

# Effects of Isentropic and Partial Molar Compressibility of Propiophenone with 1-Alkanols Binary Mixtures at 303.15 to 318.15 K

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**Abstract:** Densities ( $\rho$ ), ultrasonic speeds of sound ( $u$ ) of binary mixtures of propiophenone (PPH) with 1-propanol, 1-butanol and 1-pentanol were measured over the entire composition range at temperatures from 303.15 to 318.15 K and at atmospheric pressure 0.1 MPa. From the experimental data, excess isentropic compressibility  $K_s^E$ , partial molar compressibility (PMC)  $\bar{K}_{sm,1}^o$ ,  $\bar{K}_{sm,2}^o$ , excess partial molar compressibility  $\bar{K}_{sm,1}^{o,E}$ ,  $\bar{K}_{sm,2}^{o,E}$  over the whole composition range and  $\bar{K}_{sm,1}^{o,E,\infty}$ ,  $\bar{K}_{sm,2}^{o,E,\infty}$  at infinite dilution were calculated. The excess isentropic compressibility values correlated using Redlich-Kister polynomial equation. The variation of these parameters with composition and temperature of the mixtures have been discussed in terms of molecular interactions in these mixtures. The observed trend in excess isentropic compressibility values indicates the presence of specific interactions between propiophenone and 1-alkanol molecules. It is observed that excess isentropic values depend upon the number of hydroxyl groups and alkyl chain length in these binary mixtures.

**Keywords:** Densities, Ultrasonic speed of sound, Excess isentropic compressibility, Partial molar compressibility, Excess partial molar compressibility

## Introduction

Excess properties of the investigated binary liquid mixtures are useful for various engineering applications in the process industry, heat transfer and design of equipment, fluid flow and in chemical applications. Study on excess thermodynamic and transport properties of the binary mixtures is essential to understand more on the molecular interactions. Non-ideal behavior results when compounds are mixed with various complex molecular structures<sup>1-5</sup>. The current research study is on the binary mixtures of propiophenone with 1-propanol, 1-butanol and 1-pentanol. Propiophenone is widely used component in perfumes industries and in the synthesis of ephedrine which is used to treat bronchiole asthma. Propiophenone is also used in the synthesis of ketoamphetamines such as cathinone and

methcathinone. Propiophenone can be converted to synthetic aryl alkenes such as cinnamic acids. It is also used as a volatile low toxicity solvent in glues, paints and nail polish removers<sup>6</sup>.

Literature survey reveals some research was done on the variations in density, speed of sound, viscosity and thermodynamic properties of the benzylalcohol with 1-alkanols<sup>6</sup>, thermodynamic excess properties and FTIR spectroscopic studies on propiophenone with alkoxy ethanols at temperatures from 303.15 K to 318.15 K<sup>7</sup>, literature further provides studies on excess isentropic compressibility of binary mixtures of chloroform<sup>9</sup>, *n*-butyl acetate<sup>10</sup>, dimethyl sulphoxide (DMSO)<sup>11</sup> with 1-alkanols. Apparently no studies were made on the partial molar isentropic compressibility and excess partial molar isentropic compressibility at infinite dilution of the binary mixtures of propiophenone with 1-alkanols. Hence, this study has such importance to know much about the strength of association in 1-alkanols with respect to carbon chain length in the molecules that may induce changes in sign and magnitude of excess thermodynamic functions. Alcohols are widely used in chemical industries as reagents, solvents and fuels. Alcohols are used as solvents in the green technology, this is due to its self-association with its internal structure and they play a major role in several chemical reactions<sup>12</sup>. In chemical industries, materials are used in liquid state and therefore more study on their properties is very much essential. It imparts more weight to study the nature of molecular interactions/dynamics of the binary mixtures. There are a number of different intensive properties that are used to characterize material behavior. Partial molar property is one of it and it shows how the thermodynamic properties of the binary mixture vary with changes in the molar composition of the mixture at constant temperature and pressure.

This research paper presents the data on densities, ultrasonic velocity of binary liquid mixtures of propiophenone (PPH) with 1-propanol, 1-butanol and 1-pentanol at temperatures 303.15 K, 308.15 K, 313.15 K and 318.15 K. By using the experimental data, excess isentropic compressibility ( $K_S^E$ ), partial molar compressibility  $\bar{K}_{sm,1}^o$ ,  $\bar{K}_{sm,2}^o$ , excess partial molar compressibility  $\bar{K}_{sm,1}^{o,E}$ ,  $\bar{K}_{sm,2}^{o,E}$  over the entire composition and  $\bar{K}_{sm,1}^{o,E,\infty}$ ,  $\bar{K}_{sm,2}^{o,E,\infty}$  at infinite dilution were calculated at temperatures from 303.15 K to 318.15 K and  $K_S^E$  values are fitted to the Redlich Kister equation<sup>13</sup> to estimate the coefficients and standard deviations to analyze the molecular interactions and structural properties.

## Experimental

All required chemicals used under the current study are purchased from S.D. Fine Chemicals Ltd, India. Purities of the solvents are tabulated in Table 1.

**Table 1.** Provenance and purity of the materials used

Chemicals	CAS number	Source	Water content, %	Mass fraction purity(final)
Propiophenone	93-55-0	S.D fine Chemicals, India	0.00049	> 99.5%
1-Propanol	71-23-8	S.D fine Chemicals, India	0.0001	>99%
1-Butanol	71-36-3	S.D fine Chemicals, India	0.00035	>99%
1-Pentanol	71-41-0	S.D fine Chemicals, India	0.0004	>99%

Estimated purities of the liquid samples are greater than 99% and water content found less than 0.003 mass% (experimentally). Mixtures were prepared by mixing weighed amounts of the pure liquids adopting the method of closed system by using Mettler Toledo (ME204) balance with the precision of  $\pm 0.1$  mg. Proper care was taken to avoid air bubbles in the mixture by allowing them to stand for some time before every measurement.

Experimental and literature values of densities and ultrasonic velocities are compared at respective temperatures and are given in Table 2.

**Table 2.** Comparison of experimental values of densities, ultrasonic velocity and viscosities of pure liquids with the corresponding literature values at various temperatures.

