properties

Name	Reference	Computable	description
atom-bond connectivity index	Mordred	Descriptors index 0	...
Graovac-Ghorbani atom-bond connectivity index	Mordred	Descriptors index 1	...
[acidic/basic] group count	Mordred	Descriptors index [2-3]	...
Sp[Abs/max/Diam/AD/MAD] of adjacency matrix	Mordred	Descriptors index [4-8]	...
LogEE of adjacency matrix	Mordred	Descriptors index 9	...
V[E/R][1-3] of adjacency matrix	Mordred	Descriptors index [10-15]	...
Aromatic [atoms/bonds]	Mordred	Descriptors index [16-17]	...
Number of [all/heavy/spiro] atoms	Mordred	Descriptors index [18-20]	...
Number of [\bridgehead/hetero] atoms	Mordred	Descriptors index [21-22]	...
Number of [\H/B/C/N/O/S/P/F/Cl/Br/I] atoms	Mordred	Descriptors index [23-33]	...
Number of halogen atoms	Mordred	Descriptors index 34	...
moreau-broto autocorrelation of lag [0-8] weighted by ...	Mordred	Descriptors index [35-133]	...
... valence electrons	Mordred	Descriptors index [35-43]	...
... sigma electrons	Mordred	Descriptors index [44-52]	...
... intrinsic state	Mordred	Descriptors index [53-61]	...
... atomic number	Mordred	Descriptors index [62-70]	...
... mass	Mordred	Descriptors index [71-79]	...
... vdw volume	Mordred	Descriptors index [80-88]	...
... sanderson EN	Mordred	Descriptors index [89-97]	...

Name	Reference	Computable	description
... pauling EN	Mordred	Descriptors index [98-106]	...
... allred-rocow EN	Mordred	Descriptors index [107-115]	...
... polarizability	Mordred	Descriptors index [116-124]	...
... ionization potential	Mordred	Descriptors index [125-133]	...
averaged moreau-broto autocorrelation of lag [0-8] weighted by ...	Mordred	Descriptors index [134-232]	...
... valence electrons	Mordred	Descriptors index [134-142]	...
... sigma electrons	Mordred	Descriptors index [143-151]	...
... intrinsic state	Mordred	Descriptors index [152-160]	...
... atomic number	Mordred	Descriptors index [161-169]	...
... mass	Mordred	Descriptors index [170-178]	...
... vdw volume	Mordred	Descriptors index [179-187]	...
... sanderson EN	Mordred	Descriptors index [188-196]	...
... pauling EN	Mordred	Descriptors index [197-205]	...
... allred-rocow EN	Mordred	Descriptors index [206-214]	...
... polarizability	Mordred	Descriptors index [215-223]	...
... ionization potential	Mordred	Descriptors index [224-232]	...
centered moreau-broto autocorrelation of lag [0-8] weighted by ...	Mordred	Descriptors index [233-340]	...
... gasteiger charge	Mordred	Descriptors index [233-340]	...
... valence electrons	Mordred	Descriptors index [242-250]	...
... sigma electrons	Mordred	Descriptors index [251-259]	...
... intrinsic state	Mordred	Descriptors index	...

Name	Reference	Computable	description
		[260-268]	
... atomic number	Mordred	Descriptors index [269-277]	...
... mass	Mordred	Descriptors index [278-286]	...
... vdw volume	Mordred	Descriptors index [287-295]	...
... sanderson EN	Mordred	Descriptors index [296-304]	...
... pauling EN	Mordred	Descriptors index [305-313]	...
... allred-rocow EN	Mordred	Descriptors index [314-322]	...
... polarizability	Mordred	Descriptors index [323-331]	...
... ionization potential	Mordred	Descriptors index [332-340]	...
averaged and centered moreau-broto autocorrelation of lag [0-8] weighted by ...	Mordred	Descriptors index [341-331]	...
... gasteiger charge	Mordred	Descriptors index [341-349]	...
... valence electrons	Mordred	Descriptors index [350-358]	...
... sigma electrons	Mordred	Descriptors index [359-367]	...
... intrinsic state	Mordred	Descriptors index [368-376]	...
... atomic number	Mordred	Descriptors index [377-385]	...
... mass	Mordred	Descriptors index [386-394]	...
... vdw volume	Mordred	Descriptors index [395-403]	...
... sanderson EN	Mordred	Descriptors index [404-412]	...
... pauling EN	Mordred	Descriptors index [413-421]	...
... allred-rocow EN	Mordred	Descriptors index [422-430]	...
... polarizability	Mordred	Descriptors index [431-439]	...

Name	Reference	Computable	description
... ionization potential	Mordred	Descriptors index [440-448]	...
moran coefficient of lag [1-8] weighted by ...	Mordred	Descriptors index [449-544]	...
... gasteiger charge	Mordred	Descriptors index [449-456]	...
... valence electrons	Mordred	Descriptors index [457-464]	...
... sigma electrons	Mordred	Descriptors index [465-472]	...
... intrinsic state	Mordred	Descriptors index [473-480]	...
... atomic number	Mordred	Descriptors index [481-488]	...
... mass	Mordred	Descriptors index [489-496]	...
... vdw volume	Mordred	Descriptors index [497-504]	...
... sanderson EN	Mordred	Descriptors index [505-512]	...
... pauling EN	Mordred	Descriptors index [513-520]	...
... allred-rocow EN	Mordred	Descriptors index [521-528]	...
... polarizability	Mordred	Descriptors index [529-536]	...
... ionization potential	Mordred	Descriptors index [537-544]	...
geary coefficient of lag [1-8] weighted by ...	Mordred	Descriptors index [545-640]	...
... gasteiger charge	Mordred	Descriptors index [545-562]	...
... valence electrons	Mordred	Descriptors index [553-560]	...
... sigma electrons	Mordred	Descriptors index [561-568]	...
... intrinsic state	Mordred	Descriptors index [569-576]	...
... atomic number	Mordred	Descriptors index [577-584]	...
... mass	Mordred	Descriptors index	...

