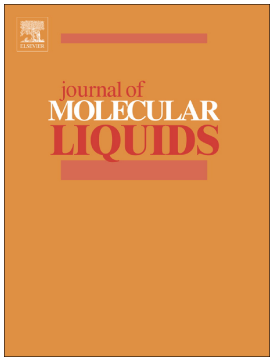


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# Investigation of the Effective Parameters on the Gas-Solvent Partition Coefficient of Trans-Stilbene using Solvent-Solubility Approaches

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**ABSTRACT**

Stilbenes and its various derivatives have been studied in different branches of science, because of their unique properties such as fluorescence, phosphorescence, photophysical, photochrome, photochemical and various biological properties. Despite of these potentials, one of the problems of stilbenes is their poor solubility which limits some of their applications. In the current study, quantitative structure property relationship (QSPR) and linear solvation energy relationship (LSER) were used to investigate the solubility of trans-stilbene as a sample solute in organic phase. LSER is an approach which deals with the effects of solvent–solute interactions on physicochemical properties and reactivity parameters. A five parametric QSPR and a LSER model contains five empirical scales was proposed to predict and descript Ostwald solubility coefficient of trans-stilbene in 44 organic solvents. The squared correlation coefficient of different training and test sets in the proposed model were above 0.84 and 0.87 respectively in the LSER model and above 0.90 and 0.86 in QSPR model. Description of scales involved in the proposed models obtained valuable information regarding the solubility of trans-stilbene in organic phase. Donor strength of solvents, solvent acidity, polarity of solvents, dipolarity and polarizability are some of important properties and thus it was concluded that polar interactions has a principal role in the solubility of trans-stilbene.

**Key Words**: trans-stilbene, gas-solvent partition coefficient, solvent-solute interactions, solvent empirical scales

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