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Enthalpy of Formation Modeling Using Third Order Group Contribution Technics and Calculation by DFT Method.

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Appendix C. Group contribution values for the three levels.

Table S1. Group contributions Values of first-order level.

N	Groups	Occurrences	Parameters
1	CH3	406	-41,41
2	CH_2	207	-20,84
3	CH	50	-9,49
4	C	26	-1,24
5	CH_2=CH	32	38,5
6	CH=CH	28	15,06
7	CH_2=C	13	14,61
8	CH=C	6	-13,99
9	C=C	3	86,81
10	CH_2=C=CH	2	203,24
11	CH_2=C=C	1	211,9
12	CH≡C	10	230,95
13	C≡C	10	229,11
14	aCH	263	15,22
15	aC fused with aromatic ring	47	26,86
16	aC fused with non-aromatic ring	36	4,72
17	aC except as above	35	2,9
18	aN in aromatic ring	40	66,25
19	aC-CH_3	76	-23,99
20	aC-CH_2	11	-4,87
21	aC-CH	23	16,43
22	aC-C	15	68,06
23	aC-CH=CH	2	43,19
24	aC-C=CH_2	2	59,37
25	aC-C≡C	2	232,33
26	OH	54	-173,18
27	aC-OH	31	-172,71
28	COOH	20	-389,91
29	aC-COOH	20	-360,66
30	CH_3CO	10	-167,39
31	CH_2CO	2	-151,43
32	CCO	1	-146,67
33	aC-CO	12	-118,89
34	CHO	10	-129,22
35	CH_3COO	5	-360,89
36	CH_2COO	6	-355,71
37	CHCOO	2	-341,67
38	HCOO	2	-297,46
39	aC-COO	4	-300,85
40	COO except as above	8	-317,37
41	CH_3O	17	-150,11
42	CH_2O	7	-143,7
43	C-O	1	-87,16
44	aC-O	9	-108,89
45	CH_2NH_2	17	-12,52
46	$CHNH_2$	7	-3,53
47	CNH_2	2	-0,01
48	CH_3NH	3	21,03
49	CH_2NH	6	20,51

50	CHNH	2	36,33
51	CH_3N	10	61,7
52	CH_2N	10	69,27
53	aC-NH_2	15	5,61
54	aC-NH	6	44,58
55	aC-N	7	96,33
56	NH_2 except as above	13	-48,79
57	CH=N	2	108,31
58	C=N	1	73,64
59	CH_2CN	16	97,25
60	CHCN	6	102,98
61	CCN	3	102,25
62	aC-CN	9	150,11
63	CN except as above	16	153,08
64	aC-NCO	2	-85,45
65	$CH2NO_2$	2	-51,4
66	$CHNO_2$	1	-55,78
67	CNO_2	7	-58,21
68	aC-NO_2	22	-5,27
69	NO_2 except as above	20	52,27
70	ONO	8	-42,24
71	ONO_2	4	-75,31
72	$CONH_2$	10	-194,66
73	$CONHCH_3$	1	-206,59
74	$CON(CH_3)_2$	3	-187,48
75	$CON(CH_2)_2$	1	-162,96
76	CONCO	1	-299,88
77	aC-$CONH_2$	3	-176,96
78	aC-N(CO)H	1	-110,28
79	aC-CONH	3	-55,01
80	NHCONH	2	-160,06
81	NH_2CONH	5	-194,66
82	NH_2CON	2	-142,48
83	NCON	1	-39,94
84	CHNOH	2	17,96
85	CNOH	3	8,8
86	aC-CHNOH	2	173,39
87	OCH_2CH_2OH	2	-345,91
88	OCH_2CHOH	3	-358,88
89	-O-OH	2	-109,08
90	C_2H_3O	1	-156,75
91	CH_2 (cyclic)	176	-23,16
92	CH (cyclic)	93	-18,2
93	C (cyclic)	42	20,12
94	CH=CH (cyclic)	41	58,89
95	CH=C (cyclic)	21	49,6
96	C=C (cyclic)	5	125,59
97	CH_2=C (cyclic)	5	55,77
98	NH (cyclic)	31	31,77
99	N (cyclic)	27	-1,25
100	CH=N (cyclic)	13	-6,59
101	C=N (cyclic)	24	-27,17
102	O (cyclic)	53	-144,48

103	CO (cyclic)	23	-159,86
104	>NH	1	-232,97
105	-O-	1	-89,7
106	N=N	13	180,29
107	C_{cyclic}=N-	1	171,26
108	C_{cyclic}=CH-	1	96,74
109	N=O	7	112,75
110	C_{cyclic}=C	2	59,4
111	N=N2	5	225,31
112	aC-CON	3	-60,25
113	aC=O	1	-147,75
114	aN-	7	220,93
115	CH=C=CH	1	215,83

Table S2. Group contributions Values of second-order level.

N°	Groups	Occurrences	Parameters
1	$(CH_3)_2CH$	34	-0,29
2	$(CH_3)_3C$	28	4,25
3	$C(CH_3)_2C(CH_3)_2$	2	53,64
4	CH_n=CH_m-CH_p=CH_k (k,m,n,p in 0..2)	14	35,16
5	CH_3-CH_m=CH_n (m,n in 0..2)	33	29,09
6	CH_2-CH_m=CH_n (m,n in 0..2)	27	26,58
7	CH_p-CH_m=CH_n (m,n in 0..2; p in 0..1)	5	28,98
8	CHCHO or CCHO	1	6,13
9	CH_3COCH_2	4	-11,22
10	CH_3COCH or CH_3COC	1	-2,58
11	CH_3COOCH or CH_3COOC	3	-42,75
12	CHOH	6	-3,43
13	COH	1	-18,18
14	OH-CH_n-COO (n in 0..2)	1	13,41
15	$CH_m(OH)CH_n(OH)$ (m,n in 0..2)	3	-5,41
16	$CH_m(OH)CH_n(NH_p)$ (m,n,p in 0..2)	2	-4,48
17	$CH_m(NH_2)CH_n(NH_2)$ (m,n in 0..2)	5	5,11
18	$CH_m(NH_n)$-COOH (m,n in 0..2)	6	18,17
19	HOOC-CH_n-COOH (n in 1..2)	1	1,91
20	HO-CH_n-COOH (n in 1..2)	1	4,29
21	NH_2-CH_n-CH_m-COOH (n, m in 1..2)	1	-0,73
22	NC-CH_n-CH_m-CN (n, m in 1..2)	3	12,31
23	NC-CH_n-COO (n in 1..2)	2	12,17
24	CH_m-O-CH_n=CH_p (m,n,p in 0..3)	3	2,57
25	CH_m=CH_n-CN (m,n in 0..2)	1	1,47
26	CH_n=CH_m-COO-CH_p (m,n,p in 0..3)	1	-12,71
27	CH_m=CH_n-CHO (m,n in 0..2)	3	14,28
28	CH_m=CH_n-COOH (m,n in 0..2)	3	19,9
29	aC-CH_n-NH_m (n in 1..2; m in 0..2))	2	65,36
30	aC-CH_n-O- (n in 1..2)	5	-43,35
31	aC-CH_n-CN (n in 1..2)	2	-23,08
32	aC-CH_n-COOH (n in 1..2)	1	-17,87
33	aC-CH_m-NO_2 (n in 1..2)	2	-83,39
34	aC-CH_n-OOC (n in 1..2)	1	18,95
35	aC-$CH(CH_3)_2$	14	0,3
36	aC-$C(CH_3)_3$	12	-39,97

37	$(CH_n=C)_{(cyc)}$-CHO (n in 0..2)	1	-61,44
38	$(CH_n=C)_{cyc}$-COO-CH_m (n,m in 0..3)	2	-54,58
39	$(CH_n=C)_{cyc}$-CH_3 (n in 0..2)	10	-28,08
40	$(CH_n=C)_{cyc}$-CN (n in 0..2)	2	-38,55
41	CH_{cyc}-CH_3	8	10,14
42	CH_{cyc}-CH_2	27	-2,69
43	CH_{cyc}-CH	4	57,26
44	CH_{cyc}-C	1	25,51
45	CH_{cyc}-CH=CH_n (n in 1..2)	2	37,01
46	CH_{cyc}-OH	5	-5,9
47	CH_{cyc}-NH_2	2	63,8
48	CH_{cyc}-CN	4	-47,35
49	CH_{cyc}-COOH	1	42,94
50	CH_{cyc}-NO_2	2	-111,53
51	CH_{cyc}-O-	1	-11,13
52	CH_{cyc}-OOC	1	-20,55
53	C_{cyc}-CH_3	22	-6,98
54	C_{cyc}-OH	3	-21,14
55	$>N_{cyc}$-CH_3	12	-2,19
56	$>N_{cyc}$-CH_2	1	66,12
57	$AROMRINGs^1s^2$	13	11,47
58	$AROMRINGs^1s^3$	13	-0,8
59	$AROMRINGs^1s^4$	31	0,85
60	$AROMRINGs^1s^2s^3$	5	33,96
61	$AROMRINGs^1s^2s^4$	8	24,71
62	$AROMRINGs^1s^3s^5$	2	10,33
63	$AROMRINGs^1s^2s^3s^4$	5	28,96
64	$AROMRINGs^1s^2s^3s^5$	10	22,84
65	$AROMRINGs^1s^2s^4s^5$	4	12,89
66	$PYRIDINEs^2$	3	-5,12
67	$PYRIDINEs^3$	5	5,3
68	$PYRIDINEs^4$	4	4,84
69	$PYRIDINEs^2s^3$	2	2,33
70	$PYRIDINEs^2s^4$	2	6,53
71	$PYRIDINEs^2s^5$	3	3,58
72	$PYRIDINEs^2s^6$	1	-5,23
73	$PYRIDINEs^3s^4$	1	6,07
74	$PYRIDINEs^3s^5$	1	8,87
75	$(CH^n=CH^m)^{cyc}$-COOH	1	28,32
76	$AROMRINGs^1s^2s^3s^4s^5$	4	41,2
77	$(N=C)_{cyc}$-CH_3	10	4,6

Table S3. Group contributions Values of third-order level.

