Research Article

Binary mixtures of 2-ethyl-1-hexanol with various functional groups (benzyl chloride, 3-methylaniline, 3-methoxyaniline and 2,6-dimethylcyclohexanone)

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Abstract
In the binary mixtures of 2-ethyl-1-hexanol with various functional groups (benzyl chloride, 3-methyl aniline, 3-methoxy aniline and 2,6-dimethyl cyclohexanone) densities, speeds of sound and viscosities including those of pure liquids were measured over the entire composition range at different temperatures (303.15, 308.15 and 313.15) K and atmospheric pressure 0.1 MPa. Using this experimentally determined data, the excess/deviation parameters (molar volume, isentropic compressibility and deviation in viscosity) partial molar volumes, partial molar isentropic compressibilities of these components at infinite dilution were calculated. The results are discussed in terms of intermolecular forces between different component molecules in the binary mixture are more than the average intermolecular forces existing between the similar molecules of pure components.

Keywords 2-ethyl-1-hexanol · Binary mixtures · Functional groups

1 Introduction

The study of thermodynamic properties of binary mixtures contributes to an understanding of the behavior of different liquids and their functional groups. This information is very useful in the design of industrial process and in the development of theories for the liquid state and predictive methods. Excess thermodynamic parameters of different mixtures are useful in the study of molecular interactions and arrangements.

The knowledge of physicochemical properties of non-aqueous binary liquid mixtures has relevance in theoretical and applied areas of research, and such results are frequently used in design process (flow, mass transfer or heat transfer calculations) in many chemical and industrial processes [1]. The excess properties derived from these physical property data reflect the physicochemical behavior of the liquid mixtures with respect to the solution structure and intermolecular interactions between the component molecules of the mixture [2, 3].

Study of hydrogen-bonded systems is essential and helpful as hydrogen bond plays a vital role in chemical, physical and biological process. Organic compounds containing electronegative group can interact with compounds containing active hydrogen through hydrogen bond. This type of hydrogen bond takes part in role in the stability of biologically important molecules. Alkanols are polar and self-associated liquids and the dipolar association of alkanols decreases when they are mixed with polar compounds containing various functional groups due to formation of hydrogen bonds between 2-ethyl-1-hexanol and various functional groups in the mixtures

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over the rupture of hydrogen bonds present in pure 2-ethyl-1-hexanol.

We report here a study of excess/deviation functions in four non-component molecules with 2-ethyl-1-hexanol systems. This is in continuation of our earlier work [4–6] on excess/deviation functions of polar liquids with amines. However, in this work a systematic study is reported on excess/deviation functions of non-component molecules with 2-ethyl-1-hexanol over the entire composition range and at temperature (T) ranging from 303.15 to 313.15 K. The results are discussed in terms of intermolecular forces between the different components molecules in the binary mixture are more than the average intermolecular forces existing between the similar molecules of pure components.

2 Procedure

2.1 Materials

The 3-methoxyaniline, benzyl chloride and 3-methylaniline liquids were sigma Aldrich samples. Table 1 contains information regarding their source, purification method, final purity and analysis method. Values of density, speed of sound, and viscosity are presented in Table 2. These values are in good agreement with the data available in the literature [7–14].

2.2 Apparatus and procedure

All the binary liquid mixtures were prepared by weighing required amounts of pure liquids in an electric balance (ER-120A, Afoset) with a precision of ± 0.01 mg by syringing each component into air-tight stopper bottles to minimize evaporation losses. The uncertainty of the mole fraction was $\pm 1 \times 10^{-4}$.

The details of the density, speed of sound and viscosity methods and their measurement techniques were described elsewhere [15]. The uncertainty of density measurement for liquid mixtures is $\pm 0.2 \times 10^{-4}$ g cm^3. The uncertainty in the measured speed of sound is ± 0.053 m s^{-1}. The experimental uncertainty of viscosity estimated as ± 1.13%. The temperature of the liquids during the measurements was maintained within an uncertainty of ± 0.01 K in an electronically controlled thermostatic water bath.

2.3 Theory

The excess thermodynamic/deviation functions were calculated by using the following equations

$$V^E = V - (x_1 V_1 + x_2 V_2) \tag{1}$$

$$\Delta h = h - (x_1 h_1 + x_1 h_1) \tag{2}$$

$$G^{*E} = RT[\ln hV - (x_1 \ln h_1 V_1 + x_2 \ln h_2 V_2) \tag{3}$$

where η, η_1,η_2, V, V_1 and V_2 are viscosities and mixture molar volumes and pure components respectively.

The isentropic compressibilities were calculated from the relation

$$\kappa_s = \left(u^2 \rho\right)^{-1} \tag{4}$$

where ρ is the density and u is the speed of sound of the binary mixture.

