

DRAGON Plus version - No. of variables: 1497

No.	Rel.No.	Symbol	Definition	Class
1	1	MW	molecular weight	constitutional descriptors
2	2	AMW	average molecular weight	constitutional descriptors
3	3	Sv	sum of atomic van der Waals volumes (scaled on Carbon atom)	constitutional descriptors
4	4	Se	sum of atomic Sanderson electronegativities (scaled on Carbon atom)	constitutional descriptors
5	5	Sp	sum of atomic polarizabilities (scaled on Carbon atom)	constitutional descriptors
6	6	Ss	sum of Kier-Hall electrotopological states	constitutional descriptors
7	7	Mv	mean atomic van der Waals volume (scaled on Carbon atom)	constitutional descriptors
8	8	Me	mean atomic Sanderson electronegativity (scaled on Carbon atom)	constitutional descriptors
9	9	Mp	mean atomic polarizability (scaled on Carbon atom)	constitutional descriptors
10	10	Ms	mean electrotopological state	constitutional descriptors
11	11	nAT	number of atoms	constitutional descriptors
12	12	nSK	number of non-H atoms	constitutional descriptors
13	13	nBT	number of bonds	constitutional descriptors
14	14	nBO	number of non-H bonds	constitutional descriptors
15	15	nBM	number of multiple bonds	constitutional descriptors
16	16	SCBO	sum of conventional bond orders (H-depleted)	constitutional descriptors
17	17	nCIC	number of rings	constitutional descriptors
18	18	nCIR	number of circuits	constitutional descriptors
19	19	RBN	number of rotatable bonds	constitutional descriptors
20	20	RBF	rotatable bond fraction	constitutional descriptors
21	21	nDB	number of double bonds	constitutional descriptors
22	22	nTB	number of triple bonds	constitutional descriptors
23	23	nAB	number of aromatic bonds	constitutional descriptors
24	24	nH	number of Hydrogen atoms	constitutional descriptors
25	25	nC	number of Carbon atoms	constitutional descriptors
26	26	nN	number of Nitrogen atoms	constitutional descriptors
27	27	nO	number of Oxygen atoms	constitutional descriptors
28	28	nP	number of Phosphorous atoms	constitutional descriptors
29	29	nS	number of Sulfur atoms	constitutional descriptors
30	30	nF	number of Fluorine atoms	constitutional descriptors
31	31	nCL	number of Chlorine atoms	constitutional descriptors
32	32	nBR	number of Bromine atoms	constitutional descriptors
33	33	nI	number of Iodine atoms	constitutional descriptors
34	34	nB	number of Boron atoms	constitutional descriptors
35	35	nHM	number of heavy atoms	constitutional descriptors
36	36	nX	number of halogen atoms	constitutional descriptors
37	37	nR03	number of 3-membered rings	constitutional descriptors

No.	Rel.No.	Symbol	Definition	Class
38	38	nR04	number of 4-membered rings	constitutional descriptors
39	39	nR05	number of 5-membered rings	constitutional descriptors
40	40	nR06	number of 6-membered rings	constitutional descriptors
41	41	nR07	number of 7-membered rings	constitutional descriptors
42	42	nR08	number of 8-membered rings	constitutional descriptors
43	43	nR09	number of 9-membered rings	constitutional descriptors
44	44	nR10	number of 10-membered rings	constitutional descriptors
45	45	nR11	number of 11-membered rings	constitutional descriptors
46	46	nR12	number of 12-membered rings	constitutional descriptors
47	47	nBnz	number of benzene-like rings	constitutional descriptors
48	1	ISIZ	information index on molecular size	topological descriptors
49	2	IAC	total information index of atomic composition	topological descriptors
50	3	AAC	mean information index on atomic composition	topological descriptors
51	4	ZM1	first Zagreb index M1	topological descriptors
52	5	ZM1V	first Zagreb index by valence vertex degrees	topological descriptors
53	6	ZM2	second Zagreb index M2	topological descriptors
54	7	ZM2V	second Zagreb index by valence vertex degrees	topological descriptors
55	8	Qindex	Quadratic index	topological descriptors
56	9	SNar	Narumi simple topological index (log)	topological descriptors
57	10	HNar	Narumi harmonic topological index	topological descriptors
58	11	GNar	Narumi geometric topological index	topological descriptors
59	12	Xt	Total structure connectivity index	topological descriptors
60	13	Dz	Pogliani index	topological descriptors
61	14	Ram	ramification index	topological descriptors
62	15	Pol	polarity number	topological descriptors
63	16	LPRS	log of product row sums (PRS)	topological descriptors
64	17	VDA	average vertex distance degree	topological descriptors
65	18	MSD	mean square distance index (Balaban)	topological descriptors
66	19	SMTI	Schultz Molecular Topological Index (MTI)	topological descriptors
67	20	SMTIV	Schultz MTI by valence vertex degrees	topological descriptors
68	21	GMTI	Gutman Molecular Topological Index	topological descriptors
69	22	GMTIV	Gutman MTI by valence vertex degrees	topological descriptors
70	23	Xu	Xu index	topological descriptors
71	24	SPI	superpendentic index	topological descriptors
72	25	W	Wiener W index	topological descriptors
73	26	WA	mean Wiener index	topological descriptors
74	27	RDSUM	reciprocal distance Wiener-type index	topological descriptors
75	28	Har	Harary H index	topological descriptors
76	29	QW	quasi-Wiener index (Kirchhoff number)	topological descriptors

No.	Rel.No.	Symbol	Definition	Class
77	30	Tl1	first Mohar index Tl1	topological descriptors
78	31	Tl2	second Mohar index Tl2	topological descriptors
79	32	HyDp	hyper-distance-path index	topological descriptors
80	33	RHyDp	reciprocal hyper-distance-path index	topological descriptors
81	34	w	detour index	topological descriptors
82	35	ww	hyper-detour index	topological descriptors
83	36	Rww	reciprocal hyper-detour index	topological descriptors
84	37	D/D	distance/detour index	topological descriptors
85	38	Wap	all-path Wiener index	topological descriptors
86	39	WhetZ	Wiener-type index from Z weighted distance matrix (Barysz matrix)	topological descriptors
87	40	Whetm	Wiener-type index from mass weighted distance matrix	topological descriptors
88	41	Whetv	Wiener-type index from van der Waals weighted distance matrix	topological descriptors
89	42	Whete	Wiener-type index from electronegativity weighted distance matrix	topological descriptors
90	43	Whetp	Wiener-type index from polarizability weighted distance matrix	topological descriptors
91	44	J	Balaban J index	topological descriptors
92	45	JhetZ	Balaban-type index from Z weighted distance matrix (Barysz matrix)	topological descriptors
93	46	Jhetm	Balaban-type index from mass weighted distance matrix	topological descriptors
94	47	Jhetv	Balaban-type index from van der Waals weighted distance matrix	topological descriptors
95	48	Jhete	Balaban-type index from electronegativity weighted distance matrix	topological descriptors
96	49	Jhetp	Balaban-type index from polarizability weighted distance matrix	topological descriptors
97	50	MAXDN	maximal electrotopological negative variation	topological descriptors
98	51	MAXDP	maximal electrotopological positive variation	topological descriptors
99	52	DELS	molecular electrotopological variation	topological descriptors
100	53	TIE	E-state topological parameter	topological descriptors
101	54	X0	connectivity index chi-0	topological descriptors
102	55	X1	connectivity index chi-1 (Randic connectivity index)	topological descriptors
103	56	X2	connectivity index chi-2	topological descriptors
104	57	X3	connectivity index chi-3	topological descriptors
105	58	X4	connectivity index chi-4	topological descriptors
106	59	X5	connectivity index chi-5	topological descriptors
107	60	X0A	average connectivity index chi-0	topological descriptors
108	61	X1A	average connectivity index chi-1	topological descriptors
109	62	X2A	average connectivity index chi-2	topological descriptors
110	63	X3A	average connectivity index chi-3	topological descriptors
111	64	X4A	average connectivity index chi-4	topological descriptors
112	65	X5A	average connectivity index chi-5	topological descriptors
113	66	X0v	valence connectivity index chi-0	topological descriptors
114	67	X1v	valence connectivity index chi-1	topological descriptors
115	68	X2v	valence connectivity index chi-2	topological descriptors

No.	Rel.No.	Symbol	Definition	Class
116	69	X3v	valence connectivity index chi-3	topological descriptors
117	70	X4v	valence connectivity index chi-4	topological descriptors
118	71	X5v	valence connectivity index chi-5	topological descriptors
119	72	X0Av	average valence connectivity index chi-0	topological descriptors
120	73	X1Av	average valence connectivity index chi-1	topological descriptors
121	74	X2Av	average valence connectivity index chi-2	topological descriptors
122	75	X3Av	average valence connectivity index chi-3	topological descriptors
123	76	X4Av	average valence connectivity index chi-4	topological descriptors
124	77	X5Av	average valence connectivity index chi-5	topological descriptors
125	78	X0sol	solvation connectivity index chi-0	topological descriptors
126	79	X1sol	solvation connectivity index chi-1	topological descriptors
127	80	X2sol	solvation connectivity index chi-2	topological descriptors
128	81	X3sol	solvation connectivity index chi-3	topological descriptors
129	82	X4sol	solvation connectivity index chi-4	topological descriptors
130	83	X5sol	solvation connectivity index chi-5	topological descriptors
131	84	XMOD	modified Randic chi-1 index	topological descriptors
132	85	RDCHI	reciprocal distance Randic-type index	topological descriptors
133	86	RDSQ	reciprocal distance squared Randic-type index	topological descriptors
134	87	S0K	Kier symmetry index	topological descriptors
135	88	S1K	1-path Kier alpha-modified shape index	topological descriptors
136	89	S2K	2-path Kier alpha-modified shape index	topological descriptors
137	90	S3K	3-path Kier alpha-modified shape index	topological descriptors
138	91	PHI	Kier flexibility index	topological descriptors
139	92	BLI	Kier benzene-likeliness index	topological descriptors
140	93	PW2	path/walk 2 - Randic shape index	topological descriptors
141	94	PW3	path/walk 3 - Randic shape index	topological descriptors
142	95	PW4	path/walk 4 - Randic shape index	topological descriptors
143	96	PW5	path/walk 5 - Randic shape index	topological descriptors
144	97	PJI2	2D Petitjean shape index	topological descriptors
145	98	CSI	eccentric connectivity index	topological descriptors
146	99	ECC	eccentricity	topological descriptors
147	100	AECC	average eccentricity	topological descriptors
148	101	DECC	eccentric	topological descriptors
149	102	MDDD	mean distance degree deviation	topological descriptors
150	103	UNIP	unipolarity	topological descriptors
151	104	CENT	centralization	topological descriptors
152	105	VAR	variation	topological descriptors
153	106	BAC	Balaban centric index	topological descriptors
154	107	Lop	Lopping centric index	topological descriptors

No.	Rel.No.	Symbol	Definition	Class
155	108	ICR	radial centric information index	topological descriptors
156	109	IDE	mean information content on the distance equality	topological descriptors
157	110	IDM	mean information content on the distance magnitude	topological descriptors
158	111	IDDE	mean information content on the distance degree equality	topological descriptors
159	112	IDDM	mean information content on the distance degree magnitude	topological descriptors
160	113	IDET	total information content on the distance equality	topological descriptors
161	114	IDMT	total information content on the distance magnitude	topological descriptors
162	115	IVDE	mean information content vertex degree equality	topological descriptors
163	116	IVDM	mean information content vertex degree magnitude	topological descriptors
164	117	HVcpx	graph vertex complexity index	topological descriptors
165	118	HDcpx	graph distance complexity index (log)	topological descriptors
166	119	Uindex	Balaban U index	topological descriptors
167	120	Vindex	Balaban V index	topological descriptors
168	121	Xindex	Balaban X index	topological descriptors
169	122	Yindex	Balaban Y index	topological descriptors
170	123	IC0	information content index (neighborhood symmetry of 0-order)	topological descriptors
171	124	TIC0	total information content index (neighborhood symmetry of 0-order)	topological descriptors
172	125	SIC0	structural information content (neighborhood symmetry of 0-order)	topological descriptors
173	126	CIC0	complementary information content (neighborhood symmetry of 0-order)	topological descriptors
174	127	BIC0	bond information content (neighborhood symmetry of 0-order)	topological descriptors
175	128	IC1	information content index (neighborhood symmetry of 1-order)	topological descriptors
176	129	TIC1	total information content index (neighborhood symmetry of 1-order)	topological descriptors
177	130	SIC1	structural information content (neighborhood symmetry of 1-order)	topological descriptors
178	131	CIC1	complementary information content (neighborhood symmetry of 1-order)	topological descriptors
179	132	BIC1	bond information content (neighborhood symmetry of 1-order)	topological descriptors
180	133	IC2	information content index (neighborhood symmetry of 2-order)	topological descriptors
181	134	TIC2	total information content index (neighborhood symmetry of 2-order)	topological descriptors
182	135	SIC2	structural information content (neighborhood symmetry of 2-order)	topological descriptors
183	136	CIC2	complementary information content (neighborhood symmetry of 2-order)	topological descriptors
184	137	BIC2	bond information content (neighborhood symmetry of 2-order)	topological descriptors
185	138	IC3	information content index (neighborhood symmetry of 3-order)	topological descriptors
186	139	TIC3	total information content index (neighborhood symmetry of 3-order)	topological descriptors
187	140	SIC3	structural information content (neighborhood symmetry of 3-order)	topological descriptors
188	141	CIC3	complementary information content (neighborhood symmetry of 3-order)	topological descriptors
189	142	BIC3	bond information content (neighborhood symmetry of 3-order)	topological descriptors
190	143	IC4	information content index (neighborhood symmetry of 4-order)	topological descriptors
191	144	TIC4	total information content index (neighborhood symmetry of 4-order)	topological descriptors
192	145	SIC4	structural information content (neighborhood symmetry of 4-order)	topological descriptors
193	146	CIC4	complementary information content (neighborhood symmetry of 4-order)	topological descriptors

No.	Rel.No.	Symbol	Definition	Class
194	147	BIC4	bond information content (neighborhood symmetry of 4-order)	topological descriptors
195	148	IC5	information content index (neighborhood symmetry of 5-order)	topological descriptors
196	149	TIC5	total information content index (neighborhood symmetry of 5-order)	topological descriptors
197	150	SIC5	structural information content (neighborhood symmetry of 5-order)	topological descriptors
198	151	CIC5	complementary information content (neighborhood symmetry of 5-order)	topological descriptors
199	152	BIC5	bond information content (neighborhood symmetry of 5-order)	topological descriptors
200	153	LP1	Lovasz-Pelikán index (leading eigenvalue)	topological descriptors
201	154	STN	spanning tree number (log)	topological descriptors
202	155	Eig1Z	Leading eigenvalue from Z weighted distance matrix (Barysz matrix)	topological descriptors
203	156	Eig1m	Leading eigenvalue from mass weighted distance matrix	topological descriptors
204	157	Eig1v	Leading eigenvalue from van der Waals weighted distance matrix	topological descriptors
205	158	Eig1e	Leading eigenvalue from electronegativity weighted distance matrix	topological descriptors
206	159	Eig1p	Leading eigenvalue from polarizability weighted distance matrix	topological descriptors
207	160	SEigZ	Eigenvalue sum from Z weighted distance matrix (Barysz matrix)	topological descriptors
208	161	SEigm	Eigenvalue sum from mass weighted distance matrix	topological descriptors
209	162	SEigv	Eigenvalue sum from van der Waals weighted distance matrix	topological descriptors
210	163	SEige	Eigenvalue sum from electronegativity weighted distance matrix	topological descriptors
211	164	SEigp	Eigenvalue sum from polarizability weighted distance matrix	topological descriptors
212	165	AEigZ	Absolute eigenvalue sum from Z weighted distance matrix (Barysz matrix)	topological descriptors
213	166	AEigm	Absolute eigenvalue sum from mass weighted distance matrix	topological descriptors
214	167	AEigv	Absolute eigenvalue sum from van der Waals weighted distance matrix	topological descriptors
215	168	AEige	Absolute eigenvalue sum from electronegativity weighted distance matrix	topological descriptors
216	169	AEigp	Absolute eigenvalue sum from polarizability weighted distance matrix	topological descriptors
217	170	VEA1	eigenvector coefficient sum from adjacency matrix	topological descriptors
218	171	VEA2	average eigenvector coefficient sum from adjacency matrix	topological descriptors
219	172	VRA1	Randic-type eigenvector-based index from adjacency matrix	topological descriptors
220	173	VRA2	average Randic-type eigenvector-based index from adjacency matrix	topological descriptors
221	174	VED1	eigenvector coefficient sum from distance matrix	topological descriptors
222	175	VED2	average eigenvector coefficient sum from distance matrix	topological descriptors
223	176	VRD1	Randic-type eigenvector-based index from distance matrix	topological descriptors
224	177	VRD2	average Randic-type eigenvector-based index from distance matrix	topological descriptors
225	178	VEZ1	eigenvector coefficient sum from Z weighted distance matrix (Barysz matrix)	topological descriptors
226	179	VEZ2	average eigenvector coefficient sum from Z weighted distance matrix (Barysz matrix)	topological descriptors
227	180	VRZ1	Randic-type eigenvector-based index from Z weighted distance matrix (Barysz matrix)	topological descriptors
228	181	VRZ2	average Randic-type eigenvector-based index from Z weighted distance matrix (Barysz matrix)	topological descriptors
229	182	VEm1	eigenvector coefficient sum from mass weighted distance matrix	topological descriptors
230	183	VEm2	average eigenvector coefficient sum from mass weighted distance matrix	topological descriptors
231	184	VRm1	Randic-type eigenvector-based index from mass weighted distance matrix	topological descriptors
232	185	VRm2	average Randic-type eigenvector-based index from mass weighted distance matrix	topological descriptors

