

Index	Descriptor Name	Type	Description	Dimension	Extended class
1	BalabanJ	Balaban's J index	Balaban's J value for a molecule, Chem. Phys. Lett. 89:399-404 (1982).	2	Topological descriptors
2	BertzCT	BertzCT	A topological index meant to quantify "complexity" of molecules. J. Am. Chem. Soc. 103:3599-601 (1981).	2	Topological descriptors
3	Chi0	Chi indices	From equations (1),(9) and (10) of Rev. Comp. Chem. vol 2, 367-422, (1991)	2	Connectivity descriptors
4	Chi1	Chi indices	From equations (1),(11) and (12) of Rev. Comp. Chem. vol 2, 367-422, (1991)	2	Connectivity descriptors
5	Chi0v	Chi indices	From equations (5),(9) and (10) of Rev. Comp. Chem. vol 2, 367-422, (1991)	2	Connectivity descriptors
6	Chi1v	Chi indices	From equations (5),(11) and (12) of Rev. Comp. Chem. vol 2, 367-422, (1991)	2	Connectivity descriptors
7	Chi2v	Chi indices	From equations (5),(15) and (16) of Rev. Comp. Chem. vol 2, 367-422, (1991)	2	Connectivity descriptors
8	Chi3v	Chi indices	From equations (5),(15) and (16) of Rev. Comp. Chem. vol 2, 367-422, (1991)	2	Connectivity descriptors
9	Chi4v	Chi indices	From equations (5),(15) and (16) of Rev. Comp. Chem. vol 2, 367-422, (1991)	2	Connectivity descriptors
10	Chi0n	Chi indices	Similar to Hall Kier Chi0v, but uses nVal instead of valence This makes a big difference after we get out of the first row. Rev. Comput. Chem. 2:367-422 (1991).	2	Connectivity descriptors
11	Chi1n	Chi indices	Similar to Hall Kier Chi1v, but uses nVal instead of valence. Rev. Comput. Chem. 2:367-422 (1991).	2	Connectivity descriptors
12	Chi2n	Chi indices	Similar to Hall Kier Chi2v, but uses nVal instead of valence This makes a big difference after we get out of the first row. Rev. Comput. Chem. 2:367-422 (1991).	2	Connectivity descriptors
13	Chi3n	Chi indices	Similar to Hall Kier Chi3v, but uses nVal instead of valence This makes a big difference after we get out of the first row. Rev. Comput. Chem. 2:367-422 (1991).	2	Connectivity descriptors
14	Chi4n	Chi indices	Similar to Hall Kier Chi4v, but uses nVal instead of valence. This makes a big difference after we get out of the first row. Rev. Comput. Chem. 2:367-422 (1991).	2	Connectivity descriptors
15	EState_VSA1	EState_VSA	MOE-type descriptors using EState indices and surface area contributions (developed at RD, not described in the CCG paper).	2	MOE-type descriptors
16	EState_VSA2	EState_VSA	MOE-type descriptors using EState indices and surface area contributions (developed at RD, not described in the CCG paper).	2	MOE-type descriptors
17	EState_VSA3	EState_VSA	MOE-type descriptors using EState indices and surface area contributions (developed at RD, not described in the CCG paper).	2	MOE-type descriptors