N°	Groups	Occurrences	Parameters
1	NH_n-$(CH_n)_m$-COOH (m>2, n in 0..2)	2	3,93
2	OH-$(CH_n)_m$-OH (m>2, n in 0..2)	2	2,1
3	NC-$(CH_n)_m$-CN (m>2)	1	-3,81
4	aC-$(CH_n=CH_m)_{cyc}$ (fused rings) (n,m in 0..1)	2	20,24
5	aC-aC (different rings)	12	22,53
6	aC-CH_{ncyc} (different rings) (n in 0..1)	5	-5,62
7	aC-CH_{ncyc} (fused rings) (n in 0..1)	20	14,07
8	aC-$(CH_n)_m$-aC (different rings) (m>1; n in 0..2)	1	-6,85

9	CH_{cyc}-CH_{cyc} (different rings)	6	29,66
10	$CH_{multiring}$	36	1,17
11	$C_{multiring}$	20	-34,73
12	aC-CH_m-aC (different rings) (m in 0..2)	3	8,52
13	aC-(CH_m=CH_n)-aC (different rings) (m,n in 0..2)	1	21,31
14	aC-CO_{cyc} (fused rings)	3	38,03
15	aC-CO-NH_n-aC (different rings) (n in 0..1)	3	-54,84
16	aC-NH_{ncyc} (fused rings) (n in 0..1)	12	-0,37
17	aC-(C=N)$_{cyc}$ (different rings)	2	-39,19
18	aC-(N=CH_n)$_{cyc}$ (fused rings) (n in 0..1)	2	12,93
19	aC-(CH_n=N)$_{cyc}$ (fused rings) (n in 0..1)	1	39,23
20	aC-O_{cyc} (fused rings)	3	27,12
21	AROM.FUSED[2]	48	-23,1
22	AROM.FUSED[2]s^1	8	6,58
23	AROM.FUSED[2]s^2	9	-12,35
24	AROM.FUSED[2]s^2s^3	3	-0,88
25	AROM.FUSED[2]s^1s^4	4	-9,86
26	AROM.FUSED[2]s^1s^2	2	31,81
27	AROM.FUSED[2]s^1s^3	2	17,67
28	AROM.FUSED[3]	4	-19,55
29	AROM.FUSED[4a]	8	-34,96
30	AROM.FUSED[4a]s^1	1	25,11
31	AROM.FUSED[4a]s^1s^4	1	68,67
32	AROM.FUSED[4p]	12	-10,86
33	AROM.FUSED[4p]s^3s^4	2	42,83
34	AROM.FUSED[4a]s15	5	-7,36
35	PYRIDINE.FUSED[2-iso]	1	1,2
36	N multiring	2	41,26

Table S4. Group contributions values of the new propositions.

N°	Groups	Occurrences	Parameters
1	NH=CH	1	65,41
2	N=CH2	1	85,41
3	OH=C=CH	3	-53,08
4	>N-	2	86,25
5	(-N=C=O)	1	-40,17
6	O=C=C=C=O	1	-93,64
7	aC-C=[N+][O-]	3	75,41
8	-C≡C-cyc	1	233,58
9	aC-N=[N+][O-]	2	182,71
10	N=[N+][O-]	3	134,98
11	(N=[N+])cycl [O-]	4	98,36
12	aC-[O-][N+]=[N+][O-]	2	174,42
13	[O-][N+]=[N+][O-]	1	148,73
14	(aC=[N+]-[O])aromatic	5	-7,58
15	aFC=[N+]-[O]	1	35,27
16	aC-C#[N+]-[O-]	1	155,69
17	(C=[N+]([O-])-O cyc	4	85,74
18	([C-]-[N+2]-[0-])cyc	1	28
19	(C=[N+])cyc-[O-]	4	86,22
20	(C=[N+])cyc-$[O-]_c$-CH_3	1	-26,4

21	aC-NNN	1	333,24
22	NNN	2	290,81
23	(-[N+]#[C-]	3	204,73
24	(C=C=C)	1	192,14
25	N#C-[C-]-C#N	1	225,97
26	O-O-	2	175,72
27	(-O-CH2-O-)cyc	3	-7,5
28	(-O-CHn-O-)cyc n=0,1	3	-5,17
29	(O-CO-O-)cyc	2	-54,95
30	(O-CO-C-)cyc	2	-10,87
31	(CO-O-CO-)cyc	2	-49,11
32	(C-CO-C-)cyc	1	105,01
33	(-CO-CO-)	1	-137,29
34	(-C=C-O-)	2	22,98
35	(-C=C-O-C=C-)	1	-83,64
36	N-N ALIPHATC	2	129,79
37	(N-N)cycl	3	81,68
38	(N-N-N)cycl	3	40,87
39	(C=N-N-C=N	1	137,44
40	(N=N-N-C=N)	6	157,26
41	(N=N-N-N=C)	1	162,88
42	(N=C-C=N)	1	132,56
43	(C=N-N)	4	55,6
44	(N=C-N)	6	27,7
45	NHn-(C=N)	5	53,87
46	(C=N-C)	1	102,39
47	(N=N-N)	1	19,68
48	(-AC-N=C-N-AC)	1	32,38
49	(-AC-N=N-N-AC)	1	20,25
50	(N-C=N-N)	2	30,54
51	(ac-C=N-N-ac-)	1	39,48
52	C-(NO2)2	3	-70,42
53	C-(NO2)3	3	-52,57
54	(C=N-O)	12	169,64
55	(N=C-O)	3	91,13
56	(-C=N-O-N=O-)	1	3,51
57	(C-CO-)cyc	1	-47,27
58	(-N-CO-)n cycl	8	-28,21
59	(N-O-)cyc	8	149,22
60	(N-)cyc-O	5	212,98
61	(-N-O-N-)	6	-12,81
62	(aC-N-O-N-aC)	4	9,04
63	N-OH	1	85,81
64	(-N=N-O-)	1	77,11
65	(aC-N=N-O-aC)	1	76,78
66	(AC-N=C-O-AC)	1	-18,86
67	(aC=[N+]-[O])aromatic	4	24,01
68	Carboaliphatic 3	20	117,17
69	Carboaliphatic 4	12	162,78
70	Carboaliphatic 5	48	50,36

71	Carboaliphatic 6	60	26,82
72	Carboaliphatic 7	4	37,65
73	Carboaliphatic 8	6	78,13
74	Carboaliphatic 10	3	64,47
75	Carboaliphatic 11	2	109,76
76	Carboaliphatic 12	3	138,27
77	Carboaliphatic 14	3	78,25
78	Carboaliphatic 18	1	-249,97
79	Carboaliphatic 17	1	40,54
80	Hetero ring 3	4	137,26
81	Hetero ring 4	6	125,68
82	Hetero ring 5	68	36,68
83	Hetero ring 6	22	58,81
84	Hetero ring 7	2	33,95
85	Hetero ring 8	2	78,39
86	Hetero ring 15	1	154,5

Appendix D. Prediction results of standard enthalpies of formation in gaseous stat using new group contribution method.

- ***No***: number of the compounds.
- ***Name***: name of the compounds.
- ***Formula***: chemical formula of the compound.
- ***EXP***: Experimental values.
- ***Statues***: Training statues or test statues.
- ***CAS***: CAS number of the compounds, (Chemical Abstracts Service).
- ***CAL***: Calculated formation enthalpy using the new group contribution method (kJ/mol).
- ***AAD***: Mean absolute error for the new group contribution method (kJ/mol).
- **ARD**: Average relative error (%).
  Note:
- C-H compounds are marked in black color, C-H-O compounds are marked in red color, C-H-N compounds are marked in blue color and C-H-O-N compounds are marked in brown color.

Table S5. Prediction results of standard enthalpies of formation in gaseous stat using new group contribution method.

						kJ/mol			%
N0	***N0***	***Names***	**Formula**	***CAS***	***Statues***	***EXP .***	***CAL.***	***AAD***	ARD
1	*1*	Propyne	C3H4	74-99-7	Training	185.4	189.54	4.14	0.00
2	*2*	1,3-Butadiyne	C4H2	460-12-8	Training	464	461.9	-2.1	0.00
3	*3*	1,2-Butadiene	C4H6	590-19-2	Training	162.2	161.82	-0.38	0.00
4	*4*	2-Butyne	C4H6	503-17-3	Training	145.1	146.28	1.18	0.00
5	*5*	cis-2-Butene	C4H8	590-18-1	Test	-7.7	-9.59	-1.89	-0.03
6	*6*	3-Methyl-1,2-butadiene	C5H8	598-25-4	Training	129.07	129.07	0	0.00
7	*7*	1,2-Pentadiene	C5H8	591-95-7	Training	140.6	140.98	0.38	0.00
8	*8*	trans-1,3-Pentadiene	C5H8	2004-70-8	Test	75.77	76.39	0.62	0.00
9	*9*	2,3-Pentadiene	C5H8	591-96-8	Training	133	133	0	0.00
10	*10*	1-Butyne, 3-methyl-	C5H8	598-23-2	Training	136.4	138.34	1.94	0.00
11	*11*	Cyclopropane,ethenyl-	C5H8	693-86-7	Training	127	128.16	1.16	0.00
12	*12*	Cyclopentane	C5H10	287-92-3	Training	-76.4	-65.44	10.96	-0.02
13	*13*	1,1-Dimethylcyclopropane	C5H10	1630-94-0	Test	-8.2	-5.81	2.39	-0.04
14	*14*	2-Methyl-1-butene	C5H10	563-46-2	Training	-35.1	-33.39	1.71	-0.01
15	*15*	3-Methyl-1-butene	C5H10	563-45-1	Training	-25.5	-25.13	0.37	0.00
16	*16*	2-Methyl-2-butene	C5H10	513-35-9	Training	-41.5	-50.95	-9.45	-0.03
17	*17*	trans-2-Pentene	C5H10	646-04-8	Test	-32	-32.94	-0.94	0.00

