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# Thermophysical properties of N-isopropyl-2-propanamine+alkanol (C1-C3) mixtures as absorbents for carbon dioxide capture

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**Abstract**−As N-isopropyl-2-propanamine+alkanol ($C_1$-$C_3$) systems are potential absorbents for $CO_2$ capture, we measured density ($\rho$), viscosity ($\eta$) and the ultrasonic speed data (u) for N-isopropyl-2-propanamine (DIPA) with alkanol ($C_1$-$C_3$) at T=(298.15 and 308.15) K and 0.1 MPa. The experimental density ($\rho$), viscosity ($\eta$) and ultrasonic speed (u) data were used to derive excess molar volume ($V_m^E$), apparent, partial, and excess partial molar volume, deviation in viscosity and deviation in ultrasonic speed, excess isentropic compressibility ($\kappa_s^E$). We predicted the $V_m^E$ values using the Prigogine-Flory-Patterson theory (PFP) and by Nakata and Sakurai model. An *Ab initio* approach was proposed for the excess isentropic compressibility ($\kappa_s^E$) and $\Delta\eta$ data which not only reproduces the experimental data but also gives important parameters that describe the extent of depolymerization on mixing and strength of intermolecular interactions.

Keywords: $CO_2$ Capture, Viscosity, Excess Isentropic Compressibility, Excess Molar Volume, N-isopropyl-2-propanamine, Alkanol

## INTRODUCTION

Increased discharge of industrial pollutants results in greenhouse gas emissions into the atmosphere and causes significant environmental changes [1,2]. This issue garners researchers interest in capturing $CO_2$ more efficiently [3,4]. The current policies and mitigation strategies proposed by the International Energy Agency (IEA) suggest $CO_2$ emissions reach ~45 gigatonnes by 2035, consequently leading to an increase of 5.6 °C in the global temperature [5,6]. These situations will aggravate further, unless considerable efforts are made to stabilize the GHG concentration to 450 ppm $CO_2$ [7]. Solvent-based $CO_2$ removal is an extensively used technology for economically and sustainably mitigating carbon emission reduction targets [8]. So to capture $CO_2$, researchers are searching for novel solvent amines for such capturing process [7-14]. Many workers have studied the N-isopropyl-2-propanamine (DIPA) absorbent for $CO_2$ capture from flue gases [15-17]. Due to intermolecular H-bonding between the two components chosen under study, it enhances the solubility of amine on mixing with the alkanol [18,19]. As a result, DIPA+alkanol binary mixtures may be excellent absorbents for removing acid gases. Such systems thermophysical properties have significant importance in interpreting intermolecular interactions. Such factors encouraged us to measure the density ($\rho$), viscosity ($\eta$) and ultrasonic speed (u) for DIPA (1)+alkanol ($C_1$-$C_3$) (2) mixtures in the whole composition range and at T=298.15 and 308.15 K temperature and 0.1 MPa. The partial ($\overline{V}_i$), excess partial ($\overline{V}_i^E$) and apparent ($V_{\varphi i}$) molar volume were derived from ($V_m^E$) and provided an understanding of the intermolecular interactions. The Prigogine-Flory-Patterson theory (PFP) and Nakata and Sakurai model were used to analyze the $V_m^E$ data. Using ultrasonic speed (u) and viscosity ($\eta$) data the deviation in ultrasonic speed ($\Delta$u) as well as viscosity and excess isentropic compressibility ($\kappa_s^E$) were derived. Further to study interactions deeply, the Ab initio approach was applied to $\kappa_s^E$ and $\Delta\eta$.

## EXPERIMENTAL

### 1. Materials

Distillation processes were used to purify DIPA (1) and alkanol (2) from Sigma-Aldrich and Merck [20-24]. The chemical specification of chemicals, purification methods and purity analysis results with GC, i.e., gas chromatography remain listed in Table 1. We confirmed the sample purity by comparing the measured density ($\rho$) and viscosity ($\eta$) data to the literature at T=(298.15 and 308.15) K

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**Table 1. Details of chemical source, purification method, purity and analysis method**

| Chemical name | CAS number | Source | Initial mole fraction purity (%) | Purification method | Final mole fraction purity | Analysis method |
|---|---|---|---|---|---|---|
| DIPA | 108-18-9 | Sigma | ≥99.5 | Distillation | 0.996 | GC |
| Methanol | 67-56-1 | Merck | ≥99.80 | Distillation | 0.998 | GC |
| Ethanol | 64-17-5 | Merck | ≥99.80 | Distillation | 0.998 | GC |
| 1-Propanol | 71-23-8 | Sigma | ≥99.50 | Distillation | 0.996 | GC |
| 2-Propanol | 67-63-0 | Sigma | ≥99.50 | Distillation | 0.996 | GC |

**Table 2. Densities ($\rho$/g cm$^{-3}$), speed of sound (u/m s$^{-1}$) and viscosity ($\eta$/mPa s) of the pure compound at different temperature and at 0.1 MPa pressure**

| Compound | T/K | $\rho$/g cm$^{-3}$ |  | u/m s$^{-1}$ |  | $\eta$/mPa·s |  |
|---|---|---|---|---|---|---|---|
|  |  | This work | Literature | This work | Literature | This work | Literature |
| DIPA | 298.15 | 0.71474 | 0.7148 [25] | 1096.1 | 1096 [26] | 0.386 | 0.382 [27] |
|  | 308.15 | 0.70502 | 0.70518 [25] | 1046.1 | 1046 [26] | 0.352 | 0.347 [27] |
| Methanol | 298.15 | 0.78666 | 0.7866 [28] | 1102.1 | 1102.3 [29] | 0.577 | 0.5570 [30] |
|  | 308.15 | 0.77714 | 0.7771 [31] | 1069.5 | 1069.78 [29] | 0.489 | 0.474 [32] |
| Ethanol | 298.15 | 0.78463 | 0.78497 [33]<br>0.7851 [28] | 1142.1 | 1142.9 [29] | 1.066 | 1.0789 [30] |
|  | 308.15 | 0.77729 | 0.77794 [34] | 1107.3 | 1109.16 [29] | 0.896 | 0.907 [32] |
| 1-Propanol | 298.15 | 0.79871 | 0.7995 [35] | 1205.6 | 1205.4 [29] | 1.988 | 1.95 [36] |
|  | 308.15 | 0.79152 | 0.7915 [34] | 1173.9 | 1171.41 [29] | 1.591 | 1.537 [32] |
| 2-Propanol | 298.15 | 0.78130 | 0.78123 [37] | 1143.9 | 1144 [38] | 2.079 | 2.0763 [39] |
|  | 308.15 | 0.77248 | 0.77267 [37] | 1102.1 | 1102.3 [38] | 1.589 | 1.543 [32] |

Standard uncertainties $u_c$: $u_c$ (T)=0.01 K; $u_c$ (p)=0.04 MPa; $u_c$ ($\rho$)=5×10$^{-5}$ gcm$^{-3}$; $u_c$ (u)=0.5 ms$^{-1}$; $u_c$ ($\eta$)=0.003 mPa·s

as demonstrated in Table 2.

## 2. Apparatus and Procedure

We used a vibrating tube densimeter (Anton Paar DSA-5000 M model) integrated with a micro viscometer (LOVIS 2000 ME model) for measuring the ($\rho$), ($\eta$) and (u) of the pure component and their binaries at 298.15 K and 308.15 K respectively, with temperature controlled to approximately ±0.01 K.

Standard uncertainties in these measurements were $u_c$: $u_c$ (T)= 0.01 K; $u_c$ (p)=0.04 MPa; $u_c$ ($\rho$)=5×10$^{-5}$ g cm$^{-3}$; $u_c$ (u)=0.5 m s$^{-1}$; $u_c$ ($\eta$)=0.003 mPa·s.

## RESULTS AND DISCUSSION

The ($V_m^E$) were derived using the experimentally determined value of densities (mixture density $\rho$, pure component density $\rho_i$) and molar masses ($M_i$) using Eq. (1) as shown in Fig. 1 and Table 3 at T=298.15 K and 308.15 K

$$V_m^E = \frac{M_1x_1+M_2x_2}{\rho} - \frac{M_1x_1}{\rho_1} - \frac{M_2x_2}{\rho_2} \qquad (1)$$

The Redlich-Kister (RK) polynomial equation was used to fit the $V_m^E$ data:

$$X(V_m^E, \Delta u, \Delta\eta \text{ or } \kappa_s^E) = x_1(1-x_1)\left[\sum_{j=1}^{4} A^{(j)}(2x_1-1)^{(j-1)}\right] \qquad (2)$$

We calculated the adjustable parameters $A^{(j)}$ with their standard deviations $\sigma$(X) by using the least square method as shown below

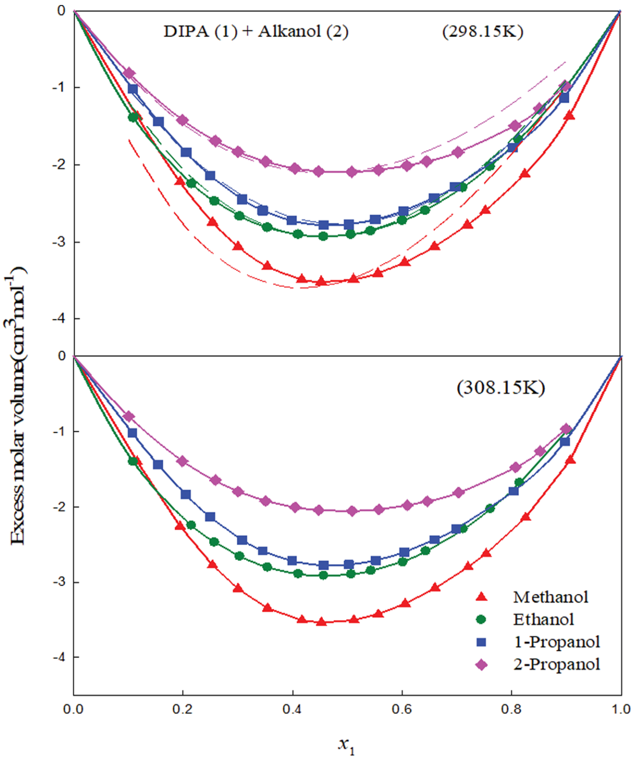

**Fig. 1.** Excess molar volume as a function of mole fraction of $x_1$, where as middle dash line at T=298.15 K curve represents the predicted excess molar volume through PFP.

