CDK

Summary of the currently available descriptors listing the descriptor type and the names of the individual values

Descriptor Type	*Descriptor Class*	*Definition*	*Descriptor Name*
ALOGP	Constitutional Descriptor	Calculates atom additive logP and molar refractivity values as described by Ghose and Crippen	ALogP ALogp2 AMR
APol	Electronic Descriptor	Descriptor that calculates the sum of the atomic polarizabilities (including implicit hydrogens).	apol
AminoAcidCount	Protein Descriptor Constitutional Descriptor	Returns the number of amino acids found in the system	nA nR nN nD nC nF nQ nE nG nH nI nP nL nK nM nS nT nY nV nW
AromaticAtomsCount	Constitutional Descriptor	Descriptor based on the number of aromatic atoms of a molecule.	naAromAtom
AromaticBondsCount	Constitutional Descriptor	Descriptor based on the number of aromatic bonds of a molecule.	nAromBond
AtomCount	Constitutional Descriptor	Descriptor based on the number of atoms of a certain element type.	nAtom
AutocorrelationCharge	Topological Descriptor	The Moreau-Broto autocorrelation descriptors using partial charges	ATSc1 ATSc2 ATSc3 ATSc4 ATSc5
AutocorrelationMass	Topological Descriptor	The Moreau-Broto autocorrelation descriptors using atomic weight	ATSm1 ATSm2 ATSm3 ATSm4 ATSm5
AutocorrelationPolarizability	Topological Descriptor	The Moreau-Broto autocorrelation descriptors using polarizability	ATSp1 ATSp2 ATSp3 ATSp4 ATSp5
BCUT	Hybrid Descriptor	Eigenvalue based descriptor noted for its utility in chemical diversity described by Pearlman et al. .	BCUTw-1l BCUTw-1h BCUTc-1l BCUTc-1h BCUTp-1l BCUTp-1h

BPol	Electronic Descriptor	Descriptor that calculates the sum of the absolute value of the difference between atomic polarizabilities of all bonded atoms in the molecule (including implicit hydrogens).	bpol
BondCount	Constitutional Descriptor	Descriptor based on the number of bonds of a certain bond order.	nB
CPSA	Electronic Descriptor Geometrical Descriptor	A variety of descriptors combining surface area and partial charge information	PPSA-1 PPSA-2 PPSA-3 PNSA-1 PNSA-2 PNSA-3 DPSA-1 DPSA-2 DPSA-3 FPSA-1 FPSA-2 FPSA-3 FNSA-1 FNSA-2 FNSA-3 WPSA-1 WPSA-2 WPSA-3 WNSA-1 WNSA-2 WNSA-3 RPCG RNCG RPCS RNCS THSA TPSA RHSA RPSA
CarbonTypes	Topological Descriptor	Characterizes the carbon connectivity in terms of hybridization	C1SP1 C2SP1 C1SP2 C2SP2 C3SP2 C1SP3 C2SP3 C3SP3 C4SP3
ChiChain	Topological Descriptor	Evaluates the Kier & Hall Chi chain indices of orders 3,4,5 and 6	SCH-3 SCH-4 SCH-5 SCH-6 SCH-7 VCH-3 VCH-4 VCH-5 VCH-6 VCH-7
ChiCluster	Topological Descriptor	Evaluates the Kier & Hall Chi cluster indices of orders 3,4,5,6 and 7	SC-3 SC-4 SC-5 SC-6 VC-3 VC-4 VC-5 VC-6
ChiPathCluster	Topological Descriptor	Evaluates the Kier & Hall Chi path cluster indices of orders 4,5 and 6	SPC-4 SPC-5 SPC-6 VPC-4 VPC-5 VPC-6
ChiPath	Topological Descriptor	Evaluates the Kier & Hall Chi path indices of orders 0,1,2,3,4,5,6 and 7	SP-0 SP-1 SP-2 SP-3 SP-4 SP-5 SP-6 SP-7 VP-0 VP-1 VP-2 VP-3 VP-4 VP-5 VP-6 VP-7
EccentricConnectivityIndex	Topological Descriptor	A topological descriptor combining distance and adjacency information.	ECCEN
FragmentComplexity	Topological Descriptor	Class that returns the complexity of a system. The complexity is defined as @cdk.cite{Nilakantan06}	fragC