18	*18*	Isopentane	C5H12	78-78-4	Test	-153.7	-154.86	-1.16	0.00
19	*19*	Pentane	C5H12	109-66-0	Test	-146.8	-145.35	1.45	0.00
20	*20*	Cyclohexene	C6H10	110-83-8	Training	-4.32	-6.94	-2.62	-0.08
21	*21*	1,5-Hexadiene	C6H10	592-42-7	Test	85	88.48	3.48	0.01
22	*22*	3-Methylcyclopentene	C6H10	1120-62-3	Training	9.67	13.45	3.78	0.05
23	*23*	1-Hexyne	C6H10	693-02-7	Training	122.3	127.01	4.71	0.01
24	*24*	2-Hexyne	C6H10	764-35-2	Training	107.7	104.6	-3.1	0.00
25	*25*	Cyclopentane, methylene-	C6H10	1528-30-9	Training	10.2	13.49	3.29	0.04
26	*26*	3-Hexyne	C6H10	928-49-4	Training	105.4	104.6	-0.8	0.00
27	*27*	Bicyclo[3,1,0]hexane	C6H10	285-58-5	Test	39	40.84	1.84	0.01
28	*28*	1,1-Bicyclopropyl	C6H10	5685-46-1	Training	130	134.97	4.97	0.01
29	*29*	1,3-Butadiene, 2-ethyl-	C6H10	3404-63-5	Test	63.6	52.59	-11.01	0.02
30	*30*	(E)-1,3-Hexadiene	C6H10	20237-34-7	Test	54	53.04	-0.96	0.00
31	*31*	cis-1,3-hexadiene	C6H10	14596-92-0	Test	59	53.04	-5.96	0.01
32	*32*	trans-1,4-Hexadiene	C6H10	7319-00-8	Test	74	73.56	-0.44	0.00
33	*33*	cis-2-Methyl-1-vinylcyclopropane	C6H10	2628-57-1	Training	103	101.84	-1.16	0.00
34	*34*	Cyclohexane	C6H12	110-82-7	Test	-123.3	-112.14	11.16	-0.01
35	*35*	2,3-Dimethyl-1-butene	C6H12	563-78-0	Training	-65.9	-61.34	4.56	-0.01
36	*36*	cis-2-Hexene	C6H12	7688-21-3	Training	-47	-53.78	-6.78	-0.02
37	*37*	trans-2-Hexene	C6H12	4050-45-7	Training	-51	-53.78	-2.78	-0.01
38	*38*	Bicyclo[6,2,0]decapentaene	C10H8	20455-01-0	Training	514.2	516.76	2.56	0.00
39	*39*	Benzene, 1-butynyl-	C10H10	622-76-4	Training	248.6	246.17	-2.43	0.00
40	*40*	1,4-Dicyclopropylbuta-1,3-diyne	C10H10	114546-62-	Training	561.8	563.52	1.72	0.00
41	*41*	3,4-Dimethylenebicyclo[4,2,0]octa-1,5-diene	C10H10	136846-72-	Training	359	354.01	-4.99	0.00
42	*42*	cis-Decahydronaphthalene	C10H18	493-01-6	Training	-169.2	-165.69	3.51	0.00
43	*43*	Butylbenzene	C10H14	104-51-8	Test	-12.8	-11.87	0.93	-0.01
44	*44*	Benzene, (1-methylpropyl)-	C10H14	135-98-8	Test	-17.4	-11.14	6.26	-0.05
45	*45*	1,2,4,5-Tetramethylbenzene	C10H14	95-93-2	Training	-47.1	-52.63	-5.53	-0.02
46	*46*	Benzene, 1,2,3,4-tetramethyl-	C10H14	488-23-3	Training	-36	-36.55	-0.55	0.00
47	*47*	Camphene	C10H16	79-92-5	Training	-28	-23.7	4.3	-0.02
48	*48*	Adamantane	C10H16	281-23-2	Test	-134.4	-126.6	7.8	-0.01
49	*49*	trans-1-Methyl-1,2-dicyclopropylcyclopropane	C10H16	150895-64-	Training	179.2	182.51	3.31	0.00
50	*50*	cis-1-Methyl-1,2-dicyclopropylcyclopropane	C10H16	150895-65-	Training	181	182.51	1.51	0.00

51	*51*	1,3-Cyclopentadiene, 1,2,3,4,5-pentamethyl-	C10H16	4045-44-7	Training	-25	-25.9	-0.9	0.00
52	*52*	Spiro[5,5]undecane	C11H20	180-43-8	Test	-188.3	-192.57	-4.27	0.00
53	*53*	Cyclohexene, 1-methyl-4-(1-methylethyl)-	C10H18	5502-88-5	Training	-110.8	-116.11	-5.31	-0.01
54	*54*	5-Decyne	C10H18	1942-46-7	Training	18.7	21.23	2.53	0.02
55	*55*	4-Decyne	C10H18	2384-86-3	Training	19.9	21.23	1.33	0.01
56	*56*	2-Decyne	C10H18	2384-70-5	Training	23.6	21.23	-2.37	0.01
57	*57*	Bicyclo[5,3,0]decane	C10H18	5661-80-3	Training	-130.1	-131.32	-1.22	0.00
58	*58*	Cyclopentane, pentyl-	C10H20	3741-00-2	Training	-188.9	-187.94	0.96	0.00
59	*59*	trans-1,2-di-tert-butylethylene	C10H20	692-48-8	Training	-167	-169.46	-2.46	0.00
60	*60*	1,1,4-Trimethylcycloheptane	C10H20	2158-55-6	Training	-210.3	-204.29	6.01	0.00
61	*61*	Bicyclo[4,4,1]undeca-1,3,5,7,9-pentaene	C11H10	2443-46-1	Training	323	327.98	4.98	0.00
62	*62*	1a,7b-Dihydrocyclopropa[a]naphthalene	C11H10	3463-79-4	Training	238	227.19	-10.81	0.01
63	*63*	Bicyclo[4,4,1]undeca-1,3,5,8-tetralene	C11H12	6074-99-3	Training	261	253.63	-7.37	0.00
64	*64*	1,1-Dimethylindan	C11H14	4912-92-9	Test	-1.6	2.73	4.33	-0.36
65	*65*	1H-Indene, 2,3-dihydro-4,7-dimethyl-	C11H14	6682-71-9	Training	-7.4	-8.95	-1.55	-0.03
66	*66*	1-tert-Butyl-3-methylbenzene	C11H16	1075-38-3	Test	-54	-60.07	-6.07	-0.01
67	*67*	Pentamethylbenzene	C11H16	700-12-9	Training	-67.2	-63.52	3.68	-0.01
68	*68*	Tetracyclo[6,2,1,0(2,7),o(3,5)]undecane	C11H16	1777-44-2	Test	59	50.31	-8.69	0.02
69	*69*	1-Methyladamantane	C11H18	768-91-2	Test	-171.7	-165.6	6.1	0.00
70	*70*	Bicyclo[2,2,2]oct-2-ene, 5-(1-methylethyl)-, (1α,4α,5β)-	C11H18	106562-31-	Training	-51.9	-44.56	7.34	-0.02
71	*71*	Bicyclo[2,2,2]oct-2-ene,5-(1-methylethyl)-,(1α,4α,5α)-	C11H18	106623-87-	Training	-50.6	-44.56	6.04	-0.02
72	*72*	Bicyclo[3,3,3]undecane	C11H20	29415-95-0	Training	-89	-86.22	2.78	0.00
73	*73*	Cyclohexane, pentyl-	C11H22	4292-92-6	Test	-233.8	-234.65	-0.85	0.00
74	*74*	Acenaphthylene	C12H8	208-96-8	Training	259.7	265.11	5.41	0.00
75	*75*	Acenaphthene	C12H10	83-32-9	Training	156	147.55	-8.45	0.01
76	*76*	Biphenyl	C12H10	92-52-4	Test	180	180.54	0.54	0.00
77	*77*	Naphthalene, 2,3-dimethyl-	C12H12	581-40-8	Training	76.1	73.09	-3.01	0.01
78	*78*	Naphthalene, 2,7-dimethyl-	C12H12	582-16-1	Training	79.5	72.37	-7.13	0.01
79	*79*	Tricyclo[4,4,2,0(1,6)dodeca-2,4,8-triene	C12H14	60329-21-7	Test	276.6	271.22	-5.38	0.00
80	*80*	Anti tricyclo[4.2.2.2(2,5)]dodeca-3,7-diene	C12H16	69349-54-8	Training	143	143.44	0.44	0.00
81	*81*	Syn tricyclo[4.2.2.2(2,5)]dodeca-3,7-diene	C12H16	67278-00-6	Training	154	143.44	-10.56	0.01
82	*82*	(Z) 3,3-Bis-(1-cyclohexenylidene)	C12H16	132911-35-	Training	92.5	91.85	-0.65	0.00
83	*83*	(E) 3,3-Bis-(1-cyclohexenylidene)	C12H16	132911-34-	Training	91.2	91.85	0.65	0.00