**Table 3. Experimental density $\rho$ (g cm$^{-3}$), excess molar volume $V_m^E$ (cm$^3$mol$^{-1}$), ultrasonic speed u (ms$^{-1}$), deviation in ultrasonic speed $\Delta$u (m s$^{-1}$), viscosity ($\eta$/mPa s) and deviation in viscosity ($\Delta\eta$/mPa s) for DIPA (1)+alkanol (2) mixtures**

| $x_1$ | $\rho$ | $V_m^E$ | u | $\Delta$u | $\eta$ | $\Delta\eta$ | $\rho$ | $V_m^E$ | u | $\Delta$u | $\eta$ | $\Delta\eta$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | T=298.15 K | | | | | | T=308.15 K | | | | | |
| DIPA (1)+Methanol (2) | | | | | | | | | | | | |
| 0.1158 | 0.78471 | −1.373 | 1152.1 | 50.6 | 0.732 | 0.177 | 0.77500 | −1.400 | 1114.5 | 48.0 | 0.683 | 0.210 |
| 0.1940 | 0.78275 | −2.223 | 1174.6 | 73.6 | 0.813 | 0.273 | 0.77285 | −2.259 | 1133.9 | 69.2 | 0.712 | 0.249 |
| 0.2534 | 0.78007 | −2.748 | 1185.0 | 84.4 | 0.847 | 0.318 | 0.76989 | −2.775 | 1142.3 | 79.0 | 0.703 | 0.249 |
| 0.3001 | 0.77717 | −3.065 | 1189.3 | 89.0 | 0.855 | 0.335 | 0.76686 | −3.087 | 1145.2 | 83.0 | 0.686 | 0.238 |
| 0.3540 | 0.77309 | −3.320 | 1190.4 | 90.4 | 0.844 | 0.335 | 0.76278 | −3.345 | 1145.0 | 84.0 | 0.659 | 0.218 |
| 0.4168 | 0.76774 | −3.488 | 1187.3 | 87.7 | 0.809 | 0.311 | 0.75734 | −3.503 | 1140.8 | 81.3 | 0.624 | 0.192 |
| 0.4523 | 0.76446 | −3.517 | 1184.0 | 84.6 | 0.780 | 0.289 | 0.75411 | −3.536 | 1136.9 | 78.2 | 0.603 | 0.176 |
| 0.5118 | 0.75888 | −3.486 | 1176.4 | 77.3 | 0.722 | 0.243 | 0.74856 | −3.503 | 1128.7 | 71.4 | 0.570 | 0.151 |
| 0.5562 | 0.75474 | −3.409 | 1169.6 | 70.8 | 0.674 | 0.204 | 0.74448 | −3.429 | 1121.7 | 65.4 | 0.546 | 0.133 |
| 0.6053 | 0.75018 | −3.266 | 1161.7 | 63.2 | 0.622 | 0.160 | 0.73996 | −3.285 | 1113.6 | 58.4 | 0.520 | 0.114 |
| 0.6596 | 0.74532 | −3.062 | 1152.9 | 54.7 | 0.568 | 0.117 | 0.73514 | −3.077 | 1104.6 | 50.6 | 0.492 | 0.093 |
| 0.7201 | 0.74013 | −2.781 | 1143.4 | 45.6 | 0.517 | 0.077 | 0.73004 | −2.797 | 1095.0 | 42.4 | 0.462 | 0.071 |
| 0.7531 | 0.73736 | −2.598 | 1138.5 | 40.9 | 0.494 | 0.061 | 0.72737 | −2.624 | 1090.0 | 38.2 | 0.445 | 0.059 |
| 0.8251 | 0.73139 | −2.121 | 1128.4 | 31.2 | 0.458 | 0.039 | 0.72147 | −2.143 | 1079.5 | 29.4 | 0.410 | 0.034 |
| 0.9067 | 0.72429 | −1.365 | 1116.2 | 19.5 | 0.431 | 0.027 | 0.71447 | −1.384 | 1066.8 | 18.5 | 0.375 | 0.010 |
| DIPA (1)+Ethanol (2) | | | | | | | | | | | | |
| 0.1086 | 0.78488 | −1.390 | 1175.0 | 37.9 | 1.179 | 0.187 | 0.77676 | −1.404 | 1138.9 | 36.0 | 1.005 | 0.168 |
| 0.2152 | 0.77970 | −2.247 | 1186.4 | 54.2 | 1.185 | 0.265 | 0.77083 | −2.247 | 1146.6 | 50.5 | 0.942 | 0.163 |
| 0.2572 | 0.77683 | −2.473 | 1187.0 | 56.7 | 1.159 | 0.268 | 0.76777 | −2.472 | 1145.9 | 52.5 | 0.895 | 0.138 |
| 0.3033 | 0.77344 | −2.668 | 1185.9 | 57.7 | 1.115 | 0.255 | 0.76414 | −2.659 | 1143.5 | 53.1 | 0.836 | 0.105 |
| 0.3541 | 0.76942 | −2.814 | 1182.9 | 57.1 | 1.050 | 0.225 | 0.75998 | −2.805 | 1139.4 | 52.2 | 0.768 | 0.065 |
| 0.4103 | 0.76479 | −2.905 | 1178.2 | 54.9 | 0.964 | 0.177 | 0.75519 | −2.891 | 1133.6 | 49.9 | 0.696 | 0.023 |
| 0.4566 | 0.76094 | −2.933 | 1173.4 | 52.3 | 0.887 | 0.131 | 0.75122 | −2.914 | 1128.1 | 47.3 | 0.641 | −0.007 |
| 0.5069 | 0.75664 | −2.904 | 1167.6 | 48.8 | 0.801 | 0.080 | 0.74693 | −2.896 | 1121.6 | 44.1 | 0.587 | −0.033 |
| 0.5429 | 0.75359 | −2.859 | 1163.1 | 46.0 | 0.741 | 0.044 | 0.74382 | −2.848 | 1116.8 | 41.6 | 0.554 | −0.047 |
| 0.6012 | 0.74859 | −2.723 | 155.6 | 41.1 | 0.650 | −0.007 | 0.73896 | −2.739 | 1,108.8 | 37.2 | 0.508 | −0.061 |
| 0.6432 | 0.74505 | −2.593 | 1149.9 | 37.4 | 0.592 | −0.036 | 0.73526 | −2.590 | 1102.8 | 34.0 | 0.481 | −0.065 |
| 0.7116 | 0.73920 | −2.295 | 1140.5 | 31.1 | 0.517 | −0.065 | 0.72941 | −2.295 | 1092.9 | 28.4 | 0.446 | −0.063 |
| 0.7612 | 0.73498 | −2.022 | 1133.5 | 26.4 | 0.478 | −0.070 | 0.72522 | −2.028 | 1085.5 | 24.2 | 0.426 | −0.056 |
| 0.8143 | 0.73046 | −1.674 | 1125.7 | 21.1 | 0.450 | −0.063 | 0.72071 | −1.682 | 1077.3 | 19.4 | 0.409 | −0.044 |
| 0.9018 | 0.72307 | −0.980 | 1112.3 | 11.7 | 0.424 | −0.029 | 0.71332 | −0.984 | 1063.2 | 10.8 | 0.382 | −0.023 |
| DIPA (1)+1-Propanol (2) | | | | | | | | | | | | |
| 0.1073 | 0.79297 | −1.013 | 1214.0 | 20.6 | 1.743 | −0.073 | 0.78515 | −1.022 | 1180.1 | 18.9 | 1.430 | −0.028 |
| 0.1544 | 0.79055 | −1.438 | 1216.2 | 27.9 | 1.617 | −0.124 | 0.78242 | −1.445 | 1180.7 | 25.5 | 1.354 | −0.046 |
| 0.2051 | 0.78757 | −1.839 | 1217.0 | 34.2 | 1.480 | −0.179 | 0.77914 | −1.842 | 1179.7 | 31.1 | 1.266 | −0.071 |
| 0.2487 | 0.78475 | −2.136 | 1216.2 | 38.2 | 1.366 | −0.224 | 0.77606 | −2.131 | 1177.5 | 34.5 | 1.187 | −0.096 |
| 0.3075 | 0.78046 | −2.447 | 1213.0 | 41.4 | 1.220 | −0.275 | 0.77154 | −2.444 | 1172.7 | 37.3 | 1.078 | −0.132 |
| 0.3452 | 0.77744 | −2.593 | 1209.7 | 42.2 | 1.139 | −0.296 | 0.76833 | −2.583 | 1168.5 | 37.9 | 1.008 | −0.155 |
| 0.3988 | 0.77280 | −2.725 | 1203.6 | 41.9 | 1.031 | −0.318 | 0.76357 | −2.718 | 1161.2 | 37.6 | 0.910 | −0.187 |
| 0.4565 | 0.76753 | −2.783 | 1195.4 | 40.0 | 0.929 | −0.327 | 0.75817 | −2.777 | 1152.0 | 35.8 | 0.810 | −0.215 |
| 0.5026 | 0.76317 | −2.773 | 1188.0 | 37.7 | 0.859 | −0.324 | 0.75371 | −2.767 | 1143.9 | 33.6 | 0.737 | −0.232 |
| 0.5516 | 0.75842 | −2.706 | 1179.6 | 34.6 | 0.790 | −0.314 | 0.74898 | −2.713 | 1134.8 | 30.9 | 0.667 | −0.241 |
| 0.6037 | 0.75344 | −2.598 | 1170.2 | 30.9 | 0.728 | −0.293 | 0.74390 | −2.603 | 1124.9 | 27.7 | 0.604 | −0.239 |
| 0.6591 | 0.74812 | −2.429 | 1160.2 | 26.9 | 0.663 | −0.269 | 0.73854 | −2.436 | 1114.3 | 24.2 | 0.550 | −0.224 |
| 0.6981 | 0.74441 | −2.282 | 1153.2 | 24.2 | 0.622 | −0.248 | 0.73483 | −2.295 | 1106.9 | 21.8 | 0.520 | −0.206 |
| 0.8034 | 0.73456 | −1.776 | 1134.9 | 17.3 | 0.517 | −0.184 | 0.72492 | −1.793 | 1087.4 | 15.9 | 0.467 | −0.129 |
| 0.8969 | 0.72564 | −1.127 | 1118.3 | 10.9 | 0.436 | −0.115 | 0.71595 | −1.139 | 1069.7 | 10.3 | 0.432 | −0.048 |