No.	Rel.No.	Symbol	Definition	Class
233	186	VEv1	eigenvector coefficient sum from van der Waals weighted distance matrix	topological descriptors
234	187	VEv2	average eigenvector coefficient sum from van der Waals weighted distance matrix	topological descriptors
235	188	VRv1	Randic-type eigenvector-based index from van der Waals weighted distance matrix	topological descriptors
236	189	VRv2	average Randic-type eigenvector-based index from van der Waals weighted distance matrix	topological descriptors
237	190	VEe1	eigenvector coefficient sum from electronegativity weighted distance matrix	topological descriptors
238	191	VEe2	average eigenvector coefficient sum from electronegativity weighted distance matrix	topological descriptors
239	192	VRe1	Randic-type eigenvector-based index from electronegativity weighted distance matrix	topological descriptors
240	193	VRe2	average Randic-type eigenvector-based index from electronegativity weighted distance matrix	topological descriptors
241	194	VEp1	eigenvector coefficient sum from polarizability weighted distance matrix	topological descriptors
242	195	VEp2	average eigenvector coefficient sum from polarizability weighted distance matrix	topological descriptors
243	196	VRp1	Randic-type eigenvector-based index from polarizability weighted distance matrix	topological descriptors
244	197	VRp2	average Randic-type eigenvector-based index from polarizability weighted distance matrix	topological descriptors
245	198	NGS	Gordon-Scantlebury index (molecular path count of order 2)	topological descriptors
246	199	MPC03	molecular path count of order 03	topological descriptors
247	200	MPC04	molecular path count of order 04	topological descriptors
248	201	MPC05	molecular path count of order 05	topological descriptors
249	202	MPC06	molecular path count of order 06	topological descriptors
250	203	MPC07	molecular path count of order 07	topological descriptors
251	204	MPC08	molecular path count of order 08	topological descriptors
252	205	MPC09	molecular path count of order 09	topological descriptors
253	206	MPC10	molecular path count of order 10	topological descriptors
254	207	piPC03	molecular multiple path count of order 03	topological descriptors
255	208	piPC04	molecular multiple path count of order 04	topological descriptors
256	209	piPC05	molecular multiple path count of order 05	topological descriptors
257	210	piPC06	molecular multiple path count of order 06	topological descriptors
258	211	piPC07	molecular multiple path count of order 07	topological descriptors
259	212	piPC08	molecular multiple path count of order 08	topological descriptors
260	213	piPC09	molecular multiple path count of order 09	topological descriptors
261	214	piPC10	molecular multiple path count of order 10	topological descriptors
262	215	TPC	total path count	topological descriptors
263	216	piID	conventional bond-order ID number	topological descriptors
264	217	PCR	ratio of multiple path counts to path counts	topological descriptors
265	218	PCD	difference of multiple path counts to path counts	topological descriptors
266	219	CID	Randic ID number	topological descriptors
267	220	BID	Balaban ID number	topological descriptors
268	221	D/Dr03	distance/detour ring index of order 3	topological descriptors
269	222	D/Dr04	distance/detour ring index of order 4	topological descriptors
270	223	D/Dr05	distance/detour ring index of order 5	topological descriptors
271	224	D/Dr06	distance/detour ring index of order 6	topological descriptors

No.	Rel.No.	Symbol	Definition	Class
272	225	D/Dr07	distance/detour ring index of order 7	topological descriptors
273	226	D/Dr08	distance/detour ring index of order 8	topological descriptors
274	227	D/Dr09	distance/detour ring index of order 9	topological descriptors
275	228	D/Dr10	distance/detour ring index of order 10	topological descriptors
276	229	D/Dr11	distance/detour ring index of order 11	topological descriptors
277	230	D/Dr12	distance/detour ring index of order 12	topological descriptors
278	231	T(N..N)	sum of topological distances between N..N	topological descriptors
279	232	T(N..O)	sum of topological distances between N..O	topological descriptors
280	233	T(N..S)	sum of topological distances between N..S	topological descriptors
281	234	T(N..P)	sum of topological distances between N..P	topological descriptors
282	235	T(N..F)	sum of topological distances between N..F	topological descriptors
283	236	T(N..Cl)	sum of topological distances between N..Cl	topological descriptors
284	237	T(N..Br)	sum of topological distances between N..Br	topological descriptors
285	238	T(N..I)	sum of topological distances between N..I	topological descriptors
286	239	T(O..O)	sum of topological distances between O..O	topological descriptors
287	240	T(O..S)	sum of topological distances between O..S	topological descriptors
288	241	T(O..P)	sum of topological distances between O..P	topological descriptors
289	242	T(O..F)	sum of topological distances between O..F	topological descriptors
290	243	T(O..Cl)	sum of topological distances between O..Cl	topological descriptors
291	244	T(O..Br)	sum of topological distances between O..Br	topological descriptors
292	245	T(O..I)	sum of topological distances between O..I	topological descriptors
293	246	T(S..S)	sum of topological distances between S..S	topological descriptors
294	247	T(S..P)	sum of topological distances between S..P	topological descriptors
295	248	T(S..F)	sum of topological distances between S..F	topological descriptors
296	249	T(S..Cl)	sum of topological distances between S..Cl	topological descriptors
297	250	T(S..Br)	sum of topological distances between S..Br	topological descriptors
298	251	T(S..I)	sum of topological distances between S..I	topological descriptors
299	252	T(P..P)	sum of topological distances between P..P	topological descriptors
300	253	T(P..F)	sum of topological distances between P..F	topological descriptors
301	254	T(P..Cl)	sum of topological distances between P..Cl	topological descriptors
302	255	T(P..Br)	sum of topological distances between P..Br	topological descriptors
303	256	T(P..I)	sum of topological distances between P..I	topological descriptors
304	257	T(F..F)	sum of topological distances between F..F	topological descriptors
305	258	T(F..Cl)	sum of topological distances between F..Cl	topological descriptors
306	259	T(F..Br)	sum of topological distances between F..Br	topological descriptors
307	260	T(F..I)	sum of topological distances between F..I	topological descriptors
308	261	T(Cl..Cl)	sum of topological distances between Cl..Cl	topological descriptors
309	262	T(Cl..Br)	sum of topological distances between Cl..Br	topological descriptors
310	263	T(Cl..I)	sum of topological distances between Cl..I	topological descriptors

No.	Rel.No.	Symbol	Definition	Class
311	264	T(Br..Br)	sum of topological distances between Br..Br	topological descriptors
312	265	T(Br..I)	sum of topological distances between Br..I	topological descriptors
313	266	T(I..I)	sum of topological distances between I..I	topological descriptors
314	1	MWC01	molecular walk count of order 01	molecular walk counts
315	2	MWC02	molecular walk count of order 02	molecular walk counts
316	3	MWC03	molecular walk count of order 03	molecular walk counts
317	4	MWC04	molecular walk count of order 04	molecular walk counts
318	5	MWC05	molecular walk count of order 05	molecular walk counts
319	6	MWC06	molecular walk count of order 06	molecular walk counts
320	7	MWC07	molecular walk count of order 07	molecular walk counts
321	8	MWC08	molecular walk count of order 08	molecular walk counts
322	9	MWC09	molecular walk count of order 09	molecular walk counts
323	10	MWC10	molecular walk count of order 10	molecular walk counts
324	11	TWC	total walk count	molecular walk counts
325	12	SRW01	self-returning walk count of order 01	molecular walk counts
326	13	SRW02	self-returning walk count of order 02	molecular walk counts
327	14	SRW03	self-returning walk count of order 03	molecular walk counts
328	15	SRW04	self-returning walk count of order 04	molecular walk counts
329	16	SRW05	self-returning walk count of order 05	molecular walk counts
330	17	SRW06	self-returning walk count of order 06	molecular walk counts
331	18	SRW07	self-returning walk count of order 07	molecular walk counts
332	19	SRW08	self-returning walk count of order 08	molecular walk counts
333	20	SRW09	self-returning walk count of order 09	molecular walk counts
334	21	SRW10	self-returning walk count of order 10	molecular walk counts
335	1	BEHm1	highest eigenvalue n. 1 of Burden matrix / weighted by atomic masses	BCUT descriptors
336	2	BEHm2	highest eigenvalue n. 2 of Burden matrix / weighted by atomic masses	BCUT descriptors
337	3	BEHm3	highest eigenvalue n. 3 of Burden matrix / weighted by atomic masses	BCUT descriptors
338	4	BEHm4	highest eigenvalue n. 4 of Burden matrix / weighted by atomic masses	BCUT descriptors
339	5	BEHm5	highest eigenvalue n. 5 of Burden matrix / weighted by atomic masses	BCUT descriptors
340	6	BEHm6	highest eigenvalue n. 6 of Burden matrix / weighted by atomic masses	BCUT descriptors
341	7	BEHm7	highest eigenvalue n. 7 of Burden matrix / weighted by atomic masses	BCUT descriptors
342	8	BEHm8	highest eigenvalue n. 8 of Burden matrix / weighted by atomic masses	BCUT descriptors
343	9	BELm1	lowest eigenvalue n. 1 of Burden matrix / weighted by atomic masses	BCUT descriptors
344	10	BELm2	lowest eigenvalue n. 2 of Burden matrix / weighted by atomic masses	BCUT descriptors
345	11	BELm3	lowest eigenvalue n. 3 of Burden matrix / weighted by atomic masses	BCUT descriptors
346	12	BELm4	lowest eigenvalue n. 4 of Burden matrix / weighted by atomic masses	BCUT descriptors
347	13	BELm5	lowest eigenvalue n. 5 of Burden matrix / weighted by atomic masses	BCUT descriptors
348	14	BELm6	lowest eigenvalue n. 6 of Burden matrix / weighted by atomic masses	BCUT descriptors
349	15	BELm7	lowest eigenvalue n. 7 of Burden matrix / weighted by atomic masses	BCUT descriptors

No.	Rel.No.	Symbol	Definition	Class
350	16	BELm8	lowest eigenvalue n. 8 of Burden matrix / weighted by atomic masses	BCUT descriptors
351	17	BEHv1	highest eigenvalue n. 1 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
352	18	BEHv2	highest eigenvalue n. 2 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
353	19	BEHv3	highest eigenvalue n. 3 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
354	20	BEHv4	highest eigenvalue n. 4 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
355	21	BEHv5	highest eigenvalue n. 5 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
356	22	BEHv6	highest eigenvalue n. 6 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
357	23	BEHv7	highest eigenvalue n. 7 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
358	24	BEHv8	highest eigenvalue n. 8 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
359	25	BELv1	lowest eigenvalue n. 1 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
360	26	BELv2	lowest eigenvalue n. 2 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
361	27	BELv3	lowest eigenvalue n. 3 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
362	28	BELv4	lowest eigenvalue n. 4 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
363	29	BELv5	lowest eigenvalue n. 5 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
364	30	BELv6	lowest eigenvalue n. 6 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
365	31	BELv7	lowest eigenvalue n. 7 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
366	32	BELv8	lowest eigenvalue n. 8 of Burden matrix / weighted by atomic van der Waals volumes	BCUT descriptors
367	33	BEHe1	highest eigenvalue n. 1 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
368	34	BEHe2	highest eigenvalue n. 2 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
369	35	BEHe3	highest eigenvalue n. 3 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
370	36	BEHe4	highest eigenvalue n. 4 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
371	37	BEHe5	highest eigenvalue n. 5 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
372	38	BEHe6	highest eigenvalue n. 6 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
373	39	BEHe7	highest eigenvalue n. 7 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
374	40	BEHe8	highest eigenvalue n. 8 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
375	41	BELe1	lowest eigenvalue n. 1 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
376	42	BELe2	lowest eigenvalue n. 2 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
377	43	BELe3	lowest eigenvalue n. 3 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
378	44	BELe4	lowest eigenvalue n. 4 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
379	45	BELe5	lowest eigenvalue n. 5 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
380	46	BELe6	lowest eigenvalue n. 6 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
381	47	BELe7	lowest eigenvalue n. 7 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
382	48	BELe8	lowest eigenvalue n. 8 of Burden matrix / weighted by atomic Sanderson electronegativities	BCUT descriptors
383	49	BEHp1	highest eigenvalue n. 1 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
384	50	BEHp2	highest eigenvalue n. 2 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
385	51	BEHp3	highest eigenvalue n. 3 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
386	52	BEHp4	highest eigenvalue n. 4 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
387	53	BEHp5	highest eigenvalue n. 5 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
388	54	BEHp6	highest eigenvalue n. 6 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors

No.	Rel.No.	Symbol	Definition	Class
389	55	BEHp7	highest eigenvalue n. 7 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
390	56	BEHp8	highest eigenvalue n. 8 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
391	57	BELp1	lowest eigenvalue n. 1 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
392	58	BELp2	lowest eigenvalue n. 2 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
393	59	BELp3	lowest eigenvalue n. 3 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
394	60	BELp4	lowest eigenvalue n. 4 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
395	61	BELp5	lowest eigenvalue n. 5 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
396	62	BELp6	lowest eigenvalue n. 6 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
397	63	BELp7	lowest eigenvalue n. 7 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
398	64	BELp8	lowest eigenvalue n. 8 of Burden matrix / weighted by atomic polarizabilities	BCUT descriptors
399	1	GGI1	topological charge index of order 1	Galvez topol. charge indices
400	2	GGI2	topological charge index of order 2	Galvez topol. charge indices
401	3	GGI3	topological charge index of order 3	Galvez topol. charge indices
402	4	GGI4	topological charge index of order 4	Galvez topol. charge indices
403	5	GGI5	topological charge index of order 5	Galvez topol. charge indices
404	6	GGI6	topological charge index of order 6	Galvez topol. charge indices
405	7	GGI7	topological charge index of order 7	Galvez topol. charge indices
406	8	GGI8	topological charge index of order 8	Galvez topol. charge indices
407	9	GGI9	topological charge index of order 9	Galvez topol. charge indices
408	10	GGI10	topological charge index of order 10	Galvez topol. charge indices
409	11	JGI1	mean topological charge index of order1	Galvez topol. charge indices
410	12	JGI2	mean topological charge index of order2	Galvez topol. charge indices
411	13	JGI3	mean topological charge index of order3	Galvez topol. charge indices
412	14	JGI4	mean topological charge index of order4	Galvez topol. charge indices
413	15	JGI5	mean topological charge index of order5	Galvez topol. charge indices
414	16	JGI6	mean topological charge index of order6	Galvez topol. charge indices
415	17	JGI7	mean topological charge index of order7	Galvez topol. charge indices
416	18	JGI8	mean topological charge index of order8	Galvez topol. charge indices
417	19	JGI9	mean topological charge index of order9	Galvez topol. charge indices
418	20	JGI10	mean topological charge index of order10	Galvez topol. charge indices
419	21	JGT	global topological charge index	Galvez topol. charge indices
420	1	ATS1m	Broto-Moreau autocorrelation of a topological structure - lag 1 / weighted by atomic masses	2D autocorrelations
421	2	ATS2m	Broto-Moreau autocorrelation of a topological structure - lag 2 / weighted by atomic masses	2D autocorrelations
422	3	ATS3m	Broto-Moreau autocorrelation of a topological structure - lag 3 / weighted by atomic masses	2D autocorrelations
423	4	ATS4m	Broto-Moreau autocorrelation of a topological structure - lag 4 / weighted by atomic masses	2D autocorrelations
424	5	ATS5m	Broto-Moreau autocorrelation of a topological structure - lag 5 / weighted by atomic masses	2D autocorrelations
425	6	ATS6m	Broto-Moreau autocorrelation of a topological structure - lag 6 / weighted by atomic masses	2D autocorrelations
426	7	ATS7m	Broto-Moreau autocorrelation of a topological structure - lag 7 / weighted by atomic masses	2D autocorrelations
427	8	ATS8m	Broto-Moreau autocorrelation of a topological structure - lag 8 / weighted by atomic masses	2D autocorrelations

