Chemical Simulations

Chapter 5

Continuum Solvent Models

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The GB/SA solvation model

Details: Qiu, D., et al.¹

$$G_{\text{pol},i}' = \frac{-166.0}{R_{\text{vdW},i} + \phi + P_1} + \sum^{1,2} \frac{P_2 \, V_j}{r_{ij}^4} + \sum^{1,3} \frac{P_3 \, V_j}{r_{ij}^4} + \sum^{1,\geq 4} \frac{P_4 \, V_j CCF}{r_{ij}^4}$$

¹ J. Phys. Chem. A **1997**, 101, 3005.