Further, the excess isentropic compressibilities (k_s^E) are calculated from the following relations recommended by Benson and Kiyohara [16]

$$k_s^E = k_s - k_s^{id} \tag{5}$$

$$k_s^{id} = \sum_{i=1}^{2} \varphi_i \left[\kappa_{s,i} + \frac{TV_i\left(\alpha_i^2\right)}{C_{p,i}}\right] - \left\{\frac{T\left(\sum_{i=1}^{2} x_i V_i\right)\left(\sum_{i=1}^{2} \varphi_i \alpha_i\right)^2}{\sum_{i=1}^{2} x_i C_{p,i}}\right\} \tag{6}$$

Table 1 List of chemicals with details of source, CAS number, purity and water content

Name of the chemical	Source	CAS number	Purification method	Mass fraction purity	Water content[b] (%)	Analysis method[a]
2-Ethyl-1-hexanol	Sigma Aldrich, India	104-76-7	None	0.996	0.045	GC
Benzyl chloride	S.D. fine Chemicals, India	536-90-3	Fractional distillation	0.993	0.039	GC
3-Methylaniline	S.D. fine Chemicals, India	108-44-1	None	0.996	0.042	GC
3-Methoxyaniline	Sigma Aldrich, India	536-90-3	None	0.995	0.042	GC
2,6-Dimethylcyclohexanone	S.D. fine Chemicals, India	2816-57-1	None	0.995	0.043	GC

[a]Gas chromatography

[b]Karl–Fischer method

Table 2 Densities, viscosity and speeds of sounds data of pure components at different temperatures and 0.1 MPa pressure

Component (K)	Density (ρ/g cm^{-3})		Speed of sound (u/m s^{-1})			Viscosity (η/mPa s)	
	Experimental	Literature	Experimental	Literature	C_P (J K^{-1} mol^{-1})	Experimental	Literature
2-Ethyl-1-hexanol							
303.15	0.82529	0.82539 [7]	1302	1301 [7]	317.5[a] [27]	7.146	7.144 [7]
		0.82528 [8]					
308.15	0.82159	0.82168 [7]	1282	1283 [7]		6.012	6.090 [7]
		0.82158 [8]					
313.15	0.81788		1261			4.774	–
Benzyl chloride							
303.15	1.09492	1.0948 [14]	1357.6	1356.6 [14]	182.4[a] [28]	1.114	1.1121 [14]
308.15	0.84892		1342.5			1.058	
313.15	0.60292		1327.4			1.002	
3-Methylaniline							
303.15	0.98032	0.9808 [10]	1568.2	1567.0 [10]	228.0 [11, 12]	3.018	
		0.98096 [12]					
308.15	0.97611	0.9727 [10]	1530.6	1533.0 [10]	230..0 [11, 12]	2.707	
313.15	0.97186	0.9646 [10]	1491.7	1492.0 [10]	232.0 [11, 12]	2.396	
3-Methoxyaniline							
303.15	1.09025		1579.9		228.0 [11]	5.593	
308.15	1.08705		1552.0		230.5 [11]	5.160	
313.15	1.08320		1523.4		232.6 [11]	4.733	
2,6-Dimethyl cyclohexanone							
303.15	0.90890 [13]		1305.4 [13]		195.2 [9]	3.709 [13]	
308.15	0.90460 [13]		1285.1 [13]		197.5 [9]	3.237 [13]	
313.15	0.90040 [13]		1265.2 [13]		199.6 [9]	2.765 [13]	

The standard uncertainties are $(x_1) = 1 \times 10^{-4}$, u (ρ) ± 0.2×10^{-4} g cm^{-3}, u (u) = 0.5%, u (η) = 1.03%, u (T) = 0.01 K for density, viscosity and speed of sound, u (T) = 0.02 K for viscosity and u (p) = 1 kPa

[a]298.15 K

where φ_i, $C_{p,i}$, V_i, $\kappa_{s,i}$ and α_i are the volume fraction, molar heat capacity, molar volume, isentropic compressibility and coefficient of isobaric thermal expansion of pure components respectively.

Excess/deviation functions (V^E, $\Delta\eta$ and κ_s^E) values are fitted to a Redlich–Kister polynomial equation [17]

$$Y^{E} = x_1 x_2 \sum_{i=0}^{j} A_i \left(1 - 2x_1\right)^i \tag{7}$$

where Y^E is the V^E, $\Delta\eta$ and κ_s^E. Coefficientsn values A_i are determined by using the method of least-squares. The standard deviation σ (Y^E) were calculated by the formula as follows

$$\sigma(Y^E) = [\,\Sigma(Y_{exp}^E - Y_{cal}^E)^2/(m-n)]^{1/2} \tag{8}$$

where m is the total number of experimental points and n is the number of parameters. The coefficients, A_i and corresponding standard deviation values (σ) are presented in Table 3.

3 Results and discussion

The experimental density, speed of sound and viscosity data and their excess/deviation values for the 2-ethyl-1-hexanol with various functional groups at various temperatures are given in Tables 2 and 4. All the excess/deviation values of these parameters V^E, κ_s^E $\Delta\eta$ and G^{*E} at various temperatures are represented graphically in Figs. 1, 2, 3 and 4.