No.	Rel.No.	Symbol	Definition	Class
428	9	ATS1v	Broto-Moreau autocorrelation of a topological structure - lag 1 / weighted by atomic van der Waals volumes	2D autocorrelations
429	10	ATS2v	Broto-Moreau autocorrelation of a topological structure - lag 2 / weighted by atomic van der Waals volumes	2D autocorrelations
430	11	ATS3v	Broto-Moreau autocorrelation of a topological structure - lag 3 / weighted by atomic van der Waals volumes	2D autocorrelations
431	12	ATS4v	Broto-Moreau autocorrelation of a topological structure - lag 4 / weighted by atomic van der Waals volumes	2D autocorrelations
432	13	ATS5v	Broto-Moreau autocorrelation of a topological structure - lag 5 / weighted by atomic van der Waals volumes	2D autocorrelations
433	14	ATS6v	Broto-Moreau autocorrelation of a topological structure - lag 6 / weighted by atomic van der Waals volumes	2D autocorrelations
434	15	ATS7v	Broto-Moreau autocorrelation of a topological structure - lag 7 / weighted by atomic van der Waals volumes	2D autocorrelations
435	16	ATS8v	Broto-Moreau autocorrelation of a topological structure - lag 8 / weighted by atomic van der Waals volumes	2D autocorrelations
436	17	ATS1e	Broto-Moreau autocorrelation of a topological structure - lag 1 / weighted by atomic Sanderson electronegativities	2D autocorrelations
437	18	ATS2e	Broto-Moreau autocorrelation of a topological structure - lag 2 / weighted by atomic Sanderson electronegativities	2D autocorrelations
438	19	ATS3e	Broto-Moreau autocorrelation of a topological structure - lag 3 / weighted by atomic Sanderson electronegativities	2D autocorrelations
439	20	ATS4e	Broto-Moreau autocorrelation of a topological structure - lag 4 / weighted by atomic Sanderson electronegativities	2D autocorrelations
440	21	ATS5e	Broto-Moreau autocorrelation of a topological structure - lag 5 / weighted by atomic Sanderson electronegativities	2D autocorrelations
441	22	ATS6e	Broto-Moreau autocorrelation of a topological structure - lag 6 / weighted by atomic Sanderson electronegativities	2D autocorrelations
442	23	ATS7e	Broto-Moreau autocorrelation of a topological structure - lag 7 / weighted by atomic Sanderson electronegativities	2D autocorrelations
443	24	ATS8e	Broto-Moreau autocorrelation of a topological structure - lag 8 / weighted by atomic Sanderson electronegativities	2D autocorrelations
444	25	ATS1p	Broto-Moreau autocorrelation of a topological structure - lag 1 / weighted by atomic polarizabilities	2D autocorrelations
445	26	ATS2p	Broto-Moreau autocorrelation of a topological structure - lag 2 / weighted by atomic polarizabilities	2D autocorrelations
446	27	ATS3p	Broto-Moreau autocorrelation of a topological structure - lag 3 / weighted by atomic polarizabilities	2D autocorrelations
447	28	ATS4p	Broto-Moreau autocorrelation of a topological structure - lag 4 / weighted by atomic polarizabilities	2D autocorrelations
448	29	ATS5p	Broto-Moreau autocorrelation of a topological structure - lag 5 / weighted by atomic polarizabilities	2D autocorrelations
449	30	ATS6p	Broto-Moreau autocorrelation of a topological structure - lag 6 / weighted by atomic polarizabilities	2D autocorrelations
450	31	ATS7p	Broto-Moreau autocorrelation of a topological structure - lag 7 / weighted by atomic polarizabilities	2D autocorrelations
451	32	ATS8p	Broto-Moreau autocorrelation of a topological structure - lag 8 / weighted by atomic polarizabilities	2D autocorrelations
452	33	MATS1m	Moran autocorrelation - lag 1 / weighted by atomic masses	2D autocorrelations
453	34	MATS2m	Moran autocorrelation - lag 2 / weighted by atomic masses	2D autocorrelations
454	35	MATS3m	Moran autocorrelation - lag 3 / weighted by atomic masses	2D autocorrelations
455	36	MATS4m	Moran autocorrelation - lag 4 / weighted by atomic masses	2D autocorrelations
456	37	MATS5m	Moran autocorrelation - lag 5 / weighted by atomic masses	2D autocorrelations
457	38	MATS6m	Moran autocorrelation - lag 6 / weighted by atomic masses	2D autocorrelations
458	39	MATS7m	Moran autocorrelation - lag 7 / weighted by atomic masses	2D autocorrelations
459	40	MATS8m	Moran autocorrelation - lag 8 / weighted by atomic masses	2D autocorrelations
460	41	MATS1v	Moran autocorrelation - lag 1 / weighted by atomic van der Waals volumes	2D autocorrelations
461	42	MATS2v	Moran autocorrelation - lag 2 / weighted by atomic van der Waals volumes	2D autocorrelations
462	43	MATS3v	Moran autocorrelation - lag 3 / weighted by atomic van der Waals volumes	2D autocorrelations
463	44	MATS4v	Moran autocorrelation - lag 4 / weighted by atomic van der Waals volumes	2D autocorrelations
464	45	MATS5v	Moran autocorrelation - lag 5 / weighted by atomic van der Waals volumes	2D autocorrelations
465	46	MATS6v	Moran autocorrelation - lag 6 / weighted by atomic van der Waals volumes	2D autocorrelations
466	47	MATS7v	Moran autocorrelation - lag 7 / weighted by atomic van der Waals volumes	2D autocorrelations

No.	Rel.No.	Symbol	Definition	Class
467	48	MATS8v	Moran autocorrelation - lag 8 / weighted by atomic van der Waals volumes	2D autocorrelations
468	49	MATS1e	Moran autocorrelation - lag 1 / weighted by atomic Sanderson electronegativities	2D autocorrelations
469	50	MATS2e	Moran autocorrelation - lag 2 / weighted by atomic Sanderson electronegativities	2D autocorrelations
470	51	MATS3e	Moran autocorrelation - lag 3 / weighted by atomic Sanderson electronegativities	2D autocorrelations
471	52	MATS4e	Moran autocorrelation - lag 4 / weighted by atomic Sanderson electronegativities	2D autocorrelations
472	53	MATS5e	Moran autocorrelation - lag 5 / weighted by atomic Sanderson electronegativities	2D autocorrelations
473	54	MATS6e	Moran autocorrelation - lag 6 / weighted by atomic Sanderson electronegativities	2D autocorrelations
474	55	MATS7e	Moran autocorrelation - lag 7 / weighted by atomic Sanderson electronegativities	2D autocorrelations
475	56	MATS8e	Moran autocorrelation - lag 8 / weighted by atomic Sanderson electronegativities	2D autocorrelations
476	57	MATS1p	Moran autocorrelation - lag 1 / weighted by atomic polarizabilities	2D autocorrelations
477	58	MATS2p	Moran autocorrelation - lag 2 / weighted by atomic polarizabilities	2D autocorrelations
478	59	MATS3p	Moran autocorrelation - lag 3 / weighted by atomic polarizabilities	2D autocorrelations
479	60	MATS4p	Moran autocorrelation - lag 4 / weighted by atomic polarizabilities	2D autocorrelations
480	61	MATS5p	Moran autocorrelation - lag 5 / weighted by atomic polarizabilities	2D autocorrelations
481	62	MATS6p	Moran autocorrelation - lag 6 / weighted by atomic polarizabilities	2D autocorrelations
482	63	MATS7p	Moran autocorrelation - lag 7 / weighted by atomic polarizabilities	2D autocorrelations
483	64	MATS8p	Moran autocorrelation - lag 8 / weighted by atomic polarizabilities	2D autocorrelations
484	65	GATS1m	Geary autocorrelation - lag 1 / weighted by atomic masses	2D autocorrelations
485	66	GATS2m	Geary autocorrelation - lag 2 / weighted by atomic masses	2D autocorrelations
486	67	GATS3m	Geary autocorrelation - lag 3 / weighted by atomic masses	2D autocorrelations
487	68	GATS4m	Geary autocorrelation - lag 4 / weighted by atomic masses	2D autocorrelations
488	69	GATS5m	Geary autocorrelation - lag 5 / weighted by atomic masses	2D autocorrelations
489	70	GATS6m	Geary autocorrelation - lag 6 / weighted by atomic masses	2D autocorrelations
490	71	GATS7m	Geary autocorrelation - lag 7 / weighted by atomic masses	2D autocorrelations
491	72	GATS8m	Geary autocorrelation - lag 8 / weighted by atomic masses	2D autocorrelations
492	73	GATS1v	Geary autocorrelation - lag 1 / weighted by atomic van der Waals volumes	2D autocorrelations
493	74	GATS2v	Geary autocorrelation - lag 2 / weighted by atomic van der Waals volumes	2D autocorrelations
494	75	GATS3v	Geary autocorrelation - lag 3 / weighted by atomic van der Waals volumes	2D autocorrelations
495	76	GATS4v	Geary autocorrelation - lag 4 / weighted by atomic van der Waals volumes	2D autocorrelations
496	77	GATS5v	Geary autocorrelation - lag 5 / weighted by atomic van der Waals volumes	2D autocorrelations
497	78	GATS6v	Geary autocorrelation - lag 6 / weighted by atomic van der Waals volumes	2D autocorrelations
498	79	GATS7v	Geary autocorrelation - lag 7 / weighted by atomic van der Waals volumes	2D autocorrelations
499	80	GATS8v	Geary autocorrelation - lag 8 / weighted by atomic van der Waals volumes	2D autocorrelations
500	81	GATS1e	Geary autocorrelation - lag 1 / weighted by atomic Sanderson electronegativities	2D autocorrelations
501	82	GATS2e	Geary autocorrelation - lag 2 / weighted by atomic Sanderson electronegativities	2D autocorrelations
502	83	GATS3e	Geary autocorrelation - lag 3 / weighted by atomic Sanderson electronegativities	2D autocorrelations
503	84	GATS4e	Geary autocorrelation - lag 4 / weighted by atomic Sanderson electronegativities	2D autocorrelations
504	85	GATS5e	Geary autocorrelation - lag 5 / weighted by atomic Sanderson electronegativities	2D autocorrelations
505	86	GATS6e	Geary autocorrelation - lag 6 / weighted by atomic Sanderson electronegativities	2D autocorrelations

No.	Rel.No.	Symbol	Definition	Class
506	87	GATS7e	Geary autocorrelation - lag 7 / weighted by atomic Sanderson electronegativities	2D autocorrelations
507	88	GATS8e	Geary autocorrelation - lag 8 / weighted by atomic Sanderson electronegativities	2D autocorrelations
508	89	GATS1p	Geary autocorrelation - lag 1 / weighted by atomic polarizabilities	2D autocorrelations
509	90	GATS2p	Geary autocorrelation - lag 2 / weighted by atomic polarizabilities	2D autocorrelations
510	91	GATS3p	Geary autocorrelation - lag 3 / weighted by atomic polarizabilities	2D autocorrelations
511	92	GATS4p	Geary autocorrelation - lag 4 / weighted by atomic polarizabilities	2D autocorrelations
512	93	GATS5p	Geary autocorrelation - lag 5 / weighted by atomic polarizabilities	2D autocorrelations
513	94	GATS6p	Geary autocorrelation - lag 6 / weighted by atomic polarizabilities	2D autocorrelations
514	95	GATS7p	Geary autocorrelation - lag 7 / weighted by atomic polarizabilities	2D autocorrelations
515	96	GATS8p	Geary autocorrelation - lag 8 / weighted by atomic polarizabilities	2D autocorrelations
516	1	qpmax	maximum positive charge	charge descriptors
517	2	qnmax	maximum negative charge	charge descriptors
518	3	Qpos	total positive charge	charge descriptors
519	4	Qneg	total negative charge	charge descriptors
520	5	Qtot	total absolute charge (electronic charge index - ECI)	charge descriptors
521	6	Qmean	mean absolute charge (charge polarization)	charge descriptors
522	7	Q2	total squared charge	charge descriptors
523	8	RPCG	relative positive charge	charge descriptors
524	9	RNCG	relative negative charge	charge descriptors
525	10	SPP	subpolarity parameter	charge descriptors
526	11	TE1	topographic electronic descriptor	charge descriptors
527	12	TE2	topographic electronic descriptor (bond restricted)	charge descriptors
528	13	PCWTe	partial charge weighted topological electronic charge	charge descriptors
529	14	LDip	local dipole index	charge descriptors
530	1	HOMA	Harmonic Oscillator Model of Aromaticity index	aromaticity indices
531	2	RCI	Jug RC index	aromaticity indices
532	3	AROM	aromaticity (trial)	aromaticity indices
533	4	HOMT	HOMA total (trial)	aromaticity indices
534	1	DP01	molecular profile no. 01	Randic molecular profiles
535	2	DP02	molecular profile no. 02	Randic molecular profiles
536	3	DP03	molecular profile no. 03	Randic molecular profiles
537	4	DP04	molecular profile no. 04	Randic molecular profiles
538	5	DP05	molecular profile no. 05	Randic molecular profiles
539	6	DP06	molecular profile no. 06	Randic molecular profiles
540	7	DP07	molecular profile no. 07	Randic molecular profiles
541	8	DP08	molecular profile no. 08	Randic molecular profiles
542	9	DP09	molecular profile no. 09	Randic molecular profiles
543	10	DP10	molecular profile no. 10	Randic molecular profiles
544	11	DP11	molecular profile no. 11	Randic molecular profiles

No.	Rel.No.	Symbol	Definition	Class
545	12	DP12	molecular profile no. 12	Randic molecular profiles
546	13	DP13	molecular profile no. 13	Randic molecular profiles
547	14	DP14	molecular profile no. 14	Randic molecular profiles
548	15	DP15	molecular profile no. 15	Randic molecular profiles
549	16	DP16	molecular profile no. 16	Randic molecular profiles
550	17	DP17	molecular profile no. 17	Randic molecular profiles
551	18	DP18	molecular profile no. 18	Randic molecular profiles
552	19	DP19	molecular profile no. 19	Randic molecular profiles
553	20	DP20	molecular profile no. 20	Randic molecular profiles
554	21	SP01	shape profile no. 01	Randic molecular profiles
555	22	SP02	shape profile no. 02	Randic molecular profiles
556	23	SP03	shape profile no. 03	Randic molecular profiles
557	24	SP04	shape profile no. 04	Randic molecular profiles
558	25	SP05	shape profile no. 05	Randic molecular profiles
559	26	SP06	shape profile no. 06	Randic molecular profiles
560	27	SP07	shape profile no. 07	Randic molecular profiles
561	28	SP08	shape profile no. 08	Randic molecular profiles
562	29	SP09	shape profile no. 09	Randic molecular profiles
563	30	SP10	shape profile no. 10	Randic molecular profiles
564	31	SP11	shape profile no. 11	Randic molecular profiles
565	32	SP12	shape profile no. 12	Randic molecular profiles
566	33	SP13	shape profile no. 13	Randic molecular profiles
567	34	SP14	shape profile no. 14	Randic molecular profiles
568	35	SP15	shape profile no. 15	Randic molecular profiles
569	36	SP16	shape profile no. 16	Randic molecular profiles
570	37	SP17	shape profile no. 17	Randic molecular profiles
571	38	SP18	shape profile no. 18	Randic molecular profiles
572	39	SP19	shape profile no. 19	Randic molecular profiles
573	40	SP20	shape profile no. 20	Randic molecular profiles
574	41	SHP2	average shape profile index of order 2	Randic molecular profiles
575	1	W3D	3D-Wiener index	geometrical descriptors
576	2	J3D	3D-Balaban index	geometrical descriptors
577	3	H3D	3D-Harary index	geometrical descriptors
578	4	AGDD	average geometric distance degree	geometrical descriptors
579	5	DDI	D/D index	geometrical descriptors
580	6	ADDD	average distance/distance degree	geometrical descriptors
581	7	G1	gravitational index G1	geometrical descriptors
582	8	G2	gravitational index G2 (bond-restricted)	geometrical descriptors
583	9	RGyr	radius of gyration (mass weighted)	geometrical descriptors

