

Determination of the Solute Descriptors for Eugenol Acetate by Gas Chromatography and Liquid-Liquid Partition Systems

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Eugenol acetate is a naturally occurring phytochemical compound found in a wide variety of plants including Cinnamon. The pleasant aroma makes it useful in the cosmetic and food industries as a fragrance and as a food flavoring agent. Furthermore, it is useful as an antioxidant and anti-inflammatory agent in the traditional medicine. It is important to determine the toxicological and environmental properties considering its uses. The conventional methods to determine these properties are costly and time consuming. Instead the Abrahams solvation parameter model which is based on the quantitative structure-property relationships can be used. This theory can be summarized with the following equations. $\log SP = c + eE + sS + aA + bB + lL$ for transfers from gas phase to a condensed phase, and $\log SP = c + eE + sS + aA + bB + vV$ for transfers between two condensed phases. Here, SP is a solute property. The simple letters are system constants and the capital letters are solute descriptors. Here V is the Characteristic volume descriptor, and E is the Excess molar refraction descriptor. L is the Gas-Hexadecane Partition coefficient. S is the Dipolarity/polarizability descriptor and A and B are, the Hydrogen bonding descriptors. The retention factor values of solutes in chromatographic methods and equilibrium constants in partition systems can be used as solute properties to determine descriptor values. In this research, the descriptor values of Eugenol acetate were determined using gas chromatography. Seven stationary phases with different polarities were used to obtain standard retention factor values at different temperatures. Also partition coefficient values in eleven organic biphasic systems were determined. The obtained standard retention factor values and the partition coefficient values were used to determine descriptor values using the Solver algorithm in MS excel® with minimum standard deviation. The determined descriptor values for Eugenol acetate are, E= 0.9161, S = 1.3293, A = 0.000, L= 6.3943, B= 0.7928 and V= 1.6519 respectively with a 0.064 standard deviation.

Keywords: Eugenol acetate, Descriptors, Solvation parameter model, Gas chromatography

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