Table 3 Coefficients of Redlich–Kister equation and standard deviation (σ) values for liquid mixtures of 2-ethyl-1-hexanol with various functional groups at T = (303.15–313.15) K

T (K)	A_0	A_1	A_2	σ
2-Ethyl-1-hexanol (1) + benzyl chloride (2)				
V^E (cm^3 mol^{-1})				
303.15	−0.4085	−0.4731	−0.5329	0.001
308.15	0.0642	0.0887	0.1081	0.001
313.15	0.0317	−0.1143	−0.2181	0.001
κ_s^E (TPa^{-1})				
303.15	−77.93	−0.638	21.61	0.001
308.15	−79.94	0.559	7.987	0.066
313.15	−81.94	1.755	−5.625	0.002
$\Delta\eta$ (mPa s)				
303.15	0.101	−0.019	−0.005	0.001
308.15	0.105	−0.026	0.011	0.001
313.15	0.107	−0.019	0.031	0.001
2-Ethyl-1-hexanol (1) + 3-methylaniline (2)				
V^E (cm^3 mol^{-1})				
303.15	−0.4201	−0.4853	−0.5468	0.001
308.15	0.0636	0.0877	0.1017	0.001
313.15	−0.0021	−0.1404	−0.2746	0.001
κ_s^E (TPa^{-1})				
303.15	−80.69	16.24	−14.09	0.001
308.15	−82.69	17.78	−23.47	0.134
313.15	−84.25	16.48	−38.10	0.104
$\Delta\eta$ (mPa s)				
303.15	0.051	−0.031	0.007	0.001
308.15	0.053	−0.034	0.014	0.001
313.15	0.0547	−0.038	0.024	0.001
2-Ethyl-1-hexanol (1) + 3-methoxyaniline (2)				
V^E (cm^3 mol^{-1})				
303.15	−0.4262	−0.4954	−0.5649	0.001
308.15	0.0767	0.0904	0.1037	0.001
313.15	−0.0705	−0.1964	−0.3210	0.001
κ_s^E (TPa^{-1})				
303.15	−82.98	16.71	−20.96	0.001
308.15	−84.37	17.37	−31.84	0.001
313.15	−86.56	16.47	−43.24	0.109
$\Delta\eta$ (mPa s)				
303.15	0.107	−0.018	0.231	0.001
308.15	0.111	−0.025	0.031	0.001
313.15	0.115	−0.018	0.049	0.001
2-Ethyl-1-hexanol (1) + 2,6-dimethylcyclohexanone (2)				
V^E (cm^3 mol^{-1})				
303.15	−0.4353	−0.5167	−0.5861	0.001
308.15	0.0812	0.0848	0.1068	0.001
313.15	−0.1282	−0.2206	−0.3707	0.001
κ_s^E (TPa^{-1})				
303.15	−14.061	−2.154	0.898	0.005
308.15	−14.339	−2.246	−0.270	0.001
313.15	−14.617	−2.340	−1.445	0.005
$\Delta\eta$ (mPa s)				
303.15	0.112	−0.017	0.036	0.001
308.15	0.114	−0.025	0.051	0.001
313.15	0.119	−0.016	0.070	0.001

All the excess/deviation values of these parameters may be explained qualitatively in terms of

1. molecular interactions between like/unlike molecules and the difference in size and shape of the unlike components
2. Possible H-bond interaction between 2-ethyl-1-hexanol and various functional groups in the mixtures having 2-ethyl-1-hexanol as a proton donor
3. Dipole–dipole interactions between polar–polar components

The magnitude of excess values of V^E and κ_s^E from ideality of the systems that can be negative, positive, or zero may be explained as a balance between positive contributions (hydrogen bond rupture and dispersive interactions between unlike molecules) and negative contributions (intermolecular dipolar interactions, geometrical fitting between components, intermolecular association complexes between unlike molecules)

The experimental values indicate that the negative effects are dominant over positive ones in all the mixtures, since the excess values of V^E and κ_s^E for all the binary systems is negative over the whole concentration range at various temperatures. In the present systems, negative sign of V^E shows that the predominance of formation of hydrogen bonds between 2-ethyl-1-hexanol and various functional groups in the mixtures over the rupture of hydrogen bonds present in pure 2-ethyl-1-hexanol [18, 19].

The negative values of V^E for the four systems are in the following order:

2-Ethyl-1-hexanol + 2, 6-dimethylcyclohexanone > 2-ethyl-1-hexanol + 3-methoxyaniline > 2-ethyl-1-hexanol +3-methylaniline > 2-ethyl-1-hexanol + benzyl chloride

The value at the minima for the system (2-ethyl-1-hexanol + 2,6-dimethylcyclohexanone) is slightly more negative than that of remaining various functional groups, and this may be due to the ability of 2,6-dimethylcyclohexanone to form stronger hydrogen bonds with 2-ethyl-1-hexanol than various functional groups with

Table 4 Density (ρ), excess molar volumes (V^E), speed of sound (u), excess isentropic compressibility (κ_s^E), viscosity (η), deviation in viscosity ($\Delta\eta$) and excess Gibbs energy of activation of viscous flow (G^{*E}) of binary liquid mixtures of 2-ethyl-1-hexanol with various functional groups at T = (303.15 to 313.15) K and 0.1 MPa pressure

