



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Application of Quantitative Structure-Retention Relationships (QSRR) to a Set of Organic Bromo and Nitrile Derivatives

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Abstract: The retention times are studied for two sets of 1-bromo-2-aryloxyetanes and 3-aryloxypropionitriles derivatives by means of Quantitative Structure-Retention Relationships (QSRR). Five quantum mechanical molecular descriptors are used to calculate the regression equations. The fitting polynomials are computed in several-variable at first, second, and third order equations. Results are only significant when resorting to several-variable formulae which seems to point out the rather complex physical chemistry nature of the property under study.

Key Words: QSRR - Quantum mechanical molecular descriptors - Retention Index - Bromo and Nitrile Derivatives

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