Compound	T, K	Density ( $\rho$ )		Ultrasonic speed (u)	
		Experimental $\text{g/cm}^{-3}$	Literature [Ref] $\text{g/cm}^{-3}$	Experimental $\text{m. s}^{-1}$	Literature [Ref] $\text{m. s}^{-1}$
Propiophenone	303.15	1.0045	1.00437 <sup>[14]</sup> 1.00724 <sup>[18]</sup>	1446.41	1458 <sup>[18]</sup> ; 1440 <sup>[14]</sup>
	308.15	1.0015	1.00896 <sup>[15]</sup> 1.00870 <sup>[16]</sup> 1.00600 <sup>[14]</sup>	1427.038	1438 <sup>[18]</sup> ; 1432 <sup>[19]</sup>
	313.15	0.9985		1403.95	
	318.15	0.9955		1380	
1-Propanol	303.15	0.7953	0.79559 <sup>[7]</sup> , 0.79557 <sup>[17]</sup> , 0.7966 <sup>[9]</sup> , 0.7963 <sup>[20]</sup> , 0.80632 <sup>[22]</sup> , 0.806 <sup>[23]</sup>	1197.9	1192 <sup>[7]</sup> , 1189 <sup>[17]</sup> 1193 <sup>[9]</sup> , 1191 <sup>[21]</sup> 1205.45 <sup>[22]</sup> ; 202.47 <sup>[23]</sup>
	308.15	0.7914	0.7917 <sup>[25]</sup> , 0.7915 <sup>[24]</sup> , 0.7915 <sup>[29]</sup>	1166.28	1172.04 <sup>[25]</sup> , 1171.41 <sup>[26]</sup>
	313.15	0.7873	0.7872 <sup>[7]</sup> , 0.7877 <sup>[17]</sup>	1135.71	1158 <sup>[7]</sup> , 1155 <sup>[17]</sup>
	318.15	0.7834		1109.83	
1-Butanol	303.15	0.8022	0.80231 <sup>[9]</sup> , 0.80195 <sup>[28]</sup> , 0.8023 <sup>[32]</sup> , 0.80206 <sup>[7]</sup> , 0.80209 <sup>[17]</sup>	1230.114	1226 <sup>[7]</sup> , 1222 <sup>[17]</sup> , 1227 <sup>[9]</sup> , 1224 <sup>[21]</sup>
	308.15	0.7982		1215.873	
	313.15	0.7943	0.79409 <sup>[7]</sup> , 0.7943 <sup>[17]</sup>	1201.797	1191 <sup>[7]</sup> , 1189 <sup>[17]</sup>
	318.15	0.7904		1188.308	
1-Pentanol	303.15	0.8076	0.80656 <sup>[7]</sup>	1264.786	1262 <sup>[7]</sup> , 1265 <sup>[27]</sup>
	308.15	0.804	0.8033 <sup>[25]</sup> , 0.8036 <sup>[30]</sup> , 0.80345 <sup>[31]</sup>	1243.6	1243.67 <sup>[25]</sup>
	313.15	0.8002	0.79905 <sup>[7]</sup> 0.79905 <sup>[27]</sup>	1220.231	1225 <sup>[7]</sup> , 1225 <sup>[27]</sup>
	318.15	0.796		1196.24	

Proper care was taken to avoid any evaporation loss while doing the experiment. The densities of liquids and their mixtures were measured using bi-capillary pycnometer having a capillary diameter of 0.85 mm, which was calibrated using double distilled water. The necessary buoyancy corrections were applied. The density ( $\rho$ ) values were reproducible within  $\pm 0.2 \text{ Kg m}^{-3}$ . The ultrasonic velocity (u) measurements were measured by a single frequency (2 MHz) variable path interferometer with an error of  $\pm 0.0001\%$  ultrasonic interferometer model F-05(s.no.1415342) Mittal Enterprises, New Delhi. The mole fraction of each mixture measured with the masses of the components. Averages of three consecutive measurements were taken for all the values at the temperatures from 303.15 K to 318.15 K with an increment of 5 K under atmospheric pressure.

## Results and Discussion

The experimental values of ultrasonic velocity and density of three binary mixtures at temperatures 303.15, 308.15, 313.15 and 318.15 K with respective mole fractions ( $x_1$ ) are reported in Table 3. The following relations are used to determine the respective parameters.

**Table 3.** Experimental values at temperatures T=303.15, 308.15, 313.15 and 318.15 K. densities ( $\rho/\text{g}\cdot\text{cm}^{-3}$ ) and ultrasonic velocities ( $u/\text{m}\cdot\text{s}^{-1}$ ) of binary mixtures of propiophenone with 1-propanol, 1-butanol and 1-pentanol at T=303.15, 308.15, 313.15 and 318.15 K

$X_1$	303.15K		308.15 K		313.15 K		318.15 K	
	$\rho$ $\text{g cm}^{-3}$	U $\text{m}\cdot\text{s}^{-1}$	$\rho$ $\text{g cm}^{-3}$	U $\text{m}\cdot\text{s}^{-1}$	$\rho$ $\text{g cm}^{-3}$	U $\text{m}\cdot\text{s}^{-1}$	$\rho$ $\text{g cm}^{-3}$	U $\text{m}\cdot\text{s}^{-1}$
PPH+1-Propanol								
0	0.7953	1197.90	0.7914	1166.28	0.7873	1135.71	0.7834	1109.83
0.0588	0.8179	1213.06	0.8146	1182.45	0.8111	1152.50	0.8083	1126.88
0.1233	0.8404	1229.69	0.8372	1199.90	0.8338	1170.51	0.8311	1145.07
0.1943	0.8627	1247.77	0.8596	1218.82	0.8562	1189.99	0.8536	1164.73
0.2728	0.8846	1267.53	0.8815	1239.52	0.8783	1211.27	0.8756	1186.20
0.3601	0.9060	1289.35	0.9030	1262.39	0.8998	1234.77	0.8972	1209.80
0.4577	0.9267	1313.58	0.9237	1287.81	0.9207	1260.89	0.9181	1236.11
0.5676	0.9466	1340.65	0.9437	1316.20	0.9407	1290.10	0.9383	1265.60
0.6924	0.9657	1371.22	0.9629	1348.28	0.9601	1323.16	0.9577	1298.90
0.8351	0.9845	1406.10	0.9819	1384.91	0.9792	1360.80	0.9769	1336.86
1	1.0045	1446.41	1.0015	1427.04	0.9985	1403.95	0.9955	1380.00
PPH+1-Butanol								
0	0.8022	1230.11	0.7982	1215.87	0.7943	1201.80	0.7904	1188.31
0.0710	0.8236	1246.38	0.8199	1232.06	0.8164	1217.62	0.8128	1203.66
0.1468	0.8449	1263.48	0.8415	1248.74	0.8382	1233.87	0.8348	1219.12
0.2278	0.8662	1281.47	0.8629	1266.36	0.8596	1250.57	0.8563	1235.17
0.3145	0.8872	1300.48	0.8839	1284.91	0.8807	1268.45	0.8774	1252.02
0.4077	0.9077	1320.73	0.9045	1304.68	0.9013	1287.34	0.8981	1269.89
0.5080	0.9276	1342.34	0.9245	1325.82	0.9213	1307.57	0.9182	1289.16
0.6163	0.9468	1365.59	0.9438	1348.55	0.9408	1329.37	0.9378	1309.94
0.7336	0.9656	1390.59	0.9628	1373.04	0.9600	1352.86	0.9571	1332.25
0.8610	0.9845	1417.52	0.9817	1399.35	0.9791	1377.91	0.9763	1355.92
1	1.0045	1446.41	1.0015	1427.04	0.9985	1403.95	0.9955	1380.00
PPH+1-Pentanol								
0	0.8076	1264.79	0.8040	1243.60	0.8002	1220.23	0.7960	1196.24
0.0836	0.8279	1280.92	0.8246	1260.49	0.8212	1237.59	0.8174	1214.11
0.1703	0.8484	1297.42	0.8453	1277.15	0.8420	1254.27	0.8384	1230.79
0.2602	0.8689	1314.29	0.8658	1294.18	0.8626	1271.33	0.8591	1247.85
0.3537	0.8891	1331.59	0.8860	1311.65	0.8829	1288.83	0.8794	1265.35
0.4508	0.9090	1349.37	0.9060	1329.60	0.9028	1306.81	0.8994	1283.34
0.5518	0.9285	1367.71	0.9255	1348.12	0.9224	1325.36	0.9191	1301.89
0.6570	0.9474	1386.53	0.9446	1367.13	0.9416	1344.40	0.9385	1320.93
0.7665	0.9662	1405.87	0.9634	1386.67	0.9606	1363.97	0.9577	1340.51
0.8808	0.9850	1425.73	0.9823	1406.74	0.9795	1384.07	0.9767	1360.62
1	1.0045	1446.41	1.0015	1427.04	0.9985	1403.95	0.9955	1380.00