x_1	Density (ρ) (g cm^{-3})	V^E (cm^3 mol^{-1})	u (m s^{-1})	κ_s^E (TPa^{-1})	Viscosity (η) (mPa s)	$\Delta\eta$ (mPa s)	G^{*E} (J mol^{-1})
2-Ethyl-1-hexanol (1) + + benzyl chloride (2)							
303.15 K							
0.0000	1.09492	0.0000	1357.0	0.000	1.114	0.000	0.000
0.0905	1.06300	−0.0362	1349.0	−5.179	1.669	0.009	5.981
0.1896	1.03021	−0.0670	1342.8	−10.63	2.275	0.017	9.180
0.2577	1.00889	−0.0827	1339.5	−13.88	2.689	0.020	10.24
0.3423	0.98366	−0.0958	1335.7	−17.02	3.203	0.024	10.71
0.4351	0.95746	−0.1023	1331.5	−19.05	3.764	0.025	10.46
0.5296	0.93226	−0.1008	1327.0	−19.41	4.333	0.025	9.590
0.6229	0.90872	−0.0918	1322.2	−18.04	4.894	0.023	8.282
0.7201	0.88551	−0.0754	1316.7	−14.92	5.476	0.019	6.543
0.8312	0.86049	−0.0494	1310.4	−9.664	6.140	0.012	4.181
1.0000	0.82529	0.0000	1302.0	0.000	7.146	0.000	0.000
308.15 K							
0.0000	0.84892	0.0000	1342.0	0.000	1.058	0.000	0.000
0.0905	0.84659	−0.0512	1341.7	−6.180	1.516	0.010	5.124
0.1896	0.84396	−0.0872	1340.5	−11.87	2.016	0.018	7.965
0.2577	0.84213	−0.1039	1338.9	−14.96	2.357	0.022	8.925
0.3423	0.83982	−0.1145	1336.1	−17.91	2.779	0.025	9.375
0.4351	0.83727	−0.1195	1331.7	−19.51	3.240	0.026	9.180
0.5296	0.83466	−0.1165	1326.1	−19.93	3.708	0.026	8.440
0.6229	0.83208	−0.1066	1319.3	−18.71	4.168	0.024	7.301
0.7201	0.82940	−0.0921	1310.8	−15.74	4.645	0.020	5.773
0.8312	0.82631	−0.0648	1300.0	−10.66	5.189	0.013	3.691
1.0000	0.82159	0.0000	1282.0	0.000	6.012	0.000	0.000
313.15 K							
0.0000	0.60292	0.0000	1327.2	0.000	1.002	0.000	0.000
0.0905	0.61819	−0.0633	1324.3	−7.174	1.355	0.012	4.192
0.1896	0.63565	−0.1051	1320.3	−13.09	1.737	0.020	6.662
0.2577	0.64812	−0.1214	1317.0	−16.09	1.997	0.023	7.555
0.3423	0.66421	−0.1325	1312.5	−18.70	2.319	0.026	8.034
0.4351	0.68268	−0.1353	1306.8	−20.22	2.670	0.027	7.957
0.5296	0.70243	−0.1315	1300.5	−20.39	3.027	0.027	7.393
0.6229	0.72296	−0.1221	1293.8	−19.23	3.377	0.025	6.451
0.7201	0.74550	−0.1067	1286.2	−16.58	3.739	0.021	5.144
0.8312	0.77284	−0.0779	1276.8	−11.68	4.152	0.015	3.320
1.0000	0.81788	0.0000	1261.0	0.000	4.774	0.000	0.000
2-Ethyl-1-hexanol (1) + 3-methylaniline (2)							
303.15 K							
0.0000	0.98032	0.0000	1568.2	0.000	3.018	0.000	0.000
0.0951	0.96024	−0.0405	1529.0	−8.867	3.421	0.011	1.233
0.1616	0.94708	−0.0630	1504.0	−13.29	3.701	0.016	1.846
0.2417	0.93211	−0.0840	1476.2	−17.01	4.037	0.021	2.363
0.3403	0.91486	−0.0983	1445.3	−19.60	4.448	0.025	2.721
0.4388	0.89884	−0.1055	1417.8	−20.41	4.856	0.026	2.819
0.5389	0.88365	−0.1029	1392.8	−19.76	5.268	0.026	2.697
0.6281	0.87097	−0.0943	1372.6	−18.09	5.635	0.024	2.425

Table 4 (continued)

