## Molecular Descriptors

| **Abbrev** | **Descriptor Name** | **Type** | **Reference** |
| --- | --- | --- | --- |
| natom | Number of atoms | Constitutional | none |
| nC | Number of C atoms | Constitutional | none |
| nH | Number of H atoms | Constitutional | none |
| nO | Number of O atoms | Constitutional | none |
| nN | Number of N atoms | Constitutional | none |
| nS | Number of S atoms | Constitutional | none |
| nF | Number of F atoms | Constitutional | none |
| nCl | Number of Cl atoms | Constitutional | none |
| nBr | Number of Br atoms | Constitutional | none |
| nI | Number of I atoms | Constitutional | none |
| nP | Number of P atoms | Constitutional | none |
| nb | Number of bonds | Constitutional | none |
| nsb | Number of single bonds | Constitutional | none |
| ndb | Number of double bonds | Constitutional | none |
| ntb | Number of triple bonds | Constitutional | none |
| narb | Number of aromatic bonds | Constitutional | none |
| nring | Number of rings | Constitutional | none |
| nbenz | Number of benzene rings | Constitutional | none |
| Gib | Gravitation index (all bonds) | Geometrical | none |
| Gia | Gravitation index (all pairs) | Geometrical | none |
| Wien | Wiener index | Topological | Wiener, 1947 |
| Ran0 | Randic index (order 0) | Topological | Randic, 1975 |
| Ran1 | Randic index (order 1) | Topological | Randic, 1975 |
| Ran2 | Randic index (order 2) | Topological | Randic, 1975 |
| Ran3 | Randic index (order 3) | Topological | Randic, 1975 |
| KH0 | Kier&Hall index (order 0) | Topological | Kier, 1976 |
| KH1 | Kier&Hall index (order 1) | Topological | Kier, 1976 |
| KH2 | Kier&Hall index (order 2) | Topological | Kier, 1976 |
| KH3 | Kier&Hall index (order 3) | Topological | Kier, 1976 |
| shap1 | Kier shape index (order 1) | Topological | Kier, 1990 |
| shap2 | Kier shape index (order 2) | Topological | Kier, 1990 |
| shap3 | Kier shape index (order 3) | Topological | Kier, 1990 |
| flex | Kier flexibility index | Topological | Kier, 1990 |
| IC0 | Information content (order 0) | Topological | Kier, 1980 |
| SIC0 | Structural Information content (order 0) | Topological | Basak, 1984 |
| CIC0 | Complementary Information content (order 0) | Topological | Basak, 1984 |
| BIC0 | Bonding Information content (order 0) | Topological | Basak, 1984 |
| IC1 | Information content (order 1) | Topological | Kier, 1980 |
| SIC1 | Structural Information content (order 1) | Topological | Basak, 1984 |
| CIC1 | Complementary Information content (order 1) | Topological | Basak, 1984 |
| BIC1 | Bonding Information content (order 1) | Topological | Basak, 1984 |
| IC2 | Information content (order 2) | Topological | Kier, 1980 |
| SIC2 | Structural Information content (order 2) | Topological | Basak, 1984 |
| CIC2 | Complementary Information content (order 2) | Topological | Basak, 1984 |
| BIC2 | Bonding Information content (order 2) | Topological | Basak, 1984 |
| Bal | Balaban index | Topological | Balaban, 1982 |
| Sxy | XY Shadow | Geometrical | Rohrbaugh, 1987 |
| Sxyr | XY Shadow / XY Rectangle | Geometrical | Rohrbaugh, 1987 |
| Syz | YZ Shadow | Geometrical | Rohrbaugh, 1987 |
| Syzr | YZ Shadow / YZ Rectangle | Geometrical | Rohrbaugh, 1987 |
| Szx | ZX Shadow | Geometrical | Rohrbaugh, 1987 |
| Szxr | ZX Shadow / ZX Rectangle | Geometrical | Rohrbaugh, 1987 |
| MV | Molecular volume | Geometrical | none |
| Mvbox | Molecular volume / XYZ Box | Geometrical | none |
