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A method for calculating the enthalpy of hydrophobic effect

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Abstract

A new method for calculating the enthalpy of hydrophobic effect for compounds incapable of specific interactions with water was suggested. The method is based on separating the enthalpy of hydration into the contributions from nonspecific hydration and hydrophobic effect. The contribution from nonspecific hydration was determined by a method described previously. The enthalpies of hydrophobic effect for inert gases, alkanes, aromatic hydrocarbons, and their derivatives were determined. It was found that the enthalpy of hydrophobic effect for inert gases and alkanes is negative and independent of the size of the molecule dissolved in water. For aromatic compounds, the enthalpy is positive; it increases with the molecular size. © Pleiades Publishing, Inc., 2006.

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