**Table 3. Continued**

| $x_1$ | $\rho$ | $V_m^E$ | u | $\Delta u$ | $\eta$ | $\Delta\eta$ | $\rho$ | $V_m^E$ | u | $\Delta u$ | $\eta$ | $\Delta\eta$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | T=298.15 K | | | | | | T=308.15 K | | | | | |
| | | | | | | DIPA (1)+2-Propanol (2) | | | | | | |
| 0.1004 | 0.77752 | −0.811 | 1156.7 | 17.5 | 1.751 | −0.158 | 0.76825 | −0.801 | 1111.7 | 15.2 | 1.370 | −0.095 |
| 0.1983 | 0.77270 | −1.419 | 1161.5 | 27.0 | 1.407 | −0.336 | 0.76307 | −1.396 | 1114.3 | 23.3 | 1.128 | −0.215 |
| 0.2588 | 0.76913 | −1.689 | 1161.5 | 29.9 | 1.222 | −0.418 | 0.75924 | −1.647 | 1113.4 | 25.8 | 0.988 | −0.281 |
| 0.3002 | 0.76651 | −1.831 | 1160.6 | 31.0 | 1.110 | −0.461 | 0.75663 | −1.799 | 1111.9 | 26.6 | 0.902 | −0.315 |
| 0.3505 | 0.76314 | −1.958 | 1158.5 | 31.3 | 0.992 | −0.494 | 0.75320 | −1.925 | 1109.4 | 26.9 | 0.811 | −0.345 |
| 0.4044 | 0.75940 | −2.045 | 1155.5 | 30.9 | 0.884 | −0.510 | 0.74937 | −2.007 | 1106.1 | 26.6 | 0.729 | −0.360 |
| 0.4474 | 0.75637 | −2.085 | 1152.6 | 30.1 | 0.819 | −0.503 | 0.74632 | −2.046 | 1103.0 | 25.9 | 0.674 | −0.362 |
| 0.5084 | 0.75198 | −2.091 | 1148.1 | 28.4 | 0.737 | −0.481 | 0.74192 | −2.055 | 1098.2 | 24.6 | 0.610 | −0.350 |
| 0.5574 | 0.74850 | −2.067 | 1144.1 | 26.8 | 0.687 | −0.448 | 0.73846 | −2.037 | 1094.2 | 23.3 | 0.570 | −0.330 |
| 0.6092 | 0.74483 | −2.012 | 1139.7 | 24.9 | 0.640 | −0.407 | 0.73478 | −1.982 | 1089.8 | 21.8 | 0.534 | −0.302 |
| 0.6456 | 0.74226 | −1.954 | 1136.6 | 23.5 | 0.612 | −0.374 | 0.73223 | −1.928 | 1086.7 | 20.7 | 0.510 | −0.280 |
| 0.7029 | 0.73824 | −1.835 | 1131.5 | 21.1 | 0.565 | −0.324 | 0.72823 | −1.812 | 1081.6 | 18.9 | 0.477 | −0.243 |
| 0.8070 | 0.73083 | −1.491 | 1121.5 | 16.1 | 0.476 | −0.236 | 0.72090 | −1.477 | 1071.7 | 14.8 | 0.418 | −0.173 |
| 0.8520 | 0.72749 | −1.271 | 1116.7 | 13.5 | 0.438 | −0.198 | 0.71761 | −1.264 | 1066.9 | 12.5 | 0.393 | −0.142 |
| 0.8990 | 0.72379 | −0.974 | 1111.1 | 10.1 | 0.410 | −0.147 | 0.71394 | −0.967 | 1061.3 | 9.6 | 0.371 | −0.106 |

Standard uncertainties $u_c$: $u_c$ (T)=0.01 K; $u_c$ (p)=0.04 MPa; $u_c$ ($\rho$)=$5\times10^{-5}$ gcm$^{-3}$; $u_c$ (u)=0.5 ms$^{-1}$; $u_c$ ($\eta$)=0.003 mPa·s

and reported in Table 4.

$$\sigma(X)=\left(\frac{\sum(X_{expt1}-X_{calcd.})^2}{(m-n)}\right)^{1/2} \tag{3}$$

where m or n is the number of experimental points or adjustable parameters.

We observed that the ($V_m^E$) values for DIPA (1)+alkanol (2) were negative across the whole composition range. The ($V_m^E$) sum of two opposite factors was positive due to the breaking of like interactions on mixing of pure components and negative due to the establishment of unlike interactions. At equimolar composition, it follows the pattern of DIPA (1) with alkanol (2) as 2-propanol>1-propanol>ethanol>methanol. The negative impact is owing to ($V_m^E$) strong interactions (H-bonding) between unlike molecules and changes in free volume. In such interactions amine behaves as an electron pair donor (Lewis base). In contrast, alcohol is an electron pair acceptor (Lewis acid), which results in the formation of electron donor-acceptor (Lewis acid-Lewis base) interactions [40]. Strong interactions between the two components of DIPA and alkanol result in negative values ($V_m^E$) leading to volume contraction on mixing DIPA with alkanol. It shows maximum interaction in the case of methanol due to its small size, which offers less steric hindrance and interacts effectively with DIPA. DIPA is a secondary amine and weakly self-associated [41]. Thus, DIPA can donate electrons easily and interacts strongly with the alkanol group even though alkanol is strongly associated. The increases in carbon chain length decrease the degree of self-association and polarity; hence, unlike interactions decrease. In the case of propanol -secondary alcohol interacts weakly owing to repulsions affected by the branched propyl group compared to the linear chain. It was observed that temperature has no significant effect on excess molar volume.

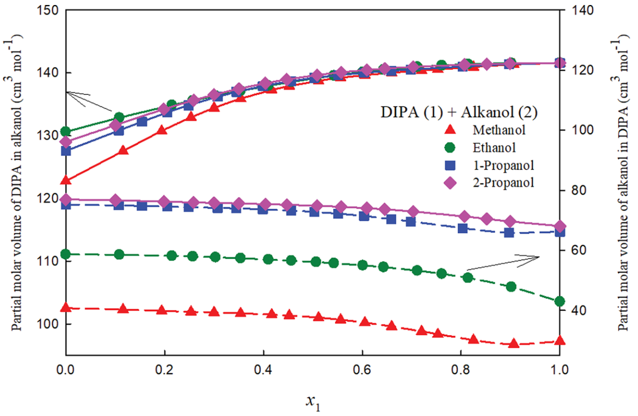

**Fig. 2. Partial molar volume of DIPA and alkanol in a binary mixture as a function of mole fraction $x_1$ at T=298.15 K.**

Using $V_m^E$ data we have derived the partial ($\bar{V}_i$), excess partial ($\bar{V}_i^E$) and apparent molar volume ($V_{\varphi i}$) for DIPA (1)+alkanol (2) mixtures, as such properties provide us data about the solute - solute and the solute - solvent molecular interactions and shown in supplementary Table S1 and Fig. 2 to Fig. 4 [42,43].

The following equations were used to calculate the excess partial molar volumes, $\bar{V}_1^E$ and $\bar{V}_2^E$ data:

$$\bar{V}_1^E=(\bar{V}_1-\bar{V}_1^o) \tag{4}$$

$$\bar{V}_2^E=(\bar{V}_2-\bar{V}_2^o) \tag{5}$$

$$\bar{V}_1=\bar{V}_m^E+\bar{V}_1^o+(1-x_1)(\partial\bar{V}_m^E/\partial x_1)_{p,\,T} \tag{6}$$

$$\bar{V}_2=\bar{V}_m^E+\bar{V}_2^o-x_1(\partial\bar{V}_m^E/\partial x_1)_{p,\,T} \tag{7}$$

Figs. 2 and 3 show the partial molar volume ($\bar{V}_1$) and excess partial molar volume ($\bar{V}_1^E$) as a function of mole fractions. Such prop-

**Table 4. Adjustable parameters for excess molar volume ($V_m^E$/cm$^3$mol$^{-1}$), deviation in ultrasonic speed Δu/m s$^{-1}$, deviation in viscosity Δ$\eta$/mPa s and excess isentropic compressibility $\kappa_s^E$/TPa$^{-1}$ along with standard deviation ($\sigma$)**

| Property | T/K | A$^{(1)}$ | A$^{(2)}$ | A$^{(3)}$ | A$^{(4)}$ | $\sigma$ |
|---|---|---|---|---|---|---|
| | | | DIPA (1)+Methanol (2) | | | |
| $V_m^E$/cm$^3$ mol$^{-1}$ | 298.15 | −14.007 | 2.036 | −0.893 | −5.950 | 0.002 |
| | 308.15 | −14.072 | 2.062 | −1.177 | −5.891 | 0.003 |
| Δu/m s$^{-1}$ | 298.15 | 315.6 | −264.4 | 74.0 | 150.0 | 0.002 |
| | 308.15 | 291.5 | −247.4 | 83.3 | 136.6 | 0.002 |
| Δ$\eta$/mPa s | 298.15 | 1.010 | −1.663 | 0.004 | 1.235 | 0.001 |
| | 308.15 | 0.624 | −0.844 | 0.811 | −0.657 | 0.001 |
| $\kappa_s^E$/TPa$^{-1}$ | 298.15 | −76.3 | 52.6 | −24.4 | −22.0 | 0.053 |
| | | | DIPA (1)+Ethanol (2) | | | |
| $V_m^E$/cm$^3$ mol$^{-1}$ | 298.15 | −11.648 | 1.699 | −1.711 | 0.680 | 0.002 |
| | 308.15 | −11.608 | 1.565 | −1.919 | 1.012 | 0.005 |
| Δu/m s$^{-1}$ | 298.15 | 197.1 | −146.9 | 106.1 | −29.6 | 0.002 |
| | 308.15 | 178.2 | −134.3 | 113.0 | −40.6 | 0.002 |
| Δ$\eta$/mPa s | 298.15 | 0.347 | −2.049 | 0.724 | 0.971 | 0.002 |
| | 308.15 | −0.120 | −0.929 | 1.393 | −0.568 | 0.002 |
| $\kappa_s^E$/TPa$^{-1}$ | 298.15 | −57.4 | 30.4 | −24.1 | 9.6 | 0.03 |
| | | | DIPA (1)+1-Propanol (2) | | | |
| $V_m^E$/cm$^3$ mol$^{-1}$ | 298.15 | −11.094 | 1.445 | −0.425 | −3.935 | 0.002 |
| | 308.15 | −11.081 | 1.300 | −0.626 | −3.724 | 0.002 |
| Δu/m s$^{-1}$ | 298.15 | 151.2 | −115.3 | 23.9 | 86.8 | 0.002 |
| | 308.15 | 135.1 | −103.7 | 30.0 | 78.7 | 0.002 |
| Δ$\eta$/mPa s | 298.15 | −1.300 | 0.266 | 0.483 | −0.919 | 0.001 |
| | 308.15 | −0.923 | −0.570 | 0.830 | 0.669 | 0.002 |
| $\kappa_s^E$/TPa$^{-1}$ | 298.15 | −53.5 | 20.9 | −6.1 | −16.3 | 0.02 |
| | | | DIPA (1)+2-Propanol (2) | | | |
| $V_m^E$/cm$^3$ mol$^{-1}$ | 298.15 | −8.373 | 0.272 | −2.327 | −2.138 | 0.001 |
| | 308.15 | −8.228 | 0.176 | −2.396 | −2.047 | 0.004 |
| Δu/m s$^{-1}$ | 298.15 | 114.7 | −59.8 | 59.9 | 13.1 | 0.001 |
| | 308.15 | 99.2 | −47.9 | 58.7 | 14.1 | 0.002 |
| Δ$\eta$/mPa s | 298.15 | −1.939 | 1.039 | 0.364 | −1.518 | 0.001 |
| | 308.15 | −1.408 | 0.582 | 0.472 | −1.029 | 0.001 |
| $\kappa_s^E$/TPa$^{-1}$ | 298.15 | −44.6 | 13.9 | −14.6 | −4.1 | 0.01 |

