

**Title:** Solution enthalpies of 1,4-dioxane: Study of solvent effects through quantitative structure-property relationships

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**Abstract:** Solution enthalpies of 1,4-dioxane have been obtained in 15 protic and aprotic solvents at 298.15 K. Breaking the overall process through the use of Solomonov's methodology the cavity term was calculated and interaction enthalpies ( $\Delta H_{int}$ ) were determined. Main factors involved in the interaction enthalpy have been identified and quantified using a QSPR approach based on the TAKA model equation. The relevant descriptors were found to be  $\pi^*$  and  $\beta$ , which showed, respectively, exothermic and endothermic contributions.

The magnitude of  $\pi^*$  coefficient points toward non-specific solute-solvent interactions playing a major role in the solution process. The positive value of the  $\beta$  coefficient reflects the endothermic character of the solvents' hydrogen bond acceptor (HBA) basicity contribution, indicating that solvent molecules engaged in hydrogen bonding preferentially interact with each other rather than with 1,4-dioxane. (C) 2013 Elsevier B.V. All rights reserved.

**Keywords:** Solution enthalpy; Interaction enthalpy; Cavity term; Kamlet-Taft parameters; QSPR

**KeyWords Plus:** Carbon-Atom Replacement; Acetone Molecule Can; Base-Acid Properties; Cyclic Ethers; T= 298.15 K; Thermochemical Behavior; Preferential Solvation; Macrocycle Interation; Binary-Mixtures; Crown-Ethers

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