84	*84*	Benzene, 1,2,4-trimethyl-5-(1-methylethyl)-	C12H18	10222-95-4	Training	-103.3	-94.73	8.57	-0.01
85	*85*	Tricyclo[4,2,2,2(2,5)]dodec-3-ene	C12H18	69122-74-3	Training	33	38.23	5.23	0.02
86	*86*	Adamantane, 1,3-dimethyl-	C12H20	702-79-4	Test	-219	-204.59	14.41	-0.01
87	*87*	2,2-dimethyladamantane	C12H20	19740-34-2	Test	-183	-180.11	2.89	0.00
88	*88*	Cyclohexane, hexyl-	C12H24	4292-75-5	Test	-254.4	-255.49	-1.09	0.00
89	*89*	(Z) 2,3-Di-tert-butyl-2-butene	C12H24	54429-93-5	Training	-123.1	-122.35	0.75	0.00
90	*90*	9H-Fluorene	C13H10	86-73-7	Test	175	172.3	-2.7	0.00
91	*91*	Diphenylmethane	C13H12	101-81-5	Training	165	158.75	-6.25	0.01
92	*92*	1H-Indene, 2,3-dihydro-1,1,4,7-tetramethyl-	C13H18	1078-04-2	Training	-62.5	-62.45	0.05	0.00
93	*93*	1,3,5-Trimethyladamantane	C13H22	707-35-7	Test	-255	-243.59	11.41	-0.01
94	*94*	Cyclopentane, octyl-	C13H26	1795-20-6	Test	-250.7	-250.46	0.24	0.00
95	*95*	Tridecane	C13H28	629-50-5	Training	-311.5	-312.08	-0.58	0.00
96	*96*	Diphenylacetylene	C14H10	501-65-5	Training	385	387.43	2.43	0.00
97	*97*	Phenanthrene	C14H10	85-01-8	Test	201.2	202.58	1.38	0.00
98	*98*	trans-Stilbene	C14H12	103-30-0	Training	219.6	219.6	0	0.00
99	*99*	9H-Fluorene, 9-methyl-	C14H12	2523-37-7	Training	148	145.98	-2.02	0.00
100	*100*	Pyracene	C14H12	567-79-3	Training	174.3	176.12	1.82	0.00
101	*101*	Octalene	C14H12	257-55-6	Training	551.5	549.89	-1.61	0.00
102	*102*	1,2-Diphenylethane	C14H14	103-29-7	Training	135.6	135.6	0	0.00
103	*103*	Phenanthrene, 1,2,3,4-tetrahydro-	C14H14	1013-08-7	Test	92.3	82.83	-9.47	0.01
104	*104*	n-Nonylcyclohexane	C14H14	2883-02-5 -	Test	-316.2	-318.01	-1.81	0.00
105	*105*	Cyclotetradecane	C14H28	295-17-0	Training	-239.2	-245.99	-6.79	0.00
106	*106*	Cyclopentane, nonyl-	C14H28	2882-98-6	Test	-271.3	-271.31	-0.01	0.00
107	*107*	(E)-3,4-Di-tert-butyl-3-hexene	C14H28	75245-21-5	Training	-168.3	-169.05	-0.75	0.00
108	*108*	2,2,3,3,4,4,5,5-Octamethylhexane	C14H30	65149-84-0	Training	-248.3	-249.7	-1.4	0.00
109	*109*	Phenanthrene, 4-methyl-	C15H12	832-64-4	Training	195.8	193.05	-2.75	0.00
110	*110*	4-Methyldiadamantane	C15H22	30545-28-9	Test	-182.1	-180.06	2.04	0.00
111	*111*	6-(tert-butyl)-1,1-dimethylindan	C15H22	3605-31-0	Training	-104	-97.9	6.1	-0.01
112	*112*	Pentadecane	C15H32	629-62-9	Test	-354.8	-353.76	1.04	0.00
113	*113*	Phenanthrene, 2,7-dimethyl-	C16H14	1576-69-8	Training	143	145.67	2.67	0.00
114	*114*	Phenanthrene, 9,10-dimethyl-	C16H14	604-83-1	Training	167	177.85	10.85	0.01
115	*115*	[2,2]Paracyclophane	C16H16	1633-22-3	Training	244.7	242.53	-2.17	0.00
116	*116*	(2,2)Metacyclophane	C16H16	2319-97-3	Training	170	168.73	-1.27	0.00

117	*117*	2,2-Metaparacyclophane	C16H16	5385-36-4	Training	218.3	214.02	-4.28	0.00
118	*118*	Tricyclo[8,2,2,24,7]-hexadecane	C16H28	283-68-1	Training	-152	-154.11	-2.11	0.00
119	*119*	1-Hexadecene	C16H32	629-73-2	Test	-248.4	-247.26	1.14	0.00
120	*120*	Cyclopentane, undecyl-	C16H32	6785-23-5	Training	-312.5	-312.99	-0.49	0.00
121	*121*	Hexadecane	C16H34	544-76-3	Test	-374.9	-374.6	0.3	0.00
122	*122*	n-Dodecylcyclopentane	C17H34	5634-30-0	Test	-333.2	-333.83	-0.63	0.00
123	*123*	Chrysene	C18H12	218-01-9	Training	268.7	275.89	7.19	0.00
124	*124*	Triphenylene	C18H12	217-59-4	Training	270.1	274.49	4.39	0.00
125	*125*	p-Terphenyl	C18H14	92-94-4	Test	279	270.61	-8.39	0.00
126	*126*	Naphthacene, 5,12-dihydro-	C18H14	959-02-4	Training	224.9	227.67	2.77	0.00
127	*127*	Phenanthrene, 2,4,5,7-tetramethyl-	C18H18	7396-38-5	Training	130	127.3	-2.7	0.00
128	*128*	Phenanthrene, 3,4,5,6-tetramethyl-	C18H18	7343-06-8 -	Training	160	155.58	-4.42	0.00
129	*129*	[18]-Annulene	C18H18	2040-73-5	Training	280	280	0	0.00
130	*130*	2,5-Diphenyl-1,5-hexadiene	C18H18	7283-49-0	Training	285	282.42	-2.58	0.00
131	*131*	Tricyclo[10,2,2,2(5,8)]octadeca-5,7,12,14,15,17-hexaene	C18H20	2913-24-8	Training	129.4	136.19	6.79	0.01
132	*132*	Octadecane	C18H38	593-45-3	Training	-414.6	-416.28	-1.68	0.00
133	*133*	Triphenylmethane	C19H16	519-73-3	Training	276.1	276.11	0.01	0.00
134	*134*	2,6-Diphenyl-1,6-heptadiene	C19H20	27905-65-3	Training	259	261.58	2.58	0.00
135	*135*	1,5-Diphenylbicyclo[3,2,0]heptane	C19H22	94383-67-2	Training	215	214.9	-0.1	0.00
136	*136*	Perylene	C20H12	198-55-0	Training	318.3	319.32	1.02	0.00
137	*137*	Benzo[k]fluoranthene	C20H12	207-08-9	Training	306.2	307.21	1.01	0.00
138	*138*	Chrysene, 5,6-dimethyl-	C20H16	3697-27-6	Training	262	251.15	-10.85	0.01
139	*139*	Benz[a]anthracene, 7,12-dimethyl-	C20H16	56-56-4	Training	277	277	0	0.00
140	*140*	Hexacyclopropylethane	C20H30	26902-55-6	Training	466.5	466.5	0	0.00
141	*141*	Pentalene,1,3,5-tris(1,1-dimethylethyl)-	C20H30	50356-52-0	Training	14	11.39	-2.61	0.02
142	*142*	meso-3,4-Dicyclohexyl-2,5-dimethylhexane	C20H38	62678-52-8	Training	-300	-304.04	-4.04	0.00
143	*143*	Cyclohexane, tetradecyl-	C20H40	1795-18-2	Test	-419.3	-422.21	-2.91	0.00
144	*144*	Eicosane	C20H42	112-95-8	Test	-455.8	-457.96	-2.16	0.00
145	*145*	1,8-Paracyclophane	C21H26	6169-94-4	Training	29	29	0	0.00
146	*146*	Benzo[b]triphenylene	C22H14	215-58-7	Training	331	323.69	-7.31	0.00
147	*147*	1,1-Diphenyl-1,1-bicyclopentyl	C22H26	59358-70-2	Training	111	102.45	-8.55	0.01
148	*148*	Benzene, 1,1,1,1-(1,2-ethanediylidene)tetrakis-	C26H22	632-50-8	Training	357	360.12	3.12	0.00
149	*149*	Pentacyclo[18,2,2,2(9,12),0(4,15),0(6,17)]hexacosa-	C26H26	35117-21-6	Training	326	330.28	4.28	0.00

150	*150*	5-Butyldocosane	C26H54	55282-16-1	Test	-587.6	-592.23	-4.63	0.00
151	*151*	11-Butyldocosane	C26H54	13475-76-8	Test	-593.3	-592.23	1.07	0.00
152	*152*	9,9-Bianthracene	C28H18	1055-23-8	Training	475	475	0	0.00
153	*153*	11-Decylheneicosane	C31H64	55320-06-4	Test	-700	-696.43	3.57	0.00
154	*154*	1,8-Cyclotetradecadiyne	C14H20	1540-80-3	Training	313.8	313.8	0	0.00
155	*155*	Oxiniacic acid	C6H5NO3	2398-81-4	Training	-225.1	-225.1	0	0.00
156	*156*	1,2,6,7-Cyclodecatetraene	C10H12	3451-55-6	Training	356.1	356.1	0	0.00
157	*157*	9,10[1,2]-Benzenoanthracene, 9,10-dihydro-	C20H14	477-75-8	Test	322	328.22	6.22	0.00
158	*158*	Hexane, 2,2,5,5-tetramethyl-	C10H22	1071-81-4	Training	-285	-284.15	0.85	0.00
159	*159*	o-Terphenyl	C18H14	84-15-1	Test	282.8	281.23	-1.57	0.00
160	*160*	3,3-Dimethyl-1-butyne	C6H10	917-92-0	Training	106.1	109.71	3.61	0.00
161	*161*	m-Terphenyl	C18H14	92-06-8	Test	280	268.95	-11.05	0.01
162	*162*	1,1-Biphenyl, 4-methyl-	C13H12	644-08-6	Test	138.2	142.18	3.98	0.00
163	*163*	3,9-Dimethylbenz[a]anthracene	C20H16	316-51-8	Training	189	194.87	5.87	0.00
164	*164*	2-Ethyl-1-butene	C6H12	760-21-4	Training	-56.07	-56.74	-0.67	0.00
165	*165*	1,1-Biphenyl, 2-methyl-	C13H12	643-58-3	Training	152.8	152.8	0	0.00
166	*166*	Cyclohexane, ethyl-	C8H16	1678-91-7	Training	-172.6	-172.13	0.47	0.00
167	*167*	Cyclohexane, propyl-	C9H18	1678-92-8	Test	-192.4	-192.97	-0.57	0.00
168	*168*	Butylcyclohexane	C10H20	1678-93-9	Test	-213.2	-213.81	-0.61	0.00
169	*169*	Benzene, 1,2,3,5-tetramethyl-	C10H14	527-53-7	Training	-43.2	-42.67	0.53	0.00
170	*170*	Heptylcyclohexane	C13H26	5617-41-4	Training	-275	-276.33	-1.33	0.00
171	*171*	Cyclohexane, octyl-	C14H28	1795-15-9	Test	-295.6	-297.17	-1.57	0.00
172	*172*	1-Butene	C4H8	106-98-9	Test	-0.63	2.83	3.46	-0.73
173	*173*	Cyclohexane, decyl-	C16H32	1795-16-0	Test	-336.9	-338.85	-1.95	0.00
174	*174*	1-Hexene	C6H12	592-41-6	Test	-42	-38.85	3.15	-0.01
175	*175*	4,4-Dimethylbiphenyl	C14H14	613-33-2	Test	111.3	103.83	-7.47	0.01
176	*176*	Butane	C4H10	106-97-8	Training	-125.6	-124.51	1.09	0.00
177	*177*	Cyclopropane	C3H6	75-19-4	Training	53.3	47.69	-5.61	0.01
178	*178*	1-Butyne	C4H6	107-00-6	Training	165.2	168.7	3.5	0.00
179	*179*	Neopentane	C5H12	463-82-1	Test	-167.9	-158.4	9.5	-0.01
180	*180*	1,4-Pentadiene	C5H8	591-93-5	Training	106.3	109.33	3.03	0.00
181	*181*	Dodecylcyclohexane	C18H36	1795-17-1	Test	-378.1	-380.53	-2.43	0.00
182	*182*	Cyclohexane, undecyl-	C17H34	54105-66-7	Test	-357	-359.69	-2.69	0.00