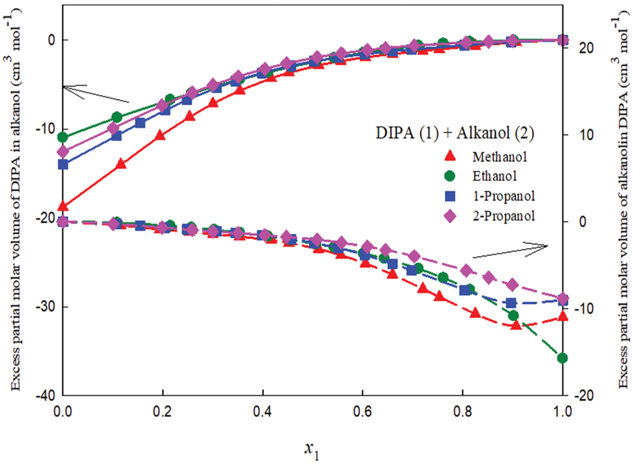

**Fig. 3. Excess Partial molar volume of DIPA and alkanol in a binary mixture as a function of mole fraction $x_1$ at T=298.15 K.**

erties depend upon the component size, shape, interactions and structural effect. But our interest lies in measuring partial molar volume ($\overline{V}_i$) value at infinite dilution where solute-solute interactions totally vanish because at that point it only gives the value corresponding to solute-solvent interactions independent of its entire composition.

$$\overline{V}_1^\infty = \overline{V}_1^o + \sum_{j=0}^{j=n} A_j \tag{8}$$

$$\overline{V}_2^\infty = \overline{V}_2^o + \sum_{j=0}^{j=n} A_j(-1)^j \tag{9}$$

where $\overline{V}_1^\infty$, $\overline{V}_2^\infty$ represents the partial molar volume of DIPA and partial molar volume of alkanol at infinite dilution demonstrated in Table 5. A contraction in molar volumes of pure alkanols ($V_2$) at mentioned temperature has been shown at infinite dilution. In sighting the data it is concluded that $V_2$ is considered as the sum

**Table 5. Molar volume ($V_i$/cm$^3$ mol$^{-1}$), partial molar volume ($\overline{V}_i^{\infty}$/cm$^3$ mol$^{-1}$) and excess partial molar volume ($\overline{V}_i^{E\infty}$/cm$^3$ mol$^{-1}$) at infinite dilution of binary liquid mixtures**

| Binary system | T/K | $V_1$ | $V_2$ | $\overline{V}_1^{\infty}$ | $\overline{V}_2^{\infty}$ | $\overline{V}_1^{E\infty}$ | $\overline{V}_2^{E\infty}$ |
|---|---|---|---|---|---|---|---|
| DIPA (1)+Methanol (2) | 298.15 | 141.576 | 40.729 | 122.761 | 29.743 | −18.815 | −10.986 |
| | 308.15 | 143.528 | 41.228 | 124.450 | 29.807 | −19.078 | −11.421 |
| DIPA (1)+Ethanol (2) | 298.15 | 141.576 | 58.626 | 130.596 | 42.888 | −10.980 | −15.737 |
| | 308.15 | 143.528 | 59.180 | 132.577 | 43.076 | -10.950 | −16.104 |
| DIPA (1)+1-Propanol (2) | 298.15 | 141.576 | 75.233 | 127.567 | 66.203 | −14.009 | −9.030 |
| | 308.15 | 143.528 | 75.917 | 129.397 | 66.635 | −14.131 | −9.282 |
| DIPA (1)+2-Propanol (2) | 298.15 | 141.576 | 76.909 | 129.010 | 68.075 | −12.566 | −8.834 |
| | 308.15 | 143.528 | 77.788 | 131.033 | 69.036 | −12.494 | −8.753 |

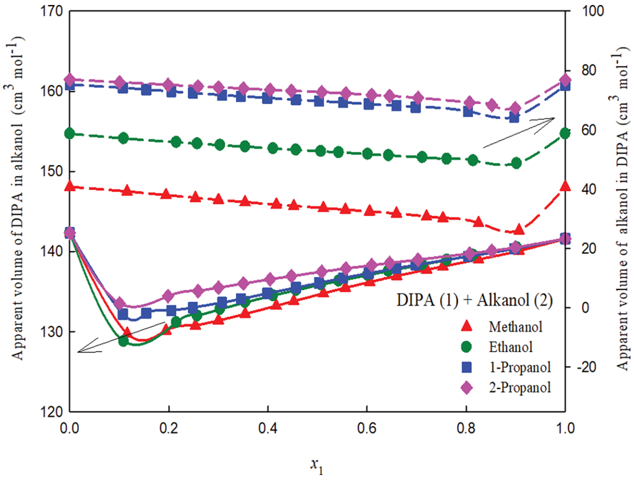

**Fig. 4. Apparent molar volume of DIPA and alkanol in a binary mixture as a function of mole fraction $x_1$ at T=298.15 K.**

of the empty volume and the actual molar volumes that appears due to H-bonding between their molecules [44]. The $\overline{V}_i^{\infty E}$ values for the DIPA (1)+alkanol (2) binary mixtures are negative at the mentioned temperature, which is shown in Table 5, so it justifies that there is a contraction in volume due to interactions that develops between the two components on mixing [31].

$\overline{V}_1^{\infty}$ and $\overline{V}_2^{\infty}$ were analyzed using the RK equation and its derivatives, neither of which provides us the best indication for measuring solute-solvent interactions. So as an alternative to utilizing the RK equation, we have an alternative method to measure it precisely and appropriately, by using the $V_{\phi i}$ to calculate the $\overline{V}_i^{\infty}$; the results acquired in the case of this approach were better and have been presented in Table S1, Fig. 4; the apparent molar volume ($V_{\phi 1}$) of DIPA in alkanol and alkanol in DIPA ($V_{\phi 2}$) are expressed as

$$V_{\phi 1}=(V_m-x_2V_2^o)/x_1 \tag{10}$$

$$V_{\phi 2}=(V_m-x_1V_1^o)/x_2 \tag{11}$$

Using Eqs. (1), (10) and (11), we get

$$V_{\phi 1}=V_1^o+(V_m^E/x_1) \tag{12}$$

$$V_{\phi 2}=V_2^o+(V_m^E/x_2) \tag{13}$$

Based on the method described above, the $\overline{V}_i$ values at infinite dilution were compared, and through the apparent molar volume $V_{\phi i}$, we found that the results obtained in the case of the latter approach are accurate. So, to measure the interactions at infinite dilution we had to use the $V_{\phi i}$ approach. Then, finally the resulting excess molar volume was further analyzed based on PFP theory.

## 1. PFP Theory [45-48]

In accordance with PFP theory, $V_m^E$ values depend upon the contributions of three terms:

1) interactions between dissimilar molecules (Inter), 2) free volume (fv) change and 3) internal pressure ($P^*$) and reduced volume change.

The PFP predicted $V_m^E$ values are expressed as the equation shown below:

$$V_m^E=V_{Inter}^E+V_{fv}^E+V_{P^*}^E \tag{14}$$

$$\frac{V_m^E}{x_1V_1^*+x_2V_2^*}=\frac{(\tilde{V}^{1/3}-1)\tilde{V}^{2/3}\psi_1\theta_2(\chi_{12}^*/P_1^*)}{((4/3)\tilde{V}^{-1/3}-1)} -\frac{(\tilde{V}_1-\tilde{V}_2)((14/9)\tilde{V}^{-1/3}-1)\psi_1\psi_2}{((4/3)\tilde{V}^{-1/3}-1)\tilde{V}}+\frac{(\tilde{V}_1-\tilde{V}_2)(P_1^*-P_2^*)\psi_1\psi_2}{P_2^*\psi_1+P_1^*\psi_2} \tag{15}$$

A comparison of the experimental value and the PFP theory predicts a good agreement, as shown in Table S2 and Fig. 1 for DIPA (1)+alkanol (2) mixtures except for methanol. This may be due to the difference in $V^*$ and $P^*$ values of binary constituents (Table S3). At equimolar composition ($x_1$=0.5), the values of three contributions to $V_m^E$ are given in Table S4.

## 2. Nakata and Sakurai Model [49]

According to Nakata and Sakurai model the $V_m^E$ and $n_D$ are correlated using Eq. (16).

$$V_m^E=-n_D[f'(n_{D1})/f(n_{D1})][\sum(V_ix_i)][\sum(n_{Di}\varphi_i)] \tag{16}$$

Using $n_D$ data for pure components and their binaries [50], $V_m^E$ values were predicted (details given in Supplementary Material) based on L-L, G-D, Eyk, H, Nw and A-B mixing rules. The results obtained from these mixing rules were reported in terms of $\sigma(V_m^E)$ (Table 6 and Fig. 6). Out of all mixing rules the best predictability was found in the case of Newton (Nw) mixing rule (minimum standard deviation), although the comparison was not very impressive (Fig. 5).