No.	Rel.No.	Symbol	Definition	Class
584	10	SPAN	span R	geometrical descriptors
585	11	SPAM	average span R	geometrical descriptors
586	12	MEcc	molecular eccentricity	geometrical descriptors
587	13	SPH	sphericity	geometrical descriptors
588	14	ASP	asphericity	geometrical descriptors
589	15	FDI	folding degree index	geometrical descriptors
590	16	PJI3	3D Petijean shape index	geometrical descriptors
591	17	L/Bw	length-to-breadth ratio by WHIM	geometrical descriptors
592	18	SEig	absolute eigenvalue sum on geometry matrix	geometrical descriptors
593	19	DISPm	d COMMA2 value / weighted by atomic masses	geometrical descriptors
594	20	QXXm	Qxx COMMA2 value / weighted by atomic masses	geometrical descriptors
595	21	QYYm	Qyy COMMA2 value / weighted by atomic masses	geometrical descriptors
596	22	QZZm	Qzz COMMA2 value / weighted by atomic masses	geometrical descriptors
597	23	DISPv	d COMMA2 value / weighted by atomic van der Waals volumes	geometrical descriptors
598	24	QXXv	Qxx COMMA2 value / weighted by atomic van der Waals volumes	geometrical descriptors
599	25	QYYv	Qyy COMMA2 value / weighted by atomic van der Waals volumes	geometrical descriptors
600	26	QZZv	Qzz COMMA2 value / weighted by atomic van der Waals volumes	geometrical descriptors
601	27	DISPe	d COMMA2 value / weighted by atomic Sanderson electronegativities	geometrical descriptors
602	28	QXXe	Qxx COMMA2 value / weighted by atomic Sanderson electronegativities	geometrical descriptors
603	29	QYYe	Qyy COMMA2 value / weighted by atomic Sanderson electronegativities	geometrical descriptors
604	30	QZZe	Qzz COMMA2 value / weighted by atomic Sanderson electronegativities	geometrical descriptors
605	31	DISPp	d COMMA2 value / weighted by atomic polarizabilities	geometrical descriptors
606	32	QXXp	Qxx COMMA2 value / weighted by atomic polarizabilities	geometrical descriptors
607	33	QYYp	Qyy COMMA2 value / weighted by atomic polarizabilities	geometrical descriptors
608	34	QZZp	Qzz COMMA2 value / weighted by atomic polarizabilities	geometrical descriptors
609	35	G(N..N)	sum of geometrical distances between N..N	geometrical descriptors
610	36	G(N..O)	sum of geometrical distances between N..O	geometrical descriptors
611	37	G(N..S)	sum of geometrical distances between N..S	geometrical descriptors
612	38	G(N..P)	sum of geometrical distances between N..P	geometrical descriptors
613	39	G(N..F)	sum of geometrical distances between N..F	geometrical descriptors
614	40	G(N..Cl)	sum of geometrical distances between N..Cl	geometrical descriptors
615	41	G(N..Br)	sum of geometrical distances between N..Br	geometrical descriptors
616	42	G(N..I)	sum of geometrical distances between N..I	geometrical descriptors
617	43	G(O..O)	sum of geometrical distances between O..O	geometrical descriptors
618	44	G(O..S)	sum of geometrical distances between O..S	geometrical descriptors
619	45	G(O..P)	sum of geometrical distances between O..P	geometrical descriptors
620	46	G(O..F)	sum of geometrical distances between O..F	geometrical descriptors
621	47	G(O..Cl)	sum of geometrical distances between O..Cl	geometrical descriptors
622	48	G(O..Br)	sum of geometrical distances between O..Br	geometrical descriptors

No.	Rel.No.	Symbol	Definition	Class
623	49	G(O..I)	sum of geometrical distances between O..I	geometrical descriptors
624	50	G(S..S)	sum of geometrical distances between S..S	geometrical descriptors
625	51	G(S..P)	sum of geometrical distances between S..P	geometrical descriptors
626	52	G(S..F)	sum of geometrical distances between S..F	geometrical descriptors
627	53	G(S..Cl)	sum of geometrical distances between S..Cl	geometrical descriptors
628	54	G(S..Br)	sum of geometrical distances between S..Br	geometrical descriptors
629	55	G(S..I)	sum of geometrical distances between S..I	geometrical descriptors
630	56	G(P..P)	sum of geometrical distances between P..P	geometrical descriptors
631	57	G(P..F)	sum of geometrical distances between P..F	geometrical descriptors
632	58	G(P..Cl)	sum of geometrical distances between P..Cl	geometrical descriptors
633	59	G(P..Br)	sum of geometrical distances between P..Br	geometrical descriptors
634	60	G(P..I)	sum of geometrical distances between P..I	geometrical descriptors
635	61	G(F..F)	sum of geometrical distances between F..F	geometrical descriptors
636	62	G(F..Cl)	sum of geometrical distances between F..Cl	geometrical descriptors
637	63	G(F..Br)	sum of geometrical distances between F..Br	geometrical descriptors
638	64	G(F..I)	sum of geometrical distances between F..I	geometrical descriptors
639	65	G(Cl..Cl)	sum of geometrical distances between Cl..Cl	geometrical descriptors
640	66	G(Cl..Br)	sum of geometrical distances between Cl..Br	geometrical descriptors
641	67	G(Cl..I)	sum of geometrical distances between Cl..I	geometrical descriptors
642	68	G(Br..Br)	sum of geometrical distances between Br..Br	geometrical descriptors
643	69	G(Br..I)	sum of geometrical distances between Br..I	geometrical descriptors
644	70	G(I..I)	sum of geometrical distances between I..I	geometrical descriptors
645	1	RDF010u	Radial Distribution Function - 1.0 / unweighted	RDF descriptors
646	2	RDF015u	Radial Distribution Function - 1.5 / unweighted	RDF descriptors
647	3	RDF020u	Radial Distribution Function - 2.0 / unweighted	RDF descriptors
648	4	RDF025u	Radial Distribution Function - 2.5 / unweighted	RDF descriptors
649	5	RDF030u	Radial Distribution Function - 3.0 / unweighted	RDF descriptors
650	6	RDF035u	Radial Distribution Function - 3.5 / unweighted	RDF descriptors
651	7	RDF040u	Radial Distribution Function - 4.0 / unweighted	RDF descriptors
652	8	RDF045u	Radial Distribution Function - 4.5 / unweighted	RDF descriptors
653	9	RDF050u	Radial Distribution Function - 5.0 / unweighted	RDF descriptors
654	10	RDF055u	Radial Distribution Function - 5.5 / unweighted	RDF descriptors
655	11	RDF060u	Radial Distribution Function - 6.0 / unweighted	RDF descriptors
656	12	RDF065u	Radial Distribution Function - 6.5 / unweighted	RDF descriptors
657	13	RDF070u	Radial Distribution Function - 7.0 / unweighted	RDF descriptors
658	14	RDF075u	Radial Distribution Function - 7.5 / unweighted	RDF descriptors
659	15	RDF080u	Radial Distribution Function - 8.0 / unweighted	RDF descriptors
660	16	RDF085u	Radial Distribution Function - 8.5 / unweighted	RDF descriptors
661	17	RDF090u	Radial Distribution Function - 9.0 / unweighted	RDF descriptors

No.	Rel.No.	Symbol	Definition	Class
662	18	RDF095u	Radial Distribution Function - 9.5 / unweighted	RDF descriptors
663	19	RDF100u	Radial Distribution Function - 10.0 / unweighted	RDF descriptors
664	20	RDF105u	Radial Distribution Function - 10.5 / unweighted	RDF descriptors
665	21	RDF110u	Radial Distribution Function - 11.0 / unweighted	RDF descriptors
666	22	RDF115u	Radial Distribution Function - 11.5 / unweighted	RDF descriptors
667	23	RDF120u	Radial Distribution Function - 12.0 / unweighted	RDF descriptors
668	24	RDF125u	Radial Distribution Function - 12.5 / unweighted	RDF descriptors
669	25	RDF130u	Radial Distribution Function - 13.0 / unweighted	RDF descriptors
670	26	RDF135u	Radial Distribution Function - 13.5 / unweighted	RDF descriptors
671	27	RDF140u	Radial Distribution Function - 14.0 / unweighted	RDF descriptors
672	28	RDF145u	Radial Distribution Function - 14.5 / unweighted	RDF descriptors
673	29	RDF150u	Radial Distribution Function - 15.0 / unweighted	RDF descriptors
674	30	RDF155u	Radial Distribution Function - 15.5 / unweighted	RDF descriptors
675	31	RDF010m	Radial Distribution Function - 1.0 / weighted by atomic masses	RDF descriptors
676	32	RDF015m	Radial Distribution Function - 1.5 / weighted by atomic masses	RDF descriptors
677	33	RDF020m	Radial Distribution Function - 2.0 / weighted by atomic masses	RDF descriptors
678	34	RDF025m	Radial Distribution Function - 2.5 / weighted by atomic masses	RDF descriptors
679	35	RDF030m	Radial Distribution Function - 3.0 / weighted by atomic masses	RDF descriptors
680	36	RDF035m	Radial Distribution Function - 3.5 / weighted by atomic masses	RDF descriptors
681	37	RDF040m	Radial Distribution Function - 4.0 / weighted by atomic masses	RDF descriptors
682	38	RDF045m	Radial Distribution Function - 4.5 / weighted by atomic masses	RDF descriptors
683	39	RDF050m	Radial Distribution Function - 5.0 / weighted by atomic masses	RDF descriptors
684	40	RDF055m	Radial Distribution Function - 5.5 / weighted by atomic masses	RDF descriptors
685	41	RDF060m	Radial Distribution Function - 6.0 / weighted by atomic masses	RDF descriptors
686	42	RDF065m	Radial Distribution Function - 6.5 / weighted by atomic masses	RDF descriptors
687	43	RDF070m	Radial Distribution Function - 7.0 / weighted by atomic masses	RDF descriptors
688	44	RDF075m	Radial Distribution Function - 7.5 / weighted by atomic masses	RDF descriptors
689	45	RDF080m	Radial Distribution Function - 8.0 / weighted by atomic masses	RDF descriptors
690	46	RDF085m	Radial Distribution Function - 8.5 / weighted by atomic masses	RDF descriptors
691	47	RDF090m	Radial Distribution Function - 9.0 / weighted by atomic masses	RDF descriptors
692	48	RDF095m	Radial Distribution Function - 9.5 / weighted by atomic masses	RDF descriptors
693	49	RDF100m	Radial Distribution Function - 10.0 / weighted by atomic masses	RDF descriptors
694	50	RDF105m	Radial Distribution Function - 10.5 / weighted by atomic masses	RDF descriptors
695	51	RDF110m	Radial Distribution Function - 11.0 / weighted by atomic masses	RDF descriptors
696	52	RDF115m	Radial Distribution Function - 11.5 / weighted by atomic masses	RDF descriptors
697	53	RDF120m	Radial Distribution Function - 12.0 / weighted by atomic masses	RDF descriptors
698	54	RDF125m	Radial Distribution Function - 12.5 / weighted by atomic masses	RDF descriptors
699	55	RDF130m	Radial Distribution Function - 13.0 / weighted by atomic masses	RDF descriptors
700	56	RDF135m	Radial Distribution Function - 13.5 / weighted by atomic masses	RDF descriptors

No.	Rel.No.	Symbol	Definition	Class
701	57	RDF140m	Radial Distribution Function - 14.0 / weighted by atomic masses	RDF descriptors
702	58	RDF145m	Radial Distribution Function - 14.5 / weighted by atomic masses	RDF descriptors
703	59	RDF150m	Radial Distribution Function - 15.0 / weighted by atomic masses	RDF descriptors
704	60	RDF155m	Radial Distribution Function - 15.5 / weighted by atomic masses	RDF descriptors
705	61	RDF010v	Radial Distribution Function - 1.0 / weighted by atomic van der Waals volumes	RDF descriptors
706	62	RDF015v	Radial Distribution Function - 1.5 / weighted by atomic van der Waals volumes	RDF descriptors
707	63	RDF020v	Radial Distribution Function - 2.0 / weighted by atomic van der Waals volumes	RDF descriptors
708	64	RDF025v	Radial Distribution Function - 2.5 / weighted by atomic van der Waals volumes	RDF descriptors
709	65	RDF030v	Radial Distribution Function - 3.0 / weighted by atomic van der Waals volumes	RDF descriptors
710	66	RDF035v	Radial Distribution Function - 3.5 / weighted by atomic van der Waals volumes	RDF descriptors
711	67	RDF040v	Radial Distribution Function - 4.0 / weighted by atomic van der Waals volumes	RDF descriptors
712	68	RDF045v	Radial Distribution Function - 4.5 / weighted by atomic van der Waals volumes	RDF descriptors
713	69	RDF050v	Radial Distribution Function - 5.0 / weighted by atomic van der Waals volumes	RDF descriptors
714	70	RDF055v	Radial Distribution Function - 5.5 / weighted by atomic van der Waals volumes	RDF descriptors
715	71	RDF060v	Radial Distribution Function - 6.0 / weighted by atomic van der Waals volumes	RDF descriptors
716	72	RDF065v	Radial Distribution Function - 6.5 / weighted by atomic van der Waals volumes	RDF descriptors
717	73	RDF070v	Radial Distribution Function - 7.0 / weighted by atomic van der Waals volumes	RDF descriptors
718	74	RDF075v	Radial Distribution Function - 7.5 / weighted by atomic van der Waals volumes	RDF descriptors
719	75	RDF080v	Radial Distribution Function - 8.0 / weighted by atomic van der Waals volumes	RDF descriptors
720	76	RDF085v	Radial Distribution Function - 8.5 / weighted by atomic van der Waals volumes	RDF descriptors
721	77	RDF090v	Radial Distribution Function - 9.0 / weighted by atomic van der Waals volumes	RDF descriptors
722	78	RDF095v	Radial Distribution Function - 9.5 / weighted by atomic van der Waals volumes	RDF descriptors
723	79	RDF100v	Radial Distribution Function - 10.0 / weighted by atomic van der Waals volumes	RDF descriptors
724	80	RDF105v	Radial Distribution Function - 10.5 / weighted by atomic van der Waals volumes	RDF descriptors
725	81	RDF110v	Radial Distribution Function - 11.0 / weighted by atomic van der Waals volumes	RDF descriptors
726	82	RDF115v	Radial Distribution Function - 11.5 / weighted by atomic van der Waals volumes	RDF descriptors
727	83	RDF120v	Radial Distribution Function - 12.0 / weighted by atomic van der Waals volumes	RDF descriptors
728	84	RDF125v	Radial Distribution Function - 12.5 / weighted by atomic van der Waals volumes	RDF descriptors
729	85	RDF130v	Radial Distribution Function - 13.0 / weighted by atomic van der Waals volumes	RDF descriptors
730	86	RDF135v	Radial Distribution Function - 13.5 / weighted by atomic van der Waals volumes	RDF descriptors
731	87	RDF140v	Radial Distribution Function - 14.0 / weighted by atomic van der Waals volumes	RDF descriptors
732	88	RDF145v	Radial Distribution Function - 14.5 / weighted by atomic van der Waals volumes	RDF descriptors
733	89	RDF150v	Radial Distribution Function - 15.0 / weighted by atomic van der Waals volumes	RDF descriptors
734	90	RDF155v	Radial Distribution Function - 15.5 / weighted by atomic van der Waals volumes	RDF descriptors
735	91	RDF010e	Radial Distribution Function - 1.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
736	92	RDF015e	Radial Distribution Function - 1.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
737	93	RDF020e	Radial Distribution Function - 2.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
738	94	RDF025e	Radial Distribution Function - 2.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
739	95	RDF030e	Radial Distribution Function - 3.0 / weighted by atomic Sanderson electronegativities	RDF descriptors

