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]	...

Name	Reference	Computable	description
... mass	Mordred	[Descriptors] index [71-79]	...
... vdw volume	Mordred	[Descriptors] index [80-88]	...
... sanderson EN	Mordred	[Descriptors] index [89-97]	...
... 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]	...

Name	Reference	Computable	description
... 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 [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]	...

Name	Reference	Computable	description
... 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]	...
... ionization potential	Mordred	[Descriptors] index [440-448]	...

Name	Reference	Computable	description
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]	...

Name	Reference	Computable	description
... 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 [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]	...

Name	Reference	Computable	description
... 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	...
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	...

Name	Reference	Computable	description
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 [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]	...

Name	Reference	Computable	description
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]	...
hybridization ratio	Mordred	[Descriptors] index 828	...

Name	Reference	Computable	description
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	...

Name	Reference	Computable	description
... 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	...
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	...

Name	Reference	Computable	description
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	...
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	...

Name	Reference	Computable	description
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]	...

Name	Reference	Computable	description
number of [ssNH2/dNH/ssNH/aaNH/tN/sssNH/dsN/aaN/sssN/ddsN/aasN]	Mordred	[Descriptors] index [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]	...

Name	Reference	Computable	description
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]	...
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]	...

Name	Reference	Computable	description
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 [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

Name	Reference	Computable	description
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]	...
[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]	...

Name	Reference	Computable	description
[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 1516-1528]	...
... (-inf < x <-0.3)	Mordred	[Descriptors] index 1516	...

Name	Reference	Computable	description
... (-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	...

Name	Reference	Computable	description
... (-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	...
... (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	...

Name	Reference	Computable	description
... (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	...
... (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	...

Name	Reference	Computable	description
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 1587-1598]	...
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

Name	Reference	Computable	description
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
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
NumHDonators	RDKit	Lipinski module	Number of bonds in the molecule that are weak enough to give off a proton.

Name	Reference	Computable	description
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.
Num{Aromatic,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
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” 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

Name	Reference	Computable	description
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
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

Name	Reference	Computable	description
fr_amide	RDKit	fragments module	Number of amides
fr_amidine	RDKit	fragments module	Number of amidine groups
fr_aniline	RDKit	fragments module	Number of 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
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

Name	Reference	Computable	description
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 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
fr_thiocyan	RDKit	fragments module	Number of thiocyanates

Name	Reference	Computable	description
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	...	...

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

[Descriptors]: Calculator(descriptors, ignore_3D=False).descriptors