## 3. Viscosity

The $\Delta\eta$ data were obtained from Eq. (17), (Table 3 and Fig. 7) and fitted value is based on the RK Eq. (2). The $A^{(j)}$ parameters

**Table 6. Standard deviations of excess molar volume values, at 298.15 K, predicted from refractive index values using Nakata and Sakurai Model based on various mixing rules**

| Binary system | AB | GD | H | N | LL | Eyk |
|---|---|---|---|---|---|---|
| DIPA (1)+Methanol (2) | 2.161 | 0.813 | 1.331 | 0.538 | 1.018 | 1.371 |
| DIPA (1)+Ethanol (2) | 1.866 | 0.820 | 1.220 | 0.607 | 0.978 | 1.251 |
| DIPA (1)+1-Propanol (2) | 1.639 | 0.483 | 0.910 | 0.321 | 0.645 | 0.945 |
| DIPA (1)+2-Propanol (2) | 1.336 | 0.583 | 0.868 | 0.437 | 0.695 | 0.890 |

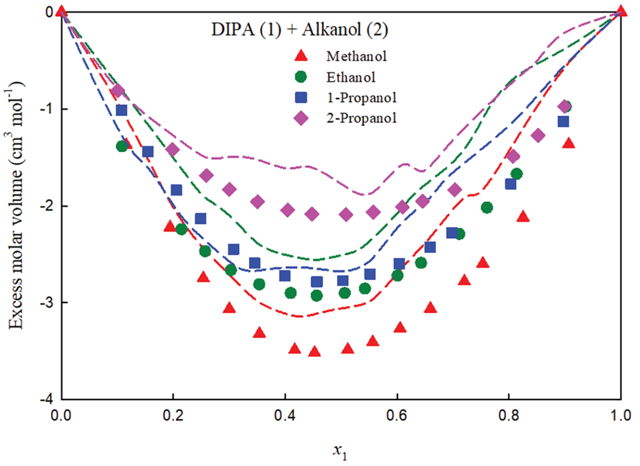

**Fig. 5. Excess molar volume a function of mole fraction $x_1$ where the symbol represents the experimental value and the dashed line represents the predicted value using the Nakata and Sakurai model based on Newton mixing rule at T=298.15 K.**

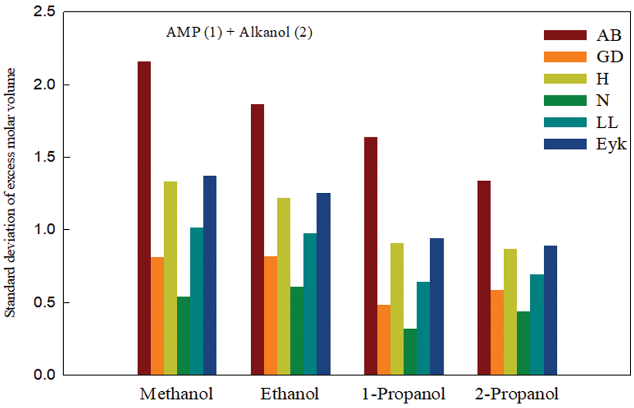

**Fig. 6. Standard deviations of excess molar volume predicted using the Nakata and Sakurai model based on various mixing rules at T=298.15 K.**

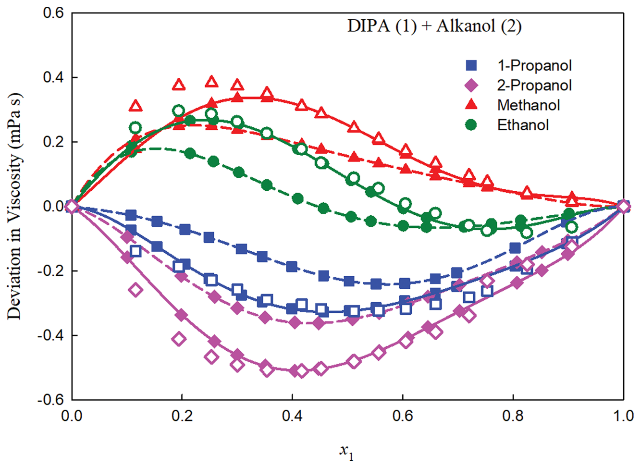

**Fig. 7. Deviation in viscosity as a function of mole fraction of DIPA ($x_1$) at T=298.15 K (solid line) and 308.15 K (dash line) where symbols represent experimental values and hollow symbol represents the value predicted by Ab initio approach.**

and $\sigma(\Delta\eta)$ are described in Table 4.

$$\Delta\eta = \eta_{mix} - \sum_i x_i \eta_i \tag{17}$$

Here $\eta_{mix}$ and $\eta_i$ signifies the $\eta$ data of binaries and pure components.

We observed that the $\Delta\eta$ values are positive for DIPA+methanol and negative for DIPA+propanol, whereas as the concentration of DIPA increases, the sign of $\Delta\eta$ changes for from positive to negative for ethanol mixtures. At equimolar concentration, the trend is as: 2-propanol<1-propanol<ethanol<methanol. In contrast to ethanol, the methanol $\Delta\eta$ values were more positive due to the relatively stronger unlike interactions. However, in the case of propanol, it was found that the value $\Delta\eta$ for 1-propanol was significantly greater than that for 2-propanol due to steric hindrance associated with branching in the propyl group. For methanol and ethanol mixtures, the $\Delta\eta$ values decrease with a rise in temperature, although it increases for propanol mixtures.

## 4. Ultrasonic Speed

The $\Delta u$ were obtained from Eq. (18), (Table 3 and Fig. 8) and fitted to RK Eq. (2). The $A^{(j)}$ parameters and $\sigma(\Delta u)$ are mentioned in Table 4.

$$\Delta u = u - \sum_{i=1}^{2} x_i u_i \tag{18}$$

where u and $u_i$ indicate the ultrasonic speed of pure component and mixture, respectively.

The deviation in ultrasonic speed data is positive for DIPA (1)+alkanol (2) across the whole composition range and it follows the order DIPA (1) with alkanol (2) as 2-propanol<1-propanol<ethanol<methanol. The ultrasonic speed values depend upon the medium for the sound to propagate; it is faster in the case of a denser medium. When DIPA is mixed with alkanol as discussed above, it results in interactions caused due to formation of H-bonding due to which the density of the medium increases. So, the trend for $\Delta u$ and that of $V_m^E$ follows the same trend as discussed in terms of interaction. As demonstrated in Fig. 8, the $\Delta u$ values decrease as the tempera-

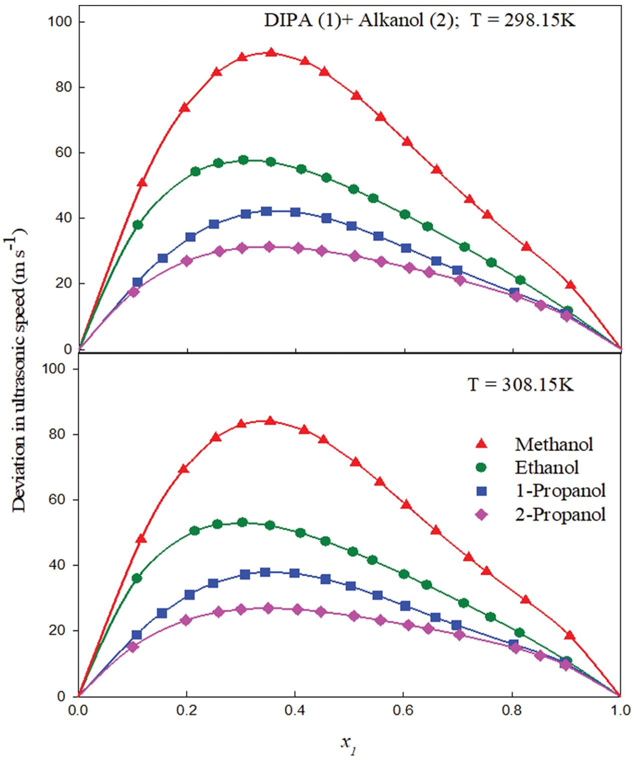

**Fig. 8. Deviation in ultrasonic speed as a function of mole fraction $x_1$.**

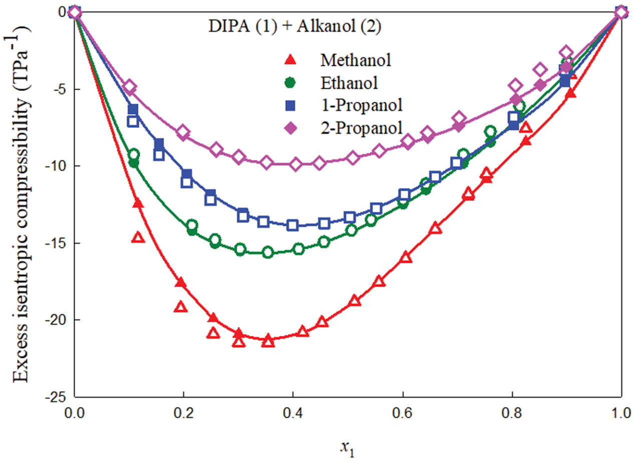

**Fig. 9. Excess isentropic compressibility as a function of mole fraction $x_1$. Hollow symbols represent value predicted through the Ab initio approach at T=298.15 K.**

ture rises.

The $\kappa_s^E$ values, were also calculated using the following relation:

$$\kappa_s^E = \kappa_s - \kappa_s^{id} \tag{19}$$

$$u^E = u - (\rho^{id}\kappa_s^{id})^{-\frac{1}{2}} \tag{20}$$

$$\kappa_s = (u^2\rho)^{-1} \tag{21}$$

The $\kappa_s^E$ depends upon the interactional strength between the two components. $\kappa_s^E$ values are negative across the entire compositional range as demonstrated in Table S5 and Fig. 9 and it follows the order of DIPA (1) with alkanol (2) as methanol<ethanol<1-propanol<2-propanol. The value of compressibility is mutually dependent upon two available factors: volume and intermolecular distance. The negative value of $K_s^E$ reflects the stronger interaction between the two components.