No.	Rel.No.	Symbol	Definition	Class
740	96	RDF035e	Radial Distribution Function - 3.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
741	97	RDF040e	Radial Distribution Function - 4.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
742	98	RDF045e	Radial Distribution Function - 4.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
743	99	RDF050e	Radial Distribution Function - 5.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
744	100	RDF055e	Radial Distribution Function - 5.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
745	101	RDF060e	Radial Distribution Function - 6.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
746	102	RDF065e	Radial Distribution Function - 6.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
747	103	RDF070e	Radial Distribution Function - 7.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
748	104	RDF075e	Radial Distribution Function - 7.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
749	105	RDF080e	Radial Distribution Function - 8.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
750	106	RDF085e	Radial Distribution Function - 8.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
751	107	RDF090e	Radial Distribution Function - 9.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
752	108	RDF095e	Radial Distribution Function - 9.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
753	109	RDF100e	Radial Distribution Function - 10.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
754	110	RDF105e	Radial Distribution Function - 10.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
755	111	RDF110e	Radial Distribution Function - 11.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
756	112	RDF115e	Radial Distribution Function - 11.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
757	113	RDF120e	Radial Distribution Function - 12.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
758	114	RDF125e	Radial Distribution Function - 12.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
759	115	RDF130e	Radial Distribution Function - 13.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
760	116	RDF135e	Radial Distribution Function - 13.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
761	117	RDF140e	Radial Distribution Function - 14.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
762	118	RDF145e	Radial Distribution Function - 14.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
763	119	RDF150e	Radial Distribution Function - 15.0 / weighted by atomic Sanderson electronegativities	RDF descriptors
764	120	RDF155e	Radial Distribution Function - 15.5 / weighted by atomic Sanderson electronegativities	RDF descriptors
765	121	RDF010p	Radial Distribution Function - 1.0 / weighted by atomic polarizabilities	RDF descriptors
766	122	RDF015p	Radial Distribution Function - 1.5 / weighted by atomic polarizabilities	RDF descriptors
767	123	RDF020p	Radial Distribution Function - 2.0 / weighted by atomic polarizabilities	RDF descriptors
768	124	RDF025p	Radial Distribution Function - 2.5 / weighted by atomic polarizabilities	RDF descriptors
769	125	RDF030p	Radial Distribution Function - 3.0 / weighted by atomic polarizabilities	RDF descriptors
770	126	RDF035p	Radial Distribution Function - 3.5 / weighted by atomic polarizabilities	RDF descriptors
771	127	RDF040p	Radial Distribution Function - 4.0 / weighted by atomic polarizabilities	RDF descriptors
772	128	RDF045p	Radial Distribution Function - 4.5 / weighted by atomic polarizabilities	RDF descriptors
773	129	RDF050p	Radial Distribution Function - 5.0 / weighted by atomic polarizabilities	RDF descriptors
774	130	RDF055p	Radial Distribution Function - 5.5 / weighted by atomic polarizabilities	RDF descriptors
775	131	RDF060p	Radial Distribution Function - 6.0 / weighted by atomic polarizabilities	RDF descriptors
776	132	RDF065p	Radial Distribution Function - 6.5 / weighted by atomic polarizabilities	RDF descriptors
777	133	RDF070p	Radial Distribution Function - 7.0 / weighted by atomic polarizabilities	RDF descriptors
778	134	RDF075p	Radial Distribution Function - 7.5 / weighted by atomic polarizabilities	RDF descriptors

No.	Rel.No.	Symbol	Definition	Class
779	135	RDF080p	Radial Distribution Function - 8.0 / weighted by atomic polarizabilities	RDF descriptors
780	136	RDF085p	Radial Distribution Function - 8.5 / weighted by atomic polarizabilities	RDF descriptors
781	137	RDF090p	Radial Distribution Function - 9.0 / weighted by atomic polarizabilities	RDF descriptors
782	138	RDF095p	Radial Distribution Function - 9.5 / weighted by atomic polarizabilities	RDF descriptors
783	139	RDF100p	Radial Distribution Function - 10.0 / weighted by atomic polarizabilities	RDF descriptors
784	140	RDF105p	Radial Distribution Function - 10.5 / weighted by atomic polarizabilities	RDF descriptors
785	141	RDF110p	Radial Distribution Function - 11.0 / weighted by atomic polarizabilities	RDF descriptors
786	142	RDF115p	Radial Distribution Function - 11.5 / weighted by atomic polarizabilities	RDF descriptors
787	143	RDF120p	Radial Distribution Function - 12.0 / weighted by atomic polarizabilities	RDF descriptors
788	144	RDF125p	Radial Distribution Function - 12.5 / weighted by atomic polarizabilities	RDF descriptors
789	145	RDF130p	Radial Distribution Function - 13.0 / weighted by atomic polarizabilities	RDF descriptors
790	146	RDF135p	Radial Distribution Function - 13.5 / weighted by atomic polarizabilities	RDF descriptors
791	147	RDF140p	Radial Distribution Function - 14.0 / weighted by atomic polarizabilities	RDF descriptors
792	148	RDF145p	Radial Distribution Function - 14.5 / weighted by atomic polarizabilities	RDF descriptors
793	149	RDF150p	Radial Distribution Function - 15.0 / weighted by atomic polarizabilities	RDF descriptors
794	150	RDF155p	Radial Distribution Function - 15.5 / weighted by atomic polarizabilities	RDF descriptors
795	1	Mor01u	3D-MoRSE - signal 01 / unweighted	3D-MoRSE descriptors
796	2	Mor02u	3D-MoRSE - signal 02 / unweighted	3D-MoRSE descriptors
797	3	Mor03u	3D-MoRSE - signal 03 / unweighted	3D-MoRSE descriptors
798	4	Mor04u	3D-MoRSE - signal 04 / unweighted	3D-MoRSE descriptors
799	5	Mor05u	3D-MoRSE - signal 05 / unweighted	3D-MoRSE descriptors
800	6	Mor06u	3D-MoRSE - signal 06 / unweighted	3D-MoRSE descriptors
801	7	Mor07u	3D-MoRSE - signal 07 / unweighted	3D-MoRSE descriptors
802	8	Mor08u	3D-MoRSE - signal 08 / unweighted	3D-MoRSE descriptors
803	9	Mor09u	3D-MoRSE - signal 09 / unweighted	3D-MoRSE descriptors
804	10	Mor10u	3D-MoRSE - signal 10 / unweighted	3D-MoRSE descriptors
805	11	Mor11u	3D-MoRSE - signal 11 / unweighted	3D-MoRSE descriptors
806	12	Mor12u	3D-MoRSE - signal 12 / unweighted	3D-MoRSE descriptors
807	13	Mor13u	3D-MoRSE - signal 13 / unweighted	3D-MoRSE descriptors
808	14	Mor14u	3D-MoRSE - signal 14 / unweighted	3D-MoRSE descriptors
809	15	Mor15u	3D-MoRSE - signal 15 / unweighted	3D-MoRSE descriptors
810	16	Mor16u	3D-MoRSE - signal 16 / unweighted	3D-MoRSE descriptors
811	17	Mor17u	3D-MoRSE - signal 17 / unweighted	3D-MoRSE descriptors
812	18	Mor18u	3D-MoRSE - signal 18 / unweighted	3D-MoRSE descriptors
813	19	Mor19u	3D-MoRSE - signal 19 / unweighted	3D-MoRSE descriptors
814	20	Mor20u	3D-MoRSE - signal 20 / unweighted	3D-MoRSE descriptors
815	21	Mor21u	3D-MoRSE - signal 21 / unweighted	3D-MoRSE descriptors
816	22	Mor22u	3D-MoRSE - signal 22 / unweighted	3D-MoRSE descriptors
817	23	Mor23u	3D-MoRSE - signal 23 / unweighted	3D-MoRSE descriptors

No.	Rel.No.	Symbol	Definition	Class
818	24	Mor24u	3D-MoRSE - signal 24 / unweighted	3D-MoRSE descriptors
819	25	Mor25u	3D-MoRSE - signal 25 / unweighted	3D-MoRSE descriptors
820	26	Mor26u	3D-MoRSE - signal 26 / unweighted	3D-MoRSE descriptors
821	27	Mor27u	3D-MoRSE - signal 27 / unweighted	3D-MoRSE descriptors
822	28	Mor28u	3D-MoRSE - signal 28 / unweighted	3D-MoRSE descriptors
823	29	Mor29u	3D-MoRSE - signal 29 / unweighted	3D-MoRSE descriptors
824	30	Mor30u	3D-MoRSE - signal 30 / unweighted	3D-MoRSE descriptors
825	31	Mor31u	3D-MoRSE - signal 31 / unweighted	3D-MoRSE descriptors
826	32	Mor32u	3D-MoRSE - signal 32 / unweighted	3D-MoRSE descriptors
827	33	Mor01m	3D-MoRSE - signal 01 / weighted by atomic masses	3D-MoRSE descriptors
828	34	Mor02m	3D-MoRSE - signal 02 / weighted by atomic masses	3D-MoRSE descriptors
829	35	Mor03m	3D-MoRSE - signal 03 / weighted by atomic masses	3D-MoRSE descriptors
830	36	Mor04m	3D-MoRSE - signal 04 / weighted by atomic masses	3D-MoRSE descriptors
831	37	Mor05m	3D-MoRSE - signal 05 / weighted by atomic masses	3D-MoRSE descriptors
832	38	Mor06m	3D-MoRSE - signal 06 / weighted by atomic masses	3D-MoRSE descriptors
833	39	Mor07m	3D-MoRSE - signal 07 / weighted by atomic masses	3D-MoRSE descriptors
834	40	Mor08m	3D-MoRSE - signal 08 / weighted by atomic masses	3D-MoRSE descriptors
835	41	Mor09m	3D-MoRSE - signal 09 / weighted by atomic masses	3D-MoRSE descriptors
836	42	Mor10m	3D-MoRSE - signal 10 / weighted by atomic masses	3D-MoRSE descriptors
837	43	Mor11m	3D-MoRSE - signal 11 / weighted by atomic masses	3D-MoRSE descriptors
838	44	Mor12m	3D-MoRSE - signal 12 / weighted by atomic masses	3D-MoRSE descriptors
839	45	Mor13m	3D-MoRSE - signal 13 / weighted by atomic masses	3D-MoRSE descriptors
840	46	Mor14m	3D-MoRSE - signal 14 / weighted by atomic masses	3D-MoRSE descriptors
841	47	Mor15m	3D-MoRSE - signal 15 / weighted by atomic masses	3D-MoRSE descriptors
842	48	Mor16m	3D-MoRSE - signal 16 / weighted by atomic masses	3D-MoRSE descriptors
843	49	Mor17m	3D-MoRSE - signal 17 / weighted by atomic masses	3D-MoRSE descriptors
844	50	Mor18m	3D-MoRSE - signal 18 / weighted by atomic masses	3D-MoRSE descriptors
845	51	Mor19m	3D-MoRSE - signal 19 / weighted by atomic masses	3D-MoRSE descriptors
846	52	Mor20m	3D-MoRSE - signal 20 / weighted by atomic masses	3D-MoRSE descriptors
847	53	Mor21m	3D-MoRSE - signal 21 / weighted by atomic masses	3D-MoRSE descriptors
848	54	Mor22m	3D-MoRSE - signal 22 / weighted by atomic masses	3D-MoRSE descriptors
849	55	Mor23m	3D-MoRSE - signal 23 / weighted by atomic masses	3D-MoRSE descriptors
850	56	Mor24m	3D-MoRSE - signal 24 / weighted by atomic masses	3D-MoRSE descriptors
851	57	Mor25m	3D-MoRSE - signal 25 / weighted by atomic masses	3D-MoRSE descriptors
852	58	Mor26m	3D-MoRSE - signal 26 / weighted by atomic masses	3D-MoRSE descriptors
853	59	Mor27m	3D-MoRSE - signal 27 / weighted by atomic masses	3D-MoRSE descriptors
854	60	Mor28m	3D-MoRSE - signal 28 / weighted by atomic masses	3D-MoRSE descriptors
855	61	Mor29m	3D-MoRSE - signal 29 / weighted by atomic masses	3D-MoRSE descriptors
856	62	Mor30m	3D-MoRSE - signal 30 / weighted by atomic masses	3D-MoRSE descriptors

No.	Rel.No.	Symbol	Definition	Class
857	63	Mor31m	3D-MoRSE - signal 31 / weighted by atomic masses	3D-MoRSE descriptors
858	64	Mor32m	3D-MoRSE - signal 32 / weighted by atomic masses	3D-MoRSE descriptors
859	65	Mor01v	3D-MoRSE - signal 01 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
860	66	Mor02v	3D-MoRSE - signal 02 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
861	67	Mor03v	3D-MoRSE - signal 03 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
862	68	Mor04v	3D-MoRSE - signal 04 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
863	69	Mor05v	3D-MoRSE - signal 05 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
864	70	Mor06v	3D-MoRSE - signal 06 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
865	71	Mor07v	3D-MoRSE - signal 07 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
866	72	Mor08v	3D-MoRSE - signal 08 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
867	73	Mor09v	3D-MoRSE - signal 09 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
868	74	Mor10v	3D-MoRSE - signal 10 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
869	75	Mor11v	3D-MoRSE - signal 11 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
870	76	Mor12v	3D-MoRSE - signal 12 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
871	77	Mor13v	3D-MoRSE - signal 13 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
872	78	Mor14v	3D-MoRSE - signal 14 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
873	79	Mor15v	3D-MoRSE - signal 15 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
874	80	Mor16v	3D-MoRSE - signal 16 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
875	81	Mor17v	3D-MoRSE - signal 17 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
876	82	Mor18v	3D-MoRSE - signal 18 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
877	83	Mor19v	3D-MoRSE - signal 19 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
878	84	Mor20v	3D-MoRSE - signal 20 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
879	85	Mor21v	3D-MoRSE - signal 21 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
880	86	Mor22v	3D-MoRSE - signal 22 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
881	87	Mor23v	3D-MoRSE - signal 23 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
882	88	Mor24v	3D-MoRSE - signal 24 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
883	89	Mor25v	3D-MoRSE - signal 25 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
884	90	Mor26v	3D-MoRSE - signal 26 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
885	91	Mor27v	3D-MoRSE - signal 27 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
886	92	Mor28v	3D-MoRSE - signal 28 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
887	93	Mor29v	3D-MoRSE - signal 29 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
888	94	Mor30v	3D-MoRSE - signal 30 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
889	95	Mor31v	3D-MoRSE - signal 31 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
890	96	Mor32v	3D-MoRSE - signal 32 / weighted by atomic van der Waals volumes	3D-MoRSE descriptors
891	97	Mor01e	3D-MoRSE - signal 01 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
892	98	Mor02e	3D-MoRSE - signal 02 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
893	99	Mor03e	3D-MoRSE - signal 03 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
894	100	Mor04e	3D-MoRSE - signal 04 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
895	101	Mor05e	3D-MoRSE - signal 05 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors

