SUPPLEMENTARY MATERIAL TO

Prediction of excess molar volumes of binary mixtures by Prigogine–Flory–Patterson (PFP) and extended real association solution (ERAS) models

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TABLE S-I. Parameters of the pure components used in PFP and ERAS models calculations at 298.15 K

<table>
<thead>
<tr>
<th>Subsstance</th>
<th>$K$</th>
<th>$\alpha \times 10^{12}$</th>
<th>$\kappa \times 10^{10}$</th>
<th>$P^*$</th>
<th>$V^*$</th>
<th>$\Delta h^*$</th>
<th>$\Delta v^*$</th>
<th>$S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol$^1$</td>
<td>986</td>
<td>11.89</td>
<td>11.92</td>
<td>443.6</td>
<td>32.13</td>
<td>–25.1</td>
<td>–5.6</td>
<td>16.49</td>
</tr>
<tr>
<td>Ethanol$^2$</td>
<td>317</td>
<td>11.20</td>
<td>11.53</td>
<td>411.8</td>
<td>46.90</td>
<td>–25.1</td>
<td>–5.6</td>
<td>15.43</td>
</tr>
<tr>
<td>Propan-1-ol$^2$</td>
<td>197</td>
<td>10.20</td>
<td>10.06</td>
<td>414.1</td>
<td>61.10</td>
<td>–25.1</td>
<td>–5.6</td>
<td>14.90</td>
</tr>
<tr>
<td>Butan-1-ol$^2$</td>
<td>175</td>
<td>9.32</td>
<td>9.42</td>
<td>422.7</td>
<td>75.70</td>
<td>–25.1</td>
<td>–5.6</td>
<td>14.56</td>
</tr>
<tr>
<td>Butan-2-ol$^2$</td>
<td>68</td>
<td>10.30</td>
<td>10.40</td>
<td>388.7</td>
<td>75.40</td>
<td>–25.1</td>
<td>–5.6</td>
<td>14.07</td>
</tr>
<tr>
<td>Pentan-1-ol$^3$</td>
<td>153</td>
<td>9.05</td>
<td>8.84</td>
<td>411.0</td>
<td>89.76</td>
<td>–25.1</td>
<td>–5.6</td>
<td>14.58</td>
</tr>
<tr>
<td>Acetonitrile$^4$</td>
<td>0</td>
<td>11.10</td>
<td>11.70</td>
<td>408.0</td>
<td>42.20</td>
<td>–13.2</td>
<td>–2.8</td>
<td>15.19</td>
</tr>
<tr>
<td>Hexan-1-amine$^5$</td>
<td>0.874</td>
<td>10.68</td>
<td>9.30</td>
<td>495.0</td>
<td>106.87</td>
<td>–13.2</td>
<td>–2.8</td>
<td>0</td>
</tr>
<tr>
<td>Benzene$^6$</td>
<td>0.6</td>
<td>12.18</td>
<td>9.66</td>
<td>626.3</td>
<td>69.26</td>
<td>–15.0</td>
<td>0</td>
<td>12.43</td>
</tr>
<tr>
<td>Chlorobenzene$^7$</td>
<td>0.8</td>
<td>9.91</td>
<td>7.65</td>
<td>611.0</td>
<td>82.26</td>
<td>–3.5</td>
<td>–3.0</td>
<td>12.34</td>
</tr>
</tbody>
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TABLE S-II. Interactional parameters, $\chi_{12}$, and contributions of the PFP theory, interactional, free volume and pressure contribution $P^*$ for binary mixtures at $T = 298.15$ K

<table>
<thead>
<tr>
<th>Mixture</th>
<th>$\chi_{12}$</th>
<th>Interactional</th>
<th>Free volume</th>
<th>$P^*$</th>
<th>$P^*$ effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol+benzene</td>
<td>–1.51</td>
<td>–0.01208</td>
<td>–0.00025</td>
<td>0.01210</td>
<td></td>
</tr>
<tr>
<td>Ethanol+benzene</td>
<td>–7.77</td>
<td>–0.08232</td>
<td>–0.01058</td>
<td>0.10101</td>
<td></td>
</tr>
<tr>
<td>Propan-1-ol+benzene</td>
<td>–6.87</td>
<td>–0.08524</td>
<td>–0.04066</td>
<td>0.21342</td>
<td></td>
</tr>
<tr>
<td>Butan-1-ol+benzene</td>
<td>–1.74</td>
<td>–0.02428</td>
<td>–0.07624</td>
<td>0.29901</td>
<td></td>
</tr>
<tr>
<td>Butan-2-ol+benzene</td>
<td>25.36</td>
<td>0.35358</td>
<td>–0.03830</td>
<td>0.17076</td>
<td></td>
</tr>
<tr>
<td>Methanol+chlorobenzene</td>
<td>–213.72</td>
<td>–1.55626</td>
<td>–0.02805</td>
<td>–0.09270</td>
<td></td>
</tr>
<tr>
<td>Ethanol+chlorobenzene</td>
<td>–18.62</td>
<td>–0.18219</td>
<td>–0.01087</td>
<td>–0.07843</td>
<td></td>
</tr>
<tr>
<td>Propan-1-ol+chlorobenzene</td>
<td>–15.05</td>
<td>–0.17473</td>
<td>–0.00051</td>
<td>–0.01834</td>
<td></td>
</tr>
</tbody>
</table>