a) The isentropic compressibility ( $K_s$ ) was calculated using the Laplace relation

$$K_s = U^{-2} \rho^{-1} \quad (1)$$

Where  $u$  is the ultrasonic velocity and  $\rho$  is the density.

b) Excess isentropic compressibility ( $K_s^E$ ) calculated by the relation

$$K_s^E = K_s - K_s^{iD} \quad (2)$$

$$K_s^{iD} = \sum_{i=1}^2 \Phi_i \left( K_{si} + \frac{TV_i \alpha_i^2}{C_{pi}} \right) - \frac{T \left( \sum_{i=1}^2 x_i V_i \right) \left( \sum_{i=1}^2 \phi_i \alpha_i \right)}{\sum_{i=1}^2 x_i C_{pi}} \quad (3)$$

Where  $\Phi_i$  is the ideal state volume fraction and is defined by the relation:

$$\Phi_i = \frac{x_i V_i}{\sum_{i=1}^2 x_i V_i} \quad (4)$$

$K_s^{iD}$  is the isentropic compressibility of the ideal mixture. Its values are calculated as per Benson and Kiyohara<sup>333</sup> and Acree<sup>344</sup>

Where  $\Phi_i$  is the volume fraction of component  $i$  in the mixture,  $\chi_i$  is the corresponding mole fraction of  $i$ ,  $T$  is the absolute temperature and  $K_s$ ,  $V_i$ ,  $\alpha_i$  and  $C_{pi}$  are the isentropic compressibility (the source of  $\alpha_i$  and  $C_{pi}$  values is from the book Riddick and Bunger, techniques of chemistry, Vol-II and from the literature values<sup>Error! Reference source not found.,Error! Reference source not found.</sup>), molar volume, cubic expansion coefficient and molar heat capacity of the pure component  $i$ , respectively. The cubic expansion coefficients were calculated by using experimental densities at different temperatures.

From the thermodynamic point of view, the ultrasonic velocity, excess isentropic compressibility, partial molar isentropic compressibility and excess partial molar isentropic compressibility are strongly affected by the changes of concentration and temperature, besides the type of bonding present between the molecules of the constituent liquids.

The non-linear variation is a deviation from ideal behavior which suggests the presence of intermolecular interactions between the component molecules of the mixtures, however the strength of interaction is well reflected in the excess parameters like excess isentropic compressibility ( $K_s^E$ ), partial molar compressibility and excess partial molar compressibility, as these parameters are found to be more sensitive towards intermolecular interactions in the liquid mixtures.

Hydrogen bonding causes considerable influence on these parameters, because of the fact that specific interactions between the molecules are controlled mainly by hydrogen bond that binds the molecules together. Computed parameter values of the binary mixtures ( $K_s^E$ ,  $\bar{K}_{sm,1}^o$ ,  $\bar{K}_{sm,2}^o$ ,  $\bar{K}_{sm,1}^{o,E}$ ,  $\bar{K}_{sm,2}^{o,E}$ ,  $\bar{K}_{sm,1}^{o,E,\infty}$ ,  $\bar{K}_{sm,2}^{o,E,\infty}$ ), are given in Tables 4-7 at temperatures from 303.15 K to 313.15 K for the binary mixtures of propiophenone with 1-propanol, 1-butanol and 1-pentanol.

### Excess isentropic compressibility ( $K_s^E$ )

Excess isentropic compressibility  $K_s^E$  values for the binary mixtures of propiophenone with 1-alkanols are graphically represented (3D) along with their respective mole fractions at temperatures from 303.15 K to 318.15 K in Figure 1 and the data values are tabulated in Table 4.

Computed  $K_s^E$  values are negative for all the binary mixtures over the entire composition range at temperatures from 303.15 K to 318.15 K.  $K_s^E$  values are maximum at the mole fractions 0.2728 of 1-propanol, at 0.4077 of 1-butanol and at 0.4508 of 1-pentanol and the negative values of  $K_s^E$  are increasing with increase in temperatures. Figures 2-4 shows the graphical representation of  $K_s^E$  values for the binary mixtures of propiophenone with 1-alkanols (1-propanol, 1-butanol and 1-pentanol) at temperatures from 303.15 K-318.15 K.