Name	Reference	Computable	description
		[585-592]	
... vdw volume	Mordred	Descriptors index [593-600]	...
... sanderson EN	Mordred	Descriptors index [601-608]	...
... pauling EN	Mordred	Descriptors index [609-616]	...
... allred-rocow EN	Mordred	Descriptors index [617-624]	...
... polarizability	Mordred	Descriptors index [625-632]	...
... ionization potential	Mordred	Descriptors index [633-640]	...
first [heighest/lowest] eigenvalue of Burden matrix weighted by ...	Mordred	Descriptors index [545-640]	...
... gasteiger charge	Mordred	Descriptors index [641-642]	...
... valence electrons	Mordred	Descriptors index [643-644]	...
... sigma electrons	Mordred	Descriptors index [645-646]	...
... intrinsic state	Mordred	Descriptors index [647-648]	...
... atomic number	Mordred	Descriptors index [649-650]	...
... mass	Mordred	Descriptors index [651-652]	...
... vdw volume	Mordred	Descriptors index [653-654]	...
... sanderson EN	Mordred	Descriptors index [655-656]	...
... pauling EN	Mordred	Descriptors index [657-658]	...
... allred-rocow EN	Mordred	Descriptors index [659-660]	...
... polarizability	Mordred	Descriptors index [661-662]	...
... ionization potential	Mordred	Descriptors index [663-664]	...
Balaban's J index	Mordred	Descriptors index x	...

Name	Reference	Computable	description
0: graph energy ...	Mordred	Descriptors index x	...
1: leading eigenvalue ...	Mordred	Descriptors index x	...
2: spectral diamiter ...	Mordred	Descriptors index x	...
3: spectral absolute diviation ...	Mordred	Descriptors index x	...
4: spectral mean absolute diviation...	Mordred	Descriptors index x	...
5: Estrada-like index...	Mordred	Descriptors index x	...
6: spectral moment ...	Mordred	Descriptors index x	...
7: coefficient sum of the last eigenvector ...	Mordred	Descriptors index x	...
8: average coefficient of the last eigenvector ...	Mordred	Descriptors index x	...
9: logarithmic coefficient sum of the last eigenvector ...	Mordred	Descriptors index x	...
10: Randic-like eigenvector-based index ...	Mordred	Descriptors index x	...
11: normalized Randic-like eigenvector-based index ...	Mordred	Descriptors index x	...
12: logarithmic Randic-like eigenvector-based index ...	Mordred	Descriptors index x	...
... from Barysz matrix weighted by atomic number	Mordred	Descriptors index [666-678]	...
... from Barysz matrix weighted by mass	Mordred	Descriptors index [679-691]	...
... from Barysz matrix weighted by vdw volume	Mordred	Descriptors index [692-704]	...
... from Barysz matrix weighted by sanderson EN	Mordred	Descriptors index [705-717]	...
... from Barysz matrix weighted by pauling EN	Mordred	Descriptors index [718-730]	...
... from Barysz matrix weighted by allred-rocow EN	Mordred	Descriptors index [731-743]	...
... from Barysz matrix weighted by polarizability	Mordred	Descriptors index [744-756]	...
... from Barysz matrix weighted by ionization potential	Mordred	Descriptors index	...

Name	Reference	Computable	description
		[757-769]	
Bertz CT	Mordred	Descriptors index 770	...
number of all bonds in non-kekulized structure	Mordred	Descriptors index 771	...
number of bonds connecting to heavy atom in non-kekulized structure	Mordred	Descriptors index 772	...
number of [single/double/triple] bonds in non-kekulized structure	Mordred	Descriptors index [773-775]	...
number of [Aromatic/multiple] bonds in non-kekulized structure	Mordred	Descriptors index [776-777]	...
number of [single/double] bonds in kekulized structure	Mordred	Descriptors index [778-779]	...
partial negative surface area (version [1-5])	Mordred	Descriptors index [780-784]	...
partial positive surface area (version [1-5])	Mordred	Descriptors index [785-789]	...
difference in charged partial surface area (version [1-5])	Mordred	Descriptors index [790-794]	...
fractional charged partial negative surface area (version [1-5])	Mordred	Descriptors index [795-799]	...
fractional charged partial positive surface area (version [1-5])	Mordred	Descriptors index [800-804]	...
surface weighted charged partial negative surface area (version [1-5])	Mordred	Descriptors index [805-809]	...
surface weighted charged partial positive surface area (version [1-5])	Mordred	Descriptors index [810-814]	...
relative [negative/positive] charge	Mordred	Descriptors index [815-816]	...
relative [negative/positive] charge surface area	Mordred	Descriptors index [816-817]	...
total [hydrophobic/polar] surface area	Mordred	Descriptors index [818-819]	...
relative [hydrophobic/polar] surface area	Mordred	Descriptors index [820-821]	...
SP carbon bound to [1-2] other carbon	Mordred	Descriptors index [822-823]	...
SP2 carbon bound to [1-3] other carbon	Mordred	Descriptors index [824-825]	...
SP3 carbon bound to [1-4] other carbon	Mordred	Descriptors index [826-827]	...