x_1	Density (ρ) (g cm^{-3})	V^E (cm^3 mol^{-1})	u (m s^{-1})	κ_s^E (TPa^{-1})	Viscosity (η) (mPa s)	$\Delta\eta$ (mPa s)	G^{*E} (J mol^{-1})
0.7341	0.85684	−0.0763	1350.7	−14.87	6.068	0.019	1.929
0.8347	0.84429	−0.0523	1331.5	−10.501	6.477	0.013	1.302
1.0000	0.82529	0.0000	1302.0	0.000	7.146	0.000	0.000
308.15 K							
0.0000	0.97611	0.0000	1530.6	0.000	2.707	0.000	0.000
0.0951	0.95621	−0.0555	1495.6	−9.728	3.033	0.012	1.110
0.1616	0.94313	−0.0827	1472.5	−14.30	3.258	0.017	1.660
0.2417	0.92821	−0.1050	1446.3	−17.87	3.528	0.022	2.134
0.3403	0.91100	−0.1189	1417.2	−20.22	3.858	0.026	2.466
0.4388	0.89500	−0.1220	1391.3	−20.91	4.184	0.027	2.560
0.5389	0.87985	−0.1192	1368.0	−20.43	4.515	0.027	2.460
0.6281	0.86720	−0.1095	1349.0	−18.74	4.808	0.025	2.218
0.7341	0.85312	−0.0927	1328.5	−15.56	5.154	0.021	1.768
0.8347	0.84060	−0.0678	1310.3	−11.14	5.480	0.014	1.199
1.0000	0.82159	0.0000	1282.0	0.000	6.012	0.000	0.000
313.15 K							
0.0000	0.97186	0.0000	1491.7	0.000	2.396	0.000	0.000
0.0951	0.95215	−0.0697	1460.7	−10.59	2.635	0.013	0.913
0.1616	0.93913	−0.1001	1439.5	−15.31	2.799	0.019	1.367
0.2417	0.92426	−0.1238	1415.1	−18.73	2.994	0.023	1.758
0.3403	0.90710	−0.1366	1387.8	−20.84	3.232	0.027	2.041
0.4388	0.89113	−0.1385	1363.5	−21.41	3.467	0.028	2.130
0.5389	0.87603	−0.1354	1341.7	−20.79	3.705	0.028	2.057
0.6281	0.86342	−0.1247	1324.3	−19.39	3.916	0.026	1.864
0.7341	0.84939	−0.1091	1305.4	−16.57	4.163	0.022	1.494
0.8347	0.83691	−0.0833	1288.6	−12.41	4.397	0.016	1.019
1.0000	0.81788	0.0000	1261.0	0.000	4.774	0.000	0.000
2-Ethyl-1-hexanol (1) + 3-methoxyaniline (2)							
303.15 K							
0.0000	1.09025	0.0000	1579.9	0.000	5.593	0.000	0.000
0.0981	1.05573	−0.0472	1532.1	−9.728	5.752	0.007	0.225
0.1789	1.02906	−0.0741	1497.3	−15.04	5.882	0.011	0.366
0.2587	1.00416	−0.0920	1466.8	−18.40	6.008	0.013	0.465
0.3569	0.97533	−0.1042	1434.0	−20.54	6.161	0.014	0.540
0.4412	0.95206	−0.1075	1409.6	−21.01	6.292	0.013	0.564
0.5309	0.92866	−0.1050	1387.0	−20.43	6.429	0.012	0.554
0.6399	0.90198	−0.0945	1363.2	−18.42	6.596	0.010	0.497
0.7458	0.87772	−0.0769	1343.2	−15.13	6.758	0.007	0.398
0.8498	0.85534	−0.0520	1325.6	−10.408	6.917	0.004	0.260
1.0000	0.82529	0.0000	1302.0	0.000	7.146	0.000	0.000
308.15 K							
0.0000	1.08705	0.0000	1552.0	0.000	5.160	0.000	0.000
0.0981	1.05254	−0.0615	1506.2	−10.52	5.251	0.008	0.190
0.1789	1.02582	−0.0932	1472.3	−15.96	5.324	0.012	0.307
0.2587	1.00086	−0.1121	1442.2	−19.21	5.394	0.014	0.389
0.3569	0.97195	−0.1233	1409.9	−21.10	5.479	0.015	0.449
0.4412	0.94861	−0.1254	1386.0	−21.41	5.550	0.014	0.468
0.5309	0.92517	−0.1222	1364.0	−20.78	5.625	0.013	0.459
0.6399	0.89844	−0.1119	1341.2	−18.90	5.715	0.010	0.409

Table 4 (continued)

