2020/11/09

株式会社アフィニティサイエンス

ParaSurf 20 で計算可能な記述子一覧

No	Descriptor	Description	Symbol in CSV file
1	μ	Dipole moment	**dipole**
2	μ^D	Dipolar density	**dipden**
3	α	Molecular electronic polarisabilty	**polarizability**
4	MW	Molecular weight	**MWt**
5	G	Globularity	**globularity**
6	A	Molecular surface area	**totalarea**
7	VOL	Molecular volume	**volume**
8	V_{max}	Maximum (most positive) MEP	**MEPmax**
9	V_{min}	Minimum (most negative) MEP	**MEPmin**
10	$\bar{V}_+$	Mean of the positive MEP values	**meanMEP+**
11	$\bar{V}_-$	Mean of the negative MEP values	**meanMEP-**
12	$\bar{V}$	Mean of all MEP values	**meanMEP**
13	ΔV	MEP-range	**MEP-range**
14	σ_+^2	Total variance in the positive MEP values	**MEPvar+**
15	σ_-^2	Total variance in the negative MEP values	**MEPvar-**
16	σ_{tot}^2	Total variance in the MEP	**MEPvartot**
17	ν	MEP balance parameter	**MEPbalance**
18	$\sigma_{tot}^2\nu$	Product of the total variance in the MEP and the balance parameter	**var*balance**
19	γ_1^V	Skewness of the MEP-distribution	**MEPskew**
20	γ_2^V	Kurtosis of the MEP-distribution	**MEPkurt**
21	$\int_V$	Integrated MEP over the surface	**MEPint**
22	IE_L^{max}	Maximum value of the local ionization energy	**IELmax**
23	IE_L^{min}	Minimum value of the local ionization energy	**IELmin**
24	$\overline{IE_L}$	Mean value of the local ionization energy	**IELbar**
25	ΔIE_L	Range of the local ionization energy	**IELrange**
26	σ_{IE}^2	Variance in the local ionization energy	**IELvar**
27	$\gamma_1^{IE_L}$	Skewness of the local ionization energy distribution	**IELskew**
28	$\gamma_2^{IE_L}$	Kurtosis of the local ionization energy distribution	**IELkurt**

29	$\int_{IE_L}$	Integrated local ionization energy over the surface	**IELint**
30	EA_L^{max}	Maximum of the local electron affinity	**EALmax**
31	EA_L^{min}	Minimum of the local electron affinity	**EALmin**
32	$\overline{EA_{L+}}$	Mean of the positive values of the local electron affinity	**EALbar+**
33	$\overline{EA_{L-}}$	Mean of the negative values of the local electron affinity	**EALbar-**
34	$\overline{EA_L}$	Mean value of the local electron affinity	**EALbar**
35	ΔEA_L	Range of the local electron affinity	**EALrange**
36	σ_{EA+}^2	Variance in the local electron affinity for all positive values	**EALvar+**
37	σ_{EA-}^2	Variance in the local electron affinity for all negative values	**EALvar-**
38	σ_{EAtot}^2	Sum of the positive and negative variances in the local electron affinity	**EALvartot**
39	ν_{EA}	Local electron affinity balance parameter	**EALbalance**
40	δA_{EA}^+	Fraction of the surface area with positive local electron affinity	**EALfraction+**
41	A_{EA}^+	Surface area with positive local electron affinity	**EALarea+**
42	$\gamma_1^{EA_L}$	Skewness of the local electron affinity distribution	**EALskew**
43	$\gamma_2^{EA_L}$	Kurtosis of the local electron affinity distribution	**EALkurt**
44	$\int_{EA_L}$	Integrated local electron affinity over the surface	**EALint**
45	α_L^{max}	Maximum value of the local polarizability	**POLmax**
46	α_L^{min}	Minimum value of the local polarizability	**POLmin**
47	$\overline{\alpha_L}$	Mean value of the local polarizability	**POLbar**
48	$\Delta\alpha_L$	Range of the local polarizability	**POLrange**
49	σ_α^2	Variance in the local polarizability	**POLvar**
50	$\gamma_1^{\alpha_L}$	Skewness of the local polarizability distribution	**POLskew**
51	$\gamma_2^{\alpha_L}$	Kurtosis of the local polarizability distribution	**POLkurt**
52	$\int_{\alpha_L}$	Integrated local polarizability over the surface	**POLint**
53	χ_L^{max}	Maximum value of the local electronegativity	**ENEGmax**
54	χ_L^{min}	Minimum value of the local electronegativity	**ENEGmin**
55	$\overline{\chi_L}$	Mean value of the local electronegativity	**ENEGbar**
56	$\Delta\chi_L$	Range of the local electron electronegativity	**ENEGrange**
57	σ_χ^2	Variance in the local electronegativity	**ENEGvar**
58	$\gamma_1^{\chi_L}$	Skewness of the local electronegativity distribution	**ENEGskew**
59	$\gamma_2^{\chi_L}$	Kurtosis of the local electronegativity distribution	**ENEGkurt**