18	EState_VSA4	EState_VSA	MOE-type descriptors using EState indices and surface area contributions (developed at RD, not described in the CCG paper).	2	MOE-type descriptors
19	EState_VSA5	EState_VSA	MOE-type descriptors using EState indices and surface area contributions (developed at RD, not described in the CCG paper).	2	MOE-type descriptors
20	EState_VSA6	EState_VSA	MOE-type descriptors using EState indices and surface area contributions (developed at RD, not described in the CCG paper).	2	MOE-type descriptors
21	EState_VSA7	EState_VSA	MOE-type descriptors using EState indices and surface area contributions (developed at RD, not described in the CCG paper).	2	MOE-type descriptors
22	EState_VSA8	EState_VSA	MOE-type descriptors using EState indices and surface area contributions (developed at RD, not described in the CCG paper).	2	MOE-type descriptors
23	EState_VSA9	EState_VSA	MOE-type descriptors using EState indices and surface area contributions (developed at RD, not described in the CCG paper).	2	MOE-type descriptors
24	EState_VSA10	EState_VSA	MOE-type descriptors using EState indices and surface area contributions (developed at RD, not described in the CCG paper).	2	MOE-type descriptors
25	EState_VSA11	EState_VSA	MOE-type descriptors using EState indices and surface area contributions (developed at RD, not described in the CCG paper).	2	MOE-type descriptors
26	ExactMolWt	ExactMolWt	The molecule's exact molecular weight.	2	Molecular property descriptors
27	FractionCSP3	FractionCSP3	The fraction of C atoms that are SP3 hybridized.	1	Constitutional descriptors
28	HallKierAlpha	HallKierAlpha	The Hall-Kier alpha value for a molecule.Rev. Comput. Chem. 2:367-422 (1991).	2	Topological descriptors
29	HeavyAtomCount	HeavyAtomCount	Number of heavy atoms of a molecule.	1	Constitutional descriptors
30	HeavyAtomMolWt	HeavyAtomMolWt	The average molecular weight of the molecule ignoring hydrogens	1	Constitutional descriptors
31	Ipc	Ipc	the information content of the coefficients of the characteristic polynomial of the adjacency matrix of a hydrogen-suppressed graph of a molecule.	2	Topological descriptors
32	Kappa1	Kappa descriptors	Hall-Kier Kappa1 value	2	Topological descriptors
33	Kappa2	Kappa descriptors	Hall-Kier Kappa2 value	2	Topological descriptors
34	Kappa3	Kappa descriptors	Hall-Kier Kappa2 value	2	Topological descriptors
35	LabuteASA	LabuteASA	Labute's Approximate Surface Area (ASA from MOE)	2	MOE-type descriptors

36	MolLogP	MolLogP	Wildman-Crippen LogP value.Wildman and Crippen JCICS 39:868-73 (1999)	2	Molecular property descriptors
37	MolMR	MolMR	Wildman-Crippen MR value.Wildman and Crippen JCICS 39:868-73 (1999)	2	Molecular property descriptors
38	MolWt	MolWt	The average molecular weight of the molecule	2	Molecular property descriptors
39	NHOHCount	NHOHCount	Number of NHs or OHs	1	Constitutional descriptors
40	NOCCount	NOCCount	Number of Nitrogens and Oxygens	1	Constitutional descriptors
41	NumAliphaticCarbocycles	NumAliphaticCarbocycles	The number of aliphatic (containing at least one non-aromatic bond) carbocycles for a molecule	1	Constitutional descriptors
42	NumAliphaticHeterocycles	NumAliphaticHeterocycles	The number of aliphatic (containing at least one non-aromatic bond) heterocycles for a molecule	1	Constitutional descriptors
43	NumAliphaticRings	NumAliphaticRings	The number of aliphatic (containing at least one non-aromatic bond) rings for a molecule	1	Constitutional descriptors
44	NumAromaticCarbocycles	NumAromaticCarbocycles	The number of aromatic carbocycles for a molecule	1	Constitutional descriptors
45	NumAromaticHeterocycles	NumAromaticHeterocycles	The number of aromatic heterocycles for a molecule	1	Constitutional descriptors
46	NumAromaticRings	NumAromaticRings	The number of aromatic rings for a molecule	1	Constitutional descriptors
47	NumHAcceptors	NumHAcceptors	Number of Hydrogen Bond Acceptors	1	Constitutional descriptors
48	NumHDonors	NumHDonors	Number of Hydrogen Bond Donors	1	Constitutional descriptors
49	NumHeteroatoms	NumHeteroatoms	Number of Heteroatoms	1	Constitutional descriptors
50	NumRadicalElectrons	NumRadicalElectrons	The number of radical electrons the molecule has (says nothing about spin state)	1	Constitutional descriptors
51	NumRotatableBonds	NumRotatableBonds	Number of Rotatable Bonds	1	Constitutional descriptors
52	NumSaturatedCarbocycles	NumSaturatedCarbocycles	The number of saturated carbocycles for a molecule	1	Constitutional descriptors
53	NumSaturatedHeterocycles	NumSaturatedHeterocycles	The number of saturated heterocycles for a molecule	1	Constitutional descriptors