**Table 4.** The values of excess isentropic compressibility of the components propiophenone with 1-alkanols at temperatures from T=303.15 K to 318.15 K

$X_1$	$K_s^E = K_s - K_s^{iD}$			
	303.15 K	308.15 K	313.15 K	318.15 K
PPH+1-Propanol				
0.0000	0.0000	0.0000	0.0000	0.0000
0.0588	-6.0223	-7.9445	-9.7337	-12.1406
0.1233	-10.5237	-13.0492	-15.5083	-18.4838
0.1943	-13.2661	-16.1472	-18.9424	-22.2120
0.2728	-14.4144	-17.3722	-20.2664	-23.6085
0.3601	-14.1361	-17.0349	-19.8339	-22.9646
0.4577	-12.5608	-15.2526	-17.8054	-20.6741
0.5676	-9.8755	-12.1725	-14.3736	-16.9130
0.6924	-6.4920	-8.2617	-10.0084	-12.0261
0.8351	-2.8969	-4.0270	-5.1248	-6.5530
1.0000	0.0000	0.0000	0.0000	0.0000
PPH+1-Butanol				
0.0000	0.0000	0.0000	0.0000	0.0000
0.0710	-8.0939	-9.0283	-9.8690	-10.6555
0.1468	-14.1328	-15.3033	-16.6622	-17.6585
0.2278	-18.1540	-19.4534	-20.5685	-21.8289
0.3145	-20.1583	-21.4058	-22.5762	-23.6565
0.4077	-20.3350	-21.4896	-22.5226	-23.4614
0.5080	-18.7571	-19.8482	-20.7559	-21.6993
0.6163	-15.6613	-16.6559	-17.5430	-18.5312
0.7336	-11.2536	-12.1927	-13.0700	-13.9828
0.8610	-5.9055	-6.6368	-7.2832	-8.0125
1.0000	0.0000	0.0000	0.0000	0.0000
PPH+1-Pentanol				
0.0000	0.0000	0.0000	0.0000	0.0000
0.0836	-8.3932	-9.9361	-11.4393	-13.2250
0.1703	-14.7750	-16.7314	-18.7093	-21.0665
0.2602	-19.0851	-21.2313	-23.3910	-26.0483
0.3537	-21.3685	-23.5280	-25.7683	-28.4693
0.4508	-21.7190	-23.8192	-25.9608	-28.5989
0.5518	-20.2812	-22.2213	-24.2432	-26.6889
0.6570	-17.0942	-18.8465	-20.6446	-22.8202
0.7665	-12.4360	-13.9043	-15.3773	-17.1419
0.8808	-6.5619	-7.5929	-8.6141	-9.8304
1.0000	0.0000	0.0000	0.0000	0.0000

**Table 5.** Coefficients of Redlich-Kister polynomial equation

Property	Temp, K	A0	A1	A2	$\sigma$
PPH+1-PROPANOL					
$K_S^E$	303.15	-46.156	50.112	-21.302	0.134
	308.15	-55.829	58.574	-33.020	0.349
	313.15	-65.141	66.691	-44.586	0.548
	318.15	-75.438	75.801	-61.552	0.872
PPH+1-Butanol					
$K_S^E$	303.15	-75.723	44.265	-11.400	0.037
	308.15	-79.904	46.490	-18.965	0.111
	313.15	-83.492	48.872	-27.302	0.200
	318.15	-87.205	50.287	-34.798	0.242
PPH+1-Pentanol					
$K_S^E$	303.15	-84.956	29.327	-0.321	0.025
	308.15	-92.829	33.027	-9.228	0.119
	313.15	-100.991	36.763	-17.404	0.225
	318.15	-110.960	41.352	-26.736	0.342

**Table 6.** The values of the partial molar isentropic compressibility of the components propiophenone with 1-alkanols at temperatures T= 303.15 K to 318.15 K

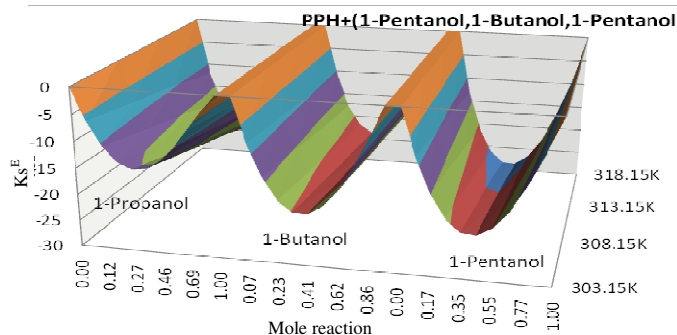
$x_1$	303.15 K		308.15 K		313.15 K		318.15 K	
	$\overline{K}_{s,m,1}^E$	$\overline{K}_{s,m,2}^E$	$\overline{K}_{s,m,1}^E$	$\overline{K}_{s,m,2}^E$	$\overline{K}_{s,m,1}^E$	$\overline{K}_{s,m,2}^E$	$\overline{K}_{s,m,1}^E$	$\overline{K}_{s,m,2}^E$
Propiophenone+ 1-Propanol								
0.0000	-0.1735	0.0000	-0.3027	0.0000	-0.4304	0.0000	-0.6119	0.0000
0.0588	-0.1967	0.0014	-0.2951	0.0009	-0.3918	0.0004	-0.5226	-0.0006
0.1233	-0.2221	0.0060	-0.2978	0.0044	-0.3717	0.0027	-0.4652	-0.0003
0.1943	-0.2460	0.0137	-0.3069	0.0111	-0.3658	0.0085	-0.4345	0.0035
0.2728	-0.2636	0.0231	-0.3162	0.0203	-0.3669	0.0175	-0.4220	0.0118
0.3601	-0.2686	0.0294	-0.3176	0.0274	-0.3645	0.0252	-0.4145	0.0206
0.4577	-0.2538	0.0216	-0.3005	0.0197	-0.3453	0.0176	-0.3943	0.0149
0.5676	-0.2121	-0.0242	-0.2541	-0.0317	-0.2945	-0.0390	-0.3408	-0.0453
0.6924	-0.1413	-0.1568	-0.1722	-0.1889	-0.2020	-0.2196	-0.2380	-0.2517
0.8351	-0.0535	-0.4747	-0.0665	-0.5809	-0.0792	-0.6835	-0.0950	-0.8039
1.0000	0.0000	-1.1757	0.0000	-1.4742	0.0000	-1.7642	0.0000	-2.1279
Propiophenone+ 1-Butanol								
0.0000	-0.4286	0.0000	-0.5238	0.0000	-0.6192	0.0000	-0.7172	0.0000
0.0710	-0.4404	0.0009	-0.5029	0.0001	-0.5633	-0.0007	-0.6263	-0.0016
0.1468	-0.4424	0.0025	-0.4822	0.0000	-0.5189	-0.0026	-0.5576	-0.0054
0.2278	-0.4314	0.0020	-0.4573	-0.0023	-0.4799	-0.0065	-0.5034	-0.0113
0.3145	-0.4044	-0.0059	-0.4233	-0.0111	-0.4393	-0.0158	-0.4551	-0.0219
0.4077	-0.3590	-0.0299	-0.3755	-0.0350	-0.3899	-0.0390	-0.4030	-0.0451
0.5080	-0.2943	-0.0844	-0.3103	-0.0893	-0.3253	-0.0923	-0.3381	-0.0980
0.6163	-0.2127	-0.1923	-0.2275	-0.2001	-0.2421	-0.2049	-0.2543	-0.2126
0.7336	-0.1219	-0.3899	-0.1327	-0.4104	-0.1439	-0.4275	-0.1533	-0.4457
0.8610	-0.0394	-0.7342	-0.0439	-0.7905	-0.0485	-0.8447	-0.0525	-0.8947
1.0000	0.0000	-1.3139	0.0000	-1.4536	0.0000	-1.5967	0.0000	-1.7229

Contd....