## 5. Ab Initio Approach

According to this approach, the values for the present DIPA $(1_n)$+alkanol $(2_n)$ mixtures were assumed to show changes caused due to the following processes.

(a) The formation of $(1_n)$---$(2_n)$ interactions between binary components with the interactional parameter $\chi_{12}^{\dagger}$ per mole:

$$\Delta X_a = x_1\chi_{12}^{\dagger}S_2 \tag{22}$$

$$S_2 = \frac{x_2V_2}{\sum x_1V_i} \tag{23}$$

Here $S_2$ is referred to as the surface fraction of alkanol in (1)---(2) interaction.

(b) These $(1_n)$---$(2_n)$ interactions result in rupturing/depolymerization of (i) intermolecular association (H-bonding) in pure DIPA and alkanol molecules to yield their monomers with interactional parameter as $\chi_{11}$ and $\chi_{22}$ per mole:

$$\Delta X_{b(i)} = x_1\chi_{11}S_2' \tag{24}$$

$$\Delta X_{b(ii)} = x_1\chi_{22}S_2' \tag{25}$$

$$S_2' \propto x_1S_2 = \frac{Kx_1x_2V_2}{\sum x_iV_i} \tag{26}$$

Here $S_2'$ is stated as the surface fraction of alkanol that causes the changes in DIPA [51,52].

and (c) The monomers would then interact with one another to form (1)---(2) interactions with interactional energy parameters as $\chi_{12}$ per mole.

$$\Delta X_c = \chi_{12}S_2'x_2 \tag{27}$$

Therefore, the total difference in ΔX owing to all three processes (a), (b) and (c) would be given as

$$\Delta X = \left[\frac{x_1x_2V_2}{\sum x_1V}\right][\chi_{12}^{*} + Kx_1\chi_{11} + Kx_1\chi_{22} + Kx_2\chi_{12}] \tag{28}$$

It would be reasonable to assume that for the present mixtures: $\chi_{12}^{\dagger} = K\chi_{12} = \chi_{12}^{*}$ and $K\chi_{11} = K\chi_{22} = \chi^{*}$ so the Eq. (28) reduces to

$$\Delta X = \left[\frac{x_1x_2V_2}{\sum x_1V}\right][\chi_{12}^{*}(1+x_2) + x_1\chi^{*}] \tag{29}$$

The experimental values at two compositions ($x_1 \approx 0.4$ and 0.5) were used to compute parameter $\chi_{12}^{*}$ and $\chi^{*}$ from Eq. (29) (Table 7). Using the $\chi_{12}^{*}$ and $\chi^{*}$, we calculated the $\kappa_s^E$ and $\Delta\eta$ values at other mole fractions as indicated in Figs. 7 and 9 and its standard deviations are reported in Table 7. As $\chi^{*}$ is a measure of the extent of depolymerization of DIPA or alkanol on mixing, the magnitude of $\chi^{*}$ clearly indicates (Table 7) that depolymerization is maximum in the case of methanol and in minimum in 2-propanol. The further magnitude of $\chi_{12}^{*}$ which is a measure of unlike interactions

**Table 7. Interactional parameters for deviation in viscosity ($\Delta\eta$) and excess isentropic compressibility ($\kappa_s^E$) at T=298.15 K based on Ab initio approach along with its standard deviation**

| Binary system | $\Delta\eta$ | | | $\kappa_s^E$ | | |
|---|---|---|---|---|---|---|
| | $\chi_{12}^*$ | $\chi^*$ | $\sigma(\Delta\eta)$ | $\chi_{12}^*$ | $\chi^*$ | $\sigma(\Delta\eta)$ |
| DIPA (1)+Methanol (2) | 2.184 | −2.053 | 0.052 | −94.513 | −58.625 | 0.940 |
| DIPA (1)+Ethanol (2) | 1.761 | −4.005 | 0.023 | −57.155 | −24.038 | 0.422 |
| DIPA (1)+1-Propanol (2) | −0.753 | −1.477 | 0.031 | −41.162 | −30.686 | 0.443 |
| DIPA (1)+2-Propanol (2) | −1.594 | −0.726 | 0.040 | −29.404 | −20.103 | 0.501 |

between DIPA and alkanol, also shows that methanol and ethanol interact strongly with DIPA as compared to propanol and weakly with 2-propanol owing to steric hindrance offered by a branched propyl group. If this is true, the $V_m^E$ of these mixtures should also follow the above sequence as both $\eta$ and excess volume are the measure of the packing effect. This is indeed true in our case [53].

## CONCLUSION

We measured the density, viscosity, and ultrasonic speed of DIPA (1)+alkanol (2) mixtures at T=(298.15 and 308.15) K and 0.1 MPa. The $V_m^E$ values are negative, the $\Delta u$ are positive, whereas $\Delta\eta$ values are positive in methanol in case the ethanol sign changes from positive to negative at a higher mole fraction of DIPA and is negative in case of propanol. Due to stronger intermolecular interactions in DIPA+alkanol mixtures, the trend of $V_m^E$ is 2-propanol>1-propanol>ethanol>methanol, whereas in the case of $\Delta u$ and $\Delta\eta$ methanol>ethanol>1-propanol>2-propanol. Similarly, the trend observed, using the $V_m^E$ data, the volumetric properties such as partial ($\bar{V}_i$), excess partial ($\bar{V}_i^E$) and apparent molar volume ($V_{\varphi i}$) were calculated, which gives an idea of the intermolecular interaction between them. Further we interpreted the $V_m^E$ data based on Prigogine-Flory-Patterson theory (PFP) and Nakata and Sakurai model. It shows good predictability in the former case; later the error was found to be minimum in the case of the Newton mixing rule. Further to study the interactions we have proposed an ab initio approach and successfully predicted the values of $\kappa_s^E$ and $\Delta\eta$.

## ACKNOWLEDGEMENT

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## SUPPORTING INFORMATION

Additional information as noted in the text. This information is available via the Internet at http://www.springer.com/chemistry/journal/11814.

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# Supporting Information

# Thermophysical properties of N-isopropyl-2-propanamine+alkanol (C1-C3) mixtures as absorbents for carbon dioixde capture

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**Derived thermodynamic properties:** The excess molar volume, deviation in ultrasonic speed and deviation in viscosity for the present binary mixtures at T=(298.15 and 308.15) K and at pressure of 0.1 MPa were derived using the experimental densities, ultrasonic speed and the viscosities values of all pure compound and their binaries.

Using $V_m^E$ the partial molar volume, excess partial molar volume and the apparent molar volume were derived at T=(298.15 and 308.15) K as shown in Table S1. The $V_m^E$ values were also predicted using Prigogine-Flory-Patterson (PFP) theory which are shown in Table S2, and the parameters used in the PFP theory such as Isobaric expansivity ($10^3\ \alpha/\mathrm{K}^{-1}$), isothermal compressibility ($10^3\ \kappa_T/\mathrm{cm}^3\ \mathrm{J}^{-1}$), characteristic pressure ($P^*/\mathrm{J\ cm}^{-3}$), characteristic molar volume ($V^*/\mathrm{cm}^3\ \mathrm{mol}^{-1}$) and characteristic temperature ($T^*/\mathrm{K}$) shown in Table S3 and PFP interaction parameter ($\chi_{12}$) and its three contributions terms such as interactions between dissimilar molecules, free volume change and internal pressure and the reduced volume change.

at ($x_1$=0.5) at 298.15 K and at ambient pressure is shown in Table S4.

Further the $V_m^E$ data were also predicted using $n_D$ data for pure components as well as their binaries by employing Nakata and Sakurai Model.

**Nakata and Sakurai model [1]**

The $n_D$ of binary mixtures may be expressed as [2]

$$\frac{f(n_D)}{\rho}=\sum_{i=1}^{2} w_i \frac{f(n_{Di})}{\rho_i} \tag{1}$$

where $w_i$ is the mass fraction of *i* th component and f represents a function of the refractive index.

According to this model the relationship between the $V_m^E$ and $n_D$ data of the mixtures is described as

$$V_m^E=\sum_{i=1}^{2}\left[(f(n_{Di})-f(n_D))\left(\frac{x_iV_i}{f(n_D)}\right)\right] \tag{2}$$

$$V_m^E=-n_D[f'(n_{D1})/f(n_{D1})][\sum(V_ix_i)][\sum(n_{Di}\varphi_i)] \tag{3}$$

Where $\varphi_i$ represents the volume fractions ($\varphi_1$ and $\varphi_2$) and are expressed as

$$\varphi_1=\frac{x_1V_1}{\sum x_iV_i} \text{ and } \varphi_2=\frac{x_2V_2}{\sum x_iV_i} \tag{4}$$

The function of $\frac{f'(n)}{f(n)}$ is given as for various laws

Arago-Biot (A-B): $\frac{f'(n_D)}{f(n_D)}=\frac{1}{n_D}$

Gladstone-Dale (G-D): $\frac{f'(n_D)}{f(n_D)}=\frac{1}{n_D-1}$

Lorentz-Lorenz (L-L): $\frac{f'(n_D)}{f(n_D)}=\frac{6n_D}{(n_D^2-1)(n_D^2+2)}$

Heller (H): $\frac{f'(n_D)}{f(n_D)}=\frac{1}{n_D(n_D-1)}$

Newton (Nw): $\frac{f'(n_D)}{f(n_D)}=\frac{2n_D}{(n_D^2-1)}$

Eykman (Eyk): $\frac{f'(n_D)}{f(n_D)}=\frac{2.8n_D}{(n_D^2-1)(n_D^2+0.4)}$

The results obtained were analysed quantitatively in terms of standard deviation.

