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Roberto Todeschini and Viviana Consonni, Molecular Descriptors for Chemoinformatics (2 volumes), Wiley-VCH, 2009. Mati Karelson, Molecular Descriptors in QSAR/QSPR, John Wiley & Sons, 2000. James Devillers and Alexandru T. Balaban (Eds.), Topological indices and related descriptors in QSAR and QSPR.

Molecular descriptor - Wikipedia

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A molecular descriptor is a structural or physicochemical property of a molecule or part of a molecule. A QSAR model for predictive toxicology is a mathematical relationship between a chemical's quantitative molecular descriptors and its toxicological endpoint [9,44].Molecular descriptors derived from atomic or molecular properties that translate physicochemical, topological, and surface ...

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