x_1	Density (ρ) (g cm^{-3})	V^E (cm^3 mol^{-1})	u (m s^{-1})	κ_s^E (TPa^{-1})	Viscosity (η) (mPa s)	$\Delta\eta$ (mPa s)	G^{*E} (J mol^{-1})
0.7458	0.87415	−0.0945	1322.1	−15.84	5.803	0.008	0.327
0.8498	0.85174	−0.0674	1305.2	−11.21	5.889	0.005	0.213
1.0000	0.82159	0.0000	1282.0	0.000	6.012	0.000	0.000
313.15 K							
0.0000	1.08320	0.0000	1523.4	0.000	4.733	0.000	0.000
0.0981	1.04880	−0.0757	1479.6	−11.31	4.746	0.009	0.174
0.1789	1.02211	−0.1122	1446.4	−16.89	4.753	0.013	0.277
0.2587	0.99715	−0.1323	1416.8	−20.02	4.759	0.015	0.348
0.3569	0.96823	−0.1425	1385.0	−21.67	4.763	0.015	0.399
0.4412	0.94489	−0.1433	1361.8	−22.02	4.766	0.015	0.415
0.5309	0.92145	−0.1394	1340.7	−21.54	4.768	0.013	0.404
0.6399	0.89474	−0.1293	1318.4	−19.58	4.770	0.011	0.360
0.7458	0.87048	−0.1121	1300.2	−16.75	4.772	0.008	0.285
0.8498	0.84807	−0.0829	1284.2	−12.32	4.773	0.005	0.185
1.0000	0.81788	0.0000	1261.0	0.000	4.774	0.000	0.000
2-Ethyl-1-hexanol (1) + 2,6-dimethylcyclohexanone (2)							
303.15 K							
0.0000	0.90890	0.0000	1305.4	0.000	3.709	0.000	0.000
0.1012	0.89975	−0.0529	1305.2	−1.072	4.070	0.014	0.672
0.1895	0.89186	−0.0822	1305.1	−1.903	4.381	0.021	1.069
0.2695	0.88481	−0.0984	1305.1	−2.528	4.660	0.025	1.307
0.3621	0.87676	−0.1080	1305.1	−3.091	4.981	0.027	1.457
0.4569	0.86868	−0.1100	1305.0	−3.439	5.308	0.028	1.494
0.5429	0.86149	−0.1065	1304.8	−3.540	5.603	0.028	1.438
0.6235	0.85486	−0.0993	1304.5	−3.415	5.878	0.026	1.314
0.7523	0.84451	−0.0796	1303.9	−2.784	6.316	0.021	0.993
0.8523	0.83665	−0.0556	1303.2	−1.902	6.653	0.015	0.648
1.0000	0.82529	0.0000	1302.0	0.000	7.146	0.000	0.000
308.15 K							
0.0000	0.90460	0.0000	1285.1	0.000	3.237	0.000	0.000
0.1012	0.89560	−0.0659	1284.9	−1.157	3.533	0.015	0.635
0.1895	0.88780	−0.1005	1284.8	−2.004	3.785	0.023	1.006
0.2695	0.88080	−0.1187	1284.8	−2.630	4.011	0.026	1.224
0.3621	0.87282	−0.1286	1284.8	−3.174	4.270	0.028	1.362
0.4569	0.86479	−0.1304	1284.7	−3.511	4.534	0.029	1.398
0.5429	0.85765	−0.1268	1284.5	−3.607	4.772	0.029	1.346
0.6235	0.85107	−0.1195	1284.3	−3.500	4.994	0.027	1.232
0.7523	0.84078	−0.0988	1283.8	−2.896	5.347	0.023	0.937
0.8523	0.83296	−0.0713	1283.2	−2.021	5.618	0.016	0.614
1.0000	0.82159	0.0000	1282.0	0.000	6.012	0.000	0.000
313.15 K							
0.0000	0.90040	0.0000	1265.2	0.000	2.765	0.000	0.000
0.1012	0.89156	−0.0834	1264.8	−1.242	2.985	0.016	0.549
0.1895	0.88383	−0.1211	1264.6	−2.105	3.169	0.024	0.859
0.2695	0.87687	−0.1389	1264.5	−2.733	3.334	0.027	1.043
0.3621	0.86893	−0.1486	1264.3	−3.256	3.522	0.029	1.159
0.4569	0.86094	−0.1494	1264.1	−3.582	3.713	0.031	1.193
0.5429	0.85383	−0.1449	1263.8	−3.674	3.885	0.030	1.151
0.6235	0.84728	−0.1368	1263.5	−3.585	4.046	0.028	1.059

Table 4 (continued)

x_1	Density (ρ) (g cm^{-3})	V^E (cm^3 mol^{-1})	u (m s^{-1})	κ_s^E (TPa^{-1})	Viscosity (η) (mPa s)	$\Delta\eta$ (mPa s)	G^{*E} (J mol^{-1})
0.7523	0.83706	−0.1173	1262.9	−3.008	4.300	0.024	0.809
0.8523	0.82926	−0.0870	1262.3	−2.141	4.495	0.018	0.539
1.0000	0.81788	0.0000	1261.0	0.000	4.774	0.000	0.000

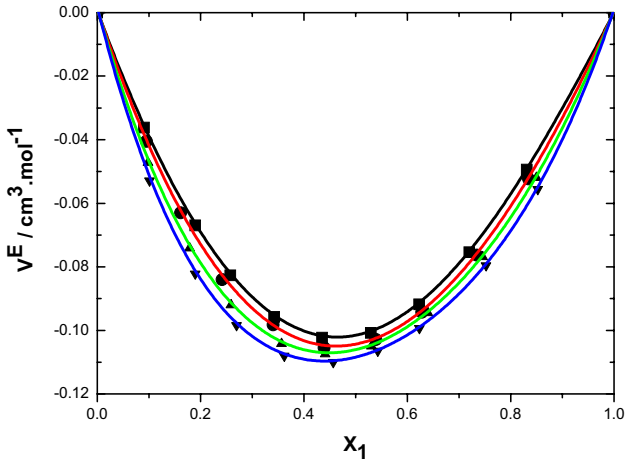

Fig. 1 Curves of excess molar volume (V^E) with mole fraction for the binary mixtures of 2-ethyl-1-hexanol with benzyl chloride (square); 3-methylaniline (circle):3-methoxyaniline (triangle) and 2,6-dimethylcyclohexanone (inverted triangle) at 303.15 K

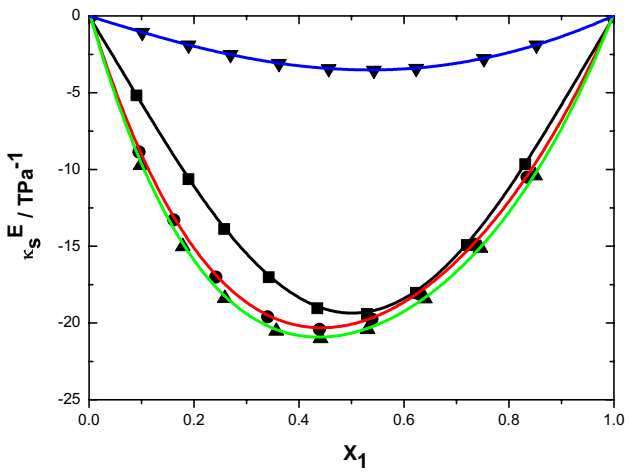

Fig. 2 Curves of excess isentropic compressibility with mole fraction for the binary mixtures of 2-ethyl-1-hexanol with benzyl chloride (square); 3-methylaniline (circle):3-methoxyaniline (triangle) and 2,6-dimethylcyclohexanone (inverted triangle) at 303.15 K