| MA | Molecular surface area | Geometrical | none |
| Z-QmaxC | Max partial charge for a C atom [Zefirov's PC] | Electrostatic | Kirpichenok, 1987 |
| Z-QminC | Min partial charge for a C atom [Zefirov's PC] | Electrostatic | Kirpichenok, 1987 |
| Z-QmaxH | Max partial charge for a H atom [Zefirov's PC] | Electrostatic | Kirpichenok, 1987 |
| Z-QminH | Min partial charge for a H atom [Zefirov's PC] | Electrostatic | Kirpichenok, 1987 |
| Z-Qmax | Max partial charge (Qmax) | Electrostatic | none |
| Z-Qmin | Min partial charge (Qmin) | Electrostatic | none |
| Z-Pol | Polarity parameter (Qmax-Qmin) | Electrostatic | none |
| Z-Polr2 | Polarity parameter / square distance | Electrostatic | none |
| Z-T1E | Topographic electronic index (all pairs)  [Zefirov's PC] | Electrostatic | Osmialowski, 1986 |
| Z-T2E | Topographic electronic index (all bonds)  [Zefirov's PC] | Electrostatic | Osmialowski, 1986 |
| Z-TMS | TMSA Total molecular surface area [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-PPSA1 | PPSA-1 Partial positive surface area [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-PNSA1 | PNSA-1 Partial negative surface area [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-PPSA2 | PPSA-2 Total charge weighted PPSA [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-PNSA2 | PNSA-2 Total charge weighted PNSA [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-PPSA3 | PPSA-3 Atomic charge weighted PPSA  [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-PNSA3 | PNSA-3 Atomic charge weighted PNSA  [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-RPCG | RPCG Relative positive charge (QMPOS/QTPLUS) [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-RPCS | RPCS Relative positive charged SA (SAMPOS\*RPCG) [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-RNCG | RNCG Relative negative charge (QMNEG/QTMINUS) [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-RNCS | RNCS Relative negative charged SA (SAMNEG\*RNCG) [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-HDSA | HDSA H-donors surface area [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-HASA | HASA H-acceptors surface area [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-HBSA | HBSA H-bonding surface area [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-HDCA | HDCA H-donors charged surface area [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-HACA | HACA H-acceptors charged surface area  [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-HBCA | HBCA H-bonding charged surface area  [Zefirov's PC] | Electrostatic | Stanton, 1990 |
| Z-minHAD | min(#HA, #HD) [Zefirov's PC] | Electrostatic | Zefirov, 1987 |
| Z-nHA | count of H-acceptor sites [Zefirov's PC] | Electrostatic | Zefirov, 1987 |
| Z-nHD | count of H-donors sites [Zefirov's PC] | Electrostatic | Zefirov, 1987 |
| Z-HDSA1 | HA dependent HDSA-1 [Zefirov's PC] | Electrostatic | Zefirov, 1987 |
| Z-HDSA2 | HA dependent HDSA-2 [Zefirov's PC] | Electrostatic | Zefirov, 1987 |
| Z-HDCA1 | HA dependent HDCA-1 [Zefirov's PC] | Electrostatic | Zefirov, 1987 |
| Z-HDCA2 | HA dependent HDCA-2 [Zefirov's PC] | Electrostatic | Zefirov, 1987 |
| Z-HASA1 | HASA-1 [Zefirov's PC] | Electrostatic | Zefirov, 1987 |
| Z-HASA2 | HASA-2 [Zefirov's PC] | Electrostatic | Zefirov, 1987 |
| Z-HACA1 | HACA-1 [Zefirov's PC] | Electrostatic | Zefirov, 1987 |
| Z-HACA2 | HACA-2 [Zefirov's PC] | Electrostatic | Zefirov, 1987 |