60	$\int_{\chi_L}$	Integrated local electronegativity over the surface	**ENEGint**
61	η_L^{max}	Maximum value of the local hardness	**HARDmax**
62	η_L^{min}	Minimum value of the local hardness	**HARDmin**
63	$\overline{\eta_L}$	Mean value of the local hardness	**HARDbar**
64	$\Delta\eta_L$	Range of the local electron hardness	**HARDrange**
65	σ_η^2	Variance in the local hardness	**HARDvar**
66	$\gamma_1^{\eta_L}$	Skewness of the local hardness distribution	**HARDskew**
67	$\gamma_2^{\eta_L}$	Kurtosis of the local hardness distribution	**HARDkurt**
68	$\int_{\eta_L}$	Integrated local hardness over the surface	**HARDint**
69	F_N^{max}	Maximum value of the electrostatic field normal to the surface	**FNmax**
70	F_N^{min}	Minimum value of the field normal to the surface	**FNmin**
71	$\overline{F_L}$	Mean value of the field normal to the surface	**FNmean**
72	σ_F^2	Variance in field normal to the surface	**FNvartot**
73	σ_{F+}^2	Variance in the field normal to the surface for all positive values	**FNvar+**
74	σ_{F-}^2	Variance in the field normal to the surface for all negative values	**FNvar-**
75	ν_F	Normal field balance parameter	**FNbal**
76	$\gamma_1^{F_N}$	Skewness of the field normal to the surface	**FNskew**
77	$\gamma_2^{F_N}$	Kurtosis of the field normal to the surface	**FNkurt**
78	$\int_{F_N}$	Integrated field normal to the surface over the surface	**FNint**
79	$\int_{F_N}^{+}$	Integrated field normal to the surface over the surface for all positive values	**FN+**
80	$\int_{F_N}^{-}$	Integrated field normal to the surface over the surface for all negative values	**FN-**
81	$\int_{\lvert F_N\rvert}$	Integrated absolute field normal to the surface over the surface	**FNabs**

Additionally if the Shannon Entropy is calculated			
i	H_{in}^{max}	Maximum value of the internal Shannon Entropy	**SHANImax**
ii	H_{in}^{min}	Minimum value of the internal Shannon Entropy	**SHANImin**
iii	$\overline{H_{in}}$	Mean value of the internal Shannon Entropy	**SHANIbar**
iv	$\sigma_{H_{in}}^2$	Variance in the internal Shannon Entropy	**SHANIvar**
v	$\int_{H_{in}}$	Integrated internal Shannon Entropy over the surface	**SHANItot**
And if the external Shannon Entropy is available			
vi	H_{ex}^{max}	Maximum value of the external Shannon Entropy	**SHANEmax**
vii	H_{ex}^{min}	Minimum value of the external Shannon Entropy	**SHANEmin**
viii	$\overline{H_{ex}}$	Mean value of the external Shannon Entropy	**SHANEbar**
ix	$\sigma_{H_{ex}}^2$	Variance in the external Shannon Entropy	**SHANEvar**
x	$\int_{H_{ex}}$	Integrated internal Shannon Entropy over the surface	**SHANEtot**