Table A – RDKit

Descriptor	Description
`NumValenceElectrons`	Total valence electron count.
`MaxPartialCharge`, `MinPartialCharge`, `MaxAbsPartialCharge`, `MinAbsPartialCharge`	Extremes of Gasteiger atomic partial charges.
`MaxEStateIndex`, `MinEStateIndex`, `MaxAbsEStateIndex`, `MinAbsEStateIndex`	Extremal electrotopological state (most electron-rich/poor atoms).
`Chi0v–Chi4v`	Valence connectivity indices (valence-weighted χ).
`BCUT2D_CHGHI`, `BCUT2D_CHGLO`	BCUT eigenvalues weighted by atomic charge.
`BCUT2D_LOGPHI`, `BCUT2D_LOGPLOW`	BCUT eigenvalues weighted by fragment logP (hydrophobic electronic environment).
`BCUT2D_MRHI`, `BCUT2D_MRLOW`	BCUT eigenvalues weighted by molar refractivity (polarizability).
`MolMR`	Global molar refractivity (electron cloud polarizability).
`MolLogP`	cLogP (overall hydrophobicity, electron density vs water).
`TPSA`	Topological polar surface area (H-bonding / polarity capacity).
`PEOE_VSA1–PEOE_VSA14`	Van der Waals surface area binned by Gasteiger partial charge.
`SMR_VSA1–SMR_VSA10`	Surface area binned by fragment molar refractivity.
`SlogP_VSA1–SlogP_VSA12`	Surface area binned by fragment logP (hydrophobic vs polar surface).
`EState_VSA1–EState_VSA11`	Surface area binned by E-state of atoms.
`VSA_EState1–VSA_EState10`	Combined surface/E-state indices (E-state distribution on surface).

Table B – ChemDes

B1. Quantum

Descriptor	Description
`HOMO_eV`	HOMO energy (eV) – electron donor ability.
`LUMO_eV`	LUMO energy (eV) – electron acceptor ability.
`HL_Gap_eV`	HOMO–LUMO energy gap – global reactivity/hardness.

B2. Global partial-charge

Descriptor	Description
Qmin, Qmax	Minimum / maximum atomic partial charge in molecule.
QCmin, QCmax, QCss	Min / max / sum of charges on carbon atoms.
QNmin, QNss	Min and sum of charges on nitrogen atoms.
QOmin, QOmax, QOss	Min / max / sum of charges on oxygen atoms.
QHmin, QHmax, QHss	Min / max / sum of charges on hydrogen atoms.
Qass	Sum of atomic charges (overall charge distribution).
Qindex	Global index summarising charge distribution pattern.

B3. Charge / valence / polar-corrected connectivity

Descriptor	Description
Chi3ch, Chi4ch, Chi5ch, Chi6ch	Charge-corrected χ connectivity (longer paths, charge-weighted).
Chi3c, Chi4c, Chi8, Chi9, Chi10	Higher-order χ indices (more global electronic topology).
Chi4pc	Polar-corrected χ index (emphasises electronegative atoms).
Chiv3c, Chiv4c	Valence/normalized χ indices (valence-weighted, higher order).
Chiv3ch, Chiv4pc, Chiv5ch, Chiv6ch	Valence + charge/polar corrected χ indices.
mChi1	Mean/modified first-order χ index.

(Here v = valence-weighted, c = charge-weighted, ch = charged, pc = polar-corrected.)

B4. Electronegativity / polarizability autocorrelations

Descriptor	Description
ATSe1–ATSe8	Broto–Moreau autocorrelation of electronegativity (lags 1–8).
ATSv1–ATSv8	Broto–Moreau autocorrelation of atomic volume.
ATSp1–ATSp8	Broto–Moreau autocorrelation of atomic polarizability.
MATSe1–MATSe8	Moran autocorrelation of electronegativity.
MATSv1–MATSv8	Moran autocorrelation of atomic volume.
MATSp1–MATSp8	Moran autocorrelation of polarizability.
GATSe1–GATSe8	Geary autocorrelation of electronegativity.
GATSv1–GATSv8	Geary autocorrelation of atomic volume.
GATSp1–GATSp8	Geary autocorrelation of polarizability.

(Number = topological distance / lag. e = electronegativity, v = volume, p = polarizability.)

B5. Single global electronic scalars

Descriptor	Description
Pol	Global molecular polarizability estimate.