Propiophenone+ 1-Pentanol								
0.0000	-0.5595	0.0000	-0.6903	0.0000	-0.8163	0.0000	-0.9634	0.0000
0.0836	-0.5510	-0.0005	-0.6379	-0.0018	-0.7237	-0.0029	-0.8252	-0.0042
0.1703	-0.5210	-0.0051	-0.5799	-0.0088	-0.6398	-0.0123	-0.7118	-0.0162
0.2602	-0.4715	-0.0188	-0.5144	-0.0249	-0.5591	-0.0307	-0.6136	-0.0373
0.3537	-0.4055	-0.0483	-0.4403	-0.0560	-0.4767	-0.0635	-0.5216	-0.0723
0.4508	-0.3272	-0.1014	-0.3578	-0.1105	-0.3895	-0.1200	-0.4285	-0.1313
0.5518	-0.2419	-0.1878	-0.2689	-0.2006	-0.2964	-0.2144	-0.3299	-0.2314
0.6570	-0.1563	-0.3194	-0.1780	-0.3430	-0.1997	-0.3681	-0.2259	-0.3990
0.7665	-0.0795	-0.5106	-0.0933	-0.5602	-0.1069	-0.6113	-0.1231	-0.6736
0.8808	-0.0227	-0.7790	-0.0276	-0.8827	-0.0323	-0.9864	-0.0379	-1.1112
1.0000	0.0000	-1.1460	0.0000	-1.3508	0.0000	-1.5516	0.0000	-1.7905

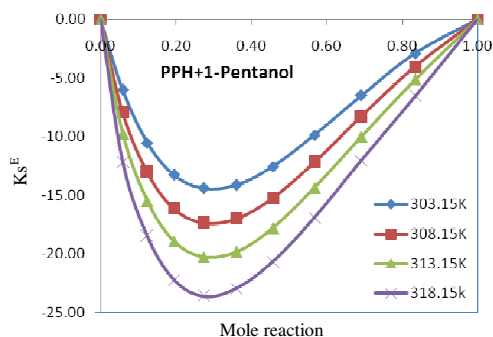
**Table 7.** The values of the partial molar compressibility at infinite dilution of the components propiophenone with 1-alkanols at temperatures T= 303.15 K to 318.15 K

T, K	$\bar{K}_{s,m,1}^o$	$\bar{K}_{s,m,1}^*$	$\bar{K}_{s,m,1}^{oE}$	$\bar{K}_{s,m,2}^o$	$\bar{K}_{s,m,2}^*$	$\bar{K}_{s,m,2}^{oE}$
Propiophenone+ 1-Propanol						
303.1500	-0.1099	6.3563	-0.1735	-1.1095	6.6217	-1.1757
308.1500	-0.2371	6.5692	-0.3027	-1.4037	7.0547	-1.4742
313.1500	-0.3621	6.8279	-0.4304	-1.6890	7.5172	-1.7642
318.1500	-0.5408	7.1096	-0.6119	-2.0484	7.9505	-2.1279
Propiophenone+ 1-Butanol						
303.1500	-0.3650	6.3563	-0.4286	-1.2378	7.6111	-1.3139
308.1500	-0.4581	6.5692	-0.5238	-1.3749	7.8693	-1.4536
313.1500	-0.5509	6.8279	-0.6192	-1.5153	8.1342	-1.5967
318.1500	-0.6461	7.1096	-0.7172	-1.6389	8.4018	-1.7229
Propiophenone+ 1-Pentanol						
303.1500	-0.4959	6.3563	-0.5595	-1.0616	8.4488	-1.1460
308.1500	-0.6246	6.5692	-0.6903	-1.2627	8.8176	-1.3508
313.1500	-0.7480	6.8279	-0.8163	-1.4591	9.2457	-1.5516
318.1500	-0.8923	7.1096	-0.9634	-1.6933	9.7221	-1.7905

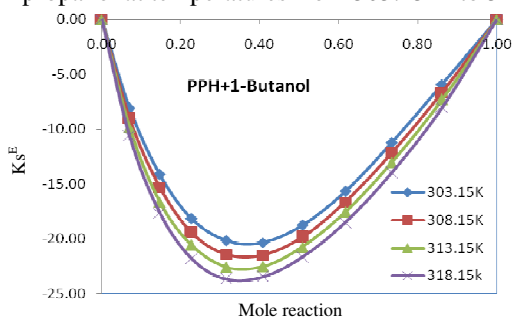


**Figure 1.** Three dimensional graph for the excess partial molar isentropic compressibility for the binary mixtures of propiophenone with 1-alkanols (1-propanol, 1-butanol and 1-pentanol) at temperatures from 303.15 K to 318.15 K

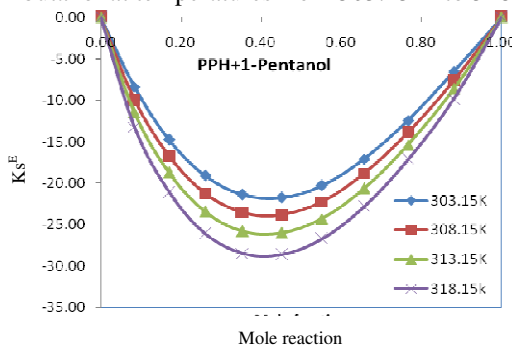




**Figure 2.** Excess partial molar isentropic compressibility for the binary mixtures of propiophenone with 1-propanol at temperatures from 303.15 K to 318.15 K



**Figure 3.** Excess partial molar isentropic compressibility for the binary mixtures of propiophenone with 1-butanol at temperatures from 303.15 K to 318.15 K



**Figure 4.** Excess partial molar isentropic compressibility for the binary mixtures of propiophenone with 1-pentanol at temperatures from 303.15 K to 318.15 K

At the equimolar concentrations,  $K_s^E$  values of 1-pentanol are more negative than 1-butanol and 1-propanol, it indicates that more number of  $-CH_2$  groups present adjacent to the  $-OH$  group, hence stronger interactions are observed. Molecules of both propiophenone and 1-alkanols are associated through hydrogen bonding due to the presence of strong proton-acceptor as well as proton-donor groups in their molecules. Mixing of propiophenone with alkanols would induce mutual dissociation of hydrogen bonded structures present in pure liquids with subsequent formation of new H-bonds between propiophenone and alkanol molecules in the mixtures. More negative values are observed for 1-pentanol than those for 1-butanol and 1-propanol and it is due to the fact that 1-pentanol is having more number of  $-CH_2$  groups resulting in stronger interaction (H-bonding) in propiophenone and 1-pentanol mixtures.