Name	Reference	Computable	description
hybridization ratio	Mordred	Descriptors index 828	...
the fraction of C atoms that are SP3 hybridized	Mordred	Descriptors index 829	...
[3-7]-ordered Chi chain weighted by sigma electrons	Mordred	Descriptors index [834-838]	...
[3-7]-ordered Chi chain weighted by valence electrons	Mordred	Descriptors index [839-843]	...
[3-6]-ordered Chi cluster weighted by sigma electrons	Mordred	Descriptors index [844-847]	...
[3-6]-ordered Chi cluster weighted by valence electrons	Mordred	Descriptors index [848-851]	...
[4-6]-ordered Chi path-cluster weighted by sigma electrons	Mordred	Descriptors index [852-854]	...
[4-6]-ordered Chi path-cluster weighted by valence electrons	Mordred	Descriptors index [855-857]	...
[0-7]-ordered Chi path weighted by sigma electrons	Mordred	Descriptors index [858-865]	...
[0-7]-ordered averaged Chi path weighted by sigma electrons	Mordred	Descriptors index [866-873]	...
[0-7]-ordered Chi path weighted by sigma electrons	Mordred	Descriptors index [874-881]	...
[0-7]-ordered averaged Chi path weighted by valence electrons	Mordred	Descriptors index [882-889]	...
sum of constitutional weighted by ...	Mordred	Descriptors index [890-897]	...
... atomic number	Mordred	Descriptors index 890	...
... mass	Mordred	Descriptors index 891	...
... vdw volume	Mordred	Descriptors index 892	...
... sanderson EN	Mordred	Descriptors index 893	...
... pauling EN	Mordred	Descriptors index 894	...
... allred-rocow EN	Mordred	Descriptors index 895	...
... polarizability	Mordred	Descriptors index 896	...
... ionization potential	Mordred	Descriptors index	...

Name	Reference	Computable	description
		897	
mean of constitutional weighted by ...	Mordred	Descriptors index [898-905]	...
... atomic number	Mordred	Descriptors index 898	...
... mass	Mordred	Descriptors index 899	...
... vdw volume	Mordred	Descriptors index 900	...
... sanderson EN	Mordred	Descriptors index 893	...
... pauling EN	Mordred	Descriptors index 894	...
... allred-rocow EN	Mordred	Descriptors index 895	...
... polarizability	Mordred	Descriptors index 896	...
... ionization potential	Mordred	Descriptors index 897	...
... ionization potential	Mordred	Descriptors index 897	...
graph energy ...	Mordred	Descriptors index 906	...
leading eigenvalue ...	Mordred	Descriptors index 907	...
spectral diamiter ...	Mordred	Descriptors index 908	...
spectral absolute diviation ...	Mordred	Descriptors index 909	...
spectral mean absolute diviation...	Mordred	Descriptors index 910	...
Estrada-like index...	Mordred	Descriptors index 911	...
spectral moment ...	Mordred	Descriptors index 912	...
coefficient sum of the last eigenvector ...	Mordred	Descriptors index 913	...
average coefficient of the last eigenvector ...	Mordred	Descriptors index 914	...
logarithmic coefficient sum of the last eigenvector ...	Mordred	Descriptors index 915	...

Name	Reference	Computable	description
Randic-like eigenvector-based index ...	Mordred	Descriptors index 916	...
normalized Randic-like eigenvector-based index ...	Mordred	Descriptors index 917	...
logarithmic Randic-like eigenvector-based index ...	Mordred	Descriptors index 918	...
... from detourn matrix	Mordred	Descriptors index [906-918]	...
detour index	Mordred	Descriptors index 919	...
graph energy ...	Mordred	Descriptors index 920	...
leading eigenvalue ...	Mordred	Descriptors index 921	...
spectral diamiter ...	Mordred	Descriptors index 922	...
spectral absolute diviation ...	Mordred	Descriptors index 923	...
spectral mean absolute diviation...	Mordred	Descriptors index 924	...
Estrada-like index...	Mordred	Descriptors index 925	...
coefficient sum of the last eigenvector ...	Mordred	Descriptors index 926	...
average coefficient of the last eigenvector ...	Mordred	Descriptors index 927	...
logarithmic coefficient sum of the last eigenvector ...	Mordred	Descriptors index 928	...
Randic-like eigenvector-based index ...	Mordred	Descriptors index 929	...
normalized Randic-like eigenvector-based index ...	Mordred	Descriptors index 930	...
logarithmic Randic-like eigenvector-based index ...	Mordred	Descriptors index 931	...
... from detourn matrix	Mordred	Descriptors index [920-931]	...
number of [sLi/ssBe/ssssBe/ssBH/sssB/ssssB/sCH3/dCH2/ssCH2/tch]	Mordred	Descriptors index [932-941]	...
number of [dsCH/aaCH/sssCH/ddC/tsC/dssC/aasC/aaaC/ssssC/sNH3/sNH2]	Mordred	Descriptors index [942-952]	...
number of	Mordred	Descriptors index	...