183	*183*	1-Pentyne	C5H8	627-19-0	Training	144.3	147.86	3.56	0.00
184	*184*	Propane	C3H8	74-98-6	Test	-103.8	-103.67	0.13	0.00
185	*185*	n-Tridecylcyclohexane	C19H38	6006-33-3	Test	-398.7	-401.37	-2.67	0.00
186	*186*	1-tert-Butyl-4-methylbenzene	C11H16	98-51-1	Test	-57	-58.41	-1.41	0.00
187	*187*	2-Methylnonane	C10H22	871-83-0	Test	-260.2	-259.07	1.13	0.00
188	*188*	Isobutane	C4H10	75-28-5	Test	-134.2	-134.31	-0.11	0.00
189	*189*	n-Pentadecylcyclohexane	C21H42	6006-95-7	Training	-439.9	-443.05	-3.15	0.00
190	*190*	5-Methylnonane	C10H22	15869-85-9	Test	-258.6	-258.78	-0.18	0.00
191	*191*	Cyclohexane, hexadecyl-	C22H44	6812-38-0	Test	-460.5	-463.89	-3.39	0.00
192	*192*	Decane	C10H22	124-18-5	Training	-249.7	-249.56	0.14	0.00
193	*193*	1-Decene	C10H20	872-05-9	Test	-123.3	-122.22	1.08	0.00
194	*194*	1-Dodecene	C12H24	112-41-4	Test	-165.4	-163.9	1.5	0.00
195	*195*	1,3-Butadiene	C4H6	106-99-0	Test	108.8	112.16	3.36	0.00
196	*196*	Undecane	C11H24	1120-21-4	Test	-270.3	-270.4	-0.1	0.00
197	*197*	Dodecane	C12H26	112-40-3	Training	-290.9	-291.24	-0.34	0.00
198	*198*	Dibenz[a,h]anthracene	C22H14	53-70-3	Training	328	325.08	-2.92	0.00
199	*199*	1-Decyne	C10H18	764-93-2	Training	41.9	43.65	1.75	0.01
200	*200*	Tetradecane	C14H30	629-59-4	Test	-332.1	-332.92	-0.82	0.00
201	*201*	Heptadecane	C17H36	629-78-7	Test	-393.9	-395.44	-1.54	0.00
202	*202*	Isobutene	C4H8	115-11-7	Training	-17.9	-10.04	7.86	-0.06
203	*203*	2-Methyl-1,3-butadiene	C5H8	78-79-5	Training	75.7	75.94	0.24	0.00
204	*204*	2-Methyladamantane	C11H18	700-56-1	Training	-152	-152.92	-0.92	0.00
205	*205*	Nonadecane	C19H40	629-92-5	Test	-435.1	-437.12	-2.02	0.00
206	*206*	Cyclopentane, heptyl-	C12H24	5617-42-5	Test	-230.1	-229.62	0.48	0.00
207	*207*	Cyclopropylacetylene	C5H6	6746-94-7	Training	292	283.6	-8.4	0.00
208	*208*	trans-3-Hexene	C6H12	13269-52-8	Test	-49.3	-56.29	-6.99	-0.02
209	*209*	Propene	C3H6	115-07-1	Training	20.41	26.18	5.77	0.04
210	*210*	3-Decyne	C10H18	2384-85-2	Training	21.8	21.23	-0.57	0.00
211	*211*	Isobutylbenzene	C10H14	538-93-2	Test	-21.5	-21.38	0.12	0.00
212	*212*	9,9-Dimethyl-9,9-bifluorenyl	C28H22	15300-82-0	Test	323.9	334.37	10.47	0.00
213	*213*	Tridecylcyclopentane	C18H36	6006-34-4	Test	-353.8	-354.67	-0.87	0.00
214	*214*	2-Pentyne	C5H8	627-21-4	Training	128.9	125.44	-3.46	0.00
215	*215*	Cyclopentane, tetradecyl-	C19H38	1795-22-8	Training	-374.4	-375.51	-1.11	0.00

216	*216*	cis-3-Hexene	C6H12	7642-09-3	Test	-45.9	-56.29	-10.39	-0.03
217	*217*	Cyclopentane, hexadecyl-	C21H42	6812-39-1	Test	-415.6	-417.19	-1.59	0.00
218	*218*	1,3,5,7-Tetramethyl-adamantane	C14H24	1687-36-1	Training	-284.6	-282.58	2.02	0.00
219	*219*	Cyclopentene	C5H8	142-29-0	Training	34	39.77	5.77	0.02
220	*220*	1,4-Hexadiene, (Z)-	C6H10	7318-67-4	Test	77	73.56	-3.44	0.01
221	*221*	1,3-Cyclopentadiene	C5H6	542-92-7	Training	139	144.97	5.97	0.01
222	*222*	Tricyclo[4,4,2,0(1,6)]dodeca-2,4-diene	C12H16	33930-87-9	Test	157.4	166.02	8.62	0.01
223	*223*	cis-1,3-Pentadiene	C5H8	1574-41-0	Test	81.72	76.39	-5.33	0.01
224	*224*	4-Methylcyclopentene	C6H10	1759-81-5	Training	15	13.45	-1.55	0.01
225	*225*	trans-2-Butene	C4H8	624-64-6	Training	-10.8	-9.59	1.21	-0.01
226	*226*	Spiro[4,5]decane	C10H18	176-63-6	Test	-145.1	-145.86	-0.76	0.00
227	*227*	1-Methylnaphthalene	C11H10	90-12-0	Training	116.9	119.75	2.85	0.00
228	*228*	4,7-Methano-1H-indene, octahydro-	C10H16	6004-38-2	Test	-60.2	-55.97	4.23	-0.01
229	*229*	2,4-Hexadiene, (E,E)-	C6H10	5194-51-4	Test	44	40.63	-3.37	0.01
230	*230*	2,4-Hexadiene, (E,Z)-	C6H10	5194-50-3	Test	48	40.63	-7.37	0.02
231	*231*	Tricyclo[4,4,2,0(1,6)dodeca-2,4,7,9-tetraene	C12H12	5181-34-0	Test	378.3	376.43	-1.87	0.00
232	*232*	Naphthalene, 1,8-dimethyl-	C12H12	569-41-5	Training	108.8	110.22	1.42	0.00
233	*233*	(Z),(Z)-2,4-Hexadiene	C6H10	6108-61-8	Test	52	40.63	-11.37	0.03
234	*234*	Tricyclo[6,2,0,03,6]deca-1(8),2,6-triene	C10H10	1610-51-1	Training	310	303.54	-6.46	0.00
235	*235*	1-Ethyl-8-methylnaphthalene	C13H14	61886-71-3	Training	98.1	87.92	-10.18	0.01
236	*236*	2,4,5,7-Tetramethyl-4,5-bis(4-tert-butylphenyl)octane	C32H50	85668-75-3	Test	-254	-242.46	11.54	-0.01
237	*237*	4,5-Diethyl-4,5-bis-(4-tert-butylphenyl)-octane	C32H50	85668-73-1	Training	-224	-223.44	0.56	0.00
238	*238*	3,4-Diethyl-3,4-bis(4-tert-butylphenyl)-hexane	C30H46	85668-74-2	Test	-170	-181.75	-11.75	-0.01
1	*239*	Acetaldehyde	C2H4O	75-07-0	Training	-170.7	-170.64	0.06	0.00
2	*240*	Oxirane	C2H4O	75-21-8	Training	-52.64	-53.54	-0.9	0.00
3	*241*	vinyl alcohol	C2H4O	557-75-5	Training	-128	-134.68	-6.68	-0.01
4	*242*	Methyl formate	C2H4O2	107-31-3	Training	-336.9	-338.88	-1.98	0.00
5	*243*	(Z) Ethene-1,2-diol	C2H4O2	65144-74-3	Test	-316	-331.3	-15.3	-0.01
6	*244*	1,2-Ethanediol	C2H6O2	107-21-1	Training	-394.4	-393.45	0.95	0.00
7	*245*	Peroxide, dimethyl	C2H6O2	690-02-8	Training	-126	-124.49	1.51	0.00
8	*246*	1,3-Dioxol-2-one	C3H2O3	872-36-6	Training	-418.61	-408.2	10.41	0.00
9	*247*	Cyclopropanone	C3H4O	5009-27-8	Training	16	16	0	0.00
10	*248*	Acrylic acid	C3H4O2	79-10-7	Training	-330.7	-331.51	-0.81	0.00

