

Molecular Descriptors in QSAR/QSPR including CD-ROM

Mati Karelson



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Molecular descriptors are mathematical values that describe the structure or shape of molecules, helping predict the activity and properties of molecules in complex experiments. This book describes the equations known as QSAR (quantitative structure-activity relationships) and QSPR (quantitative structure-property relationships), showing how they can be used productively in a wide range of industries.



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