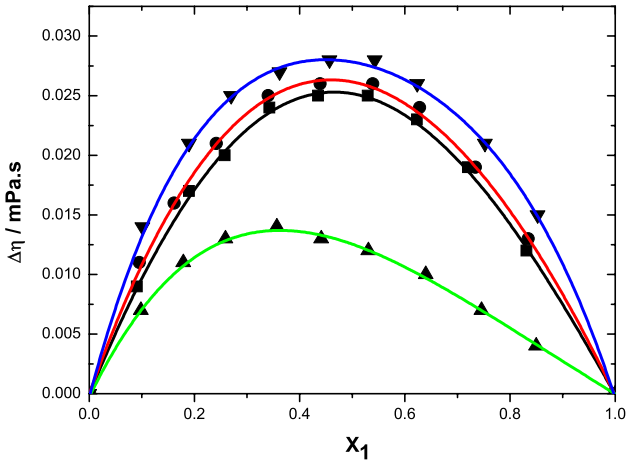

Fig. 3 Variation of deviation in viscosity (Δη) with mole fraction for the binary mixtures of 2-ethyl-1-hexanol with benzyl chloride (square); 3-methylaniline (circle):3-methoxyaniline (triangle) and 2,6-dimethylcyclohexanone (inverted triangle) at 303.15 K

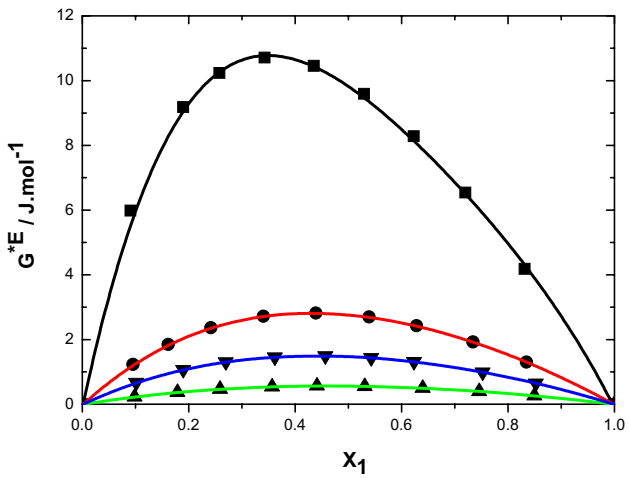

Fig. 4 Excess Gibbs energy of activation of viscous flow (G^{*E}) with mole fraction (x_1) of 2-ethyl-1-hexanol with benzyl chloride (square); 3-methylaniline (circle):3-methoxyaniline (triangle) and 2,6-dimethylcyclohexanone (inverted triangle) at 303.15 K

Table 5 The values of $\overline{V}^{\circ}_{m,1}$, $V^{*}_{m,1}$, $\overline{V}^{\circ E}_{m,1}$, $\overline{V}^{\circ}_{m,2}$, $V^{*}_{m,2}$ and $\overline{V}^{\circ E}_{m,2}$ of the components for 2-ethyl-1-hexanol with various functional groups of binary mixtures at T = (303.15–313.15) K

T (K) ($cm^3\ mol^{-1}$)	$\overline{V}^{\circ}_{m,1}$	$V^{*}_{m,1}$	$\overline{V}^{\circ E}_{m,1}$	$\overline{V}^{\circ}_{m,2}$	$V^{*}_{m,2}$	$\overline{V}^{\circ E}_{m,2}$
2-Ethyl-1-hexanol(1) + benzyl chloride (2)						
303.15	157.49	157.80	−0.313	115.17	115.61	−0.441
308.15	158.01	158.51	−0.499	148.43	149.11	−0.676
313.15	158.59	159.23	−0.643	209.09	209.94	−0.859
2-ethyl-1-hexanol(1) + 3-methylaniline (2)						
303.15	157.44	157.80	−0.359	108.82	109.30	−0.486
308.15	157.97	158.51	−0.538	109.06	109.77	−0.713
313.15	158.51	159.23	−0.720	109.33	110.25	−0.923
2-Ethyl-1-hexanol (1) + 3-methoxy aniline (2)						
303.15	157.38	157.80	−0.420	112.39	112.96	−0.573
308.15	157.91	158.51	−0.601	112.52	113.30	−0.782
313.15	158.45	159.23	−0.782	112.71	113.70	−0.990
2-Ethyl-1-hexanol (1) + 2,6-dimethylcyclohexanone (2)						
303.15	157.32	157.80	−0.482	138.20	138.85	−0.645
308.15	157.86	158.51	−0.653	138.69	139.51	−0.822
313.15	158.38	159.23	−0.850	139.10	140.16	−1.064

2-ethyl-1-hexanol. Hence, above order was justified. In the present systems, negative values of excess isentropic compressibilities shows that the interaction between the unlike molecules exceed the structure breaking effect between the like molecules.