54	NumSaturatedRings	NumSaturatedRings	The number of saturated rings for a molecule	1	Constitutional descriptors
55	NumValenceElectrons	NumValenceElectrons	The number of valence electrons the molecule has	1	Constitutional descriptors
56	PEOE_VSA1	PEOE_VSA	MOE Charge VSA Descriptor 1 (-inf < x < -0.30)	2	MOE-type descriptors
57	PEOE_VSA2	PEOE_VSA	MOE Charge VSA Descriptor 2 (-0.30 <= x < -0.25)	2	MOE-type descriptors
58	PEOE_VSA3	PEOE_VSA	MOE Charge VSA Descriptor 3 (-0.25 <= x < -0.20)	2	MOE-type descriptors
59	PEOE_VSA4	PEOE_VSA	MOE Charge VSA Descriptor 4 (-0.20 <= x < -0.15)	2	MOE-type descriptors
60	PEOE_VSA5	PEOE_VSA	MOE Charge VSA Descriptor 5 (-0.15 <= x < -0.10)	2	MOE-type descriptors
61	PEOE_VSA6	PEOE_VSA	MOE Charge VSA Descriptor 6 (-0.10 <= x < -0.05)	2	MOE-type descriptors
62	PEOE_VSA7	PEOE_VSA	MOE Charge VSA Descriptor 7 (-0.05 <= x < 0.00)	2	MOE-type descriptors
63	PEOE_VSA8	PEOE_VSA	MOE Charge VSA Descriptor 8 ( 0.00 <= x < 0.05)	2	MOE-type descriptors
64	PEOE_VSA9	PEOE_VSA	MOE Charge VSA Descriptor 9 ( 0.05 <= x < 0.10)	2	MOE-type descriptors
65	PEOE_VSA10	PEOE_VSA	MOE Charge VSA Descriptor 10 ( 0.10 <= x < 0.15)	2	MOE-type descriptors
66	PEOE_VSA11	PEOE_VSA	MOE Charge VSA Descriptor 11 ( 0.15 <= x < 0.20)	2	MOE-type descriptors
67	PEOE_VSA12	PEOE_VSA	MOE Charge VSA Descriptor 12 ( 0.20 <= x < 0.25)	2	MOE-type descriptors
68	PEOE_VSA13	PEOE_VSA	MOE Charge VSA Descriptor 13 ( 0.25 <= x < 0.30)	2	MOE-type descriptors
69	PEOE_VSA14	PEOE_VSA	MOE Charge VSA Descriptor 14 ( 0.30 <= x < inf)	2	MOE-type descriptors
70	RingCount	RingCount	The number of rings for a molecule	1	Constitutional descriptors
71	SMR_VSA1	SMR_VSA	MOE MR VSA Descriptor 1 (-inf < x < 1.29)	2	MOE-type descriptors
72	SMR_VSA2	SMR_VSA	MOE MR VSA Descriptor 2 ( 1.29 <= x < 1.82)	2	MOE-type descriptors
73	SMR_VSA3	SMR_VSA	MOE MR VSA Descriptor 3 ( 1.82 <= x < 2.24)	2	MOE-type descriptors
74	SMR_VSA4	SMR_VSA	MOE MR VSA Descriptor 4 ( 2.24 <= x < 2.45)	2	MOE-type descriptors
75	SMR_VSA5	SMR_VSA	MOE MR VSA Descriptor 5 ( 2.45 <= x < 2.75)	2	MOE-type descriptors
76	SMR_VSA6	SMR_VSA	MOE MR VSA Descriptor 6 ( 2.75 <= x < 3.05)	2	MOE-type descriptors
77	SMR_VSA7	SMR_VSA	MOE MR VSA Descriptor 7 ( 3.05 <= x < 3.63)	2	MOE-type descriptors
78	SMR_VSA8	SMR_VSA	MOE MR VSA Descriptor 8 ( 3.63 <= x < 3.80)	2	MOE-type descriptors
79	SMR_VSA9	SMR_VSA	MOE MR VSA Descriptor 9 ( 3.80 <= x < 4.00)	2	MOE-type descriptors