GravitationalIndex	Geometrical Descriptor	Descriptor characterizing the mass distribution of the molecule.	GRAV-1 GRAV-2 GRAV-3 GRAVH-1 GRAVH-2 GRAVH-3 GRAV-4 GRAV-5 GRAV-6
HBondAcceptorCount	Electronic Descriptor	Descriptor that calculates the number of hydrogen bond acceptors.	nHBAcc
HBondDonorCount	Electronic Descriptor	Descriptor that calculates the number of hydrogen bond donors.	nHBDon
KappaShapeIndices	Topological Descriptor	Descriptor that calculates Kier and Hall kappa molecular shape indices.	Kier1 Kier2 Kier3
KierHallSmarts	Topological Descriptor	Counts the number of occurrences of the E-state fragments	khs.sLi khs.ssBe khs.ssssBe khs.ssBH khs.sssB khs.ssssB khs.sCH3 khs.dCH2 khs.ssCH2 khs.tCH khs.dsCH khs.aaCH khs.sssCH khs.ddC khs.tsC khs.dssC khs.aasC khs.aaaC khs.ssssC khs.sNH3 khs.sNH2 khs.ssNH2 khs.dNH khs.ssNH khs.aaNH khs.tN khs.sssNH khs.dsN khs.aaN khs.sssN khs.ddsN khs.aasN khs.ssssN khs.sOH khs.dO khs.ssO khs.aaO khs.sF khs.sSiH3 khs.ssSiH2 khs.sssSiH khs.ssssSi khs.sPH2 khs.ssPH khs.sssP khs.dsssP khs.ssssssP khs.sSH khs.dS khs.ssS khs.aaS khs.dssS khs.ddssS khs.sCl khs.sGeH3 khs.ssGeH2 khs.sssGeH khs.ssssGe khs.sAsH2 khs.ssAsH khs.sssAs khs.sssdAs khs.sssssAs khs.sSeH khs.dSe khs.ssSe khs.aaSe khs.dssSe khs.ddssSe khs.sBr khs.sSnH3 khs.ssSnH2 khs.sssSnH khs.ssssSn khs.sI khs.sPbH3 khs.ssPbH2 khs.sssPbH khs.ssssPb
LargestChain	Constitutional Descriptor	Returns the number of atoms in the largest chain	nAtomLC
LargestPiSystem	Constitutional Descriptor	Returns the number of atoms in the largest pi chain	nAtomP
LengthOverBreadth	Geometrical Descriptor	Calculates the ratio of length to breadth.	LOBMAX LOBMIN

LongestAliphaticChain	Constitutional Descriptor	Returns the number of atoms in the longest aliphatic chain	nAtomLAC
MDE	Topological Descriptor	Evaluate molecular distance edge descriptors for C, N and O	MDEC-11 MDEC-12 MDEC-13 MDEC-14 MDEC-22 MDEC-23 MDEC-24 MDEC-33 MDEC-34 MDEC-44 MDEO-11 MDEO-12 MDEO-22 MDEN-11 MDEN-12 MDEN-13 MDEN-22 MDEN-23 MDEN-33
MomentOfInertia	Geometrical Descriptor	Descriptor that calculates the principal moments of inertia and ratios of the principal moments. Als calculates the radius of gyration.	MOMI-X MOMI-Y MOMI-Z MOMI-XY MOMI-XZ MOMI-YZ MOMI-R
PetitjeanNumber	Topological Descriptor	Descriptor that calculates the Petitjean Number of a molecule.	PetitjeanNumber
PetitjeanShapeIndex	Geometrical Descriptor Topological Descriptor	The topological and geometric shape indices described Petitjean and Bath et al. respectively. Both measure the anisotropy in a molecule.	topoShape geomShape
RotatableBondsCount	Constitutional Descriptor	Descriptor that calculates the number of nonrotatable bonds on a molecule.	nRotB
RuleOfFive	Constitutional Descriptor	This Class contains a method that returns the number failures of the Lipinski's Rule Of Five.	LipinskiFailures
TPSA	TopologicalDescriptor Electronic Descriptor	Calculation of topological polar surface area based on fragment contributions .	TopoPSA
VAdjMa	Topological Descriptor	Descriptor that calculates the vertex adjacency information of a molecule.	VAdjMat

WHIM	Hybrid Descriptor	Holistic descriptors described by Todeschini et al .	Wlambda1.unity Wlambda2.unity Wlambda3.unity Wnu1.unity Wnu2.unity Wgamma1.unity Wgamma2.unity Wgamma3.unity Weta1.unity Weta2.unity Weta3.unity WT.unity WA.unity WV.unity WK.unity WG.unity WD.unity
Weight	Constitutional Descriptor	Descriptor based on the weight of atoms of a certain element type. If no element is specified, the returned value is the Molecular Weight	MW
WeightedPath	Topological Descriptor	The weighted path (molecular ID) descriptors described by Randic. They characterize molecular branching.	WTPT-1 WTPT-2 WTPT-3 WTPT-4 WTPT-5
WienerNumbers	Topological Descriptor	This class calculates Wiener path number and Wiener polarity number.	WPATH WPOL
XLogP	Constitutional Descriptor	Prediction of logP based on the atom-type method called XLogP.	XLogP
ZagrebIndex	Topological Descriptor	The sum of the squared atom degrees of all heavy atoms.	Zagreb