| nel | No. of occupied electronic levels | Quantum-chemical | none |
| HOMO-1 | HOMO-1 energy | Quantum-chemical | none |
| HOMO | HOMO energy | Quantum-chemical | none |
| LUMO | LUMO energy | Quantum-chemical | none |
| LUMO+1 | LUMO+1 energy | Quantum-chemical | none |
| NArCmin | Min nucleoph. react. index for a C atom | Quantum-chemical | Fukui, 1975 |
| NArCmax | Max nucleoph. react. index for a C atom | Quantum-chemical | Fukui, 1975 |
| NArC | Avg nucleoph. react. index for a C atom | Quantum-chemical | Fukui, 1975 |
| EArCmin | Min electroph. react. index for a C atom | Quantum-chemical | Fukui, 1975 |
| EArCmax | Max electroph. react. index for a C atom | Quantum-chemical | Fukui, 1975 |
| EArC | Avg electroph. react. index for a C atom | Quantum-chemical | Fukui, 1975 |
| RArCmin | Min 1-electron react. index for a C atom | Quantum-chemical | Fukui, 1975 |
| RArCmax | Max 1-electron react. index for a C atom | Quantum-chemical | Fukui, 1975 |
| RArC | Avg 1-electron react. index for a C atom | Quantum-chemical | Fukui, 1975 |
| Q-QmaxC | Max net atomic charge for a C atom | Quantum-chemical | none |
| Q-QminC | Min net atomic charge for a C atom | Quantum-chemical | none |
| Q-QmaxH | Max net atomic charge for a H atom | Quantum-chemical | none |
| Q-QminH | Min net atomic charge for a H atom | Quantum-chemical | none |
| Q-Qmax | Max net atomic charge | Quantum-chemical | none |
| Q-Qmin | Min net atomic charge | Quantum-chemical | none |
| DP | Tot dipole of the molecule | Quantum-chemical | none |
| DPpc | Tot point-charge comp. of the molecular dipole | Quantum-chemical | none |
| Dphyb | Tot hybridization comp. of the molecular dipole | Quantum-chemical | none |
| Oksol | Image of the Onsager-Kirkwood solvation energy | Quantum-chemical | none |
| Q-TMS | TMSA Total molecular surface area  [Quantum-Chemical PC] | Quantum-chemical | none |
| QZ-PPSA1 | PPSA-1 Partial positive surface area  [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-PNSA1 | PNSA-1 Partial negative surface area  [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-PPSA2 | PPSA-2 Total charge weighted PPSA  [Quantum-Chemical PC] | Quantum-chemical | Pople, 1970 |
| Q-PNSA2 | PNSA-2 Total charge weighted PNSA  [Quantum-Chemical PC] | Quantum-chemical | Pople, 1970 |
| Q-PPSA3 | PPSA-3 Atomic charge weighted PPSA  [Quantum-Chemical PC] | Quantum-chemical | Pople, 1970 |
| Q-PNSA3 | PNSA-3 Atomic charge weighted PNSA  [Quantum-Chemical PC] | Quantum-chemical | Pople, 1970 |
| Q-RPCG | RPCG Relative positive charge (QMPOS/QTPLUS) [Quantum-Chemical PC] | Quantum-chemical | Pople, 1970 |
| Q-RPCS | RPCS Relative positive charged SA (SAMPOS\*RPCG) [Quantum-Chemical PC] | Quantum-chemical | Pople, 1970 |
| Q-RNCG | RNCG Relative negative charge (QMNEG/QTMINUS) [Quantum-Chemical PC] | Quantum-chemical | Pople, 1970 |
| Q-RNCS | RNCS Relative negative charged SA (SAMNEG\*RNCG) [Quantum-Chemical PC] | Quantum-chemical | Pople, 1970 |
| Q-HDSA | HDSA H-donors surface area  [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HASA | HASA H-acceptors surface area  [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HBSA | HBSA H-bonding surface area  [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HDCA | HDCA H-donors charged surface area  [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HACA | HACA H-acceptors charged surface area  [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HBCA | HBCA H-bonding charged surface area  [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-minHAD | min(#HA, #HD) [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-nHA | count of H-acceptor sites [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-nHD | count of H-donors sites [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HDSA1 | HA dependent HDSA-1 [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HDSA2 | HA dependent HDSA-2 [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HDCA1 | HA dependent HDCA-1 [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HDCA2 | HA dependent HDCA-2 [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HASA1 | HASA-1 [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HASA2 | HASA-2 [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HACA1 | HACA-1 [Quantum-Chemical PC] | Quantum-chemical | none |
| Q-HACA2 | HACA-2 [Quantum-Chemical PC] | Quantum-chemical | none |
| AOmin | Min atomic orbital electronic population | Quantum-chemical | none |
| AOmax | Max atomic orbital electronic population | Quantum-chemical | none |
| BOss | Max SIGMA-SIGMA bond order | Quantum-chemical | Sannigrahi, 1992 |
| BOpp | Max PI-PI bond order | Quantum-chemical | Sannigrahi, 1992 |
| VminC | Min valency of a C atom | Quantum-chemical | Sannigrahi, 1992 |
| VmaxC | Max valency of a C atom | Quantum-chemical | Sannigrahi, 1992 |
| VaveC | Avg valency of a C atom | Quantum-chemical | Sannigrahi, 1992 |
| BOminC | Min (>0.1) bond order of a C atom | Quantum-chemical | Sannigrahi, 1992 |
| BOmaxC | Max bond order of a C atom | Quantum-chemical | Sannigrahi, 1992 |
| BOaveC | Avg bond order of a C atom | Quantum-chemical | Sannigrahi, 1992 |
| VminH | Min valency of a H atom | Quantum-chemical | Sannigrahi, 1992 |
| VmaxH | Max valency of a H atom | Quantum-chemical | Sannigrahi, 1992 |
| VaveH | Avg valency of a H atom | Quantum-chemical | Sannigrahi, 1992 |
| BOminH | Min (>0.1) bond order of a H atom | Quantum-chemical | Sannigrahi, 1992 |
| BOmaxH | Max bond order of a H atom | Quantum-chemical | Sannigrahi, 1992 |
| BOaveH | Avg bond order of a H atom | Quantum-chemical | Sannigrahi, 1992 |
| alfa | ALFA polarizability (DIP) | Quantum-chemical | none |
| beta1 | 1X BETA polarizability (DIP) | Quantum-chemical | none |
| beta2 | (1/2)X BETA polarizability (DIP) | Quantum-chemical | none |
| zpe | Zero point vibrational energy | Thermodynamic | none |
| vibmin | Lowest normal mode vib frequency | Thermodynamic | none |
| vibmax | Highest normal mode vib frequency | Thermodynamic | none |
| IA | Principal moment of inertia A | Geometrical | Handbook of Chemistry and Physics, 1974. |
| IB | Principal moment of inertia B | Geometrical | Handbook of Chemistry and Physics, 1974. |
| IC | Principal moment of inertia C | Geometrical | Handbook of Chemistry and Physics, 1974. |
| Hvib | Vib enthalpy (300K) | Thermodynamic | Atkins, 1982 |
| Cvib | Vib heat capacity (300K) | Thermodynamic | Atkins, 1982 |
| Svib | Vib entropy (300K) | Thermodynamic | Atkins, 1982 |
| Hrot | Rot enthalpy (300K) | Thermodynamic | Atkins, 1982 |
| Crot | Rot heat capacity (300K) | Thermodynamic | Atkins, 1982 |
| Srot | Rot entropy (300K) | Thermodynamic | Atkins, 1982 |
| Ht | Translational enthalpy (300K) | Thermodynamic | Akhiezer, 1981 |
| Ct | Translational heat capacity (300K) | Thermodynamic | Akhiezer, 1981 |
| St | Translational entropy (300K) | Thermodynamic | Akhiezer, 1981 |

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