SUPPLEMENTARY MATERIAL TO

PREDICTION OF EXCESS MOLAR VOLUMES OF BINARY MIXTURES BY PRIGOGINE-FLORY-PATTERSON (PFP) AND EXTENDED REAL ASSOCIATION SOLUTION (ERAS) MODELS

Ivona R. Radović#, Nikola D. Grozdanić#, Bojan D. Djordjević[[1]](#footnote-1)#, Slobodan P. Šerbanović#, Mirjana Lj. Kijevčanin[[2]](#footnote-2)\*\*[[3]](#footnote-3)#

*Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia*

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

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Substance | *K* | *α*/10-4 K-1 | *κ*/10-10Pa-1 | *P*\*/Jcm-3 | *V*\*/cm3mol-1 | ∆*h*\*/kJmol-1 | ∆*v*\*/cm3mol-1 | *S*/nm-1 |
| Methanol20 | 986 | 11.89 | 11.92 | 443.6 | 32.13 | -25.1 | -5.6 | 16.49 |
| Ethanol21 | 317 | 11.20 | 11.53 | 411.8 | 46.90 | -25.1 | -5.6 | 15.43 |
| Propan-1-ol21 | 197 | 10.20 | 10.06 | 414.1 | 61.10 | -25.1 | -5.6 | 14.90 |
| Butan-1-ol21 | 175 | 9.32 | 9.42 | 422.7 | 75.70 | -25.1 | -5.6 | 14.56 |
| Butan-2-ol21 | 68 | 10.30 | 10.40 | 388.7 | 75.40 | -25.1 | -5.6 | 14.07 |
| Pentan-1-ol22 | 153 | 9.05 | 8.84 | 411.0 | 89.76 | -25.1 | -5.6 | 14.58 |
| Acetonitrile23 | 0 | 11.10 | 11.70 | 408.0 | 42.20 | -13.2 | -2.8 | 15.19 |
| Hexan-1-amine24 | 0.874 | 10.68 | 9.30 | 495.0 | 106.87 | -13.2 | -2.8 | 0 |
| Benzene25 | 0.6 | 12.18 | 9.66 | 626.3 | 69.26 | -15.0 | 0 | 12.43 |
| Chlorobenzene26 | 0.8 | 9.91 | 7.65 | 611.0 | 82.26 | -3.5 | -3.0 | 12.34 |

TABLE SII. Interactional parameters, *χ*12, and contributions of the PFP theory, interactional, free volume and pressure contribution *P*\* for binary mixtures at *T*=298.15 K.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Mixture | *χ*12/J cm-3 | Interactional | Free volume | *P*\* effect |
| Methanol+benzene | -1.51 | -0.01208 | -0.00025 | 0.01210 |
| Ethanol+benzene | -7.77 | -0.08232 | -0.01058 | 0.10101 |
| Propan-1-ol+benzene | -6.87 | -0.08524 | -0.04066 | 0.21342 |
| Butan-1-ol+benzene | -1.74 | -0.02428 | -0.07624 | 0.29901 |
| Butan-2-ol+benzene | 25.36 | 0.35358 | -0.03830 | 0.17076 |
| Methanol+chlorobenzene | -213.72 | -1.55626 | -0.02805 | -0.09270 |
| Ethanol+chlorobenzene | -18.62 | -0.18219 | -0.01087 | -0.07843 |
| Propan-1-ol+chlorobenzene | -15.05 | -0.17473 | -0.00051 | -0.01834 |
| Butan-1-ol+chlorobenzene | -12.12 | -0.15616 | -0.00125 | 0.03448 |
| Butan-2-ol+chlorobenzene | 11.49 | 0.15262 | -0.00212 | -0.02818 |
| Pentan-1-ol+chlorobenzene | -9.98 | -0.14546 | -0.00825 | 0.07790 |
| Butan-1-ol+n-heptane | -19.79 | 0.40173 | -0.11869 | -0.07583 |
| Butan-2-ol+n-heptane | 35.46 | 0.72049 | -0.06458 | -0.11480 |
| Butan-1-ol+hexylamine | -7.30 | -1.15015 | -0.01841 | 0.07602 |
| Methanol+acetonitrile | -18.84 | -0.15338 | -0.00375 | 0.00546 |
| Ethanol+acetonitrile | -3.13 | -0.03198 | -0.00013 | 0.00007 |
| Hexan-1-amine+n-heptane | 24.08 | 0.59286 | -0.05009 | -0.19555 |

TABLE SIII. ERAS parameters for binary mixtures at atmospheric pressure and 298.15 K

|  |  |  |  |
| --- | --- | --- | --- |
| Mixture | ∆*v*AB\*/cm3 mol-1 | *X*AB/J cm-3 | *K*AB |
| Methanol+benzene | -6.68 | -12.63 | 2.64 |
| Ethanol+benzene | -5.74 | 10.12 | 179.13 |
| Propan-1-ol+benzene | -6.00 | 17.92 | 121.92 |
| Butan-1-ol+benzene | -2.14 | -53.42 | 59.12 |
| Butan-2-ol+benzene | -4.75 | 6.53 | 22.16 |
| Methanol+chlorobenzene | -9.27 | -25.41 | 3.44 |
| Ethanol+chlorobenzene | -4.19 | -54.56 | 33.48 |
| Propan-1-ol+chlorobenzene | -3.68 | -61.65 | 28.61 |
| Butan-1-ol+chlorobenzene | -3.38 | -67.85 | 43.87 |
| butan-2-ol+chlorobenzene | -3.55 | -36.18 | 16.79 |
| Pentan-1-ol+chlorobenzene | -3.82 | -52.24 | 23.80 |
| Butan-1-ol+n-heptane | -3.28 | 7.08 | 22.72 |
| Butan-2-ol+n-heptane | -2.73 | 7.21 | 22.87 |
| Butan-1-ol+hexan-1-amine | -12.06 | 56.44 | 498.5 |
| Methanol+acetonitrile | -5.22 | -14.86 | 27.07 |
| Ethanol+acetonitrile | -5.29 | 13.25 | 13.25 |
| Hexan-1-amine+n-heptane | -0.50 | 16.64 | -0.51 |

1. The paper dedicated to Prof. Bojan D. Djordjević on the occasion of his 80th birthday [↑](#footnote-ref-1)
2. \*\* Corresponding author: [mirjana@tmf.bg.ac.rs](mailto:mirjana@tmf.bg.ac.rs) [↑](#footnote-ref-2)
3. # Serbian Chemical Society member. [↑](#footnote-ref-3)