Name	Reference	Computable	description
[ssNH2/dNH/ssNH/aaNH/tN/sssNH/dsN/aaN/sssN/ddsN/aasN]		[953-963]	
number of [ssssN/sOH/dO/ssO/aaO/sF/sSiH3/ssSiH2/sssSiH/ssssSi]	Mordred	Descriptors index [964-973]	...
number of [sPH2/ssPH/sssP/dsssP/ssssssP/sSH/dS/ssS/aaS/dssS/ddssS]	Mordred	Descriptors index [974-984]	...
number of [sCl/sGeH3/ssGeH2/sssGeH/ssssGe/sAsH2//ssAsH/sssAs]	Mordred	Descriptors index [985-992]	...
number of [sssdAs/sssssAs/sSeH/dSe/ssSe/aaSe/dssSe/ddssSe/sBr]	Mordred	Descriptors index [993-1001]	...
number of [sSnH3/ssSnH2/sssSnH/ssssSn/sI/sPbH3/ssPbH2/sssPbH/ssssPb]	Mordred	Descriptors index [1002-1010]	...
sum of [sLi/ssBe/ssssBe/ssBH/sssB/ssssB/sCH3/dCH2/ssCH2/tch]	Mordred	Descriptors index [1011-1020]	...
sum of [dsCH/aaCH/sssCH/ddC/tsC/dssC/aasC/aaaC/ssssC/sNH3/sNH2]	Mordred	Descriptors index [1021-1031]	...
sum of [ssNH2/dNH/ssNH/aaNH/tN/sssNH/dsN/aaN/sssN/ddsN/aasN]	Mordred	Descriptors index [1032-1042]	...
sum of [ssssN/sOH/dO/ssO/aaO/sF/sSiH3/ssSiH2/sssSiH/ssssSi]	Mordred	Descriptors index [1043-1052]	...
sum of [sPH2/ssPH/sssP/dsssP/ssssssP/sSH/dS/ssS/aaS/dssS/ddssS]	Mordred	Descriptors index [1053-1065]	...
sum of [sCl/sGeH3/ssGeH2/sssGeH/ssssGe/sAsH2//ssAsH/sssAs]	Mordred	Descriptors index [1066-1071]	...
sum of [sssdAs/sssssAs/sSeH/dSe/ssSe/aaSe/dssSe/ddssSe/sBr]	Mordred	Descriptors index [1072-1082]	...
sum of [sSnH3/ssSnH2/sssSnH/ssssSn/sI/sPbH3/ssPbH2/sssPbH/ssssPb]	Mordred	Descriptors index [1083-1090]	...
max of [sLi/ssBe/ssssBe/ssBH/sssB/ssssB/sCH3/dCH2/ssCH2/tch]	Mordred	Descriptors index [1090-1100]	...
max of [dsCH/aaCH/sssCH/ddC/tsC/dssC/aasC/aaaC/ssssC/sNH3/sNH2]	Mordred	Descriptors index [1101-1110]	...
max of [ssNH2/dNH/ssNH/aaNH/tN/sssNH/dsN/aaN/sssN/ddsN/aasN]	Mordred	Descriptors index [1111-1121]	...
max of [ssssN/sOH/dO/ssO/aaO/sF/sSiH3/ssSiH2/sssSiH/ssssSi]	Mordred	Descriptors index [1121-1131]	...
max of [sPH2/ssPH/sssP/dsssP/ssssssP/sSH/dS/ssS/aaS/dssS/ddssS]	Mordred	Descriptors index [1132-1142]	...
max of [sCl/sGeH3/ssGeH2/sssGeH/ssssGe/sAsH2//ssAsH/sssAs]	Mordred	Descriptors index [1143-1150]	...
max of [sssdAs/sssssAs/sSeH/dSe/ssSe/aaSe/dssSe/ddssSe/sBr]	Mordred	Descriptors index [1151-1159]	...

Name	Reference	Computable	description
max of [sSnH3/ssSnH2/sssSnH/ssssSn/sI/sPbH3/ssPbH2/sssPbH/ssssPb]	Mordred	Descriptors index [1160-1168]	...
min of [sLi/ssBe/ssssBe/ssBH/sssB/ssssB/sCH3/dCH2/ssCH2/tch]	Mordred	Descriptors index [1169-1178]	...
min of [dsCH/aaCH/sssCH/ddC/tsC/dssC/aasC/aaaC/ssssC/sNH3/sNH2]	Mordred	Descriptors index [1179-1189]	...
min of [ssNH2/dNH/ssNH/aaNH/tN/sssNH/dsN/aaN/sssN/ddsN/aasN]	Mordred	Descriptors index [1190-1200]	...
min of [ssssN/sOH/dO/ssO/aaO/sF/sSiH3/ssSiH2/sssSiH/ssssSi]	Mordred	Descriptors index [1202-1210]	...
min of [sPH2/ssPH/sssP/dsssP/ssssssP/sSH/dS/ssS/aaS/dssS/ddssS]	Mordred	Descriptors index [1211-1221]	...
min of [sCl/sGeH3/ssGeH2/sssGeH/ssssGe/sAsH2//ssAsH/sssAs]	Mordred	Descriptors index [1222-1229]	...
min of [sssdAs/sssssAs/sSeH/dSe/ssSe/aaSe/dssSe/ddssSe/sBr]	Mordred	Descriptors index [1230-1238]	...
min of [sSnH3/ssSnH2/sssSnH/ssssSn/sI/sPbH3/ssPbH2/sssPbH/ssssPb]	Mordred	Descriptors index [1239-1247]	...
eccentric connectivity index	Mordred	Descriptors index 1248	...
[/averaged] ETA core count	Mordred	Descriptors index [1249-1250]	ETA stands for Ethanolamine
ETA shape index (type: [p/y/x])	Mordred	Descriptors index [1251-1253]	ETA stands for Ethanolamine
...	Mordred	Descriptors index 1254	...
averaged ...	Mordred	Descriptors index 1255	...
sigma contribution to ...	Mordred	Descriptors index 1256	...
averaged sigma contribution to ...	Mordred	Descriptors index 1257	...
nonsigma contribution to ...	Mordred	Descriptors index 1258	...
averaged nonsigma contribution to ...	Mordred	Descriptors index 1259	...
delta contribution to ...	Mordred	Descriptors index 1260	...
averaged delta contribution to ...	Mordred	Descriptors index 1261	...
... valence electron mobile count	Mordred	Descriptors index	...