80	SMR_VSA10	SMR_VSA	MOE MR VSA Descriptor 10 ( 4.00 <= x < inf)	2	MOE-type descriptors
81	SlogP_VSA1	SlogP_VSA	MOE logP VSA Descriptor 1 (-inf < x < -0.40)	2	MOE-type descriptors
82	SlogP_VSA2	SlogP_VSA	MOE logP VSA Descriptor 2 (-0.40 <= x < -0.20)	2	MOE-type descriptors
83	SlogP_VSA3	SlogP_VSA	MOE logP VSA Descriptor 3 (-0.20 <= x < 0.00)	2	MOE-type descriptors
84	SlogP_VSA4	SlogP_VSA	MOE logP VSA Descriptor 4 ( 0.00 <= x < 0.10)	2	MOE-type descriptors
85	SlogP_VSA5	SlogP_VSA	MOE logP VSA Descriptor 5 ( 0.10 <= x < 0.15)	2	MOE-type descriptors
86	SlogP_VSA6	SlogP_VSA	MOE logP VSA Descriptor 6 ( 0.15 <= x < 0.20)	2	MOE-type descriptors
87	SlogP_VSA7	SlogP_VSA	MOE logP VSA Descriptor 7 ( 0.20 <= x < 0.25)	2	MOE-type descriptors
88	SlogP_VSA8	SlogP_VSA	MOE logP VSA Descriptor 8 ( 0.25 <= x < 0.30)	2	MOE-type descriptors
89	SlogP_VSA9	SlogP_VSA	MOE logP VSA Descriptor 9 ( 0.30 <= x < 0.40)	2	MOE-type descriptors
90	SlogP_VSA10	SlogP_VSA	MOE logP VSA Descriptor 10 ( 0.40 <= x < 0.50)	2	MOE-type descriptors
91	SlogP_VSA11	SlogP_VSA	MOE logP VSA Descriptor 11 ( 0.50 <= x < 0.60)	2	MOE-type descriptors
92	SlogP_VSA12	SlogP_VSA	MOE logP VSA Descriptor 12 ( 0.60 <= x < inf)	2	MOE-type descriptors
93	TPSA	TPSA	The polar surface area of a molecule based upon fragments	2	Molecular property descriptors
94	VSA_EState1	VSA_Estate	VSA EState Descriptor 1 (-inf < x < 4.78)	2	MOE-type descriptors
95	VSA_EState2	VSA_Estate	VSA EState Descriptor 2 ( 4.78 <= x < 5.00)	2	MOE-type descriptors
96	VSA_EState3	VSA_Estate	VSA EState Descriptor 3 ( 5.00 <= x < 5.41)	2	MOE-type descriptors
97	VSA_EState4	VSA_Estate	VSA EState Descriptor 4 ( 5.41 <= x < 5.74)	2	MOE-type descriptors
98	VSA_EState5	VSA_Estate	VSA EState Descriptor 5 ( 5.74 <= x < 6.00)	2	MOE-type descriptors
99	VSA_EState6	VSA_Estate	VSA EState Descriptor 6 ( 6.00 <= x < 6.07)	2	MOE-type descriptors
100	VSA_EState7	VSA_Estate	VSA EState Descriptor 7 ( 6.07 <= x < 6.45)	2	MOE-type descriptors
101	VSA_EState8	VSA_Estate	VSA EState Descriptor 8 ( 6.45 <= x < 7.00)	2	MOE-type descriptors
102	VSA_EState9	VSA_Estate	VSA EState Descriptor 9 ( 7.00 <= x < 11.00)	2	MOE-type descriptors
103	VSA_EState10	VSA_Estate	VSA EState Descriptor 10 ( 11.00 <= x < inf)	2	MOE-type descriptors
104	fr_AI_COO	fr_AI_COO	Number of aliphatic carboxylic acids	1	Constitutional descriptors
105	fr_AI_OH	fr_AI_OH	Number of aliphatic hydroxyl groups	1	Constitutional descriptors

106	fr_Al_OH_noTert	fr_Al_OH_noTert	Number of aliphatic hydroxyl groups excluding tert-OH	1	Constitutional descriptors
107	fr_ArN	fr_ArN	Number of N functional groups attached to aromatics	1	Constitutional descriptors
108	fr_Ar_COO	fr_Ar_COO	Number of Aromatic carboxylic acids	1	Constitutional descriptors
109	fr_Ar_N	fr_Ar_N	Number of aromatic nitrogens	1	Constitutional descriptors
110	fr_Ar_NH	fr_Ar_NH	Number of aromatic amines	1	Constitutional descriptors
111	fr_Ar_OH	fr_Ar_OH	Number of aromatic hydroxyl groups	1	Constitutional descriptors
112	fr_COO	fr_COO	Number of carboxylic acids	1	Constitutional descriptors
113	fr_COO2	fr_COO2	Number of carboxylic acids	1	Constitutional descriptors
114	fr_C_O	fr_C_O	Number of carbonyl O	1	Constitutional descriptors
115	fr_C_O_noCOO	fr_C_O_noCOO	Number of carbonyl O, excluding COOH	1	Constitutional descriptors
116	fr_C_S	fr_C_S	Number of thiocarbonyl	1	Constitutional descriptors
117	fr_HOCCN	fr_HOCCN	Number of C(OH)CCN-Ctert-alkyl or C(OH)CCNcyclic	1	Constitutional descriptors
118	fr_Iimine	fr_Iimine	Number of Imines	1	Constitutional descriptors
119	fr_NH0	fr_NH0	Number of Tertiary amines	1	Constitutional descriptors
120	fr_NH1	fr_NH1	Number of Secondary amines	1	Constitutional descriptors
121	fr_NH2	fr_NH2	Number of Primary amines	1	Constitutional descriptors
122	fr_N_O	fr_N_O	Number of hydroxylamine groups	1	Constitutional descriptors
123	fr_Ndealkylation1	fr_Ndealkylation1	Number of XCCNR groups	1	Constitutional descriptors

