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$AMW = MW / n_{AT}$ (3) where n_{AT} is the number of atoms. The mean volume (Mv) is calculated by dividing the sum of the van der Waals volumes by the number of atoms: $Mv = Sv / n_{AT}$ (4) The mean electronegativity (Me) and mean polarizability (Mp) are calculated using formulas similar to equation 4.

Molecular Descriptors Guide September 2012

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

A molecular descriptor is a structural or physicochemical property of a molecule or part of a

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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 ...

Molecular Descriptor - an overview | ScienceDirect Topics

There are currently a large number of molecular descriptors, which can be classified into three broad categories: 1-, 2-, and 3D descriptors that encode chemical composition, topology, and 3D shape and functionality, respectively. 2 A descriptor can be simple, like molecular volume, which encode only one feature of a compound, or can be complex, like 3D-MoRSE, which encode multiple physicochemical and structural properties of a compound.

PaDEL-descriptor: An open source software to calculate ...

Molecular descriptors are widely employed to present molecular characteristics in cheminformatics. Various molecular-descriptor-calculation software programs have been developed. However, users of those programs must contend with several issues, including software bugs, insufficient update frequencies, and software licensing constraints.

Mordred: a molecular descriptor calculator | Journal of ...

Meanwhile, the types of the descriptors are of high diversity. Applying different kinds of molecular descriptors are very necessary for a specific research problem. For example, molecular volume descriptors or those characterizing molecular polarity would be more relevant to study the LogD.

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The integrals $V(n_1, n_2, n_3) = \int dr x^{n_1} y^{n_2} z^{n_3}$, where $\int dr$ represents integration over the volume of a body, such as a molecule, where x , y , and z are Cartesian coordinates of a point in the interior of the body relative to an arbitrary reference frame, and where n_1 , n_2 , and n_3 are integers greater than or equal to zero, constitute moments of the volume distribution of the body ...

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