Name	Reference	Computable	description
		[1254-1261]	
[/averaged/local/averaged local] ETA composite index for reference graph	Mordred	Descriptors [index 1262-1269]	ETA stands for Ethanolamine
[/averaged/local/averaged local] ETA functionality index	Mordred	Descriptors [index 1270-1273]	ETA stands for Ethanolamine
[/averaged] ETA branching index [/(use ring count)]	Mordred	Descriptors [index 1274-1277]	ETA stands for Ethanolamine
ETA delta alpha (type: [A/B])	Mordred	Descriptors [index 1278-1279]	ETA stands for Ethanolamine
ETA epsilon (type: [1-5])	Mordred	Descriptors [index 1280-1284]	ETA stands for Ethanolamine
ETA delta epsilon (type: [A/B/C/D])	Mordred	Descriptors [index 1285-1288]	ETA stands for Ethanolamine
[/averaged] ETA delta beta	Mordred	Descriptors [index 1289-1290]	ETA stands for Ethanolamine
ETA psi	Mordred	Descriptors index 1291	ETA stands for Ethanolamine
ETA delta psi (type: [A/B])	Mordred	Descriptors [index 1292-1293]	ETA stands for Ethanolamine
fragment complexity	Mordred	Descriptors index 1294	...
molecular framework ratio	Mordred	Descriptors index 1295	...
geometric [diameter/radius]	Mordred	Descriptors [index 1296-1297]	...
[geometrical shape/geometric Petitjean] index	Mordred	Descriptors [index 1298-1299]	...
[heavy atom//heavy atom pair/pair] gravitational index	Mordred	Descriptors [index 1300-1303]	...
number of hydrogen bond [acceptor/donor]	Mordred	Descriptors [index 1304-1305]	...

Name	Reference	Computable	description
[0-5]-ordered neighborhood [/total] ...	Mordred	Descriptors [index 1306-1317]	...
[0-5]-ordered structural ...	Mordred	Descriptors [index 1318-1323]	...
[0-5]-ordered bonding ...	Mordred	Descriptors [index 1324-1329]	...
[0-5]-ordered complementary ...	Mordred	Descriptors [index 1330-1335]	...
[0-5]-ordered modified ...	Mordred	Descriptors [index 1336-1341]	...
[0-5]-ordered Z-modified ...	Mordred	Descriptors [index 1342-1347]	...
... information content	Mordred	Descriptors index [1306-1347]	...
kappa shape index [1-3]	Mordred	Descriptors [index 1348-1350]	...
Lipinski rule of five	Mordred	Descriptors index 1351	...
Ghose filter	Mordred	Descriptors index 1352	...
Filter-it™ LogS	Mordred	Descriptors index 1353	...
McGowan volume	Mordred	Descriptors index 1354	...
3D-MoRSE (distance = [1-32])	Mordred	Descriptors [index 1355-1386]	...
3D-MoRSE weighted by [mass/vdw volume](distance = [1-32])	Mordred	Descriptors [index 1387-1450]	...
3D-MoRSE weighted by [sanderson EN/polarizability](distance = [1-32])	Mordred	Descriptors [index 1451-1514]	...
Labute's Approximate Surface Area	Mordred	Descriptors index 1515	...
MOE Charge VSA Descriptor [1-13] ...	Mordred	Descriptors [index 1516-	...

Name	Reference	Computable	description
		1528]	
... (-inf < x <-0.3)	Mordred	Descriptors index 1516	...
... (-0.3 <= x <-0.25)	Mordred	Descriptors index 1517	...
... (-0.25 <= x <-0.2)	Mordred	Descriptors index 1518	...
MOE MR VSA Descriptor [1-9] ...	Mordred	Descriptors [index 1529-1537]	...
... (-inf < x < 1.29)	Mordred	Descriptors index 1529	...
... (1.29 <= x < 1.82)	Mordred	Descriptors index 1530	...
... (1.82 <= x < 2.24)	Mordred	Descriptors index 1531	...
... (2.24 <= x < 2.45)	Mordred	Descriptors index 1532	...
... (2.45 <= x < 2.75)	Mordred	Descriptors index 1533	...
... (2.75 <= x < 3.05)	Mordred	Descriptors index 1534	...
... (3.05 <= x < 3.63)	Mordred	Descriptors index 1535	...
... (3.63 <= x < 3.80)	Mordred	Descriptors index 1536	...
... (3.80 <= x < 4.00)	Mordred	Descriptors index 1537	...
MOE logP VSA Descriptor [1-11] ...	Mordred	Descriptors [index 1538-1548]	...
... (-inf < x < -0.40)	Mordred	Descriptors index 1538	...
... (-0.40 <= x < -0.20)	Mordred	Descriptors index 1539	...
... (-0.20 <= x < 0.00)	Mordred	Descriptors index 1540	...
... (0.00 <= x < 0.10)	Mordred	Descriptors index 1541	...
... (0.10 <= x < 0.15)	Mordred	Descriptors index 1542	...