The negative values of  $K_S^E$  indicates that the mixture is less compressible than the ideal mixture and suggests strong chemical and specific interactions between the components of analysed binary mixture, which are larger in the case of propiophenone + 1-pentanol

Kiyohara and Benson<sup>35</sup> suggested that  $K_S^E$  is the resultant of several opposing effects.  $K_S^E$  negative values are due to strong molecular interaction through hydrogen bonding, dipole-dipole interactions, dipole-induced dipole interactions, interstitial accommodation and orientation and complex charge transfer<sup>36</sup>. The magnitude of the various contributions depends mainly on the relative molecular size of the components. The negative values of  $K_S^E$  further indicate that the dipole interaction between the components is not only the cause of deviations but donor-acceptor properties of the components play an important role.

### Redlich-Kister equation

The values of  $K_S^E$  with respect to mole fraction were fitted to the Redlich–Kister equation of the type:

$$Y^E = x_1 x_2 \{a_0 + a_1(x_1 - x_2) + a_2(x_1 - x_2)^2\} \quad (5)$$

Where  $Y^E$  is for values of  $K_S^E$  in the polynomial degree. The values of  $a_0$ ,  $a_1$  and  $a_2$  are the coefficients of the polynomial equation and were obtained by the method of least-squares and are given in Table 4 along with standard deviation values. The standard deviations are calculated by using the equation:

$$\sigma(Y^E) = \frac{\{\sum_{i=1}^n (Y_{obs}^E - Y_{cal}^E)^2\}^{1/2}}{n - m} \quad (6)$$

Where  $n$  is the total number of experimental points and  $m$  is the number of coefficients. Standard deviation values are below 1.00 for all the studied binary mixtures.

### Partial molar isentropic compressibility (PMC)

The partial molar isentropic compressibility  $\bar{K}_{sm,1}^o$  of component 1 (propiophenone) and  $\bar{K}_{sm,2}^o$  of component 2 (*1-propanol*, *1-butanol*, *1-pentanol*) in the mixture over entire composition range are calculated using the following relations.

$$\bar{K}_{sm,1}^o = K_S^E + K_{sm,1}^* + x_2 \left( \frac{\partial K_S^E}{\partial x_1} \right) T.P \quad (7)$$

$$\bar{K}_{sm,2}^o = K_S^E + K_{sm,2}^* - x_1 \left( \frac{\partial K_S^E}{\partial x_1} \right) T.P \quad (8)$$

Where  $K_{sm,1}^*$ ,  $K_{sm,2}^*$  are molar isentropic compressibility of pure components propiophenone with *1-propanol*, *1-butanol* and *1-pentanol*. The derivative of  $\left( \frac{\partial K_S^E}{\partial x_1} \right)$

obtained by using below equations.

$$\bar{K}_{sm,2}^o = K_{sm,2}^* + x_1^2 \sum_{i=0}^n A_i (1 - 2x_1)^i + 2x_1 x_2^2 \sum_{i=1}^n A_i (1 - 2x_1)^{i-1} \quad (9)$$

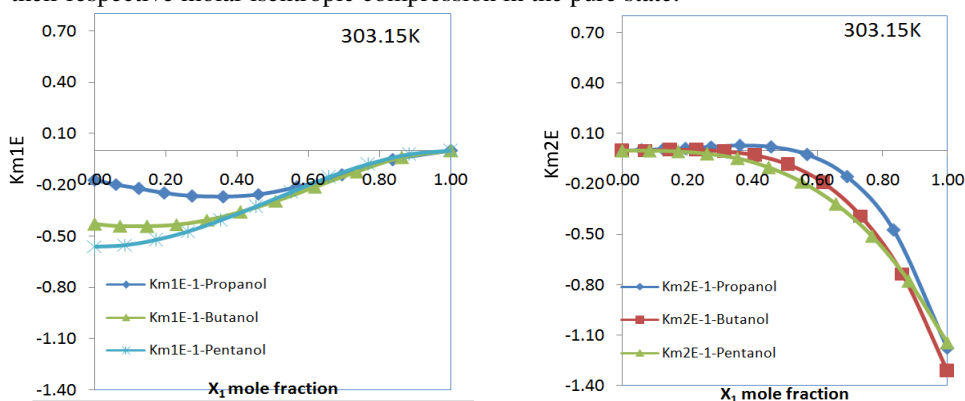
$$\bar{K}_{sm,1}^o = K_{sm,1}^* + x_2^2 \sum_{i=0}^n A_i (1 - 2x_1)^i + 2x_1 x_2^2 \sum_{i=1}^n A_i (1 - 2x_1)^{i-1} \quad (10)$$

The excess partial molar isentropic compressibility  $\overline{K}^{o,E}_{sm,1}$ ,  $\overline{K}^{o,E}_{sm,2}$  over the whole composition range is calculated by using the below relation:

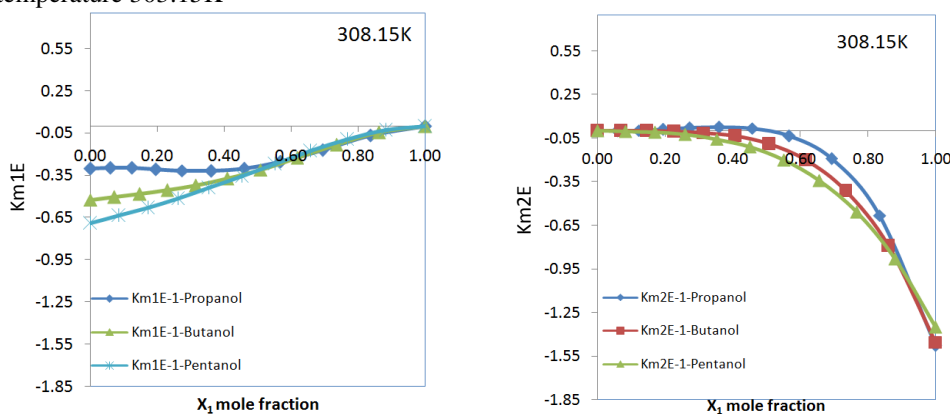
$$\overline{K}^{o,E}_{sm,1} = \overline{K}^{o}_{sm,1} - K^*_{sm,1} \quad (11)$$

