



## Abraham model correlations for describing solute transfer into 2-butoxyethanol from both water and the gas phase at 298 K



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### ABSTRACT

Infinite dilution activity coefficients ( $\gamma_{\infty}$ ) were measured at 298 K for 12 different aliphatic hydrocarbons (alkanes, cycloalkanes, alkenes), 11 different aromatic compounds (benzene, alkylbenzenes, halobenzenes, naphthalene), and 2-chloro-2-methylpropane dissolved in 2-butoxyethanol at 298 K using a headspace gas chromatographic method. As part of the experimental study solubilities of 19 crystalline nonelectrolyte solutes (2-hydroxybenzoic acid, acetylsalicylic acid, 3,5-dinitro-2-methylbenzoic acid, acenaphthene, *trans*-stilbene, xanthene, phenothiazine, 3,5-dinitrobenzoic acid, 3-chlorobenzoic acid, 2-methylbenzoic acid, 4-chloro-3-nitrobenzoic acid, 2-chloro-5-nitrobenzoic acid, benzoic acid, 4-aminobenzoic acid, benzil, thioxanthene-9-one, 3-nitrobenzoic acid, fluoranthene, and diphenyl sulfone) were determined in 2-butoxyethanol at 298 K using a static, spectrophotometric method. The experimental values were converted to gas-to-2-butoxyethanol and water-to-2-butoxyethanol partition coefficients, and molar solubility ratios using standard thermodynamic relationships. Abraham model correlations for solute transfer into 2-butoxyethanol were derived from the calculated partition coefficients and solubility ratios. The derived Abraham model describes the observed partition coefficient and solubility data to within 0.14 log units (or less).

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### 1. Introduction

Organic solvents and ionic liquids are used extensively in analytical chemistry for two-phase extractions and chemical separations based on both gas–liquid chromatography (glc) and high-performance liquid chromatography (hplc). Solvent selection is determined largely by the solvent's physical and chemical properties, and by the molecular interactions between the solvent and analyte molecule(s) present in the sample being analyzed. Differences in solvent–analyte interactions govern analyte transfer between the various phases present, and play an important role in determining solubilities, chemical selectivities, and recovery factors. For liquid–liquid extractions the organic solvent and/or ionic liquid must be partly miscible with the sample solvent media in order to establish a two-phase partitioning system. Trial-and-error methods were once used to select the most appropriate solvent for a given analytical application. Mathematical approaches based on empirical solution models, linear free energy relationships (LFERs), and quantitative structure–property relationships (QSPRs), however,

have facilitated solvent selection in the modern chemical separation methods.

Lesellier [1] recently compared several commonly used approaches for selecting solvents for chemical separations based on the Snyder solvent selectivity triangle, the Kamlet–Taft solvatochromic solvent selectivity method, the Hansen solubility parameter model, the COSMO-RS model, and the Abraham solvation parameter model. For several of the comparisons the author likely utilized solute parameters/properties rather than solvent parameters/properties because the required information was not readily available. This was particularly true in the case of the Abraham model as solvent parameters (called process or solvent equation coefficients) had been determined for about 300 water/organic solvent, air/organic solvent, and totally organic solvents biphasic partitioning systems [2–20]. Abraham model solvent equation coefficients were not available for solvents such as acetic acid, pyridine, propionitrile, diethyl phthalate, limonene,  $\alpha$ -pinene,  $\alpha$ -terpineol, glycerol and 1,3-propanediol. Even when solvent parameters were available the author still elected to use solute descriptors. We also note that one of the listed solvents in the author's discussion was paracetamol, which is a drug molecule having a melting point temperature of about 442 K.

Our contributions in the area of solvent selection have been to characterize numerous organic solvents and ionic liquids in terms of their

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