11	*249*	1,3-Dioxolan-2-one	C3H4O3	96-49-1	Training	-503	-513.41	-10.41	0.00
12	*250*	Tartronic acid	C3H4O5	80-69-3	Training	-952	-952	0	0.00
13	*251*	Acetone	C3H6O	67-64-1	Training	-218.5	-208.8	9.7	-0.01
14	*252*	Oxetane	C3H6O	503-30-0	Training	-80.54	-88.28	-7.74	-0.01
15	*253*	Propanal	C3H6O	123-38-6	Training	-188.7	-191.48	-2.78	0.00
16	*254*	Propen-2-ol	C3H6O	29456-04-0	Test	-176	-170.89	5.11	0.00
17	*255*	(Z)-1-Propenol	C3H6O	57642-96-3	Training	-174	-170.44	3.56	0.00
18	*256*	Ethyl formate	C3H6O2	109-94-4	Training	-361.7	-359.72	1.98	0.00
19	*257*	Methyl acetate	C3H6O2	79-20-9	Training	-410	-402.31	7.69	0.00
20	*258*	Propanoic acid	C3H6O2	79-09-4	Test	-455.8	-452.16	3.64	0.00
21	*259*	Acetic acid, hydroxy-, methyl ester	C3H6O3	96-35-5	Training	-556.9	-556.9	0	0.00
22	*260*	Ethyl methyl ether	C3H8O	540-67-0	Test	-216.4	-212.36	4.04	0.00
23	*261*	1-Propanol	C3H8O	71-23-8	Test	-255.1	-256.28	-1.18	0.00
24	*262*	2-Propanol	C3H8O	67-63-0	Training	-272.8	-269.21	3.59	0.00
25	*263*	2-Methoxyethanol	C3H8O2	109-86-4	Training	-376.9	-387.33	-10.43	0.00
26	*264*	1,2-Propanediol	C3H8O2	57-55-6	Training	-429.8	-423.51	6.29	0.00
27	*265*	1,3-Propanediol	C3H8O2	504-63-2	Training	-408.4	-406.78	1.62	0.00
28	*266*	Hydroperoxide, 1-methylethyl	C3H8O2	3031-75-2	Training	-197.1	-201.69	-4.59	0.00
29	*267*	Glycerol	C3H8O3	56-81-5	Training	-577.9	-581.52	-3.62	0.00
30	*268*	3-Cyclobutene-1,2-dione, 3,4-dihydroxy-	C4H2O4	2892-51-5	Training	-515	-515	0	0.00
31	*269*	Furan	C4H4O	110-00-9	Training	-27.7	-27.7	0	0.00
32	*270*	1-Buten-3-yn-2-ol	C4H4O	103905-52-	Training	83	72.38	-10.62	0.02
33	*271*	Diketene	C4H4O2	674-82-8	Training	-190.2	-195.16	-4.96	0.00
34	*272*	1,4-Dioxane-2,5-dione	C4H4O4	502-97-6	Training	-615.6	-617.92	-2.32	0.00
35	*273*	Divinyl ether	C4H6O	109-93-3	Training	-12.7	-12.7	0	0.00
36	*274*	2-Butenal	C4H6O	4170-30-3	Training	-109.7	-112.21	-2.51	0.00
37	*275*	Methacrolein	C4H6O	78-85-3	Training	-106.4	-112.66	-6.26	-0.01
38	*276*	Furan, 2,3-dihydro-	C4H6O	1191-99-7	Training	-72.25	-72.25	0	0.00
39	*277*	(Z)-1,3-Butadien-1-ol	C4H6O	70415-58-6	Test	-90	-84.47	5.53	-0.01
40	*278*	(E)-1,3-Butadien-1-ol	C4H6O	70411-98-2	Test	-88	-84.47	3.53	-0.01
41	*279*	1,3-Butadiene-2-ol	C4H6O	59120-04-6	Test	-77	-84.92	-7.92	-0.01
42	*280*	Methacrylic acid	C4H6O2	79-41-4	Training	-367.3	-367.72	-0.42	0.00
43	*281*	Methyl acrylate	C4H6O2	96-33-3	Training	-333	-333	0	0.00

44	*282*	Vinyl acetate	C4H6O2	108-05-4	Training	-313.6	-322.39	-8.79	0.00
45	*283*	Crotonic acid	C4H6O2	3724-65-0	Training	-368.5	-367.27	1.23	0.00
46	*284*	2,3-Butanedione	C4H6O2	625-34-3	Training	-326.8	-334.77	-7.97	0.00
47	*285*	Dimethyl oxalate	C4H6O4	553-90-2	Training	-709.27	-717.58	-8.31	0.00
48	*286*	2-Butanone	C4H8O	78-93-3	Training	-238.6	-240.86	-2.26	0.00
49	*287*	Ethyl vinyl ether	C4H8O	109-92-2	Training	-140.2	-144.04	-3.84	0.00
50	*288*	Isobutanal	C4H8O	78-84-2	Training	-215.7	-215.7	0	0.00
51	*289*	Cyclobutanol	C4H8O	2919-23-5	Training	-145	-141.07	3.93	0.00
52	*290*	1-Propene, 2-methoxy-	C4H8O	116-11-0	Training	-148.6	-145.25	3.35	0.00
53	*291*	Prop-1-en-1-ol, 2-methyl-	C4H8O	56640-70-1	Training	-207	-211.81	-4.81	0.00
54	*292*	But-2-en-2-ol, (Z)-	C4H8O	23169-87-1	Training	-212	-211.81	0.19	0.00
55	*293*	But-2-en-2-ol, (E)-	C4H8O	21451-76-3	Training	-214	-211.81	2.19	0.00
56	*294*	1,3-Dioxane	C4H8O2	505-22-6	Training	-340.6	-330.29	10.31	0.00
57	*295*	2-Methyl-1,3-dioxolane	C4H8O2	497-26-7	Training	-350	-353.24	-3.24	0.00
58	*296*	Ethene, 1,1-dimethoxy-	C4H8O2	922-69-0	Training	-280.7	-280.46	0.24	0.00
59	*297*	2-Methoxy-1,3-dioxolane	C4H8O3	19693-75-5	Training	-483.2	-483.2	0	0.00
60	*298*	1,3,5,7-Tetroxane	C4H8O4	293-30-1	Training	-620.24	-622.18	-1.94	0.00
61	*299*	1-Butanol	C4H10O	71-36-3	Test	-277	-277.12	-0.12	0.00
62	*300*	2-Butanol	C4H10O	78-92-2	Training	-293.1	-289.77	3.33	0.00
63	*301*	Diethyl ether	C4H10O	60-29-7	Training	-252.7	-247.37	5.33	0.00
64	*302*	2-Methyl-1-propanol	C4H10O	78-83-1	Test	-283.8	-286.63	-2.83	0.00
65	*303*	2-Methyl-2-propanol	C4H10O	75-65-0	Training	-312.6	-312.6	0	0.00
66	*304*	Methyl propyl ether	C4H10O	557-17-5	Test	-238.02	-233.2	4.82	0.00
67	*305*	2-Butanol	C4H10O	15892-23-6	Training	-292.7	-289.77	2.93	0.00
68	*306*	1,3-Butanediol	C4H10O2	107-88-0	Training	-433	-442.37	-9.37	0.00
69	*307*	1,4-Butanediol	C4H10O2	110-63-4	Training	-426	-427.62	-1.62	0.00
70	*308*	tert-Butyl hydroperoxide	C4H10O2	75-91-2	Training	-234.9	-230.31	4.59	0.00
71	*309*	Peroxide, diethyl	C4H10O2	628-37-5	Training	-193	-194.51	-1.51	0.00
72	*310*	Diethylene glycol	C4H10O3	111-46-6	Training	-571.2	-560.77	10.43	0.00
73	*311*	Cyclopentanol	C5H10O	96-41-3	Training	-243	-239.55	3.45	0.00
74	*312*	3,3-Dimethyloxetane	C5H10O	6921-35-3	Training	-148.2	-141.78	6.42	-0.01
75	*313*	3-Methyl-2-butanone	C5H10O	563-80-4	Training	-262.57	-262.57	0	0.00
76	*314*	Pentanal	C5H10O	110-62-3	Training	-228.4	-233.16	-4.76	0.00

77	*315*	1,4-Naphthalenedione	C10H6O2	130-15-4	Training	-97.5	-97.5	0	0.00
78	*316*	1,4-Naphthalenedione, 5,8-dihydroxy-	C10H6O4	475-38-7	Training	-499.1	-500.17	-1.07	0.00
79	*317*	1-Naphthol	C10H8O	90-15-3	Training	-30.8	-28.97	1.83	-0.01
80	*318*	11-Oxabicyclo[4,4,1]undeca-1,3,5,7,9-pentaene	C10H8O	4759-11-9 -	Training	200	199.28	-0.72	0.00
81	*319*	1,2-Dihydroxynaphthalene	C10H8O2	574-00-5	Training	-200.5	-191.66	8.84	-0.01
82	*320*	1,3-Naphthalenediol	C10H8O2	132-86-5	Training	-211.2	-205.8	5.4	0.00
83	*321*	3-Buten-2-one, 4-phenyl-	C10H10O	122-57-6	Training	-48.1	-48.1	0	0.00
84	*322*	1,3-Butanedione, 1-phenyl-	C10H10O2	93-91-4	Training	-244.1	-242.24	1.86	0.00
85	*323*	Homocubane-4-carboxylic acid	C10H10O2	15844-05-0	Test	3	-8.14	-11.14	0.50
86	*324*	Dimethyl isophthalate	C10H10O4	1459-93-4	Training	-629.2	-624.45	4.75	0.00
87	*325*	Dimethyl phthalate	C10H10O4	131-11-3	Training	-606.1	-612.17	-6.07	0.00
88	*326*	2,3,6-Trimethylbenzoic acid	C10H12O2	2529-36-4	Training	-371.2	-373.23	-2.03	0.00
89	*327*	Benzoic acid, 2,4,5-trimethyl-	C10H12O2	528-90-5	Training	-386.2	-389.3	-3.1	0.00
90	*328*	2,3,4-Trimethylbenzoic acid	C10H12O2	1076-47-7	Training	-377.3	-373.23	4.07	0.00
91	*329*	2,3,5-Trimethylbenzoic acid	C10H12O2	2437-66-3	Training	-382.2	-379.35	2.85	0.00
92	*330*	3,4,5-Trimethylbenzoic acid	C10H12O2	1076-88-6	Training	-389.8	-379.35	10.45	0.00
93	*331*	Benzoic acid, 2-(1-methylethyl)-	C10H12O2	2438-04-2	Training	-359.2	-354.41	4.79	0.00
94	*332*	1,3-Dioxolane, 2-methyl-2-phenyl-	C10H12O2	3674-77-9	Training	-261.9	-258.66	3.24	0.00
95	*333*	Oxirane, [(phenylmethoxy)methyl]-	C10H12O2	2930-05-4	Training	-138	-138	0	0.00
96	*334*	Thymol	C10H14O	89-83-8	Training	-184.6	-192.42	-7.82	-0.01
97	*335*	Phenol, 2-methyl-5-(1-methylethyl)-	C10H14O	499-75-2	Training	-194.2	-192.42	1.78	0.00
98	*336*	3-Methyl-4-isopropylphenol	C10H14O	3228-02-2	Training	-184	-192.42	-8.42	-0.01
99	*337*	5-Isopropyl-3-methylphenol	C10H14O	3228-03-3	Training	-210.1	-206.81	3.29	0.00
100	*338*	Phenol, 2-(1-methylpropyl)-	C10H14O	89-72-5	Training	-191.4	-187.6	3.8	0.00
101	*339*	Phenol, 4-methyl-2-(1-methylethyl)-	C10H14O	4427-56-9	Training	-198.4	-192.42	5.98	0.00
102	*340*	Phenol, 2-methyl-6-(1-methylethyl)-	C10H14O	3228-04-4	Training	-190	-183.17	6.83	0.00
103	*341*	Phenol, 2-methyl-3-(1-methylethyl)-	C10H14O	4371-48-6	Training	-182.6	-183.17	-0.57	0.00
104	*342*	2-isopropyl-m-cresol	C10H14O	3228-01-1	Training	-172	-183.17	-11.17	-0.01
105	*343*	Phenol, 4-methyl-3-(1-methylethyl)-	C10H14O	4371-46-4	Training	-185.1	-192.42	-7.32	-0.01
106	*344*	p-tert,-Butylcatechol	C10H14O2	98-29-3	Training	-374.7	-371.2	3.5	0.00
107	*345*	(1,1-dimethoxyethyl)benzene	C10H14O2	4316-35-2	Training	-288.5	-284.16	4.34	0.00
108	*346*	3-Methyl-6-isopropylcatechol	C10H14O2	490-06-2	Training	-379.1	-376.1	3	0.00
109	*347*	Benzene, (trimethoxymethyl)-	C10H14O3	707-07-3	Training	-433.3	-436.19	-2.89	0.00

