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Estimation of MOSCED parameters from the COSMO-SAC database

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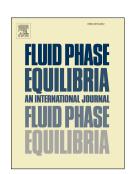
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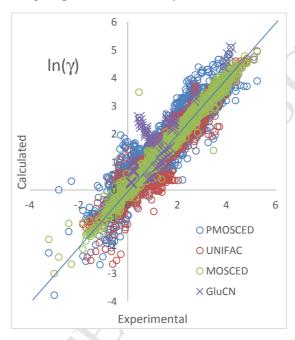
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Graphical Abstract. Natural log of infinite dilution activity coefficient for UNIFAC, PMOSCED, and original MOSCED versus 4368 experimentally measured infinite dilution activity coefficients. Values of PMOSCED for glutaronitrile (GluCN) are highlighted to show how deviations for a few compounds dominate the AAD (defined in Eqn. 8).

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