124	fr_Ndealkylation2	fr_Ndealkylation2	Number of tert-alicyclic amines (no heteroatoms, not quinine-like bridged N)	1	Constitutional descriptors
125	fr_Nhpyrrole	fr_Nhpyrrole	Number of H-pyrrole nitrogens	1	Constitutional descriptors
126	fr_SH	fr_SH	Number of thiol groups	1	Constitutional descriptors
127	fr_aldehyde	fr_aldehyde	Number of aldehydes	1	Constitutional descriptors
128	fr_alkyl_carbamate	fr_alkyl_carbamate	Number of alkyl carbamates (subject to hydrolysis)	1	Constitutional descriptors
129	fr_alkyl_halide	fr_alkyl_halide	Number of alkyl halides	1	Constitutional descriptors
130	fr_allylic_oxid	fr_allylic_oxid	Number of allylic oxidation sites excluding steroid dienone	1	Constitutional descriptors
131	fr_amide	fr_amide	Number of amides	1	Constitutional descriptors
132	fr_amidine	fr_amidine	Number of amidine groups	1	Constitutional descriptors
133	fr_aniline	fr_aniline	Number of anilines	1	Constitutional descriptors
134	fr_aryl_methyl	fr_aryl_methyl	Number of aryl methyl sites for hydroxylation	1	Constitutional descriptors
135	fr_azide	fr_azide	Number of azide groups	1	Constitutional descriptors
136	fr_azo	fr_azo	Number of azo groups	1	Constitutional descriptors
137	fr_barbitur	fr_barbitur	Number of barbiturate groups	1	Constitutional descriptors
138	fr_benzene	fr_benzene	Number of benzene rings	1	Constitutional descriptors
139	fr_benzodiazepine	fr_benzodiazepine	Number of benzodiazepines with no additional fused rings	1	Constitutional descriptors
140	fr_bicyclic	fr_bicyclic	Bicyclic	1	Constitutional descriptors
141	fr_diazo	fr_diazo	Number of diazo groups	1	Constitutional descriptors

142	fr_dihydropyridine	fr_dihydropyridine	Number of dihydropyridines	1	Constitutional descriptors
143	fr_epoxide	fr_epoxide	Number of epoxide rings	1	Constitutional descriptors
144	fr_ester	fr_ester	Number of esters	1	Constitutional descriptors
145	fr_ether	fr_ether	Number of ether oxygens (including phenoxy)	1	Constitutional descriptors
146	fr_furan	fr_furan	Number of furan rings	1	Constitutional descriptors
147	fr_guanido	fr_guanido	Number of guanidine groups	1	Constitutional descriptors
148	fr_halogen	fr_halogen	Number of halogens	1	Constitutional descriptors
149	fr_hdrzine	fr_hdrzine	Number of hydrazine groups	1	Constitutional descriptors
150	fr_hdrzone	fr_hdrzone	Number of hydrazone groups	1	Constitutional descriptors
151	fr_imidazole	fr_imidazole	Number of imidazole rings	1	Constitutional descriptors
152	fr_imide	fr_imide	Number of imide groups	1	Constitutional descriptors
153	fr_isocyan	fr_isocyan	Number of isocyanates	1	Constitutional descriptors
154	fr_isothiocyan	fr_isothiocyan	Number of isothiocyanates	1	Constitutional descriptors
155	fr_ketone	fr_ketone	Number of ketones	1	Constitutional descriptors
156	fr_ketone_Topliss	fr_ketone_Topliss	Number of ketones excluding diaryl, a,b-unsat.	1	Constitutional descriptors
157	fr_lactam	fr_lactam	Number of beta lactams	1	Constitutional descriptors
158	fr_lactone	fr_lactone	Number of cyclic esters (lactones)	1	Constitutional descriptors
159	fr_methoxy	fr_methoxy	Number of methoxy groups -OCH3	1	Constitutional descriptors