$$\overline{K}^{o,E}_{sm,2} = \overline{K}^{o}_{sm,2} - K^*_{sm,2} \quad (12)$$

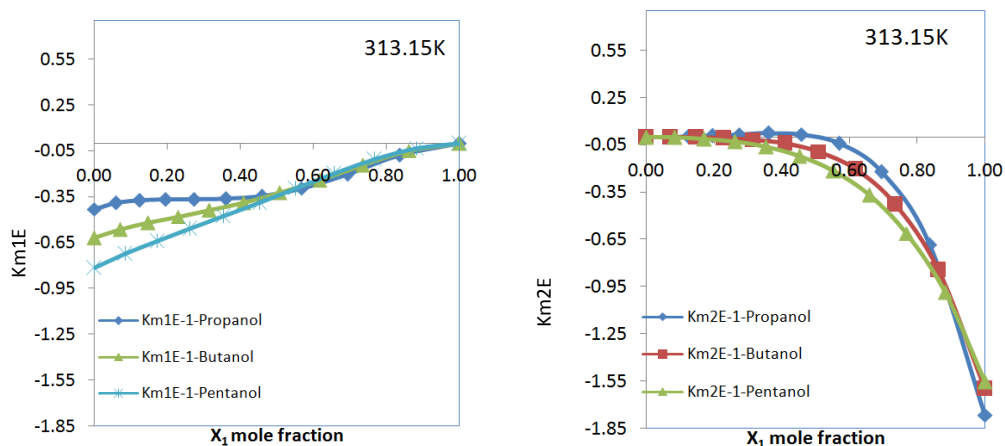
The values of excess partial molar isentropic compressibility  $\overline{K}^{o,E}_{sm,1}$ ,  $\overline{K}^{o,E}_{sm,2}$  of propiophenone with 1-alkanols are given in Table 5. Values of excess partial molar isentropic compressibility  $\overline{K}^{o,E}_{sm,1}$ ,  $\overline{K}^{o,E}_{sm,2}$  with respect to mole fraction of the entire range of composition at temperatures from 303.15 K to 318.15 K are graphically represented in Figures 5-8. Negative values of partial molar isentropic compressibility are observed and it indicates that the partial molar isentropic compressions of each component are less than their respective molar isentropic compression in the pure state.



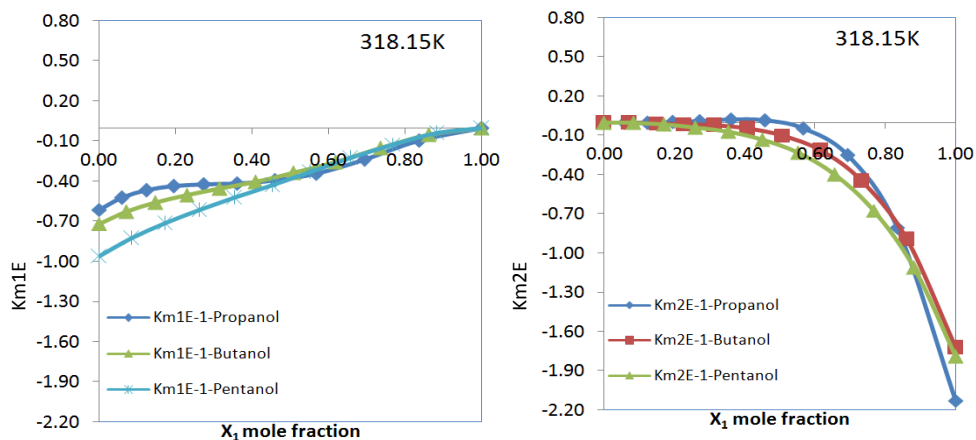
**Figure 5.** Excess partial molar isentropic compressibility at infinite dilution for the binary mixtures of propiophenone with 1-alkanols (1-pentanol, 1-butanol & 1-pentanol) at temperature 303.15K



**Figure 6.** Excess partial molar isentropic compressibility at infinite dilution for the binary mixtures of propiophenone with 1-alkanols (1-pentanol, 1-butanol & 1-pentanol) at temperature 308.15K



**Figure 7.** Excess partial molar isentropic compressibility at infinite dilution for the binary mixtures of propiophenone with 1-alkanols (1-pentanol, 1-butanol & 1-pentanol) at temperature 313.15K



**Figure 8.** Excess partial molar isentropic compressibility at infinite dilution for the binary mixtures of propiophenone with 1-alkanols (1-pentanol, 1-butanol & 1-pentanol) at temperature 318.15K

The excess partial molar isentropic compressibility of propiophenone with 1-alkanols at infinite dilution are calculated by using the relation

$$\overline{K}^{o,E,\infty}_{sm,2} = \overline{K}^{o,\infty}_{sm,2} - K_{sm,2}^* \quad (13)$$

$$\overline{K}^{o,E,\infty}_{sm,1} = \overline{K}^{o,\infty}_{sm,1} - K_{sm,1}^* \quad (14)$$

The values of excess partial molar isentropic compressibility at infinite dilution  $\overline{K}^{o,E,\infty}_{sm,1}$ ,  $\overline{K}^{o,E,\infty}_{sm,2}$  for the selected binary systems at different temperatures are presented in Table 6. Excess compressibility is important in assessing the molecular arrangement and its solidity. It provides useful information about the molecular interactions and its structure of the liquid mixture. Negative values of  $\overline{K}^{o,E,\infty}_{sm,1}$ ,  $\overline{K}^{o,E,\infty}_{sm,2}$  of propiophenone with 1-alkanols

shows stronger solute–solvent interactions at infinite dilution. The trend of the negative values of  $\overline{K}_{sm,1}^o$ ,  $\overline{K}_{sm,2}^o$ ,  $\overline{K}_{sm,1}^{o,E}$ ,  $\overline{K}_{sm,2}^{o,E}$ ,  $\overline{K}_{sm,1}^{o,E,\infty}$ ,  $\overline{K}_{sm,2}^{o,E,\infty}$  of propiophenone with 1-propanol, 1-butanol and 1-pentanol binary mixtures is increasing as the temperature increases from 303.15 K to 318.15 K.

The order of values of partial molar isentropic compressibility for propiophenone with 1-alkanols is *1-propanol*>*1-butanol*>*1-pentanol*.

## Conclusion

The excess thermodynamic properties show that molecular interactions are predominant in the binary mixtures. The negative values of  $K_s^E$  are due to the strong intermolecular attractions between unlike molecules. The current study shows that the strong dipole-dipole interactions are observed in 1-pentanol compared to that of 1-butanol and 1-propanol. From the measured experimental data, the values of excess isentropic compressibility are calculated and are correlated with Redlich–Kister type polynomial equation to derive the coefficients and standard deviation. Calculated excess partial molar isentropic compressibility of the binary mixtures and its values at infinite dilution indicate stronger solute-solvent interactions.