110	*348*	Adamantan-2-ol	C10H16O	700-57-2	Training	-299	-300.72	-1.72	0.00
111	*349*	(1α,3α,5α,7α)-3,8,8-trimethyl-4-oxatricyclo[5,1,0,03,5]octane	C10H16O	35671-18-2	Training	-98	-93.31	4.69	-0.01
112	*350*	Triethyl methanetricarboxylate	C10H16O6	6279-86-3	Training	-1173	-1163.18	9.82	0.00
113	*351*	Cyclodecanone	C10H18O	1502-06-3	Training	-305.1	-303.83	1.27	0.00
114	*352*	Beta-caran-3-ol	C10H18O	54631-17-3	Training	-259	-258.79	0.21	0.00
115	*353*	Alpha-caran-3-ol	C10H18O	38748-97-9	Training	-250	-258.79	-8.79	0.00
116	*354*	2(3H)-Furanone, 5-hexyldihydro-	C10H18O2	706-14-9	Training	-496	-491.35	4.65	0.00
117	*355*	Butanoic acid, cyclohexyl ester	C10H18O2	1551-44-6	Training	-545.7	-545.7	0	0.00
118	*356*	3,5-Heptanedione, 2,2,6-trimethyl-	C10H18O2	7333-23-5	Training	-510.7	-510.7	0	0.00
119	*357*	2,2,5,5-Tetramethyl-3-hexanone	C10H20O	868-91-7	Training	-393.9	-393.9	0	0.00
120	*358*	Methyl nonanoate	C10H20O2	1731-84-6	Training	-554.2	-563.59	-9.39	0.00
121	*359*	Octanoic acid, ethyl ester	C10H20O2	106-32-1	Training	-570	-563.59	6.41	0.00
122	*360*	15-Crown-5	C10H20O5	33100-27-5	Training	-799.5	-799.5	0	0.00
123	*361*	1-Decanol	C10H22O	112-30-1	Test	-395	-402.16	-7.16	0.00
124	*362*	1-Tert-butoxy-3-propoxy-2-propanol	C10H22O3	42991-60-6	Training	-708	-710.34	-2.34	0.00
125	*363*	2-Naphthalenecarboxylic acid	C11H8O2	93-09-4	Training	-232.5	-235.85	-3.35	0.00
126	*364*	2-Phenylbicyclo[1,1,1]pentane-2-ol	C11H12O	17684-73-0	Training	135.8	144.38	8.58	0.01
127	*365*	4-Carbomethoxyhomocubane	C11H12O2	40317-63-3	Training	26	22.98	-3.02	0.02
128	*366*	Benzal diacetate	C11H12O4	581-55-5	Training	-676.85	-676.85	0	0.00
129	*367*	Ethanone, 1-(2,4,5-trimethylphenyl)-	C11H14O	2040-07-5 -	Training	-189	-188.94	0.06	0.00
130	*368*	1-Butanone, 3-methyl-1-phenyl-	C11H14O	582-62-7	Training	-160.7	-156.24	4.46	0.00
131	*369*	Benzoic acid, p-tert-butyl-	C11H14O2	98-73-7	Test	-398.5	-395.08	3.42	0.00
132	*370*	2,3,5,6-Tetramethylbenzoic acid	C11H14O2	2604-45-7	Training	-400.1	-400.19	-0.09	0.00
133	*371*	2,3,4,5-Tetramethylbenzoic acid	C11H14O2	2529-39-7	Training	-398.7	-400.19	-1.49	0.00
134	*372*	2,3,4,6-Tetramethylbenzoic acid	C11H14O2	2408-38-0	Training	-398.1	-400.19	-2.09	0.00
135	*373*	3-Tert-butylbenzoic acid	C11H14O2	7498-54-6	Training	-400.8	-396.74	4.06	0.00
136	*374*	1,2-Propadiene-1,3-dione	C3O2	504-64-3	Training	-93.64	-93.64	0	0.00
137	*375*	Butanal	C4H8O	123-72-8	Training	-211.8	-212.32	-0.52	0.00
138	*376*	Succinic anhydride	C4H4O3	108-30-5	Training	-527.9	-522.94	4.96	0.00
139	*377*	1,3,5-Trioxane	C3H6O3	110-88-3	Training	-465.76	-466.61	-0.85	0.00
140	*378*	Benzoic acid, 3-(1-methylethyl)-	C10H12O2	5651-47-8	Test	-375.5	-366.68	8.82	0.00
141	*379*	Phenol, 2-(1,1-dimethylethyl)-	C10H14O	88-18-6	Test	-199.1	-196.52	2.58	0.00
142	*380*	Butanoic acid	C4H8O2	107-92-6	Training	-475.9	-473	2.9	0.00

143	*381*	Acetic acid	C2H4O2	64-19-7	Training	-431.9	-431.32	0.58	0.00
144	*382*	Benzoic acid, 2,4,6-trimethyl-	C10H12O2	480-63-7	Training	-374.2	-379.35	-5.15	0.00
145	*383*	2-Tert-butylbenzoic acid	C11H14O2	1077-58-3	Training	-376.1	-384.47	-8.37	0.00
146	*384*	(E)-1-Propenol	C3H6O	57642-95-2	Test	-169	-170.44	-1.44	0.00
147	*385*	Allyl alcohol	C3H6O	107-18-6	Test	-123.6	-128.94	-5.34	-0.01
148	*386*	Isopropyl methyl ether	C4H10O	598-53-8	Test	-252	-242.71	9.29	0.00
149	*387*	1,4-Dioxane	C4H8O2	123-91-1	Training	-315.3	-322.79	-7.49	0.00
150	*388*	1-Naphthalenecarboxylic acid	C11H8O2	86-55-5	Training	-223.1	-216.93	6.17	0.00
151	*389*	Phenol, 4-(1-methylpropyl)-	C10H14O	99-71-8	Training	-190.3	-198.21	-7.91	-0.01
152	*390*	Dimethyl ether	C2H6O	115-10-6	Test	-184.1	-191.52	-7.42	-0.01
153	*391*	1,2-Dimethoxyethane	C4H10O2	110-71-4	Test	-342.8	-341.89	0.91	0.00
154	*392*	2H-Inden-2-one, octahydro-3a-methyl-, cis-	C10H16O	13351-29-6	Test	-287	-294.68	-7.68	0.00
155	*393*	Camphor	C10H16O	76-22-2	Test	-267	-278.32	-11.32	-0.01
1	*394*	1H-1,2,4-Triazole	C2H3N3	288-88-0	Training	192.7	192.7	0	0.00
2	*395*	Imidazole	C3H4N2	288-32-4	Training	132.9	132.9	0	0.00
3	*396*	1H-Tetrazole, 1-methyl-	C2H4N4	16681-77-9	Training	322.9	322.79	-0.11	0.00
4	*397*	1H-Pyrazole	C3H4N2	288-13-1	Training	179.4	176.34	-3.06	0.00
5	*398*	2H-Tetrazole, 2-methyl-	C2H4N4	16681-78-0	Training	328.4	328.4	0	0.00
6	*399*	Ethyleneimine	C2H5N	151-56-4	Training	126.5	122.7	-3.8	0.00
7	*400*	5-Amino-2-methyl-2H-tetrazole	C2H5N5	6154-04-7	Training	298.8	295.74	-3.06	0.00
8	*401*	1H-Tetrazol-5-amine, 1-methyl-	C2H5N5	5422-44-6	Training	302.4	307.29	4.89	0.00
9	*402*	Dimethylamine	C2H7N	124-40-3	Training	-19	-20.38	-1.38	-0.01
10	*403*	1,2-Ethanediamine	C2H8N2	107-15-3	Training	-17	-19.93	-2.93	-0.02
11	*404*	Cyanogen	C2N2	460-19-5	Test	306.7	306.15	-0.55	0.00
12	*405*	1,3,5-Triazine	C3H3N3	290-87-9	Test	225.87	244.4	18.53	0.01
13	*406*	1H-Imidazole, 2-methyl-	C4H6N2	693-98-1	Training	89.8	91.04	1.24	0.00
14	*407*	Propanenitrile	C3H5N	107-12-0	Test	51.46	55.83	4.37	0.01
15	*408*	1H-Tetrazole, 1,5-dimethyl-	C3H6N4	5144-11-6	Training	273.2	265.39	-7.81	0.00
16	*409*	2H-Tetrazole, 2,5-dimethyl-	C3H6N4	4135-93-7	Training	251.2	251.2	0	0.00
17	*410*	Cyclopropylamine	C3H7N	765-30-0	Training	77.07	67.67	-9.4	0.02
18	*411*	Isopropylamine	C3H9N	75-31-0	Training	-83.7	-86.64	-2.94	0.00
19	*412*	Propylamine	C3H9N	107-10-8	Test	-69.9	-74.78	-4.88	-0.01
20	*413*	Trimethylamine	C3H9N	75-50-3	Training	-23.7	-21.13	2.57	-0.01