**Table S1.** Partial molar volume ($\overline{V}_i$/cm$^3$ mol$^{-1}$), excess partial molar volume ($\overline{V}_i^E$/cm$^3$ mol$^{-1}$) and apparent molar volume ($\overline{V}_{\varphi i}$/cm$^3$ mol$^{-1}$) for binary mixtures of DIPA (1)+alkanol (2)

| $x_1$ | $\overline{V}_1$ | $\overline{V}_2$ | $\overline{V}_1^E$ | $\overline{V}_2^E$ | $V_{\phi 1}$ | $V_{\phi 2}$ |
|---|---|---|---|---|---|---|
| DIPA (1)+Methanol (2); (T=298.15 K) | | | | | | |
| 0.1158 | 127.539 | 40.284 | −14.037 | −0.445 | 129.728 | 39.177 |
| 0.1940 | 130.736 | 39.836 | −10.840 | −0.893 | 130.112 | 37.969 |
| 0.2534 | 132.910 | 39.528 | −8.666 | −1.201 | 130.740 | 37.050 |
| 0.3001 | 134.407 | 39.300 | −7.169 | −1.428 | 131.369 | 36.352 |
| 0.3540 | 135.882 | 39.019 | −5.694 | −1.710 | 132.189 | 35.586 |
| 0.4168 | 137.262 | 38.597 | −4.314 | −2.132 | 133.211 | 34.751 |
| 0.4523 | 137.891 | 38.282 | −3.685 | −2.447 | 133.796 | 34.304 |
| 0.5118 | 138.730 | 37.576 | −2.846 | −3.152 | 134.760 | 33.585 |
| 0.5562 | 139.212 | 36.875 | −2.363 | −3.853 | 135.453 | 33.054 |
| 0.6053 | 139.635 | 35.915 | −1.941 | −4.814 | 136.178 | 32.453 |
| 0.6596 | 140.010 | 34.630 | −1.566 | −6.099 | 136.932 | 31.731 |
| 0.7201 | 140.363 | 32.989 | −1.213 | −7.740 | 137.716 | 30.797 |
| 0.7531 | 140.542 | 32.052 | −1.034 | −8.677 | 138.124 | 30.204 |
| 0.8251 | 140.926 | 30.113 | −0.650 | −10.616 | 139.005 | 28.603 |
| 0.9067 | 141.331 | 28.722 | −0.245 | −12.007 | 140.070 | 26.090 |
| DIPA (1)+Ethanol (2); (T=298.15 K) | | | | | | |
| 0.1086 | 132.850 | 58.501 | −8.726 | −0.125 | 128.779 | 57.067 |
| 0.2152 | 134.842 | 58.141 | −6.734 | −0.484 | 131.133 | 55.763 |
| 0.2572 | 135.572 | 57.939 | −6.004 | −0.687 | 131.961 | 55.296 |
| 0.3033 | 136.335 | 57.681 | −5.241 | −0.945 | 132.781 | 54.797 |
| 0.3541 | 137.128 | 57.353 | −4.448 | −1.273 | 133.629 | 54.269 |
| 0.4103 | 137.942 | 56.936 | −3.634 | −1.690 | 134.497 | 53.700 |
| 0.4566 | 138.558 | 56.547 | −3.018 | −2.079 | 135.153 | 53.229 |
| 0.5069 | 139.168 | 56.069 | −2.408 | −2.557 | 135.847 | 52.736 |
| 0.5429 | 139.565 | 55.686 | −2.011 | −2.940 | 136.309 | 52.370 |
| 0.6012 | 140.130 | 54.977 | −1.446 | −3.649 | 137.046 | 51.796 |
| 0.6432 | 140.478 | 54.381 | −1.098 | −4.245 | 137.544 | 51.357 |
| 0.7116 | 140.933 | 53.208 | −0.643 | −5.417 | 138.351 | 50.669 |
| 0.7612 | 141.180 | 52.156 | −0.396 | −6.470 | 138.920 | 50.161 |
| 0.8143 | 141.370 | 50.779 | −0.206 | −7.846 | 139.520 | 49.607 |
| 0.9018 | 141.537 | 47.778 | −0.039 | −10.847 | 140.489 | 48.647 |
| DIPA (1)+1-Propanol (2); (T=298.15 K) | | | | | | |
| 0.1073 | 130.801 | 74.960 | −10.775 | −0.274 | 132.143 | 74.099 |
| 0.1544 | 132.226 | 74.764 | −9.350 | −0.469 | 132.258 | 73.532 |
| 0.2051 | 133.682 | 74.551 | −7.894 | −0.683 | 132.612 | 72.920 |
| 0.2487 | 134.831 | 74.372 | −6.745 | −0.861 | 132.990 | 72.390 |
| 0.3075 | 136.198 | 74.127 | −5.378 | −1.106 | 133.618 | 71.699 |
| 0.3452 | 136.959 | 73.953 | −4.617 | −1.280 | 134.064 | 71.272 |
| 0.3988 | 137.881 | 73.658 | −3.695 | −1.575 | 134.744 | 70.701 |
| 0.4565 | 138.679 | 73.237 | −2.897 | −1.996 | 135.478 | 70.112 |
| 0.5026 | 139.190 | 72.792 | −2.386 | −2.441 | 136.059 | 69.657 |
| 0.5516 | 139.628 | 72.196 | −1.948 | −3.038 | 136.670 | 69.197 |
| 0.6037 | 140.000 | 71.409 | −1.576 | −3.825 | 137.273 | 68.678 |
| 0.6591 | 140.323 | 70.404 | −1.253 | −4.829 | 137.890 | 68.107 |
| 0.6981 | 140.520 | 69.614 | −1.056 | −5.619 | 138.307 | 67.676 |
| 0.8034 | 140.993 | 67.367 | −0.583 | −7.866 | 139.365 | 66.197 |
| 0.8969 | 141.363 | 65.871 | −0.213 | −9.362 | 140.319 | 64.300 |

**Table S1. Continued**

| $x_1$ | $\overline{V}_1$ | $\overline{V}_2$ | $\overline{V}_1^E$ | $\overline{V}_2^E$ | $V_{\phi1}$ | $V_{\phi2}$ |
|---|---|---|---|---|---|---|
| DIPA (1)+2-Propanol (2) (T=298.15 K) | | | | | | |
| 0.1004 | 131.665 | 76.664 | −9.911 | −0.245 | 133.504 | 76.008 |
| 0.1983 | 134.212 | 76.228 | −7.364 | −0.682 | 134.418 | 75.139 |
| 0.2588 | 135.633 | 75.961 | −5.942 | −0.949 | 135.050 | 74.631 |
| 0.3002 | 136.512 | 75.789 | −5.064 | −1.120 | 135.476 | 74.293 |
| 0.3505 | 137.466 | 75.588 | −4.110 | −1.321 | 135.990 | 73.895 |
| 0.4044 | 138.344 | 75.366 | −3.232 | −1.543 | 136.518 | 73.476 |
| 0.4474 | 138.940 | 75.170 | −2.636 | −1.740 | 136.915 | 73.137 |
| 0.5084 | 139.637 | 74.832 | −1.939 | −2.077 | 137.463 | 72.656 |
| 0.5574 | 140.082 | 74.488 | −1.494 | −2.421 | 137.868 | 72.241 |
| 0.6092 | 140.458 | 74.032 | −1.118 | −2.878 | 138.273 | 71.760 |
| 0.6456 | 140.672 | 73.647 | −0.904 | −3.263 | 138.549 | 71.396 |
| 0.7029 | 140.943 | 72.923 | −0.633 | −3.987 | 138.965 | 70.731 |
| 0.8070 | 141.286 | 71.277 | −0.289 | −5.633 | 139.728 | 69.181 |
| 0.8520 | 141.393 | 70.476 | −0.183 | −6.433 | 140.084 | 68.320 |
| 0.8990 | 141.483 | 69.630 | −0.093 | −7.279 | 140.493 | 67.263 |
| DIPA (1)+Methanol (2) (T=308.15 K) | | | | | | |
| 0.1158 | 129.291 | 40.773 | −14.237 | −0.454 | 143.310 | 39.644 |
| 0.1940 | 132.532 | 40.314 | −10.996 | −0.914 | 144.310 | 38.424 |
| 0.2534 | 134.739 | 40.000 | −8.789 | −1.228 | 145.310 | 37.511 |
| 0.3001 | 136.261 | 39.769 | −7.266 | −1.459 | 146.310 | 36.818 |
| 0.3540 | 137.764 | 39.487 | −5.764 | −1.740 | 147.310 | 36.049 |
| 0.4168 | 139.173 | 39.072 | −4.355 | −2.156 | 148.310 | 35.220 |
| 0.4523 | 139.816 | 38.761 | −3.712 | −2.466 | 149.310 | 34.771 |
| 0.5118 | 140.676 | 38.068 | −2.852 | −3.159 | 150.310 | 34.052 |
| 0.5562 | 141.170 | 37.378 | −2.357 | −3.850 | 151.310 | 33.501 |
| 0.6053 | 141.603 | 36.428 | −1.925 | −4.800 | 152.310 | 32.907 |
| 0.6596 | 141.984 | 35.150 | −1.544 | −6.077 | 153.310 | 32.189 |
| 0.7201 | 142.339 | 33.507 | −1.189 | −7.721 | 154.310 | 31.232 |
| 0.7531 | 142.517 | 32.561 | −1.011 | −8.666 | 155.310 | 30.604 |
| 0.8251 | 142.895 | 30.575 | −0.633 | −10.653 | 156.310 | 28.978 |
| 0.9067 | 143.290 | 29.062 | −0.238 | −12.165 | 157.310 | 26.395 |
| DIPA (1)+Ethanol (2) (T=308.15 K) | | | | | | |
| 0.1086 | 134.801 | 59.058 | −8.726 | −0.122 | 143.308 | 57.605 |
| 0.2152 | 136.754 | 58.690 | −6.773 | −0.490 | 144.308 | 56.317 |
| 0.2572 | 137.475 | 58.481 | −6.053 | −0.699 | 145.308 | 55.852 |
| 0.3033 | 138.233 | 58.214 | −5.295 | −0.966 | 146.308 | 55.364 |
| 0.3541 | 139.026 | 57.878 | −4.502 | −1.302 | 147.308 | 54.838 |
| 0.4103 | 139.848 | 57.457 | −3.680 | −1.723 | 148.308 | 54.277 |
| 0.4566 | 140.474 | 57.070 | −3.053 | −2.110 | 149.308 | 53.818 |
| 0.5069 | 141.099 | 56.602 | −2.429 | −2.578 | 150.308 | 53.307 |
| 0.5429 | 141.506 | 56.231 | −2.021 | −2.949 | 151.308 | 52.949 |
| 0.6012 | 142.089 | 55.549 | −1.438 | −3.631 | 152.308 | 52.312 |
| 0.6432 | 142.447 | 54.977 | −1.081 | −4.203 | 153.308 | 51.921 |
| 0.7116 | 142.914 | 53.844 | −0.614 | −5.336 | 154.308 | 51.223 |
| 0.7612 | 143.163 | 52.812 | −0.365 | −6.368 | 155.308 | 50.688 |
| 0.8143 | 143.349 | 51.435 | −0.178 | −7.745 | 156.308 | 50.118 |
| 0.9018 | 143.502 | 48.338 | −0.026 | −10.842 | 157.308 | 49.160 |

