

Abraham Model Expressions for Describing Water-t-Diethylene Glycol and Gas-to-Diethylene Glycol Solute Transfer Processes at 298.15 K

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Abstract

© 2017, Springer Science+Business Media New York. A gas chromatographic headspace analysis method was used to experimentally determine gas-to-liquid partition coefficients and infinite dilution activity dilution for 14 different aliphatic and cyclic hydrocarbons (alkanes, cycloalkanes, alkenes, alkynes), eight different aromatic compounds (benzene, alkylbenzenes, halobenzenes), five different chloroalkanes (dichloromethane, trichloromethane, 1-chlorobutane, 1,2-dichloropropane, isopropylbromide), tetrahydrofuran, butyl acetate, and acetonitrile dissolved in diethylene glycol at 298.15 K. Solubilities were also measured at 298.15 K for 31 crystalline nonelectrolyte organic solutes including several polycyclic aromatic hydrocarbons and substituted benzoic acid derivatives. The experimental results of the headspace chromatographic and spectroscopic solubility measurements were converted to gas-to-diethylene glycol and water-to-diethylene glycol partition coefficients, and molar solubility ratios using standard thermodynamic relationships. Expressions were derived for solute transfer into diethylene glycol from the calculated partition coefficients and solubility ratios. Mathematical correlations based on the Abraham model describe the observed partition coefficient and solubility data to within 0.14 log₁₀ units (or less).

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Keywords

Diethylene glycol solvent, Infinite dilution activity coefficients, Linear free energy relationships, Partition coefficients, Solubilities of crystalline nonelectrolyte solutes