138j A Cosmo-Based Model for Predicting Properties of Pure and Mixture Systems

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We present a refined COSMO-based model for the prediction of vapor pressure and its temperature derivative, enthalpy of vaporization. This model is successful in correlating vapor pressure and enthalpies of vaporization for hundreds of small molecules, and is also good for the predictions of the normal boiling temperature of chemical warfare agents, and for the properties of drugs with complex structures. We also consider the extension of this model to the prediction of vapor liquid equilibrium with an optimized set of parameters to unify the prediction of properties of pure and mixture system. Several hundreds of mixture systems are used to optimize the parameters and test the model. The results are compared with group contribution methods (UNIFAC) and other predictive models.