**Properties description:-**

All definitions taken from official PubChem documentation

<https://pubchemdocs.ncbi.nlm.nih.gov/pug-rest>

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| --- | --- |
| Molecular weight | The [molecular weight](https://en.wikipedia.org/wiki/Molecular_weight) is the sum of all atomic weights of the constituent atoms in a compound, measured in gr/mol. In the absence of explicit isotope labeling, averaged natural abundance (which may, for example in case of Li and U compounds, not be identical to purchasable material) is assumed. If an atom bears an explicit isotope label, 100% isotopic purity is assumed at this location, even for short-lived radioactive isotopes where this is often physically unrealistic. At this moment, it is not possible to deposit more detailed isotope composition information into the PubChem database. Pseudo-atoms which are not an element have an atomic weight of 0 g/mol. |
| Octanol-water partition coefficient | A computationally predicted octanol-water partition coefficient (or distribution coefficient).  It is used as a measure of hydrophilcity or hydrophobicity of a molecule.  From 2009, the PubChem uses version 3 of the algorithm to generate the XlogP value, which is described in the paper by [Cheng et al.](https://doi.org/10.1021/ci700257y) |
| Complexity | The complexity rating of a compound is a rough estimate of how complicated the structure is, seen from the point of view of both the elements contained and the displayed structural features including symmetry.  However, neither stereochemistry nor isotope labelling are used as auxiliary criteria.  The value is computed using the Bertz/Hendrickson/Ihlenfeldt formula, described in these papers:   * [**The first general index of molecular complexity** S.H. Bertz, J. Am. Chem. Soc., 1981, 103 (12), pp 3599–3601](https://doi.org/10.1021/ja00402a071) * [**Molecular complexity: a simplified formula adapted to individual atoms** Hendrickson et al., J. Chem. Inf. Comput. Sci., 1987, 27 (2), pp 63–67.](https://doi.org/10.1021/ci00054a004)   A scaling factor for aromaticity is used so that the complexity of benzene is the same as of cyclohexane. It is a floating point value, ranging from 0 (simple ions) to several thousand (complex natural products). Generally larger compounds are more complex than smaller ones, but highly symmetrical compounds, or compounds with few distinct atom types or elements are downgraded. Complexity is only loosely correlated with synthetic accessibility. |
| Heavy Atom Count | Number of non-hydrogen atoms. |
| Rotable Bond Count | Number of rotatable bonds. |
| TPSA | [Topological Polar Surface Area](https://en.wikipedia.org/wiki/Polar_surface_area). This is an estimate of the area (in Å2) which is polar. The implementation follows [the paper by Ertl et al. [J. Med. Chem. 2000, 43, 3714-3717](http://dx.doi.org/10.1021/jm000942e)].  It is a simple method - only N and O are considered, 3D coordinates are not used, and there are various precomputed factors for different hybridizations, charges and participation in aromatic systems. |
| Molecular Volume | Analytic volume of the first diverse conformer (default conformer) for a compound. |
| FeatureCount3D | Total number of 3D features (the sum of FeatureAcceptorCount3D, FeatureDonorCount3D, FeatureAnionCount3D, FeatureCationCount3D, FeatureRingCount3D and FeatureHydrophobeCount3D) |
| EffectiveRotorCount3D | Total number of 3D features (the sum of FeatureAcceptorCount3D, FeatureDonorCount3D, FeatureAnionCount3D, FeatureCationCount3D, FeatureRingCount3D and FeatureHydrophobeCount3D) |
| Conformer count 3D | The number of conformers in the conformer model for a compound. |
| XStericQuadrupole3D | The x component of the quadrupole moment (Qx) of the first diverse conformer (default conformer) for a compound. |
| YStericQuadrupole3D | The y component of the quadrupole moment (Qy) of the first diverse conformer (default conformer) for a compound. |
| ZStericQuadrupole3D | The y component of the quadrupole moment (Qy) of the first diverse conformer (default conformer) for a compound. |