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## References

1. Canosa J M, Rodriguez A, Iglesias M, Orge B and Tojo J, *J Therm Anal.*, 1998, **52**, 915-932.
2. Nan Z and Tan Z C, *J Therm Anal Calorim.*, 2007, **87(2)**, 539–544; DOI:10.1007/s10973-005-7295-2
3. Marongiu B, Piras A, Porcedda S and Tuveri E, *J Therm Anal Calorim.*, 2007, **91(1)**, 37-46; DOI:10.1007/s10973-007-8337-8
4. Dipali C and Anand A. *J Therm Anal Cal.*, 2012, **107**, 21-24.
5. Narendra K, Srinivasu Ch, Kalpana Ch and Narayanamurthy P, *J Therm Anal Cal.*, 2012, **107**, 25-30.
6. Bindhani S K, Roy G K, Mohanty Y K and Kubendran T R, *Russian J Phys Chem., A*, 2015, 89, 1828-1837; DOI:10.1134/S0036024415100040
7. Venkatramana L, Sreenivasulu K, Sivakumar K and Dayananda Reddy K, *J Therm Anal Calorim.*, 2014, **115(2)**, 1829-1834; DOI:10.1007/s10973-013-3473-9
8. Nanduri Gayatri Devi, Srinivasa Rao N V N B, Radha Sirija M and Ramachandran D, *IOSR Journal of Applied Chemistry (IOSR-JAC)* e-ISSN: 2278-5736, Volume 10, Issue 7 Ver. I (July. 2017), PP 44-56.
9. Ujjan B Kadam, Apoorva P Hiray, Arun B Sawant and Mehdi Hasan, *J Eng Data*, 2006, **51(1)**, 60-63; DOI:10.1021/je050169y
10. Mehdi Hasan, Apoorva P. Hiray, Ujjan B. Kadam, Dinesh F. Shirude, Keshav J. Kurhe and Arun B. Sawant, *Solution Chem.*, 2011, **40(3)**, 415-429; DOI:10.1007/s10953-011-9657-7
11. Palani R, Geetha A, Saravanan S and Sunil D. Tontapur, *R J C Rasayan J Chem.*, 2008, **1(3)**, 481-488.

12. Ali A, Nain A K, Sharma V K and Ahmad S, *Indian J Pure Appl Phys.*, 2004, **42(9)**, 666-673.
13. Redlich O and Kister A T, *Ind Engg Chem.*, 1948, **40(2)**, 345-348; DOI:10.1021/ie50458a036
14. Manukonda G S, Venkatalakshami P and Rambabu K, *Int J Phys Res.*, 2013, **3(4)**, 5.
15. Gowrisankar M, Sivarambabu S, Venkateswarlu P and Kumar K Siva, *Bull Korean Chem Soc.*, 2012, **33(5)**, 1686-1692; DOI:10.5012/bkcs.2012.33.5.1686
16. Timmermanns, J. *PhysicoChemical Constants of Pure Organic Compounds*; Elsevier Publications; Amesterdam, 1950; Vol.1.
17. Sangeeta S, Martin A and Nirmala D, *J Chem Thermodyn.*, 2013, **57**, 238-247; DOI:10.1016/j.jct.2012.08.030
18. Bindhania S K, Roya G K, Mohantya Y K and Kubendranb T R, *Russian J Phys Chem A*, 2015, **89(10)**, 1828–1837; DOI:10.1134/S0036024415100040
19. Tangeda S J, Boodida S and Nallani S, *J Chem Thermodyn.*, 2006, **38(11)**, 1438-1442; DOI:10.1016/j.jct.2006.01.009
20. Aminabhavi T M and Patil V B, *J Chem Eng Data*, 1998, **43(4)**, 497-503; DOI:10.1021/je980031y
21. Prabhakara Rao M V and Naidu P R, *Part II J Chem Thermodyn.*, 1976, **8**, 96-98; DOI:10.1016/0021-9614(76)90157-9
22. Fakruddin Babavali S K, Punyaseshudu D, Narendra K, Sridhar Yesaswi Ch and Srinivasu Ch, *J Mole Liq.*, 2016, **224(A)**, 47-52; DOI:10.1016/j.molliq.2016.09.079
23. Tridevi C M and Rana V A, *Int J Sci Res*, 2015, 22-24.
24. Riddick J A, Bunger W B and Sakano T K, *Organic Solvents: Physical Properties and Methods of Purifications*, 4<sup>th</sup> Edn., Wiley Interscience, New York, 1986.
25. Amalendu Pal, Rekha Gaba and Harsh Kumar, *J Solution Chem.*, 2011, **40(5)**, 786-802; DOI:10.1007/s10953-011-9688-0
26. Vercher E, Orchilles A V, Miguel P J, Martinez-Andreu A, *J Chem Eng Data*, 2007, **52(4)**, 1468-1482; DOI:10.1021/je7001804
27. AlTuwaim M S, Alkhaldi HAEK, Al-Jimaz S A and Mohammad A A, *J Chem Thermodyn.*, 2012, **48**, 39-47; DOI:10.1016/j.jct.2011.12.002
28. Riddick J A, Bunger W B and Sakano T K, *Organic Solvents, Physical Properties and Methods of Purification, Techniques of Chemistry*, 4<sup>th</sup> Ed., Wiley-Interscience: New York, 1986; Vol. II.
29. Peleteiro J, Gonzalez-Salgado D, Cereirina C A, Valencia J L and Romani L, *Fluid Phase Equilib.*, 2001, **191(1-2)**, 83–97; DOI:10.1016/S0378-3812(01)00614-8
30. Shan, Z and Asfour A F A, *Fluid Phase Equilib.*, 1998, **143(1-2)**, 253–262; DOI:10.1016/S0378-3812(97)00267-7
31. Al-Jimaz A S, Al-Kandary J A and Abdul-Latif A H M, *Fluid Phase Equilib.*, 2004, **218(2)**, 247-260; DOI:10.1016/j.fluid.2003.12.007
32. Nikam P S, Jadhav M C and Hasan M, *J Chem Eng Data*, 1995, **40(4)**, 931-934; DOI:10.1021/je00020a044
33. Benson G C, Kiyohara O K, *J Chem Thermodyn.*, 1979, **11(11)**, 1061-1064; DOI:10.1016/0021-9614(79)90136-8
34. Acree W E, *J Chem Eng Data*, 1983, **28(2)**, 215–216; DOI:10.1021/je00032a027
35. Kiyohara O, Benson G C, *J Chem Thermody.*, 1979, **11(9)**, 861-873; DOI:10.1016/0021-9614(79)90067-3
36. Rai R D, Shukla R, Shukla A K and Pandey J D, *J Chem Thermodyn.*, 1989, **21**, 125-129; DOI:10.1016/0021-9614(89)90122-5