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Abraham model correlations for solute transfer into 2-ethoxyethanol from water and from the gas phase

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ABSTRACT

Infinite dilution activity coefficients (γ_∞) were measured at 298 K for 13 different aliphatic hydrocarbons (alkanes, cycloalkanes, alkenes), 12 different aromatic compounds (benzene, alkylbenzenes, halobenzenes, naphthalene), and 2-chloro-2-methylpropane dissolved in 2-ethoxyethanol, along with solubilities for 11 crystalline organic compounds (xanthene, phenothiazine, acenaphthene, diphenyl sulfone, 3,5-dinitro-2-methylbenzoic acid, 3-chlorobenzoic acid, 2-methylbenzoic acid, 4-chloro-3-nitrobenzoic acid, 3,5-dinitrobenzoic acid, benzil, and thioxanthen-9-one) dissolved in 2-ethoxyethanol at 298 K. The experimental values were converted to gas-to-2-ethoxyethanol partition coefficients, water-to-2-ethoxyethanol partition coefficients, and molar solubility ratios using standard thermodynamic relationships. The calculated partition coefficient data and molar solubility ratios, combined with published literature values, were used to derive Abraham model correlations for solute transfer into 2-ethoxyethanol from both water and the gas phase. The derived Abraham model correlations predicted the observed values to within 0.15 log units (or less).

1. Introduction

Hydrogen bonding has received considerable attention over the years due to its role in determining solubilities, molecular shapes and spectral properties of biomolecules dissolved in fluid solution. Hydrogen bonding interactions can be intermolecular or intramolecular in nature, and generally result from the electrostatic attraction between a hydrogen atom bonded to a highly electronegative element (e.g., bonded to a nitrogen, oxygen or fluorine atom) and a lone electron pair residing on a nearby electronegative atom or group. C–H···Y (Y = lone-pair electron donor) interactions have also been classified as hydrogen-bonds, with the strength increasing when the C–H bond is in close proximity of electronegative atoms that are capable of withdrawing electron density from the hydrogen atom. The first ever established C–H···Y hydrogen-bond involved the participation of the acidic C–H group in the chloroform molecule [1].

Differences in hydrogen bonding interactions are important considerations in predicting solute transfer between water and hydrogen bonding solvents such as alcohols and alkoxyalcohols. If the water–solute hydrogen bonds are stronger than the organic solvent–solute hydrogen bonds then solute transfer into the organic solvent is generally not favored. If on the other hand the organic solvent–solute interactions are the stronger of the hydrogen bonding interactions, then one would predict a greater molar solute concentration in the organic solvent relative to that in the aqueous phase. Over the past two decades we have been demonstrating the applicability of the Abraham solvation parameter model to describe solute transfer into organic solvents of varying polarities and hydrogen bonding character from both water and the gas phase. The Abraham model includes not only the effects from hydrogen bonding interactions, but also contains contributions from the other types of solute–solute, solute–solvent and solvent–solvent interactions as well. Neglect of these contributions can lead to significant errors in predicting solute transfer, particularly in the case of weak H-bonded molecular solute–solvent complexes.

To date we have published correlations for describing the solubility and partitioning behavior of solutes into inert solvents (hexane–hexadecane [2,3], cyclohexane [2], methylcyclohexane [2], and isooctane [4]), into several alkylbenzene [2,5,6] and halobenzene [7] solvents, into several aprotic H-bond acceptor solvents (dibutyl ether [2], diethyl ether [2], diisopropyl ether [8], 1,4-dioxane [9], tetrahydrofuran [9], acetone [10], butanone [10], cyclohexanone [10], methyl acetate [11], ethyl acetate [11], butyl acetate [11], tributyl phosphate [12] and dimethyl sulfoxide [2]), and into several protic alcohol solvents (methanol–decanol [2,13], 2-propanol [2,14], 2-butanol [2,14], 2-methyl-1-propanol [2,14], 2-methyl-2-propanol [2,14], ethylene glycol [2,15] and propylene glycol [16]) that possess both H-bond donor and H-bond acceptor character. In total we have reported correlations for

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