	1.4565	1.3511	1.2527
1.0000	2.087	1.9092	1.7549	1.6198	1.5013	1.3966	1.3034

Table 2 Continued

Nitrobenzene + 2-Pentanol

ρ /(g·cm^{-3})

x_1	T/K=293.15	T/K=298.15	T/K=303.15	T/K=308.15	T/K=313.15	T/K=318.15	T/K=323.15
0.0000	0.8093	0.8053	0.8012	0.7970	0.7927	0.7884	0.7840
0.0810	0.8402	0.8363	0.8322	0.8280	0.8237	0.8195	0.8151
0.1601	0.8706	0.8667	0.8627	0.8585	0.8543	0.8501	0.8458
0.2400	0.9015	0.8977	0.8937	0.8895	0.8854	0.8812	0.8769
0.3500	0.9444	0.9405	0.9366	0.9325	0.9283	0.9242	0.9199
0.4401	0.9797	0.9758	0.9719	0.9678	0.9636	0.9595	0.9552
0.5600	1.0270	1.0230	1.0190	1.0150	1.0110	1.0070	1.0020
0.6503	1.0630	1.0590	1.0550	1.0500	1.0460	1.0420	1.0380
0.7402	1.0990	1.0940	1.0900	1.0860	1.0810	1.0770	1.0730
0.8504	1.1430	1.1380	1.1340	1.1290	1.1250	1.1200	1.1150
0.9404	1.1790	1.1740	1.1690	1.1650	1.1600	1.1550	1.1500
1.0000	1.2028	1.1978	1.1928	1.1879	1.1829	1.1779	1.1730
η /(mPa·s)							
0.0000	3.9739	3.2776	2.7172	2.2825	1.9312	1.6470	1.4189
0.0810	3.3231	2.7528	2.3173	1.9928	1.7114	1.4967	1.3115
0.1601	2.8268	2.3645	2.0161	1.7764	1.5454	1.3749	1.2274
0.2400	2.4440	2.0682	1.7942	1.6085	1.4170	1.2799	1.1592
0.3500	2.0955	1.8087	1.5984	1.4536	1.3007	1.1884	1.0895
0.4401	1.9315	1.6974	1.5167	1.3848	1.2490	1.1478	1.0551
0.5600	1.8632	1.6703	1.5033	1.3604	1.2395	1.1348	1.0442
0.6503	1.8668	1.6837	1.5234	1.3765	1.2586	1.1502	1.0568
0.7402	1.9142	1.7377	1.5789	1.4210	1.3020	1.1877	1.0914
0.8504	1.9993	1.8209	1.6599	1.4969	1.3776	1.2601	1.1597
0.9404	2.0545	1.8778	1.7183	1.5683	1.4509	1.3375	1.2383
1.0000	2.087	1.9092	1.7549	1.6198	1.5013	1.3966	1.3034

[a] x_1 is the mole fraction of Nitrobenzene in the (Nitrobenzene + 2-alkanol) solutions. Standard uncertainties u are u(T) = 0.01 K, u(x) = 0.0001, u(p) = 10 kPa, the combined expanded uncertainty $U_c(\rho) = 2\times10^{-4}$ g·cm^{-3} (0.95 level of confidence) and for viscosity the relative combined expanded uncertainty $U_r(\eta) = 0.02$ (0.95 level of confidence).

Table 3: Parameters A_k and Standard Deviations σ, for Binary mixtures at various temperatures

		T/K =	A_0	A_1	A_2	A_3	σ
Nitrobenzene + 2-Propanol	V_m^E /(cm^3·mol^{-1})	293.15	-3.12	0.047	-0.10		0.004
		298.15	-3.51	0.08	-0.079		0.002
		303.15	-3.87	0.17	-0.01		0.009
		308.15	-4.16	0.14	-0.057		0.005
		313.15	-4.36	0.10	0.108		0.005
		318.15	-4.67	0.076	0.164		0.006
		323.15	-4.98	0.170	0.264		0.005
	$\Delta\eta$ /(mPa·s)	293.15	-2.57	-1.31	-0.04	-0.07	0.002
		298.15	-2.15	-0.918	0.053	-0.04	0.003
		303.15	-1.80	-0.58	-0.14	0.017	0.002
		308.15	-1.50	-0.372	0.062	0.028	0.003
		313.15	-1.29	-0.47	-0.04	0.072	0.005
		318.15	-1.08	-0.41	-0.018	0.006	0.002
		323.15	-0.92	-0.32	0.005	-0.033	0.002
Nitrobenzene + 2-Butanol	V_m^E /(cm^3·mol^{-1})	293.15	-2.08	0.008	-0.047		0.004
		298.15	-2.24	0.016	-0.066		0.004
		303.15	-2.52	0.057	-0.009		0.005
		308.15	-2.74	0.026	-0.029		0.003
		313.15	-2.97	0.040	0.063		0.005
		318.15	-3.17	0.062	0.061		0.002
		323.15	-3.39	0.027	0.021		0.008
	$\Delta\eta$ /(mPa·s)	293.15	-4.09	-2.18	0.328	-0.14	0.006
		298.15	-3.44	-1.80	-0.087	0.44	0.002
		303.15	-2.47	-0.99	-0.43	0.71	0.003
		308.15	-1.86	-0.74	-0.028	0.107	0.002
		313.15	-1.62	-0.54	-0.21	0.27	0.002
		318.15	-1.28	-0.37	-0.18	0.29	0.001
		323.15	-1.07	-0.22	0.048	0.25	0.001

Table 3 Continued

		T/K =	A_0	A_1	A_2	A_3	σ
Nitrobenzene + 2 -Pentanol	V_m^E /(cm^3•mol^{-1})	293.15	-1.43	0.042	-0.01		0.003
		298.15	-1.70	-0.01	0.06		0.006
		303.15	-2.06	-0.01	0.075		0.008
		308.15	-2.24	0.065	0.071		0.006
		313.15	-2.50	0.06	0.08		0.001
		318.15	-2.80	0.021	0.13		0.008
		323.15	-3.05	0.067	0.115		0.008
	$\Delta\eta$ /(mPa•s)	293.15	-4.60	-2.52	-0.08	0.26	0.002
		298.15	-3.69	-2.15	-0.19	0.38	0.002
		303.15	-2.95	-0.90	-0.005	0.084	0.001
		308.15	-2.35	-0.59	0.02	-0.25	0.003
		313.15	-1.91	-0.66	-0.02	0.15	0.003
		318.15	-1.54	-0.27	-0.04	0.058	0.002
		323.15	-1.26	-0.024	0.021	-0.09	0.008

TABLE 4 Optimized parameters of the Free-Volume theory along with average absolute deviation (AAD %)

Compound	$\alpha \times 10^3$	B$\times$10	Lv	ADD (%)
Nitrobenzene	71.48	3.67	0.747	0.98
2-Propanol	391.43	3.05	0.041	3.1
2-Butanol	331.6	2.98	0. 031	2.01
2-Pentanol	246.94	2.49	0.022	1.4