Name	Reference	Computable	description
... (0.15 <= x < 0.20)	Mordred	Descriptors index 1543	...
... (0.20 <= x < 0.25)	Mordred	Descriptors index 1544	...
... (0.25 <= x < 0.30)	Mordred	Descriptors index 1545	...
... (0.30 <= x < 0.40)	Mordred	Descriptors index 1546	...
... (0.40 <= x < 0.50)	Mordred	Descriptors index 1547	...
... (0.50 <= x < 0.60)	Mordred	Descriptors index 1548	...
EState VSA Descriptor [1-10] ...	Mordred	Descriptors [index 1549-1558]	...
... (-inf < x < -0.39)	Mordred	Descriptors index 1549	...
... (-0.39 <= x < -0.29)	Mordred	Descriptors index 1550	...
... (-0.29 <= x < 0.72)	Mordred	Descriptors index 1551	...
... (0.72 <= x < 1.17)	Mordred	Descriptors index 1552	...
... (1.17 <= x < 1.54)	Mordred	Descriptors index 1553	...
... (1.54 <= x < 1.81)	Mordred	Descriptors index 1554	...
... (1.81 <= x < 2.05)	Mordred	Descriptors index 1555	...
... (2.05 <= x < 4.69)	Mordred	Descriptors index 1556	...
... (4.69 <= x < 9.17)	Mordred	Descriptors index 1557	...
... (9.17 <= x < 15.00)	Mordred	Descriptors index 1558	...
VSA EState Descriptor [1-9] ...	Mordred	Descriptors [index 1559-1567]	...
... (-inf < x < 4.78)	Mordred	Descriptors index 1559	...
... (4.78 <= x < 5.00)	Mordred	Descriptors index 1560	...

Name	Reference	Computable	description
... (5.00 <= x < 5.41)	Mordred	Descriptors index 1561	...
... (5.41 <= x < 5.74)	Mordred	Descriptors index 1562	...
... (5.74 <= x < 6.00)	Mordred	Descriptors index 1563	...
... (6.00 <= x < 6.07)	Mordred	Descriptors index 1564	...
... (6.07 <= x < 6.45)	Mordred	Descriptors index 1565	...
... (6.45 <= x < 7.00)	Mordred	Descriptors index 1566	...
... (7.00 <= x < 11.00)	Mordred	Descriptors index 1567	...
molecular distance edge between ...	Mordred	Descriptors [index 1568-1586]	...
... primary C and [primary C/secondary C/tertiary C/quaternary C]	Mordred	Descriptors [index 1568-1571]	...
... secondary C and [secondary C/tertiary C/quaternary C]	Mordred	Descriptors [index 1572-1574]	...
... tertiary C and [tertiary C/quaternary C]	Mordred	Descriptors [index 1575-1576]	...
... quaternary C and quaternary C	Mordred	Descriptors index 1577	...
... primary O and [primary O/secondary O]	Mordred	Descriptors [index 1578-1579]	...
... secondary O and secondary O	Mordred	Descriptors index 1580	...
... primary N and [primary N/secondary N/tertiary N]	Mordred	Descriptors [index 1581-1583]	...
... secondary N and [secondary N/tertiary N]	Mordred	Descriptors [index 1584-1585]	...
... tertiary N and tertiary N	Mordred	Descriptors index 1586	...
[/averaged] molecular ID [/on [H/C/N/O] atoms]	Mordred	Descriptors [index 1587-	...

Name	Reference	Computable	description
		1598]	
moment of inertia (axis = [X/Y/Z])	Mordred	Descriptors [index 1599-1601]	...
PBF	Mordred	Descriptors index 1602	...
[2-10]-ordred patch count	Mordred	Descriptors [index 1603-1611]	...
10-ordred total patch count	Mordred	Descriptors index 1612	...
Marsili/Gasteiger partial charges	RDKit		Electron Distribution
BalabanJ	RDKit	Graphdescriptor module	Atom indexing in molecule
BertzCT	RDKit	Graphdescriptor module	Tuple of two numbers. First number is correlated with complexity of bonds, second number is correlated with complexity of the distribution of heteroatoms.
IPC	RDKit	Graphdescriptor module	This returns the information content of the coefficients of the characteristic polynomial of the adjacency matrix of a hydrogen-suppressed graph of a molecule.
Kappa [1-3]	RDKit	Graphdescriptor module	Hallkier Kappa values. Note that these are NOT broken.
Phi	RDKit	NC	Kier Phi value for a molecule From Quantitative Structure-Activity Relationships

Name	Reference	Computable	description
Chi0n - Chi4n	RDKit	Graphdescriptor module	Similar to Hall Kier ChiXv, but uses nVal instead of valence.\ This makes a big difference after we get out of the first row.
Chi0v - Chi4v	RDKit	Graphdescriptor module	From equations (5),(9) and (10) of Rev. Comp. Chem. vol 2, 367-422, (1991)
MolLogP	RDKit	Crippen module	Wildman-Crippen LogP for a molecule
MolMR	RDKit	Crippen module	Wildman-Crippen MR for a molecule
MolWT	RDKit	Descriptors module	Sum of atomic weights in the molecule
ExactMolWT	RDKit	Descriptors module	More accurate molecular weight
Heavy Atom count	RDKit	Lipinski module	Counter of atoms with atomic weight above some threshold in the molecule
Heavy Atom MolWT	RDKit	Descriptors module	We assume this means the the ratio between the sum of heavy atom weights and the weight of the whole molecule
NHOH group count	RDKit	Lipinski module	Counts the number of NHOH groups in the molecule
NOCount	RDKit	Descriptors module	Nitrogen Oxide Grp counter
NumHAcceptors	RDKit	Lipinski module	The number of proton acceptors in the molecule

