Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

SUPPORTING INFORMATION

Using Molecular Simulation to Predict Solute Solvation and Partition Coefficients in Solvents of Different Polarity

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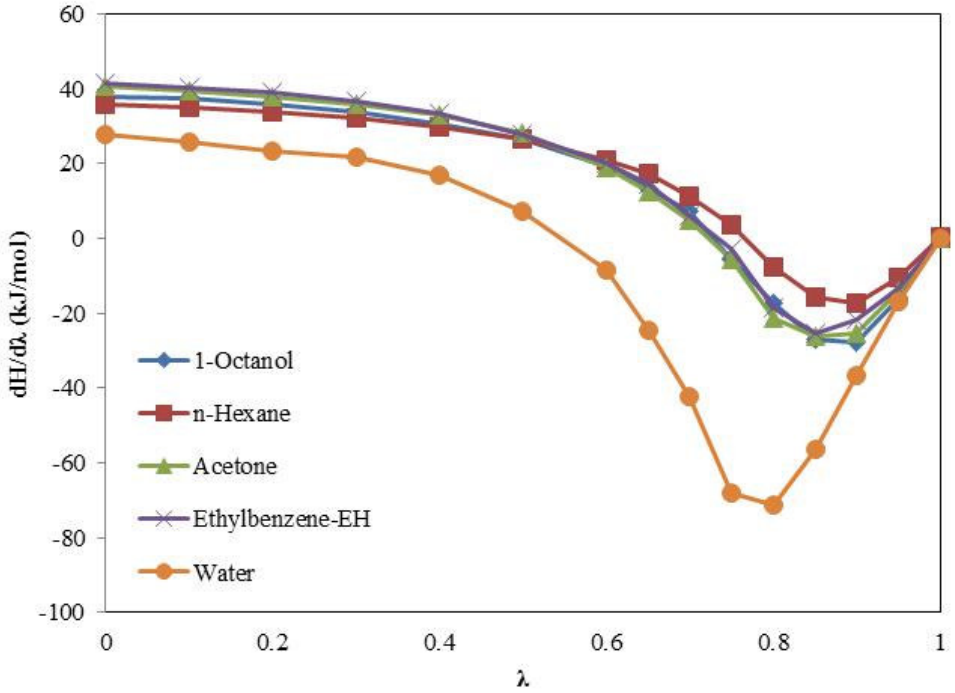

Figure S1: Derivative of the total Hamiltonian of the system with respect to the coupling parameter λ for the LJ decoupling of benzene in different solvents.

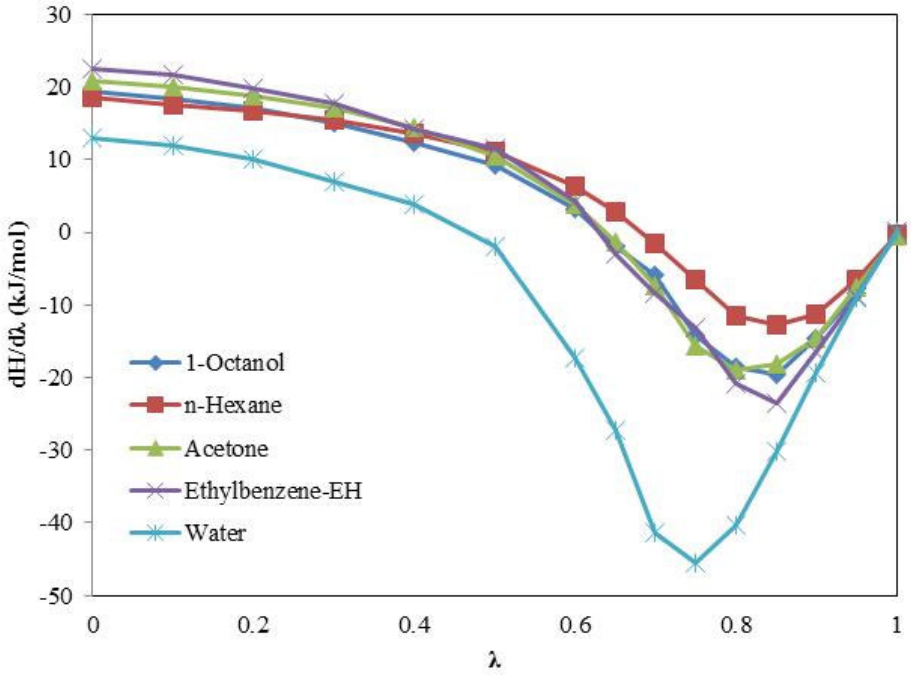

Figure S2: Derivative of the total Hamiltonian of the system with respect to the coupling parameter λ for the LJ decoupling of ethanol in different solvents

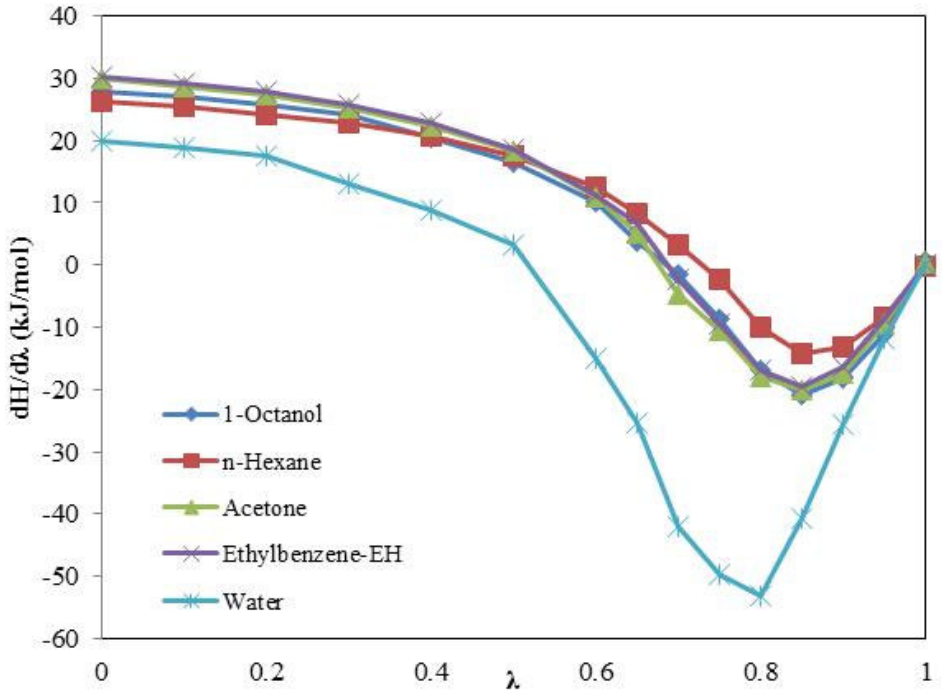

Figure S3: Derivative of the total Hamiltonian of the system with respect to the coupling parameter λ for the LJ decoupling of acetone in different solvents.