



Development of Abraham model correlations for solute transfer into both 2-propoxyethanol and 2-isopropoxyethanol at 298.15 K



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ABSTRACT

Infinite dilution activity coefficients (γ_{∞}) were measured at 298 K for 9 different aliphatic hydrocarbons (alkanes, cycloalkanes, alkenes), 7 different aromatic compounds (benzene, alkylbenzenes, halobenzenes), and for 1,2-dichloropropane, dichloromethane, acetone, acetonitrile, tetrahydrofuran, 1,4-dioxane and 2-propanol dissolved in both 2-propoxyethanol and 2-isopropoxyethanol at 298 K using a headspace gas chromatographic method. As part of the experimental study solubilities of 18 and 20 crystalline organic nonelectrolyte solutes were determined in 2-propoxyethanol and 2-isopropoxyethanol, respectively, at 298 K using a UV/visible spectrophotometric method. The experimental values were converted to gas-to-alkoxyethanol partition coefficients, water-to-alkoxyethanol partition coefficients, and molar solubility ratios using standard thermodynamic relationships. Abraham model correlations for solute transfer into both alkoxyethanols were derived from the calculated solubility ratios and partition coefficients. The derived Abraham model describes the observed solubility ratios and partition coefficients to within 0.12 log units (or less).

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1. Introduction

Organic solvents represent a significant quantity of the chemicals used in industrial manufacturing processes. Increased chemical and disposal costs, coupled with environmental concerns and governmental regulations controlling the release of hazardous materials into the environment, have prompted the manufacturing sector to find ways reduce organic solvent consumption. Implementation of solvent-free processes provides one solution to the problem; however, from a practical standpoint it is not feasible to completely eliminate organic solvents from all synthetic methods and chemical separations. Organic solvents provide a critical role in dissolving organic starting materials, in facilitating heat and mass transfer, and serve as mobile phases for chemical separations involving high-performance liquid chromatography. A more viable and more practical solution to the problem is to replace expensive solvents derived from petroleum with solvents made from renewable resources, and to replace hazardous solvents with ones that exhibit better environmental, health and safety properties.

Solvent selection includes economical, toxicological and chemical considerations. Our contributions in the area of solvent selection have focused on chemical considerations and specifically on the solubilizing

properties of potential solvent candidates. For organic synthesis the solvent must be able to dissolve the starting material(s) and provide for the convenient isolation of the synthesized product from the reaction solvent media. This can either be accomplished by selecting a solvent in which the product is not soluble or by evaporation of the solvent once the reaction is complete. In the case of purification by extraction one needs to find a two-phase partitioning system (usually water and an organic solvent) where the compounds to be separated have vastly different relative solubilities in the respective immiscible liquid phases. Purification by recrystallization is also based on solubility differences of the compound in the hot versus cold solvent, or in the dissolving solvent versus precipitating anti-solvent. The solubility of a dissolved solute in different solvents is controlled by molecular interactions between the solute and surrounding solvent molecules, as well as by solvent–solvent and solute–solute interactions.

In the past several years we have reported mathematical correlations for describing measured partition coefficient and solubility data for solutes dissolved in both traditional organic solvents and in ionic liquid solvents based on the Abraham solvation parameter model [1–7]. Solute partitioning can be between two condensed phases (a biphasic aqueous-organic or organic–organic system):

$$\log(P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V} \quad (1)$$

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