Name	Reference	Computable	description
NumHDonators	RDKit	Lipinski module	Number of bonds in the molecule that are weak enough to give off a proton.
NumHeteroatoms	RDKit	Lipinski module	Number of atoms that are NOT carbon or hydrogen
NumRotatableBonds	RDKit	Lipinski module	Counter of bonds in the molecule that can rotate. Usually single electron bonds.
NumValenceElectrons	RDKit	Descriptors module	Number of electrons in the outer most shell of an atom modulo 8.
NumAmideBonds	RDKit	NC	Amide bond counter. Google what an amide is.
NumAromaticRings	RDKit	Lipinski	Usually something like a benzene ring with delocalized electrons.
Num{Saturated,Aliphatic}Rings	RDKit	NC	Usually something like a benzene ring with delocalized electrons.
RingCount	RDKit	Lipinski module	Counter of cyclical rings in molecule
FractionCSP3	RDKit	NC	The fraction of C atoms that are SP3 hybridized
NumSpiroAtoms	RDKit	NC	Atoms shared between rings that share exactly one atom
NumBridgeheadAtoms	RDKit	NC	atoms shared between rings that share at least two bonds

Name	Reference	Computable	description
TPSA	RDKit	MolSurf module	Topological Polar Surface Area
LabuteASA	RDKit	MolSurf module	Accessible Surface Area to a solvent
PEOE_VSA [1-14]	RDKit	MolSurf module	Acronym explanation: Partial Equalization of Orbital Electronegativity and Volume, Area and Shape
SMR_VSA [1-10]	RDKit	MolSurf module	Surface-Weighted Mean Refractivity. Captures information related to the polarizability
SlogP_VSA [1-12]	RDKit	MolSurf module	the SlogP_VSA descriptors help us understand how a molecule's lipophilicity influences its behavior, especially in terms of interactions with other molecules or surfaces
EState_VSA [1-11]	RDKit	EState.EState_VSA	Used to describe the electronic state of a molecule.
MQNs	RDKit	NC	Molecular Quantum Numbers
Topliss fragments	RDKit	NC	Could not find a good description for this descriptor
Autocorr2D	RDKit	NC	From Todeschini and Consoni "Descriptors from Molecular Geometry"

Name	Reference	Computable	description
			Handbook of Chemoinformatics
BCUT2D	RDKit	NC	From Pearlman and Smith in “3D-QSAR and Drug design: Recent Advances” (1997)
fr_Al_COO	RDKit	fragments module	Number of aliphatic carboxylic acids
fr_Al_OH	RDKit	fragments module	Number of aliphatic hydroxyl groups
fr_Al_OH_noTert	RDKit	fragments module	Number of aliphatic hydroxyl groups excluding tert-OH
fr_ArN	RDKit	fragments module	Number of N functional groups attached to aromatics
fr_Ar_COO	RDKit	fragments module	Number of Aromatic carboxylic acide
fr_Ar_N	RDKit	fragments module	Number of aromatic nitrogens
fr_Ar_NH	RDKit	fragments module	Number of aromatic amines
fr_Ar_OH	RDKit	fragments module	Number of aromatic hydroxyl groups
fr_COO	RDKit	fragments module	Number of carboxylic acids
fr_COO2	RDKit	fragments module	Number of carboxylic acids
fr_C_O	RDKit	fragments module	Number of carbonyl O
fr_C_O_noCOO	RDKit	fragments module	Number of carbonyl O, excluding COOH
fr_C_S	RDKit	fragments module	Number of thiocarbonyl

Name	Reference	Computable	description
fr_HOCCN	RDKit	fragments module	Number of C(OH)CCN-Ctert-alkyl or C(OH)CCNcyclic
fr_Imine	RDKit	fragments module	Number of Imines
fr_NH0	RDKit	fragments module	Number of Tertiary amines
fr_NH1	RDKit	fragments module	Number of Secondary amines
fr_NH2	RDKit	fragments module	Number of Primary amines
fr_N_O	RDKit	fragments module	Number of hydroxylamine groups
fr_Ndealkylation1	RDKit	fragments module	Number of XCCNR groups
fr_Ndealkylation2	RDKit	fragments module	Number of tert-alicyclic amines (no heteroatoms, not quinine-like bridged N)
fr_Nhpyrrole	RDKit	fragments module	Number of H-pyrrole nitrogens
fr_SH	RDKit	fragments module	Number of thiol groups
fr_aldehyde	RDKit	fragments module	Number of aldehydes
fr_alkyl_carbamate	RDKit	fragments module	Number of alkyl carbamates (subject to hydrolysis)
fr_alkyl_halide	RDKit	fragments module	Number of alkyl halides
fr_allylic_oxid	RDKit	fragments module	Number of allylic oxidation sites excluding steroid dienone
fr_amide	RDKit	fragments module	Number of amides
fr_amidine	RDKit	fragments module	Number of amidine groups
fr_aniline	RDKit	fragments	Number of