No.	Rel.No.	Symbol	Definition	Class
896	102	Mor06e	3D-MoRSE - signal 06 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
897	103	Mor07e	3D-MoRSE - signal 07 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
898	104	Mor08e	3D-MoRSE - signal 08 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
899	105	Mor09e	3D-MoRSE - signal 09 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
900	106	Mor10e	3D-MoRSE - signal 10 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
901	107	Mor11e	3D-MoRSE - signal 11 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
902	108	Mor12e	3D-MoRSE - signal 12 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
903	109	Mor13e	3D-MoRSE - signal 13 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
904	110	Mor14e	3D-MoRSE - signal 14 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
905	111	Mor15e	3D-MoRSE - signal 15 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
906	112	Mor16e	3D-MoRSE - signal 16 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
907	113	Mor17e	3D-MoRSE - signal 17 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
908	114	Mor18e	3D-MoRSE - signal 18 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
909	115	Mor19e	3D-MoRSE - signal 19 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
910	116	Mor20e	3D-MoRSE - signal 20 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
911	117	Mor21e	3D-MoRSE - signal 21 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
912	118	Mor22e	3D-MoRSE - signal 22 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
913	119	Mor23e	3D-MoRSE - signal 23 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
914	120	Mor24e	3D-MoRSE - signal 24 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
915	121	Mor25e	3D-MoRSE - signal 25 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
916	122	Mor26e	3D-MoRSE - signal 26 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
917	123	Mor27e	3D-MoRSE - signal 27 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
918	124	Mor28e	3D-MoRSE - signal 28 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
919	125	Mor29e	3D-MoRSE - signal 29 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
920	126	Mor30e	3D-MoRSE - signal 30 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
921	127	Mor31e	3D-MoRSE - signal 31 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
922	128	Mor32e	3D-MoRSE - signal 32 / weighted by atomic Sanderson electronegativities	3D-MoRSE descriptors
923	129	Mor01p	3D-MoRSE - signal 01 / weighted by atomic polarizabilities	3D-MoRSE descriptors
924	130	Mor02p	3D-MoRSE - signal 02 / weighted by atomic polarizabilities	3D-MoRSE descriptors
925	131	Mor03p	3D-MoRSE - signal 03 / weighted by atomic polarizabilities	3D-MoRSE descriptors
926	132	Mor04p	3D-MoRSE - signal 04 / weighted by atomic polarizabilities	3D-MoRSE descriptors
927	133	Mor05p	3D-MoRSE - signal 05 / weighted by atomic polarizabilities	3D-MoRSE descriptors
928	134	Mor06p	3D-MoRSE - signal 06 / weighted by atomic polarizabilities	3D-MoRSE descriptors
929	135	Mor07p	3D-MoRSE - signal 07 / weighted by atomic polarizabilities	3D-MoRSE descriptors
930	136	Mor08p	3D-MoRSE - signal 08 / weighted by atomic polarizabilities	3D-MoRSE descriptors
931	137	Mor09p	3D-MoRSE - signal 09 / weighted by atomic polarizabilities	3D-MoRSE descriptors
932	138	Mor10p	3D-MoRSE - signal 10 / weighted by atomic polarizabilities	3D-MoRSE descriptors
933	139	Mor11p	3D-MoRSE - signal 11 / weighted by atomic polarizabilities	3D-MoRSE descriptors
934	140	Mor12p	3D-MoRSE - signal 12 / weighted by atomic polarizabilities	3D-MoRSE descriptors

No.	Rel.No.	Symbol	Definition	Class
935	141	Mor13p	3D-MoRSE - signal 13 / weighted by atomic polarizabilities	3D-MoRSE descriptors
936	142	Mor14p	3D-MoRSE - signal 14 / weighted by atomic polarizabilities	3D-MoRSE descriptors
937	143	Mor15p	3D-MoRSE - signal 15 / weighted by atomic polarizabilities	3D-MoRSE descriptors
938	144	Mor16p	3D-MoRSE - signal 16 / weighted by atomic polarizabilities	3D-MoRSE descriptors
939	145	Mor17p	3D-MoRSE - signal 17 / weighted by atomic polarizabilities	3D-MoRSE descriptors
940	146	Mor18p	3D-MoRSE - signal 18 / weighted by atomic polarizabilities	3D-MoRSE descriptors
941	147	Mor19p	3D-MoRSE - signal 19 / weighted by atomic polarizabilities	3D-MoRSE descriptors
942	148	Mor20p	3D-MoRSE - signal 20 / weighted by atomic polarizabilities	3D-MoRSE descriptors
943	149	Mor21p	3D-MoRSE - signal 21 / weighted by atomic polarizabilities	3D-MoRSE descriptors
944	150	Mor22p	3D-MoRSE - signal 22 / weighted by atomic polarizabilities	3D-MoRSE descriptors
945	151	Mor23p	3D-MoRSE - signal 23 / weighted by atomic polarizabilities	3D-MoRSE descriptors
946	152	Mor24p	3D-MoRSE - signal 24 / weighted by atomic polarizabilities	3D-MoRSE descriptors
947	153	Mor25p	3D-MoRSE - signal 25 / weighted by atomic polarizabilities	3D-MoRSE descriptors
948	154	Mor26p	3D-MoRSE - signal 26 / weighted by atomic polarizabilities	3D-MoRSE descriptors
949	155	Mor27p	3D-MoRSE - signal 27 / weighted by atomic polarizabilities	3D-MoRSE descriptors
950	156	Mor28p	3D-MoRSE - signal 28 / weighted by atomic polarizabilities	3D-MoRSE descriptors
951	157	Mor29p	3D-MoRSE - signal 29 / weighted by atomic polarizabilities	3D-MoRSE descriptors
952	158	Mor30p	3D-MoRSE - signal 30 / weighted by atomic polarizabilities	3D-MoRSE descriptors
953	159	Mor31p	3D-MoRSE - signal 31 / weighted by atomic polarizabilities	3D-MoRSE descriptors
954	160	Mor32p	3D-MoRSE - signal 32 / weighted by atomic polarizabilities	3D-MoRSE descriptors
955	1	L1u	1st component size directional WHIM index / unweighted	WHIM descriptors
956	2	L2u	2nd component size directional WHIM index / unweighted	WHIM descriptors
957	3	L3u	3rd component size directional WHIM index / unweighted	WHIM descriptors
958	4	P1u	1st component shape directional WHIM index / unweighted	WHIM descriptors
959	5	P2u	2nd component shape directional WHIM index / unweighted	WHIM descriptors
960	6	G1u	1st component symmetry directional WHIM index / unweighted	WHIM descriptors
961	7	G2u	2st component symmetry directional WHIM index / unweighted	WHIM descriptors
962	8	G3u	3st component symmetry directional WHIM index / unweighted	WHIM descriptors
963	9	E1u	1st component accessibility directional WHIM index / unweighted	WHIM descriptors
964	10	E2u	2nd component accessibility directional WHIM index / unweighted	WHIM descriptors
965	11	E3u	3rd component accessibility directional WHIM index / unweighted	WHIM descriptors
966	12	L1m	1st component size directional WHIM index / weighted by atomic masses	WHIM descriptors
967	13	L2m	2nd component size directional WHIM index / weighted by atomic masses	WHIM descriptors
968	14	L3m	3rd component size directional WHIM index / weighted by atomic masses	WHIM descriptors
969	15	P1m	1st component shape directional WHIM index / weighted by atomic masses	WHIM descriptors
970	16	P2m	2nd component shape directional WHIM index / weighted by atomic masses	WHIM descriptors
971	17	G1m	1st component symmetry directional WHIM index / weighted by atomic masses	WHIM descriptors
972	18	G2m	2st component symmetry directional WHIM index / weighted by atomic masses	WHIM descriptors
973	19	G3m	3st component symmetry directional WHIM index / weighted by atomic masses	WHIM descriptors

No.	Rel.No.	Symbol	Definition	Class
974	20	E1m	1st component accessibility directional WHIM index / weighted by atomic masses	WHIM descriptors
975	21	E2m	2nd component accessibility directional WHIM index / weighted by atomic masses	WHIM descriptors
976	22	E3m	3rd component accessibility directional WHIM index / weighted by atomic masses	WHIM descriptors
977	23	L1v	1st component size directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
978	24	L2v	2nd component size directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
979	25	L3v	3rd component size directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
980	26	P1v	1st component shape directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
981	27	P2v	2nd component shape directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
982	28	G1v	1st component symmetry directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
983	29	G2v	2st component symmetry directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
984	30	G3v	3st component symmetry directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
985	31	E1v	1st component accessibility directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
986	32	E2v	2nd component accessibility directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
987	33	E3v	3rd component accessibility directional WHIM index / weighted by atomic van der Waals volumes	WHIM descriptors
988	34	L1e	1st component size directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
989	35	L2e	2nd component size directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
990	36	L3e	3rd component size directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
991	37	P1e	1st component shape directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
992	38	P2e	2nd component shape directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
993	39	G1e	1st component symmetry directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
994	40	G2e	2st component symmetry directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
995	41	G3e	3st component symmetry directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
996	42	E1e	1st component accessibility directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
997	43	E2e	2nd component accessibility directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
998	44	E3e	3rd component accessibility directional WHIM index / weighted by atomic Sanderson electronegativities	WHIM descriptors
999	45	L1p	1st component size directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1000	46	L2p	2nd component size directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1001	47	L3p	3rd component size directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1002	48	P1p	1st component shape directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1003	49	P2p	2nd component shape directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1004	50	G1p	1st component symmetry directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1005	51	G2p	2st component symmetry directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1006	52	G3p	3st component symmetry directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1007	53	E1p	1st component accessibility directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1008	54	E2p	2nd component accessibility directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1009	55	E3p	3rd component accessibility directional WHIM index / weighted by atomic polarizabilities	WHIM descriptors
1010	56	L1s	1st component size directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1011	57	L2s	2nd component size directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1012	58	L3s	3rd component size directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors

No.	Rel.No.	Symbol	Definition	Class
1013	59	P1s	1st component shape directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1014	60	P2s	2nd component shape directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1015	61	G1s	1st component symmetry directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1016	62	G2s	2st component symmetry directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1017	63	G3s	3st component symmetry directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1018	64	E1s	1st component accessibility directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1019	65	E2s	2nd component accessibility directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1020	66	E3s	3rd component accessibility directional WHIM index / weighted by atomic electrotopological states	WHIM descriptors
1021	67	Tu	T total size index / unweighted	WHIM descriptors
1022	68	Tm	T total size index / weighted by atomic masses	WHIM descriptors
1023	69	Tv	T total size index / weighted by atomic van der Waals volumes	WHIM descriptors
1024	70	Te	T total size index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1025	71	Tp	T total size index / weighted by atomic polarizabilities	WHIM descriptors
1026	72	Ts	T total size index / weighted by atomic electrotopological states	WHIM descriptors
1027	73	Au	A total size index / unweighted	WHIM descriptors
1028	74	Am	A total size index / weighted by atomic masses	WHIM descriptors
1029	75	Av	A total size index / weighted by atomic van der Waals volumes	WHIM descriptors
1030	76	Ae	A total size index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1031	77	Ap	A total size index / weighted by atomic polarizabilities	WHIM descriptors
1032	78	As	A total size index / weighted by atomic electrotopological states	WHIM descriptors
1033	79	Gu	G total symmetry index / unweighted	WHIM descriptors
1034	80	Gm	G total symmetry index / weighted by atomic masses	WHIM descriptors
1035	81	Gs	G total symmetry index / weighted by atomic electrotopological states	WHIM descriptors
1036	82	Ku	K global shape index / unweighted	WHIM descriptors
1037	83	Km	K global shape index / weighted by atomic masses	WHIM descriptors
1038	84	Kv	K global shape index / weighted by atomic van der Waals volumes	WHIM descriptors
1039	85	Ke	K global shape index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1040	86	Kp	K global shape index / weighted by atomic polarizabilities	WHIM descriptors
1041	87	Ks	K global shape index / weighted by atomic electrotopological states	WHIM descriptors
1042	88	Du	D total accessibility index / unweighted	WHIM descriptors
1043	89	Dm	D total accessibility index / weighted by atomic masses	WHIM descriptors
1044	90	Dv	D total accessibility index / weighted by atomic van der Waals volumes	WHIM descriptors
1045	91	De	D total accessibility index / weighted by atomic Sanderson electronegativities	WHIM descriptors
1046	92	Dp	D total accessibility index / weighted by atomic polarizabilities	WHIM descriptors
1047	93	Ds	D total accessibility index / weighted by atomic electrotopological states	WHIM descriptors
1048	94	Vu	V total size index / unweighted	WHIM descriptors
1049	95	Vm	V total size index / weighted by atomic masses	WHIM descriptors
1050	96	Vv	V total size index / weighted by atomic van der Waals volumes	WHIM descriptors
1051	97	Ve	V total size index / weighted by atomic Sanderson electronegativities	WHIM descriptors

No.	Rel.No.	Symbol	Definition	Class
1052	98	Vp	V total size index / weighted by atomic polarizabilities	WHIM descriptors
1053	99	Vs	V total size index / weighted by atomic electrotopological states	WHIM descriptors
1054	1	ITH	total information content on the leverage equality	GETAWAY descriptors
1055	2	ISH	standardized information content on the leverage equality	GETAWAY descriptors
1056	3	HIC	mean information content on the leverage magnitude	GETAWAY descriptors
1057	4	HGM	geometric mean on the leverage magnitude	GETAWAY descriptors
1058	5	H0u	H autocorrelation of lag 0 / unweighted	GETAWAY descriptors
1059	6	H1u	H autocorrelation of lag 1 / unweighted	GETAWAY descriptors
1060	7	H2u	H autocorrelation of lag 2 / unweighted	GETAWAY descriptors
1061	8	H3u	H autocorrelation of lag 3 / unweighted	GETAWAY descriptors
1062	9	H4u	H autocorrelation of lag 4 / unweighted	GETAWAY descriptors
1063	10	H5u	H autocorrelation of lag 5 / unweighted	GETAWAY descriptors
1064	11	H6u	H autocorrelation of lag 6 / unweighted	GETAWAY descriptors
1065	12	H7u	H autocorrelation of lag 7 / unweighted	GETAWAY descriptors
1066	13	H8u	H autocorrelation of lag 8 / unweighted	GETAWAY descriptors
1067	14	HTu	H total index / unweighted	GETAWAY descriptors
1068	15	HATS0u	leverage-weighted autocorrelation of lag 0 / unweighted	GETAWAY descriptors
1069	16	HATS1u	leverage-weighted autocorrelation of lag 1 / unweighted	GETAWAY descriptors
1070	17	HATS2u	leverage-weighted autocorrelation of lag 2 / unweighted	GETAWAY descriptors
1071	18	HATS3u	leverage-weighted autocorrelation of lag 3 / unweighted	GETAWAY descriptors
1072	19	HATS4u	leverage-weighted autocorrelation of lag 4 / unweighted	GETAWAY descriptors
1073	20	HATS5u	leverage-weighted autocorrelation of lag 5 / unweighted	GETAWAY descriptors
1074	21	HATS6u	leverage-weighted autocorrelation of lag 6 / unweighted	GETAWAY descriptors
1075	22	HATS7u	leverage-weighted autocorrelation of lag 7 / unweighted	GETAWAY descriptors
1076	23	HATS8u	leverage-weighted autocorrelation of lag 8 / unweighted	GETAWAY descriptors
1077	24	HATSu	leverage-weighted total index / unweighted	GETAWAY descriptors
1078	25	H0m	H autocorrelation of lag 0 / weighted by atomic masses	GETAWAY descriptors
1079	26	H1m	H autocorrelation of lag 1 / weighted by atomic masses	GETAWAY descriptors
1080	27	H2m	H autocorrelation of lag 2 / weighted by atomic masses	GETAWAY descriptors
1081	28	H3m	H autocorrelation of lag 3 / weighted by atomic masses	GETAWAY descriptors
1082	29	H4m	H autocorrelation of lag 4 / weighted by atomic masses	GETAWAY descriptors
1083	30	H5m	H autocorrelation of lag 5 / weighted by atomic masses	GETAWAY descriptors
1084	31	H6m	H autocorrelation of lag 6 / weighted by atomic masses	GETAWAY descriptors
1085	32	H7m	H autocorrelation of lag 7 / weighted by atomic masses	GETAWAY descriptors
1086	33	H8m	H autocorrelation of lag 8 / weighted by atomic masses	GETAWAY descriptors
1087	34	HTm	H total index / weighted by atomic masses	GETAWAY descriptors
1088	35	HATS0m	leverage-weighted autocorrelation of lag 0 / weighted by atomic masses	GETAWAY descriptors
1089	36	HATS1m	leverage-weighted autocorrelation of lag 1 / weighted by atomic masses	GETAWAY descriptors
1090	37	HATS2m	leverage-weighted autocorrelation of lag 2 / weighted by atomic masses	GETAWAY descriptors