The negative values of κ_s^E for the four systems are in the following order:

2-Ethyl-1-hexanol + 3-methoxyaniline > 2-ethyl-1-hexanol + 3-methylaniline > 2-ethyl-1-hexanol + benzyl chloride > 2-ethyl-1-hexanol + 2, 6-dimethylcyclohexanone

Specific interactions are strong (more effect that is inductive) between 2-ethyl-1-hexanol and 3-methoxyaniline molecules thereby showing the highest negative excess isentropic compressibilities value for their binary mixture.

The sign and magnitude of Δη and G^{*E} depend on the combined effect of factors such as molecular size, shape, and intermolecular forces [20]. The positive values ofΔη and G^{*E} indicates the presence of specific interactions such as the formation of hydrogen bond between unlike molecules and negative values indicates that mutual loss of specific interactions in like molecules outweigh the specific interactions between unlike molecules [18, 21].

In the present study, the positive values of Δη and G^{*E} for these systems indicates that the strength of interaction between the components in binary mixtures and the formation of an association complex [22, 23]. This results in a liquid structure where the flow is rather difficult than would be expected on the basis of the viscosities of the pure components.

3.1 Partial molar properties

The interpretations of excess partial molar properties ($\overline{V}^{E}_{m,1}$, $\overline{V}^{E}_{m,2}$, $\overline{K}^{E}_{s,m,1}$ and $\overline{K}^{E}_{s,m,2}$) and excess partial molar properties at infinite dilution($\overline{V}^{\circ E}_{m,1}$, $\overline{V}^{\circ E}_{m,2}$, $\overline{K}^{\circ E}_{s,m,1}$ and $\overline{K}^{\circ E}_{s,m,2}$) of components 2 have previously been described [24]. Tables 5 and 6 shows that the values of $\overline{V}^{\circ E}_{m,1}$, $\overline{V}^{\circ E}_{m,2}$, $\overline{K}^{\circ E}_{s,m,1}$ and $\overline{K}^{\circ E}_{s,m,2}$ are negative over the whole composition range at experimental temperatures. The observed negative values suggest that the hetero molecular association interactions are stronger than the self-association of molecular interactions of like molecules in the mixtures [25, 26].

4 Conclusions

Densities, viscosities and speeds of sound of binary mixtures of 2-ethyl-1-hexanol with benzyl chloride,3-methylaniline,3-methoxyaniline and 2,6-dimethylcyclohexanone have been measured at different temperatures and derived parameters along with their excess/deviations values, and also excess partial molar

Table 6 The values of $\overline{K}^{\circ}_{s,m,1}$, $K^{*}_{s,m,1}$, $\overline{K}^{\circ E}_{s,m,1}$, $\overline{K}^{\circ}_{s,m,2}$, $K^{*}_{s,m,2}$ and $\overline{K}^{\circ E}_{s,m,2}$ of the components 2-ethyl-1-hexanol with various functional groups of binary mixtures at T = (303.15–313.15) K

T (K)	$\overline{K}^{\circ}_{s,m,1}$	$K^{*}_{s,m,1}$	$\overline{K}^{\circ E}_{s,m,1}$	$\overline{K}^{\circ}_{s,m,2}$	$K^{*}_{s,m,2}$	$\overline{K}^{\circ E}_{s,m,2}$
TPa^{-1}						
2-Ethyl-1-hexanol(1) + benzyl chloride (2)						
303.15	− 84.62	11.279	− 95.90	− 58.93	5.734	− 64.66
308.15	− 105.33	11.739	− 117.07	− 102.61	9.753	− 112.36
313.15	− 130.64	12.243	− 142.88	− 175.15	19.76	− 194.92
2-Ethyl-1-hexanol(1) + 3-methylaniline (2)						
303.15	− 112.46	11.279	− 123.74	− 120.22	4.534	− 124.75
308.15	− 127.43	11.739	− 139.17	− 136.77	4.800	− 141.57
313.15	− 154.02	12.243	− 166.26	− 156.28	5.098	− 161.38
2-Ethyl-1-hexanol(1) +3-methoxyaniline (2)						
303.15	− 126.03	11.279	− 137.31	− 136.70	4.151	− 140.85
308.15	− 143.96	11.739	− 155.70	− 153.49	4.327	− 157.82
313.15	− 166.64	12.243	− 178.88	− 170.49	4.523	− 175.01
2-Ethyl-1-hexanol(1) + 2,6-dimethylcyclohexanone(2)						
303.15	− 16.76	11.279	− 28.04	− 11.11	8.965	− 20.08
308.15	− 20.09	11.739	− 31.83	− 14.04	9.338	− 23.38
313.15	− 23.69	12.243	− 35.94	− 17.51	9.725	− 27.23

properties at infinite dilution ($\overline{V}^{\circ E}_{m,1}$, $\overline{V}^{\circ E}_{m,2}$, $\overline{K}^{\circ E}_{s,m,1}$ and $\overline{K}^{\circ E}_{s,m,2}$) were calculated. The results are analyzed in terms of the specific interactions through the hetero molecular association between the components of the mixtures, resulting in the formation of association complexes.

Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

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