Name	Reference	Computable	description
		module	anilines
fr_aryl_methyl	RDKit	fragments module	Number of aryl methyl sites for hydroxylation
fr_azide	RDKit	fragments module	Number of azide groups
fr_azo	RDKit	fragments module	Number of azo groups
fr_barbitur	RDKit	fragments module	Number of barbiturate groups
fr_benzene	RDKit	fragments module	Number of benzene rings
fr_benzodiazepine	RDKit	fragments module	Number of benzodiazepines with no additional fused rings
fr_bicyclic	RDKit	fragments module	Bicyclic
fr_diazo	RDKit	fragments module	Number of diazo groups
fr_dihydropyridine	RDKit	fragments module	Number of dihydropyridines
fr_epoxide	RDKit	fragments module	Number of epoxide rings
fr_ester	RDKit	fragments module	Number of esters
fr_ether	RDKit	fragments module	Number of ether oxygens (including phenoxy)
fr_furan	RDKit	fragments module	Number of furan rings
fr_guanido	RDKit	fragments module	Number of guanidine groups
fr_halogen	RDKit	fragments module	Number of halogens
fr_hdrzine	RDKit	fragments module	Number of hydrazine groups
fr_hdrzone	RDKit	fragments module	Number of hydrazone groups
fr_imidazole	RDKit	fragments module	Number of imidazole rings

Name	Reference	Computable	description
fr_imide	RDKit	fragments module	Number of imide groups
fr_isocyan	RDKit	fragments module	Number of isocyanates
fr_isothiocyan	RDKit	fragments module	Number of isothiocyanates
fr_ketone	RDKit	fragments module	Number of ketones
fr_ketone_Topliss	RDKit	fragments module	Number of ketones excluding diaryl, a,b-unsat. dienones, heteroatom on Calpha
fr_lactam	RDKit	fragments module	Number of beta lactams
fr_lactone	RDKit	fragments module	Number of cyclic esters (lactones)
fr_methoxy	RDKit	fragments module	Number of methoxy groups - OCH3
fr_morpholine	RDKit	fragments module	Number of morpholine rings
fr_nitrile	RDKit	fragments module	Number of nitriles
fr_nitro	RDKit	fragments module	Number of nitro groups
fr_nitro_arom	RDKit	fragments module	Number of nitro benzene ring substituents
fr_nitro_arom_nonortho	RDKit	fragments module	Number of non-ortho nitro benzene ring substituents
fr_nitroso	RDKit	fragments module	Number of nitroso groups, excluding NO2
fr_oxazole	RDKit	fragments module	Number of oxazole rings
fr_oxime	RDKit	fragments module	Number of oxime groups
fr_para_hydroxylation	RDKit	fragments module	Number of para-hydroxylation

Name	Reference	Computable	description
			sites
fr_phenol	RDKit	fragments module	Number of phenols
fr_phenol_noOrthoHbond	RDKit	fragments module	Number of phenolic OH excluding ortho intramolecular Hbond substituents
fr_phos_acid	RDKit	fragments module	Number of phosphoric acid groups
fr_phos_ester	RDKit	fragments module	Number of phosphoric ester groups
fr_piperdine	RDKit	fragments module	Number of piperdine rings
fr_piperzine	RDKit	fragments module	Number of piperzine rings
fr_priamide	RDKit	fragments module	Number of primary amides
fr_prisulfonamd	RDKit	fragments module	Number of primary sulfonamides
fr_pyridine	RDKit	fragments module	Number of pyridine rings
fr_quatN	RDKit	fragments module	Number of quaternary nitrogens
fr_sulfide	RDKit	fragments module	Number of thioether
fr_sulfonamd	RDKit	fragments module	Number of sulfonamides
fr_sulfone	RDKit	fragments module	Number of sulfone groups
fr_term_acetylene	RDKit	fragments module	Number of terminal acetylenes
fr_tetrazole	RDKit	fragments module	Number of tetrazole rings
fr_thiazole	RDKit	fragments module	Number of thiazole rings

Name	Reference	Computable	description
fr_thiocyan	RDKit	fragments module	Number of thiocyanates
fr_thiophene	RDKit	fragments module	Number of thiophene rings
fr_unbrch_alkane	RDKit	fragments module	Number of unbranched alkanes of at least 4 members (excludes halogenated alkanes)
fr_urea	RDKit	fragments module	Number of urea groups
Dipole moment	PyG, MolNet	Not included	...
Isotrope polarizability	PyG, MolNet	Not included	...
Highest occupied molecular orbital energy	PyG, MolNet	...	...
Lowest unoccupied molecular orbital energy	PyG, MolNet	...	...
HOMO-LUMO gap	PyG, MolNet	...	...
Electronic spatial extent	PyG, MolNet	...	...
Zero point vibration energy	PyG, MolNet	autodE/ORCA	...
Internal energy at 0K	PyG, MolNet	...	...
Internal energy at 298.15K	PyG, MolNet	autodE/ORCA	...
Enthalpy at 298.15K	PyG, MolNet	autodE/ORCA	...
Free energy at 298.15K	PyG, MolNet	autodE/ORCA	...
Heat capavity at 298.15K	PyG, MolNet	...	...
Atomization energy at 0K	PyG, MolNet	...	...
Atomization energy at 298.15K	PyG, MolNet	...	...
Atomization enthalpy at 298.15K	PyG,	...	...

Name	Reference	Computable	description
	MolNet		
Atomization free energy at 298.15K	PyG, MolNet	...	...