No.	Rel.No.	Symbol	Definition	Class
1091	38	HATS3m	leverage-weighted autocorrelation of lag 3 / weighted by atomic masses	GETAWAY descriptors
1092	39	HATS4m	leverage-weighted autocorrelation of lag 4 / weighted by atomic masses	GETAWAY descriptors
1093	40	HATS5m	leverage-weighted autocorrelation of lag 5 / weighted by atomic masses	GETAWAY descriptors
1094	41	HATS6m	leverage-weighted autocorrelation of lag 6 / weighted by atomic masses	GETAWAY descriptors
1095	42	HATS7m	leverage-weighted autocorrelation of lag 7 / weighted by atomic masses	GETAWAY descriptors
1096	43	HATS8m	leverage-weighted autocorrelation of lag 8 / weighted by atomic masses	GETAWAY descriptors
1097	44	HATSm	leverage-weighted total index / weighted by atomic masses	GETAWAY descriptors
1098	45	H0v	H autocorrelation of lag 0 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1099	46	H1v	H autocorrelation of lag 1 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1100	47	H2v	H autocorrelation of lag 2 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1101	48	H3v	H autocorrelation of lag 3 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1102	49	H4v	H autocorrelation of lag 4 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1103	50	H5v	H autocorrelation of lag 5 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1104	51	H6v	H autocorrelation of lag 6 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1105	52	H7v	H autocorrelation of lag 7 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1106	53	H8v	H autocorrelation of lag 8 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1107	54	HTv	H total index / weighted by atomic van der Waals volumes	GETAWAY descriptors
1108	55	HATS0v	leverage-weighted autocorrelation of lag 0 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1109	56	HATS1v	leverage-weighted autocorrelation of lag 1 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1110	57	HATS2v	leverage-weighted autocorrelation of lag 2 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1111	58	HATS3v	leverage-weighted autocorrelation of lag 3 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1112	59	HATS4v	leverage-weighted autocorrelation of lag 4 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1113	60	HATS5v	leverage-weighted autocorrelation of lag 5 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1114	61	HATS6v	leverage-weighted autocorrelation of lag 6 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1115	62	HATS7v	leverage-weighted autocorrelation of lag 7 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1116	63	HATS8v	leverage-weighted autocorrelation of lag 8 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1117	64	HATSV	leverage-weighted total index / weighted by atomic van der Waals volumes	GETAWAY descriptors
1118	65	H0e	H autocorrelation of lag 0 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1119	66	H1e	H autocorrelation of lag 1 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1120	67	H2e	H autocorrelation of lag 2 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1121	68	H3e	H autocorrelation of lag 3 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1122	69	H4e	H autocorrelation of lag 4 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1123	70	H5e	H autocorrelation of lag 5 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1124	71	H6e	H autocorrelation of lag 6 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1125	72	H7e	H autocorrelation of lag 7 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1126	73	H8e	H autocorrelation of lag 8 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1127	74	HTe	H total index / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1128	75	HATS0e	leverage-weighted autocorrelation of lag 0 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1129	76	HATS1e	leverage-weighted autocorrelation of lag 1 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors

No.	Rel.No.	Symbol	Definition	Class
1130	77	HATS2e	leverage-weighted autocorrelation of lag 2 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1131	78	HATS3e	leverage-weighted autocorrelation of lag 3 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1132	79	HATS4e	leverage-weighted autocorrelation of lag 4 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1133	80	HATS5e	leverage-weighted autocorrelation of lag 5 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1134	81	HATS6e	leverage-weighted autocorrelation of lag 6 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1135	82	HATS7e	leverage-weighted autocorrelation of lag 7 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1136	83	HATS8e	leverage-weighted autocorrelation of lag 8 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1137	84	HATSe	leverage-weighted total index / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1138	85	H0p	H autocorrelation of lag 0 / weighted by atomic polarizabilities	GETAWAY descriptors
1139	86	H1p	H autocorrelation of lag 1 / weighted by atomic polarizabilities	GETAWAY descriptors
1140	87	H2p	H autocorrelation of lag 2 / weighted by atomic polarizabilities	GETAWAY descriptors
1141	88	H3p	H autocorrelation of lag 3 / weighted by atomic polarizabilities	GETAWAY descriptors
1142	89	H4p	H autocorrelation of lag 4 / weighted by atomic polarizabilities	GETAWAY descriptors
1143	90	H5p	H autocorrelation of lag 5 / weighted by atomic polarizabilities	GETAWAY descriptors
1144	91	H6p	H autocorrelation of lag 6 / weighted by atomic polarizabilities	GETAWAY descriptors
1145	92	H7p	H autocorrelation of lag 7 / weighted by atomic polarizabilities	GETAWAY descriptors
1146	93	H8p	H autocorrelation of lag 8 / weighted by atomic polarizabilities	GETAWAY descriptors
1147	94	HTp	H total index / weighted by atomic polarizabilities	GETAWAY descriptors
1148	95	HATS0p	leverage-weighted autocorrelation of lag 0 / weighted by atomic polarizabilities	GETAWAY descriptors
1149	96	HATS1p	leverage-weighted autocorrelation of lag 1 / weighted by atomic polarizabilities	GETAWAY descriptors
1150	97	HATS2p	leverage-weighted autocorrelation of lag 2 / weighted by atomic polarizabilities	GETAWAY descriptors
1151	98	HATS3p	leverage-weighted autocorrelation of lag 3 / weighted by atomic polarizabilities	GETAWAY descriptors
1152	99	HATS4p	leverage-weighted autocorrelation of lag 4 / weighted by atomic polarizabilities	GETAWAY descriptors
1153	100	HATS5p	leverage-weighted autocorrelation of lag 5 / weighted by atomic polarizabilities	GETAWAY descriptors
1154	101	HATS6p	leverage-weighted autocorrelation of lag 6 / weighted by atomic polarizabilities	GETAWAY descriptors
1155	102	HATS7p	leverage-weighted autocorrelation of lag 7 / weighted by atomic polarizabilities	GETAWAY descriptors
1156	103	HATS8p	leverage-weighted autocorrelation of lag 8 / weighted by atomic polarizabilities	GETAWAY descriptors
1157	104	HATSp	leverage-weighted total index / weighted by atomic polarizabilities	GETAWAY descriptors
1158	105	RCON	Randic-type R matrix connectivity	GETAWAY descriptors
1159	106	RARS	R matrix average row sum	GETAWAY descriptors
1160	107	REIG	first eigenvalue of the R matrix	GETAWAY descriptors
1161	108	R1u	R autocorrelation of lag 1 / unweighted	GETAWAY descriptors
1162	109	R2u	R autocorrelation of lag 2 / unweighted	GETAWAY descriptors
1163	110	R3u	R autocorrelation of lag 3 / unweighted	GETAWAY descriptors
1164	111	R4u	R autocorrelation of lag 4 / unweighted	GETAWAY descriptors
1165	112	R5u	R autocorrelation of lag 5 / unweighted	GETAWAY descriptors
1166	113	R6u	R autocorrelation of lag 6 / unweighted	GETAWAY descriptors
1167	114	R7u	R autocorrelation of lag 7 / unweighted	GETAWAY descriptors
1168	115	R8u	R autocorrelation of lag 8 / unweighted	GETAWAY descriptors

No.	Rel.No.	Symbol	Definition	Class
1169	116	RTu	R total index / unweighted	GETAWAY descriptors
1170	117	R1u+	R maximal autocorrelation of lag 1 / unweighted	GETAWAY descriptors
1171	118	R2u+	R maximal autocorrelation of lag 2 / unweighted	GETAWAY descriptors
1172	119	R3u+	R maximal autocorrelation of lag 3 / unweighted	GETAWAY descriptors
1173	120	R4u+	R maximal autocorrelation of lag 4 / unweighted	GETAWAY descriptors
1174	121	R5u+	R maximal autocorrelation of lag 5 / unweighted	GETAWAY descriptors
1175	122	R6u+	R maximal autocorrelation of lag 6 / unweighted	GETAWAY descriptors
1176	123	R7u+	R maximal autocorrelation of lag 7 / unweighted	GETAWAY descriptors
1177	124	R8u+	R maximal autocorrelation of lag 8 / unweighted	GETAWAY descriptors
1178	125	RTu+	R maximal index / unweighted	GETAWAY descriptors
1179	126	R1m	R autocorrelation of lag 1 / weighted by atomic masses	GETAWAY descriptors
1180	127	R2m	R autocorrelation of lag 2 / weighted by atomic masses	GETAWAY descriptors
1181	128	R3m	R autocorrelation of lag 3 / weighted by atomic masses	GETAWAY descriptors
1182	129	R4m	R autocorrelation of lag 4 / weighted by atomic masses	GETAWAY descriptors
1183	130	R5m	R autocorrelation of lag 5 / weighted by atomic masses	GETAWAY descriptors
1184	131	R6m	R autocorrelation of lag 6 / weighted by atomic masses	GETAWAY descriptors
1185	132	R7m	R autocorrelation of lag 7 / weighted by atomic masses	GETAWAY descriptors
1186	133	R8m	R autocorrelation of lag 8 / weighted by atomic masses	GETAWAY descriptors
1187	134	RTm	R total index / weighted by atomic masses	GETAWAY descriptors
1188	135	R1m+	R maximal autocorrelation of lag 1 / weighted by atomic masses	GETAWAY descriptors
1189	136	R2m+	R maximal autocorrelation of lag 2 / weighted by atomic masses	GETAWAY descriptors
1190	137	R3m+	R maximal autocorrelation of lag 3 / weighted by atomic masses	GETAWAY descriptors
1191	138	R4m+	R maximal autocorrelation of lag 4 / weighted by atomic masses	GETAWAY descriptors
1192	139	R5m+	R maximal autocorrelation of lag 5 / weighted by atomic masses	GETAWAY descriptors
1193	140	R6m+	R maximal autocorrelation of lag 6 / weighted by atomic masses	GETAWAY descriptors
1194	141	R7m+	R maximal autocorrelation of lag 7 / weighted by atomic masses	GETAWAY descriptors
1195	142	R8m+	R maximal autocorrelation of lag 8 / weighted by atomic masses	GETAWAY descriptors
1196	143	RTm+	R maximal index / weighted by atomic masses	GETAWAY descriptors
1197	144	R1v	R autocorrelation of lag 1 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1198	145	R2v	R autocorrelation of lag 2 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1199	146	R3v	R autocorrelation of lag 3 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1200	147	R4v	R autocorrelation of lag 4 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1201	148	R5v	R autocorrelation of lag 5 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1202	149	R6v	R autocorrelation of lag 6 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1203	150	R7v	R autocorrelation of lag 7 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1204	151	R8v	R autocorrelation of lag 8 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1205	152	RTv	R total index / weighted by atomic van der Waals volumes	GETAWAY descriptors
1206	153	R1v+	R maximal autocorrelation of lag 1 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1207	154	R2v+	R maximal autocorrelation of lag 2 / weighted by atomic van der Waals volumes	GETAWAY descriptors

No.	Rel.No.	Symbol	Definition	Class
1208	155	R3v+	R maximal autocorrelation of lag 3 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1209	156	R4v+	R maximal autocorrelation of lag 4 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1210	157	R5v+	R maximal autocorrelation of lag 5 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1211	158	R6v+	R maximal autocorrelation of lag 6 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1212	159	R7v+	R maximal autocorrelation of lag 7 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1213	160	R8v+	R maximal autocorrelation of lag 8 / weighted by atomic van der Waals volumes	GETAWAY descriptors
1214	161	RTv+	R maximal index / weighted by atomic van der Waals volumes	GETAWAY descriptors
1215	162	R1e	R autocorrelation of lag 1 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1216	163	R2e	R autocorrelation of lag 2 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1217	164	R3e	R autocorrelation of lag 3 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1218	165	R4e	R autocorrelation of lag 4 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1219	166	R5e	R autocorrelation of lag 5 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1220	167	R6e	R autocorrelation of lag 6 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1221	168	R7e	R autocorrelation of lag 7 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1222	169	R8e	R autocorrelation of lag 8 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1223	170	RTe	R total index / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1224	171	R1e+	R maximal autocorrelation of lag 1 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1225	172	R2e+	R maximal autocorrelation of lag 2 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1226	173	R3e+	R maximal autocorrelation of lag 3 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1227	174	R4e+	R maximal autocorrelation of lag 4 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1228	175	R5e+	R maximal autocorrelation of lag 5 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1229	176	R6e+	R maximal autocorrelation of lag 6 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1230	177	R7e+	R maximal autocorrelation of lag 7 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1231	178	R8e+	R maximal autocorrelation of lag 8 / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1232	179	RTe+	R maximal index / weighted by atomic Sanderson electronegativities	GETAWAY descriptors
1233	180	R1p	R autocorrelation of lag 1 / weighted by atomic polarizabilities	GETAWAY descriptors
1234	181	R2p	R autocorrelation of lag 2 / weighted by atomic polarizabilities	GETAWAY descriptors
1235	182	R3p	R autocorrelation of lag 3 / weighted by atomic polarizabilities	GETAWAY descriptors
1236	183	R4p	R autocorrelation of lag 4 / weighted by atomic polarizabilities	GETAWAY descriptors
1237	184	R5p	R autocorrelation of lag 5 / weighted by atomic polarizabilities	GETAWAY descriptors
1238	185	R6p	R autocorrelation of lag 6 / weighted by atomic polarizabilities	GETAWAY descriptors
1239	186	R7p	R autocorrelation of lag 7 / weighted by atomic polarizabilities	GETAWAY descriptors
1240	187	R8p	R autocorrelation of lag 8 / weighted by atomic polarizabilities	GETAWAY descriptors
1241	188	RTp	R total index / weighted by atomic polarizabilities	GETAWAY descriptors
1242	189	R1p+	R maximal autocorrelation of lag 1 / weighted by atomic polarizabilities	GETAWAY descriptors
1243	190	R2p+	R maximal autocorrelation of lag 2 / weighted by atomic polarizabilities	GETAWAY descriptors
1244	191	R3p+	R maximal autocorrelation of lag 3 / weighted by atomic polarizabilities	GETAWAY descriptors
1245	192	R4p+	R maximal autocorrelation of lag 4 / weighted by atomic polarizabilities	GETAWAY descriptors
1246	193	R5p+	R maximal autocorrelation of lag 5 / weighted by atomic polarizabilities	GETAWAY descriptors

No.	Rel.No.	Symbol	Definition	Class
1247	194	R6p+	R maximal autocorrelation of lag 6 / weighted by atomic polarizabilities	GETAWAY descriptors
1248	195	R7p+	R maximal autocorrelation of lag 7 / weighted by atomic polarizabilities	GETAWAY descriptors
1249	196	R8p+	R maximal autocorrelation of lag 8 / weighted by atomic polarizabilities	GETAWAY descriptors
1250	197	RTp+	R maximal index / weighted by atomic polarizabilities	GETAWAY descriptors
1251	1	nCp	number of total primary C(sp3)	functional groups
1252	2	nCs	number of total secondary C(sp3)	functional groups
1253	3	nCt	number of total tertiary C(sp3)	functional groups
1254	4	nCq	number of total quaternary C(sp3)	functional groups
1255	5	nCrH2	number of ring secondary C(sp3)	functional groups
1256	6	nCrHR	number of ring tertiary C(sp3)	functional groups
1257	7	nCrR2	number of ring quaternary C(sp3)	functional groups
1258	8	nCaH	number of unsubstituted aromatic C(sp2)	functional groups
1259	9	nCaR	number of substituted aromatic C(sp2)	functional groups
1260	10	nCconjR	number of exo-conjugated C(sp2)	functional groups
1261	11	n=CH2	number of primary C(sp2)	functional groups
1262	12	n=CHR	number of secondary C(sp2)	functional groups
1263	13	n=CR2	number of tertiary C(sp2)	functional groups
1264	14	n=C=	number of allenes groups	functional groups
1265	15	n#CH	number of terminal C(sp)	functional groups
1266	16	n#CR	number of non-terminal C(sp)	functional groups
1267	17	nOCN	number of cyanates (aliphatic)	functional groups
1268	18	nOCNPh	number of cyanates (aromatic)	functional groups
1269	19	nNCO	number of isocyanates (aliphatic)	functional groups
1270	20	nNCOPh	number of isocyanates (aromatic)	functional groups
1271	21	nSCN	number of thiocyanates (aliphatic)	functional groups
1272	22	nSCNPh	number of thiocyanates (aromatic)	functional groups
1273	23	nNCS	number of isothiocyanates (aliphatic)	functional groups
1274	24	nNCSPH	number of isothiocyanates (aromatic)	functional groups
1275	25	nCOOH	number of carboxylic acids (aliphatic)	functional groups
1276	26	nCOOHPh	number of carboxylic acids (aromatic)	functional groups
1277	27	nCOOR	number of esters (aliphatic)	functional groups
1278	28	nCOORPh	number of esters (aromatic)	functional groups
1279	29	nCONH2	number of primary amides (aliphatic)	functional groups
1280	30	nCONH2Ph	number of primary amides (aromatic)	functional groups
1281	31	nCONHR	number of secondary amides (aliphatic)	functional groups
1282	32	nCONHRPh	number of secondary amides (aromatic)	functional groups
1283	33	nCONR2	number of tertiary amides (aliphatic)	functional groups
1284	34	nCONR2Ph	number of tertiary amides (aromatic)	functional groups
1285	35	nOCON	number of carbamates (aliphatic)	functional groups