**Table S1. Continued**

| $x_1$ | $\overline{V}_1$ | $\overline{V}_2$ | $\overline{V}_1^E$ | $\overline{V}_2^E$ | $V_{\phi1}$ | $V_{\phi2}$ |
|---|---|---|---|---|---|---|
| DIPA (1)+1-Propanol (2) (T=308.15 K) | | | | | | |
| 0.1073 | 132.642 | 75.641 | −10.885 | −0.276 | 143.308 | 74.772 |
| 0.1544 | 134.070 | 75.441 | −9.458 | −0.477 | 144.308 | 74.209 |
| 0.2051 | 135.529 | 75.220 | −7.999 | −0.698 | 145.308 | 73.600 |
| 0.2487 | 136.683 | 75.033 | −6.845 | −0.884 | 146.308 | 73.080 |
| 0.3075 | 138.060 | 74.778 | −5.468 | −1.139 | 147.308 | 72.388 |
| 0.3452 | 138.830 | 74.599 | −4.698 | −1.318 | 148.308 | 71.973 |
| 0.3988 | 139.767 | 74.300 | −3.761 | −1.617 | 149.308 | 71.396 |
| 0.4565 | 140.583 | 73.881 | −2.944 | −2.036 | 150.308 | 70.807 |
| 0.5026 | 141.110 | 73.444 | −2.418 | −2.473 | 151.308 | 70.355 |
| 0.5516 | 141.563 | 72.861 | −1.965 | −3.056 | 152.308 | 69.866 |
| 0.6037 | 141.950 | 72.095 | −1.577 | −3.823 | 153.308 | 69.349 |
| 0.6591 | 142.285 | 71.116 | −1.242 | −4.801 | 154.308 | 68.771 |
| 0.6981 | 142.488 | 70.344 | −1.040 | −5.573 | 155.308 | 68.316 |
| 0.8034 | 142.965 | 68.123 | −0.563 | −7.794 | 156.308 | 66.796 |
| 0.8969 | 143.324 | 66.568 | −0.204 | −9.350 | 157.308 | 64.870 |
| DIPA (1)+2-Propanol (2) (T=308.15 K) | | | | | | |
| 0.1004 | 133.669 | 77.543 | −9.859 | −0.245 | 143.309 | 76.897 |
| 0.1983 | 136.196 | 77.105 | −7.332 | −0.683 | 144.309 | 76.047 |
| 0.2588 | 137.608 | 76.836 | −5.919 | −0.952 | 145.309 | 75.566 |
| 0.3002 | 138.482 | 76.664 | −5.046 | −1.124 | 146.309 | 75.218 |
| 0.3505 | 139.432 | 76.463 | −4.096 | −1.326 | 147.309 | 74.825 |
| 0.4044 | 140.308 | 76.244 | −3.220 | −1.545 | 148.309 | 74.419 |
| 0.4474 | 140.903 | 76.052 | −2.624 | −1.736 | 149.309 | 74.086 |
| 0.5084 | 141.601 | 75.725 | −1.926 | −2.063 | 150.309 | 73.608 |
| 0.5574 | 142.047 | 75.394 | −1.481 | −2.394 | 151.309 | 73.187 |
| 0.6092 | 142.424 | 74.955 | −1.104 | −2.833 | 152.309 | 72.716 |
| 0.6456 | 142.639 | 74.585 | −0.889 | −3.204 | 153.309 | 72.349 |
| 0.7029 | 142.910 | 73.886 | −0.618 | −3.903 | 154.309 | 71.689 |
| 0.8070 | 143.250 | 72.281 | −0.278 | −5.507 | 155.309 | 70.133 |
| 0.8520 | 143.353 | 71.491 | −0.174 | −6.297 | 156.309 | 69.246 |
| 0.8990 | 143.439 | 70.646 | −0.089 | −7.142 | 157.309 | 68.206 |

**Table S2. Experimental and predicted excess molar volume using PFP theory for the binary liquid mixtures at T=298.15 K**

| $x_1$ | $V_m^E$/cm$^3$ mol$^{-1}$ | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | Expt. | PFP | Expt. | PFP | Expt. | PFP | Expt. | PFP |
| | DIPA (1)+Methanol (2) | | DIPA (1)+Ethanol (2) | | DIPA (1)+1-Propanol (2) | | DIPA (1)+2-Propanol (2) | |
| 0.1 | −1.183 | −1.678 | −1.300 | −1.189 | −0.946 | −1.011 | −0.809 | −0.850 |
| 0.2 | −2.281 | −2.769 | −2.148 | −2.057 | −1.802 | −1.804 | −1.426 | −1.472 |
| 0.3 | −3.062 | −3.377 | −2.654 | −2.618 | −2.411 | −2.363 | −1.831 | −1.875 |
| 0.4 | −3.457 | −3.597 | −2.894 | −2.894 | −2.727 | −2.685 | −2.041 | −2.076 |
| 0.5 | −3.503 | −3.503 | −2.913 | −2.913 | −2.772 | −2.772 | −2.093 | −2.093 |
| 0.6 | −3.285 | −3.155 | −2.731 | -2.701 | -2.604 | −2.632 | −2.023 | −1.945 |
| 0.7 | −2.881 | −2.598 | −2.353 | −2.282 | −2.276 | −2.274 | −1.842 | −1.648 |
| 0.8 | −2.303 | −1.869 | −1.776 | −1.680 | −1.798 | −1.708 | −1.522 | −1.216 |
| 0.9 | −1.439 | −0.995 | −0.993 | −0.913 | −1.102 | −0.947 | −0.967 | −0.663 |

**Table S3. Isobaric expansivity ($10^3\ \alpha/\mathrm{K}^{-1}$), isothermal compressibility ($10^3\ \kappa_T/\mathrm{cm}^3\ \mathrm{J}^{-1}$), characteristic pressure ($P^*/\mathrm{J\ cm}^{-3}$), characteristic molar volume ($V^*/\mathrm{cm}^3\ \mathrm{mol}^{-1}$) and characteristic temperature ($T^*/\mathrm{K}$) at T=298.15 K**

| Compound | $\alpha$ | $\kappa_T$ | $P^*$ | $V^*$ | $T^*$ |
|---|---|---|---|---|---|
| DIPA | 1.374 [3] | 1.452 [3] | 491.34 | 107.28 | 4455.2 |
| Methanol | 1.189 [4] | 1.192 [4] | 491.24 | 31.61 | 4775.5 |
| Ethanol | 1.095 [4] | 1.079 [4] | 485.61 | 46.28 | 4981.7 |
| 1-Propanol | 1.005 [5] | 0.979 [5] | 477.26 | 60.20 | 5216.8 |
| 2-Propanol | 1.064 [6] | 1.332 [6] | 378.52 | 61.02 | 5058.1 |

**Table S4. PFP interaction parameter ($\chi_{12}$) and various contributions at ($x_1$=0.5) to excess molar volume at T=298.15 K**

| System | $V^E_{Inter}$ | $V^E_{Free\ vol}$ | $V^E_{P^*}$ | $\chi_{12}$ | $V^E_m$ (PFP) |
|---|---|---|---|---|---|
| DIPA (1)+Methanol (2) | −3.482 | 0.021 | 0.000 | −199.406 | −3.503 |
| DIPA (1)+Ethanol (2) | −2.857 | 0.066 | 0.010 | −143.304 | −2.913 |
| DIPA (1)+1-Propanol (2) | −2.669 | 0.142 | 0.040 | −124.999 | −2.772 |
| DIPA (1)+2-Propanol (2) | −2.289 | 0.091 | 0.287 | −95.365 | −2.093 |

**Table S5. Values of excess isentropic compressibility ($\kappa_s^E/\mathrm{TPa}^{-1}$) at T=298.15 K**

| $x_1$ | $\kappa_s^E$ | $x_1$ | $\kappa_s^E$ | $x_1$ | $\kappa_s^E$ | $x_1$ | $\kappa_s^E$ |
|---|---|---|---|---|---|---|---|
| DIPA (1)+Methanol (2) | | DIPA (1)+Ethanol (2) | | DIPA (1)+1-Propanol (2) | | DIPA (1)+2-Propanol (2) | |
| 0.1158 | −12.475 | 0.1086 | −9.792 | 0.1073 | −6.322 | 0.1004 | −5.699 |
| 0.1940 | −17.599 | 0.2152 | −14.201 | 0.1544 | −8.548 | 0.1983 | −9.119 |
| 0.2534 | −19.915 | 0.2572 | −15.042 | 0.2051 | −10.515 | 0.2588 | −10.396 |
| 0.3001 | −20.905 | 0.3033 | −15.539 | 0.2487 | −11.831 | 0.3002 | −10.963 |
| 0.3540 | −21.270 | 0.3541 | −15.671 | 0.3075 | −13.068 | 0.3505 | −11.370 |
| 0.4168 | −20.817 | 0.4103 | −15.418 | 0.3452 | −13.552 | 0.4044 | −11.510 |
| 0.4523 | −20.221 | 0.4566 | −14.960 | 0.3988 | −13.857 | 0.4474 | −11.437 |
| 0.5118 | −18.807 | 0.5069 | −14.257 | 0.4565 | −13.738 | 0.5084 | −11.102 |
| 0.5562 | −17.500 | 0.5429 | −13.645 | 0.5026 | −13.358 | 0.5574 | −10.670 |
| 0.6053 | −15.907 | 0.6012 | −12.491 | 0.5516 | −12.727 | 0.6092 | −10.078 |
| 0.6596 | −14.056 | 0.6432 | −11.551 | 0.6037 | −11.856 | 0.6456 | −9.588 |
| 0.7201 | −11.983 | 0.7116 | −9.842 | 0.6591 | −10.759 | 0.7029 | −8.692 |
| 0.7531 | −10.868 | 0.7612 | −8.468 | 0.6981 | −9.910 | 0.8070 | −6.618 |
| 0.8251 | −8.424 | 0.8143 | −6.861 | 0.8034 | −7.347 | 0.8520 | −5.487 |
| 0.9067 | −5.304 | 0.9018 | −3.892 | 0.8969 | −4.557 | 0.8990 | −4.087 |

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