160	fr_morpholine	fr_morpholine	Number of morpholine rings	1	Constitutional descriptors
161	fr_nitrile	fr_nitrile	Number of nitriles	1	Constitutional descriptors
162	fr_nitro	fr_nitro	Number of nitro groups	1	Constitutional descriptors
163	fr_nitro_arom	fr_nitro_arom	Number of nitro benzene ring substituents	1	Constitutional descriptors
164	fr_nitro_arom_nonortho	fr_nitro_arom_nonortho	Number of non-ortho nitro benzene ring substituents	1	Constitutional descriptors
165	fr_nitroso	fr_nitroso	Number of nitroso groups, excluding NO2	1	Constitutional descriptors
166	fr_oxazole	fr_oxazole	Number of oxazole rings	1	Constitutional descriptors
167	fr_oxime	fr_oxime	Number of oxime groups	1	Constitutional descriptors
168	fr_para_hydroxylation	fr_para_hydroxylation	Number of para-hydroxylation sites	1	Constitutional descriptors
169	fr_phenol	fr_phenol	Number of phenols	1	Constitutional descriptors
170	fr_phenol_noOrthoHbond	fr_phenol_noOrthoHbond	Number of phenolic OH excluding ortho intramolecular Hbond substituents	1	Constitutional descriptors
171	fr_phos_acid	fr_phos_acid	Number of phosphoric acid groups	1	Constitutional descriptors
172	fr_phos_ester	fr_phos_ester	Number of phosphoric ester groups	1	Constitutional descriptors
173	fr_piperdine	fr_piperdine	Number of piperdine rings	1	Constitutional descriptors
174	fr_piperzine	fr_piperzine	Number of piperzine rings	1	Constitutional descriptors
175	fr_priamide	fr_priamide	Number of primary amides	1	Constitutional descriptors
176	fr_prisulfonamd	fr_prisulfonamd	Number of primary sulfonamides	1	Constitutional descriptors
177	fr_pyridine	fr_pyridine	Number of pyridine rings	1	Constitutional descriptors

178	fr_quatN	fr_quatN	Number of quarternary nitrogens	1	Constitutional descriptors
179	fr_sulfide	fr_sulfide	Number of thioether	1	Constitutional descriptors
180	fr_sulfonamd	fr_sulfonamd	Number of sulfonamides	1	Constitutional descriptors
181	fr_sulfone	fr_sulfone	Number of sulfone groups	1	Constitutional descriptors
182	fr_term_acetylene	fr_term_acetylene	Number of terminal acetylenes	1	Constitutional descriptors
183	fr_tetrazole	fr_tetrazole	Number of tetrazole rings	1	Constitutional descriptors
184	fr_thiazole	fr_thiazole	Number of thiazole rings	1	Constitutional descriptors
185	fr_thiocyan	fr_thiocyan	Number of thiocyanates	1	Constitutional descriptors
186	fr_thiophene	fr_thiophene	Number of thiophene rings	1	Constitutional descriptors
187	fr_unbrch_alkane	fr_unbrch_alkane	Number of unbranched alkanes of at least 4 members (excludes halogenated alkanes)	1	Constitutional descriptors
188	fr_urea	fr_urea	Number of urea groups	1	Constitutional descriptors
189	MaxAbsEStateIndex	Estate Index	Returns a tuple of EState indices for the molecule, Reference: Hall, Mohnney and Kier. JCICS _31_ 76-81 (1991)	2	Topological descriptors
190	MaxAbsPartialCharge	Partial Charge	Returns molecular charge descriptors	2	Topological descriptors
191	MaxEStateIndex	Estate Index	Returns a tuple of EState indices for the molecule, Reference: Hall, Mohnney and Kier. JCICS _31_ 76-81 (1991)	2	Topological descriptors
192	MaxPartialCharge	Partial Charge	Returns molecular charge descriptors	2	Topological descriptors
193	MinAbsEStateIndex	Estate Index	Returns a tuple of EState indices for the molecule, Reference: Hall, Mohnney and Kier. JCICS _31_ 76-81 (1991)	2	Topological descriptors
194	MinAbsPartialCharge	Partial Charge	Returns molecular charge descriptors	2	Topological descriptors
195	MinEStateIndex	Estate Index	Returns a tuple of EState indices for the molecule, Reference: Hall, Mohnney and Kier. JCICS _31_ 76-81 (1991)	2	Topological descriptors

196	MinPartialCharge	Partial Charge	Returns molecular charge descriptors	2	Topological descriptors
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