

Atomic Properties

Atom-properties are used in **QuBiLS software** as **Atom-Weights**. The first four atom properties are standard values for each element, *namely*:

1. Polarizability (p)
2. Atomic Mass (m) [carbon atom scaled values]
3. VdW Volumen (v)
4. Electronegativity (e)

However, other six interesting atom properties also included as Atom-weights are:

5. Charge (c)
6. TPSA (psa)
7. ALogP (a)
8. Refractivity (r)
9. Softness (s)
10. Hardness (h)

These atomic properties were taken from CDK (Chemical Development kit) implementation.