No.	Rel.No.	Symbol	Definition	Class
1286	36	nOCONPh	number of carbamates (aromatic)	functional groups
1287	37	nCOX	number of acyl halogenides (aliphatic)	functional groups
1288	38	nCOXPh	number of acyl halogenides (aromatic)	functional groups
1289	39	nCSOH	number of thioacids (aliphatic)	functional groups
1290	40	nCSOHPh	number of thioacids (aromatic)	functional groups
1291	41	nCSSH	number of dithioacids (aliphatic)	functional groups
1292	42	nCSSHPh	number of dithioacids (aromatic)	functional groups
1293	43	nCOSR	number of thioesters (aliphatic)	functional groups
1294	44	nCOSRPh	number of thioesters (aromatic)	functional groups
1295	45	nCSSR	number of dithioesters (aliphatic)	functional groups
1296	46	nCSSRPh	number of dithioesters (aromatic)	functional groups
1297	47	nCOH	number of aldehydes (aliphatic)	functional groups
1298	48	nCOHPh	number of aldehydes (aromatic)	functional groups
1299	49	nCO	number of ketones (aliphatic)	functional groups
1300	50	nCOPh	number of ketones (aromatic)	functional groups
1301	51	nCONN	number of urea derivatives	functional groups
1302	52	nNH2	number of primary amines (aliphatic)	functional groups
1303	53	nNH2Ph	number of primary amines (aromatic)	functional groups
1304	54	nNHR	number of secondary amines (aliphatic)	functional groups
1305	55	nNHRPh	number of secondary amines (aromatic)	functional groups
1306	56	nNR2	number of tertiary amines (aliphatic)	functional groups
1307	57	nNR2Ph	number of tertiary amines (aromatic)	functional groups
1308	58	nN-N	number of N hydrazines (aliphatic)	functional groups
1309	59	nN-NPh	number of N hydrazines (aromatic)	functional groups
1310	60	nN=N	number of N azo (aliphatic)	functional groups
1311	61	nN=NPh	number of N azo (aromatic)	functional groups
1312	62	nCN	number of nitriles (aliphatic)	functional groups
1313	63	nCNPh	number of nitriles (aromatic)	functional groups
1314	64	nC=N	number of immines (aliphatic)	functional groups
1315	65	nC=NPh	number of immines (aromatic)	functional groups
1316	66	nN+	number of ammonium groups (aliphatic)	functional groups
1317	67	nN+Ph	number of ammonium groups (aromatic)	functional groups
1318	68	nNHOH	number of hydroxylamines (aliphatic)	functional groups
1319	69	nNHOHPh	number of hydroxylamines (aromatic)	functional groups
1320	70	nCNOH	number of oximes (aliphatic)	functional groups
1321	71	nCNOHPh	number of oximes (aromatic)	functional groups
1322	72	nNNOx	number of N-nitroso groups (aliphatic)	functional groups
1323	73	nNNOxPh	number of N-nitroso groups (aromatic)	functional groups
1324	74	nNO	number of nitroso groups (aliphatic)	functional groups

No.	Rel.No.	Symbol	Definition	Class
1325	75	nNOPh	number of nitroso groups (aromatic)	functional groups
1326	76	nNO2	number of nitro groups (aliphatic)	functional groups
1327	77	nNO2Ph	number of nitro groups (aromatic)	functional groups
1328	78	nN(CO)2	number of imides	functional groups
1329	79	nOH	number of total hydroxyl groups	functional groups
1330	80	nOHPh	number of phenols	functional groups
1331	81	nOHp	number of primary alcohols (aliphatic)	functional groups
1332	82	nOHpPh	number of primary alcohols (aromatic)	functional groups
1333	83	nOHs	number of secondary alcohols (aliphatic)	functional groups
1334	84	nOHsPh	number of secondary alcohols (aromatic)	functional groups
1335	85	nOht	number of tertiary alcohols (aliphatic)	functional groups
1336	86	nOhtPh	number of tertiary alcohols (aromatic)	functional groups
1337	87	nROR	number of ethers (aliphatic)	functional groups
1338	88	nRORPh	number of ethers (aromatic)	functional groups
1339	89	nROX	number of hypohalogenydes (aliphatic)	functional groups
1340	90	nROXPh	number of hypohalogenydes (aromatic)	functional groups
1341	91	nH2O	number of water molecules	functional groups
1342	92	nSO	number of sulfoxides	functional groups
1343	93	nSO2	number of sulfones	functional groups
1344	94	nSO3	number of sulfates	functional groups
1345	95	nSH	number of thioles	functional groups
1346	96	nCS	number of thioketones	functional groups
1347	97	nRSR	number of solfures	functional groups
1348	98	nRSSR	number of disulfures	functional groups
1349	99	nSO3H	number of sulfonic acids	functional groups
1350	100	nSO2N	number of sulfonamides	functional groups
1351	101	nPO3	number of phosphites	functional groups
1352	102	nPO4	number of phosphates	functional groups
1353	103	nPO3S	number of phosphothionates	functional groups
1354	104	nPO2S2	number of phosphodithionates	functional groups
1355	105	nPO2SR	number of phosphothioates	functional groups
1356	106	nRCH2X	number of CH2X	functional groups
1357	107	nR2CHX	number of CR2HX	functional groups
1358	108	nR3CX	number of CR3X	functional groups
1359	109	nR=CHX	number of R=CHX	functional groups
1360	110	nR=CRX	number of R=CRX	functional groups
1361	111	nR#CX	number of R#CX	functional groups
1362	112	nRCHX2	number of CHRX2	functional groups
1363	113	nR2CX2	number of CR2X2	functional groups

No.	Rel.No.	Symbol	Definition	Class
1364	114	nR=CX2	number of R=CX2	functional groups
1365	115	nRCX3	number of RCX3	functional groups
1366	116	nPhX	number of X-C on aromatic ring	functional groups
1367	117	nCXr	number of X-C- on ring	functional groups
1368	118	nCXr=	number of X-C= on ring	functional groups
1369	119	nCconjX	number of X-C on conjugated C	functional groups
1370	120	nHDon	number of donor atoms for H-bonds (with N and O)	functional groups
1371	121	nHAcc	number of acceptor atoms for H-bonds (N O F)	functional groups
1372	1	C-001	CH3R / CH4	atom-centred fragments
1373	2	C-002	CH2R2	atom-centred fragments
1374	3	C-003	CHR3	atom-centred fragments
1375	4	C-004	CR4	atom-centred fragments
1376	5	C-005	CH3X	atom-centred fragments
1377	6	C-006	CH2RX	atom-centred fragments
1378	7	C-007	CH2X2	atom-centred fragments
1379	8	C-008	CHR2X	atom-centred fragments
1380	9	C-009	CHRX2	atom-centred fragments
1381	10	C-010	CHX3	atom-centred fragments
1382	11	C-011	CR3X	atom-centred fragments
1383	12	C-012	CR2X2	atom-centred fragments
1384	13	C-013	CRX3	atom-centred fragments
1385	14	C-014	CX4	atom-centred fragments
1386	15	C-015	=CH2	atom-centred fragments
1387	16	C-016	=CHR	atom-centred fragments
1388	17	C-017	=CR2	atom-centred fragments
1389	18	C-018	=CHX	atom-centred fragments
1390	19	C-019	=CRX	atom-centred fragments
1391	20	C-020	=CX2	atom-centred fragments
1392	21	C-021	#CH	atom-centred fragments
1393	22	C-022	#CR / R=C=R	atom-centred fragments
1394	23	C-023	#CX	atom-centred fragments
1395	24	C-024	R--CH--R	atom-centred fragments
1396	25	C-025	R--CR--R	atom-centred fragments
1397	26	C-026	R--CX--R	atom-centred fragments
1398	27	C-027	R--CH--X	atom-centred fragments
1399	28	C-028	R--CR--X	atom-centred fragments
1400	29	C-029	R--CX--X	atom-centred fragments
1401	30	C-030	X--CH--X	atom-centred fragments
1402	31	C-031	X--CR--X	atom-centred fragments

No.	Rel.No.	Symbol	Definition	Class
1403	32	C-032	X--CX--X	atom-centred fragments
1404	33	C-033	X--CH..X	atom-centred fragments
1405	34	C-034	X--CR..X	atom-centred fragments
1406	35	C-035	X--CX..X	atom-centred fragments
1407	36	C-036	Al-CH=X	atom-centred fragments
1408	37	C-037	Ar-CH=X	atom-centred fragments
1409	38	C-038	Al-C(=X)-Al	atom-centred fragments
1410	39	C-039	Ar-C(=X)-R	atom-centred fragments
1411	40	C-040	R-C(=X)-X / R-C#X / X-=C=X	atom-centred fragments
1412	41	C-041	X-C(=X)-X	atom-centred fragments
1413	42	C-042	X--CH..X	atom-centred fragments
1414	43	C-043	X--CR..X	atom-centred fragments
1415	44	C-044	X--CX..X	atom-centred fragments
1416	45	C-045	unused	atom-centred fragments
1417	46	H-046	H attached to C0(sp3) no X attached to next C	atom-centred fragments
1418	47	H-047	H attached to C1(sp3) / C0(sp2)	atom-centred fragments
1419	48	H-048	H attached to C2(sp3) / C1(sp2) / C0(sp)	atom-centred fragments
1420	49	H-049	H attached to C3(sp3) / C2(sp2) / C3(sp2) / C3(sp)	atom-centred fragments
1421	50	H-050	H attached to heteroatom	atom-centred fragments
1422	51	H-051	H attached to alfa-C	atom-centred fragments
1423	52	H-052	H attached to C0(sp3) with 1X attached to next C	atom-centred fragments
1424	53	H-053	H attached to C0(sp3) with 2X attached to next C	atom-centred fragments
1425	54	H-054	H attached to C0(sp3) with 3X attached to next C	atom-centred fragments
1426	55	H-055	H attached to C0(sp3) with 4X attached to next C	atom-centred fragments
1427	56	O-056	alcohol	atom-centred fragments
1428	57	O-057	phenol / enol / carboxyl OH	atom-centred fragments
1429	58	O-058	O=	atom-centred fragments
1430	59	O-059	Al-O-Al	atom-centred fragments
1431	60	O-060	Al-O-Ar / Ar-O-Ar / R..O..R / R-O-C=X	atom-centred fragments
1432	61	O-061	O--	atom-centred fragments
1433	62	O-062	unused	atom-centred fragments
1434	63	O-063	unused	atom-centred fragments
1435	64	O-064	unused	atom-centred fragments
1436	65	O-065	unused	atom-centred fragments
1437	66	N-066	Al-NH2	atom-centred fragments
1438	67	N-067	Al2-NH	atom-centred fragments
1439	68	N-068	Al3-N	atom-centred fragments
1440	69	N-069	Ar-NH2 / X-NH2	atom-centred fragments
1441	70	N-070	Ar-NH-Al	atom-centred fragments

No.	Rel.No.	Symbol	Definition	Class
1442	71	N-071	Ar-NAI2	atom-centred fragments
1443	72	N-072	RCO-N< / >N-X=X	atom-centred fragments
1444	73	N-073	Ar2NH / Ar3N / Ar2N-AI / R..N..R	atom-centred fragments
1445	74	N-074	R#N / R=N-	atom-centred fragments
1446	75	N-075	R--N--R / R--N--X	atom-centred fragments
1447	76	N-076	Ar-NO2 / R--N(--R)--O / RO-NO2	atom-centred fragments
1448	77	N-077	AI-NO2	atom-centred fragments
1449	78	N-078	Ar-N=X / X-N=X	atom-centred fragments
1450	79	N-079	unused	atom-centred fragments
1451	80	N-080	unused	atom-centred fragments
1452	81	F-081	F attached to C1(sp3)	atom-centred fragments
1453	82	F-082	F attached to C2(sp3)	atom-centred fragments
1454	83	F-083	F attached to C3(sp3)	atom-centred fragments
1455	84	F-084	F attached to C1(sp2)	atom-centred fragments
1456	85	F-085	F attached to C2(sp2)-C4(sp2) / C1(sp) / C4(sp3)X	atom-centred fragments
1457	86	Cl-086	Cl attached to C1(sp3)	atom-centred fragments
1458	87	Cl-087	Cl attached to C2(sp3)	atom-centred fragments
1459	88	Cl-088	Cl attached to C3(sp3)	atom-centred fragments
1460	89	Cl-089	Cl attached to C1(sp2)	atom-centred fragments
1461	90	Cl-090	Cl attached to C2(sp2)-C4(sp2) / C1(sp) / C4(sp3)X	atom-centred fragments
1462	91	Br-091	Br attached to C1(sp3)	atom-centred fragments
1463	92	Br-092	Br attached to C2(sp3)	atom-centred fragments
1464	93	Br-093	Br attached to C3(sp3)	atom-centred fragments
1465	94	Br-094	Br attached to C1(sp2)	atom-centred fragments
1466	95	Br-095	Br attached to C2(sp2)-C4(sp2) / C1(sp) / C4(sp3)X	atom-centred fragments
1467	96	I-096	I attached to C1(sp3)	atom-centred fragments
1468	97	I-097	I attached to C2(sp3)	atom-centred fragments
1469	98	I-098	I attached to C3(sp3)	atom-centred fragments
1470	99	I-099	I attached to C1(sp2)	atom-centred fragments
1471	100	I-100	I attached to C2(sp2)-C4(sp2) / C1(sp) / C4(sp3)X	atom-centred fragments
1472	101	S-101	unused	atom-centred fragments
1473	102	S-102	unused	atom-centred fragments
1474	103	S-103	unused	atom-centred fragments
1475	104	S-104	unused	atom-centred fragments
1476	105	S-105	unused	atom-centred fragments
1477	106	S-106	R-SH	atom-centred fragments
1478	107	S-107	R2S / RS-SR	atom-centred fragments
1479	108	S-108	R=S	atom-centred fragments
1480	109	S-109	R-SO-R	atom-centred fragments

No.	Rel.No.	Symbol	Definition	Class
1481	110	S-110	R-SO ₂ -R	atom-centred fragments
1482	111	S-111	unused	atom-centred fragments
1483	112	S-112	unused	atom-centred fragments
1484	113	S-113	unused	atom-centred fragments
1485	114	S-114	unused	atom-centred fragments
1486	115	S-115	unused	atom-centred fragments
1487	116	P-116	R ₃ -P=X	atom-centred fragments
1488	117	P-117	X ₃ -P=X (phosphate)	atom-centred fragments
1489	118	P-118	PX ₃ (phosphite)	atom-centred fragments
1490	119	P-119	PR ₃ (phosphine)	atom-centred fragments
1491	120	P-120	C-P(X) ₂ =X (phosphonate)	atom-centred fragments
1492	1	Ui	unsaturation index	empirical descriptors
1493	2	Hy	hydrophilic factor	empirical descriptors
1494	3	ARR	aromatic ratio	empirical descriptors
1495	1	MR	Ghose-Crippen molar refractivity	properties
1496	2	PSA	fragment-based polar surface area	properties
1497	3	MLOGP	Moriguchi octanol-water partition coeff. (logP)	properties