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Table S-II. Continued

<table>
<thead>
<tr>
<th>Mixture</th>
<th>$\chi_{12}$ / J cm$^{-3}$</th>
<th>Interactional Free volume $P^*$ effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>Butan-1-ol+chlorobenzene</td>
<td>-12.12</td>
<td>-0.15616</td>
</tr>
<tr>
<td>Butan-2-ol+chlorobenzene</td>
<td>11.49</td>
<td>0.15262</td>
</tr>
<tr>
<td>Pentan-1-ol+chlorobenzene</td>
<td>-9.98</td>
<td>-0.14546</td>
</tr>
<tr>
<td>Butan-1-ol+n-heptane</td>
<td>-19.79</td>
<td>0.40173</td>
</tr>
<tr>
<td>Butan-2-ol+n-heptane</td>
<td>35.46</td>
<td>0.72049</td>
</tr>
<tr>
<td>Butan-1-ol+hexylamine</td>
<td>-7.30</td>
<td>-1.15015</td>
</tr>
<tr>
<td>Methanol+acetonitrile</td>
<td>-18.84</td>
<td>-0.15338</td>
</tr>
<tr>
<td>Ethanol+acetonitrile</td>
<td>-3.13</td>
<td>-0.03198</td>
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</tbody>
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Table S-III. ERAS parameters for binary mixtures at atmospheric pressure and 298.15 K

<table>
<thead>
<tr>
<th>Mixture</th>
<th>$\Delta v_{AB}$ / cm$^3$ mol$^{-1}$</th>
<th>$\chi_{AB}$ / J cm$^{-3}$</th>
<th>$K_{AB}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol+benzene</td>
<td>-6.68</td>
<td>-12.63</td>
<td>2.64</td>
</tr>
<tr>
<td>Ethanol+benzene</td>
<td>-5.74</td>
<td>10.12</td>
<td>179.13</td>
</tr>
<tr>
<td>Propan-1-ol+benzene</td>
<td>-6.00</td>
<td>17.92</td>
<td>121.92</td>
</tr>
<tr>
<td>Butan-2-ol+benzene</td>
<td>-4.75</td>
<td>6.53</td>
<td>22.16</td>
</tr>
<tr>
<td>Methanol+chlorobenzene</td>
<td>-9.27</td>
<td>-25.41</td>
<td>3.44</td>
</tr>
<tr>
<td>Ethanol+chlorobenzene</td>
<td>-4.19</td>
<td>-54.56</td>
<td>33.48</td>
</tr>
<tr>
<td>Propan-1-ol+chlorobenzene</td>
<td>-3.68</td>
<td>-61.65</td>
<td>28.61</td>
</tr>
<tr>
<td>Butan-1-ol+chlorobenzene</td>
<td>-3.38</td>
<td>-67.85</td>
<td>43.87</td>
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<tr>
<td>Butan-2-ol+chlorobenzene</td>
<td>-3.55</td>
<td>-36.18</td>
<td>16.79</td>
</tr>
<tr>
<td>Pentan-1-ol+chlorobenzene</td>
<td>-3.82</td>
<td>-52.24</td>
<td>23.80</td>
</tr>
<tr>
<td>Butan-1-ol+n-heptane</td>
<td>-3.28</td>
<td>7.08</td>
<td>22.72</td>
</tr>
<tr>
<td>Butan-2-ol+n-heptane</td>
<td>-2.73</td>
<td>7.21</td>
<td>22.87</td>
</tr>
<tr>
<td>Butan-1-ol+hexylamine</td>
<td>-12.06</td>
<td>56.44</td>
<td>498.5</td>
</tr>
<tr>
<td>Methanol+acetonitrile</td>
<td>-5.22</td>
<td>-14.86</td>
<td>27.07</td>
</tr>
<tr>
<td>Ethanol+acetonitrile</td>
<td>-5.29</td>
<td>13.25</td>
<td>13.25</td>
</tr>
<tr>
<td>Hexan-1-amine+n-heptane</td>
<td>-0.50</td>
<td>16.64</td>
<td>-0.51</td>
</tr>
</tbody>
</table>

References
1. M. Bender, A. Heintz, Fluid Phase Equilib. 89 (1993) 197