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SOLUTE DESCRIPTORS FOR CINNAMYL ACETATE BY GAS CHROMATOGRAPHY AND LIQUID-LIQUID PARTITION SYSTEMS

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Cinnamyl acetate is a naturally occurring compound in Cinnamon leaf oil. It is widely used in the flavour and fragrance industry because of its sweet balsamic and floral odour. Hence, the quantification of its properties, such as toxicity, is important as it is used in cosmetics which are in direct contact with the consumer. The conventional methods of determining these properties are costly and need a significant amount of human and technical resources. However, the use of the Abraham solvation parameter model, which is based on the quantitative structure-property relationships, has become popular in estimating solute properties and the environmental distribution with significantly lower cost by using fewer resources. This model is expressed as $log\ log\ SP = c + eE + sS + aA + bB + vV$ for transfers between two condensed phases. Here, SP is a Free energy-related solute property, simple letters are system constants, and capital letters are Solute descriptors. V: McGowan's Characteristic Volume, E: excess molar refraction, S: dipolarity/polarizability, A and B: hydrogen-bond acidity and basicity. The determination of solute descriptors for cinnamyl acetate was carried out using the gas chromatographic technique with poly (dimethyldiphenylsiloxane) and poly (cyanopropylphenyldimethylsiloxane) stationary phases and organic biphasic partition systems. The stationary phases were calibrated, and isothermal retention factor values were determined at 20 °C intervals from 80 °C to 260 °C. Cinnamyl acetate was equilibrated in 19 organic biphasic systems, and the partition coefficients were determined. The descriptor values were then determined using the Solver algorithm in MS excel® such that the standard deviation would be minimum. The determined descriptor values for cinnamyl acetate are, E= 0.983 S=1.203 A= 0.000, L=5.980, B= 0.648 and V= 1.453, respectively, with a standard deviation of 0.077. The determined descriptor values can be used to estimate the distribution of cinnamyl acetate in environmental and industrial partition compartments.

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