Supporting Information

for

Trends in the Athermal Entropy of Mixing of Polymer

Solutions

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Z^{rep} Mixture Methane Hexane



Figure S1. Mixture repulsive compressibility factor for methane + ethane system

Z0 Mixture Ethane Decane



Figure S2. Mixture repulsive compressibility factor for ethane + decane system

(A0-A^{ig})/β Ethane Decane



Figure S3. Repulsive Helmholtz free energy for ethane + decane mixture



Z0 Mixture Ethane Benzene

Figure S4. Mixture repulsive compressibility factor for ethane + benzene system

Z^{rep} Mixture Methane Hexane



Figure S5. Mixture repulsive compressibility factor for methane +hexane system





Figure S6. Excess entropy of *trans*-2-butene + ACN from molecular simulations and comparing with vdW-1, $\chi_{ij}^{s} = -4.77$.

Figure S7. Excess entropy of *cis*-2-butene + ACN from molecular simulations and comparing with vdW-1, $\chi_{ij}^{s} = 2.90$.







Figure S9. Excess entropy of *trans*-2-butene + DMF from molecular simulations and comparing with vdW-1, $\chi_{ij}^{S} = -0.24$.





Figure S10. Excess entropy of *cis*-2-butene

+ DMF from molecular simulations and comparing with vdW-1, χ_{ij}^{S} = -0.24.

Figure S11. Excess entropy of 1,3-butadiene

+ DMF from molecular simulations and comparing with vdW-1, χ_{ij}^{S} = -0.24.



Figure S12. Excess entropy of ethanol





Figure S13. Excess entropy of butane

+ perfluoroC₄ from molecular simulations and comparing with vdW-1, χ_{ij}^{S} = -0.24.





Figure S14. Excess entropy of water + butane from molecular simulations and comparing with vdW-1, $\chi_{ij}^{S} = -3.29$.

Figure S15. Excess entropy of water + hexane from molecular simulations and comparing with vdW-1, $\chi_{ij}^{S} = -4.41$.



0 ٥ ٥ ٥ П -0.1 -0.2 Δ -0.3 -0.4 -Sxs/R × -0.5 X -0.6 0.1 ٥ -0.7 0.2 ж Δ 0.3 -0.8 × 0.4 ж -0.9 ж 0.5 Reg -1 0.2 0 0.4 0.6 0.8 1 Φ_1

Figure S16. Excess entropy of water + butanol from molecular simulations and comparing with vdW-1, $\chi_{ij}^{S} = -3.62$.

Figure S17. Excess entropy of water + $3MeC_5OH$ from molecular simulations and comparing with vdW-1, χ_{ij}^{s} = -4.93.





Figure S18. Excess entropy of water + C_3 Amine from molecular simulations and comparing with vdW-1, $\chi_{ij}^{S} = -3.01$.

Figure S19. Excess entropy of water + C_4 Amine from molecular simulations and comparing with vdW-1, $\chi_{ij}^{S} = -3.61$.



Figure S20. Excess entropy of water + $3C_5$ Amine from molecular simulations and comparing with vdW-1, $\chi_{ij}^{s} = -4.57$.



Figure S21. Excess entropy of hexane + butanol from molecular simulations and comparing with vdW-1, $\chi_{ij}^{S} = -0.28$.





Figure S22. Excess entropy of C₄Amine + butanol from molecular simulations and comparing with vdW-1, $\chi_{ij}^{S} = -0.04$.

Figure S23. Excess entropy of C₅Amine + propanol from molecular simulations and comparing with vdW-1, χ_{ij}^{s} = -0.05.



Figure S24. Excess entropy of octanol + $3MeC_5OH$ from molecular simulations and comparing with vdW-1, χ_{ij}^{s} = -0.21.