21	*414*	1,2-Propanediamine, (±)-	C3H10N2	10424-38-1	Training	-53.68	-52.35	1.33	0.00
22	*415*	1,2-Propanediamine	C3H10N2	78-90-0	Training	-53.6	-52.35	1.25	0.00
23	*416*	Succinonitrile	C4H4N2	110-61-2	Training	209.7	206.8	-2.9	0.00
24	*417*	3-Butenenitrile	C4H5N	109-75-1	Training	157.7	162.33	4.63	0.00
25	*418*	1H-Imidazole, 2-ethyl-	C5H8N2	1072-62-4	Training	68.3	65.6	-2.7	0.01
26	*419*	1H-Benzotriazole	C6H5N3	95-14-7	Training	335.5	335.5	0	0.00
27	*420*	2-Methyl-5-vinyltetrazole	C4H6N4	15284-39-6	Training	354	357.06	3.06	0.00
28	*421*	2-Methylpropanenitrile	C4H7N	78-82-0	Training	22.8	19.87	-2.93	0.02
29	*422*	1-Pyrroline	C4H7N	5724-81-2	Training	63	63	0	0.00
30	*423*	Piperazine	C4H10N2	110-85-0	Test	25	29.7	4.7	0.03
31	*424*	Butylamine	C4H11N	109-73-9	Training	-95	-95.62	-0.62	0.00
32	*425*	tert-Butylamine	C4H11N	75-64-9	Training	-120	-120	0	0.00
33	*426*	sec-Butylamine	C4H11N	13952-84-6	Training	-106	-107.2	-1.2	0.00
34	*427*	2-Methyl-1,2-propanediamine	C4H12N2	811-93-8	Training	-90.25	-90.25	0	0.00
35	*428*	1,2-Butanediamine	C4H12N2	4426-48-6	Training	-73.55	-73.19	0.36	0.00
36	*429*	Pyridine	C5H5N	110-86-1	Training	140.4	142.35	1.95	0.00
37	*430*	3-Methylenecyclobutanenitrile	C6H7N	15760-35-7	Training	252.4	259.75	7.35	0.00
38	*431*	4-Aminopyridine	C5H6N2	504-24-5	Training	129.9	137.58	7.68	0.01
39	*432*	2-Aminopyridine	C5H6N2	504-29-0	Training	118.1	127.62	9.52	0.01
40	*433*	3-Aminopyridine	C5H6N2	462-08-8	Training	144.2	138.04	-6.16	0.01
41	*434*	Butanenitrile, 2-methyl-	C5H9N	18936-17-9	Training	2.4	-0.69	-3.09	0.17
42	*435*	1H-Benzimidazole	C7H6N2	51-17-2	Training	181.7	181.7	0	0.00
43	*436*	Propanenitrile, 3-(dimethylamino)-	C5H10N2	1738-25-6	Training	96.7	96.69	-0.01	0.00
44	*437*	Cyclopentylamine	C5H11N	1003-03-8	Training	-54.86	-45.46	9.4	-0.02
45	*438*	Butylmethyldiazene	C5H12N2	4426-46-4	Training	78.9	79.96	1.06	0.00
46	*439*	1,3-Propanediamine, N,N-dimethyl-	C5H14N2	109-55-7	Training	-34.7	-33.92	0.78	0.00
47	*440*	Tetracyanoethene	C6N4	670-54-2	Training	705	705	0	0.00
48	*441*	3-Pyridinecarbonitrile	C6H4N2	100-54-9	Training	277.9	282.53	4.63	0.00
49	*442*	4-Pyridinecarbonitrile	C6H4N2	100-48-1	Training	283.5	282.08	-1.42	0.00
50	*443*	2-Pyridinecarbonitrile	C6H4N2	100-70-9	Training	280.7	272.11	-8.59	0.00
51	*444*	1H-Indazole	C7H6N2	271-44-3	Training	243	243	0	0.00
52	*445*	1-Cyclopentenecarbonitrile	C6H7N	3047-38-9	Training	141.8	145	3.2	0.00
53	*446*	2-Methylpyridine	C6H7N	109-06-8	Training	98.95	98.02	-0.93	0.00

54	*447*	3-Methylpyridine	C6H7N	108-99-6	Training	103.6	108.44	4.84	0.01
55	*448*	4-Methylpyridine	C6H7N	108-89-4	Training	103.8	107.98	4.18	0.01
56	*449*	2-Cyclopentene-1-carbonitrile	C6H7N	26555-56-6	Training	156.4	150.45	-5.95	0.01
57	*450*	1H-Tetrazole, 5-phenyl-	C7H6N4	18039-42-4	Training	413	418.64	5.64	0.00
58	*451*	Hexanedinitrile	C6H8N2	111-69-3	Training	149	149	0	0.00
59	*452*	Phenylhydrazine	C6H8N2	100-63-0	Training	202.9	201.68	-1.22	0.00
60	*453*	Cyclopentanecarbonitrile	C6H9N	4254-02-8	Training	48.8	45.25	-3.55	0.01
61	*454*	2-(Diethylamino)acetonitrile	C6H12N2	3010-02-4	Training	66	62.85	-3.15	0.01
62	*455*	Tetramethyldiazetine	C6H12N2	54166-22-2	Training	150.3	152.65	2.35	0.00
63	*456*	Methenamine	C6H12N4	100-97-0	Training	199	197.51	-1.49	0.00
64	*457*	Azopropane	C6H14N2	821-67-0	Training	62.4	59.12	-3.28	0.01
65	*458*	Diazene, diisopropyl	C6H14N2	3880-49-7	Training	36	40.09	4.09	0.02
66	*459*	Diisopropylamine	C6H15N	108-18-9	Training	-136.3	-139.4	-3.1	0.00
67	*460*	Dipropylamine	C6H15N	142-84-7	Training	-116.5	-124.85	-8.35	-0.01
68	*461*	Benzonitrile	C7H5N	100-47-0	Training	219	226.21	7.21	0.00
69	*462*	1H-Tetrazole, 1-phenyl-	C7H6N4	5378-52-9	Training	448	445.4	-2.6	0.00
70	*463*	Benzylamine	C7H9N	100-46-9	Training	87.8	87.8	0	0.00
71	*464*	1-Cyclohexenecarbonitrile	C7H9N	1855-63-6	Training	101.5	98.3	-3.2	0.00
72	*465*	2,3-Dimethylpyridine	C7H9N	583-61-9	Training	68.3	66.26	-2.04	0.00
73	*466*	2,4-Dimethylpyridine	C7H9N	108-47-4	Training	63.9	70.46	6.56	0.01
74	*467*	2,5-Dimethylpyridine	C7H9N	589-93-5	Training	66.4	67.51	1.11	0.00
75	*468*	2,6-Dimethylpyridine	C7H9N	108-48-5	Training	58.7	58.7	0	0.00
76	*469*	3,4-Dimethylpyridine	C7H9N	583-58-4	Training	70	70	0	0.00
77	*470*	3,5-Dimethylpyridine	C7H9N	591-22-0	Training	72.8	72.8	0	0.00
78	*471*	2-Methylaniline	C7H9N	95-53-4	Training	53.2	53.97	0.77	0.00
79	*472*	4-Methylaniline	C7H9N	106-49-0	Test	41.8	43.36	1.56	0.00
80	*473*	N-Methylaniline	C7H9N	100-61-8	Training	83.9	79.27	-4.63	0.01
81	*474*	Pyrazine, trimethyl-	C7H10N2	14667-55-1	Training	74.3	75.75	1.45	0.00
82	*475*	Hydrazine, 1-methyl-1-phenyl-	C7H10N2	618-40-6	Training	210.8	212.02	1.22	0.00
83	*476*	t-Butylmalononitrile	C7H10N2	4210-60-0	Training	126.7	134.82	8.12	0.01
84	*477*	Cyclohexanecarbonitrile	C7H11N	766-05-2	Training	-3.6	-1.46	2.14	-0.08
85	*478*	1-Piperidineacetonitrile	C7H12N2	3010-03-5	Training	83	83	0	0.00
86	*479*	Quinuclidine	C7H13N	100-76-5	Training	-4.3	1.65	5.95	-0.18

87	*480*	3,3,5,5-Tetramethyl-1-pyrazoline	C7H14N2	2721-31-5	Test	39	40.48	1.48	0.01
88	*481*	1-Butanamine, N-(1-methylethyl)-	C7H17N	39099-23-5	Training	-165	-155.2	9.8	-0.01
89	*482*	1,2-Benzenedicarbonitrile	C8H4N2	91-15-6	Training	368.3	372.56	4.26	0.00
90	*483*	1,4-Benzenedicarbonitrile	C8H4N2	623-26-7	Training	358.3	361.94	3.64	0.00
91	*484*	1,3-Dicyanobenzene	C8H4N2	626-17-5	Training	362.7	360.29	-2.41	0.00
92	*485*	Quinoxaline	C8H6N2	91-19-0	Test	240.3	254.43	14.13	0.01
93	*486*	N,N-Dimethylaniline	C8H11N	121-69-7	Training	100.5	89.6	-10.9	0.01
94	*487*	N-Ethylaniline	C8H11N	103-69-5	Training	56.1	58.43	2.33	0.01
95	*488*	Pyridine, 5-ethyl-2-methyl-	C8H11N	104-90-5	Training	34.9	45.21	10.31	0.04
96	*489*	Pyrazine, tetramethyl-	C8H12N2	1124-11-4	Test	54.7	36.54	-18.16	0.04
97	*490*	Tetramethylbutanedinitrile	C8H12N2	3333-52-6	Training	100.6	104.79	4.19	0.01
98	*491*	n-Pentylmalononitrile	C8H12N2	42046-61-7	Training	135.8	131.28	-4.52	0.00
99	*492*	1,4-Dimethyl-2,3-diaza-bicyclo[2,2,2]oct-2-ene	C8H14N2	49570-30-1	Test	92.4	93.23	0.83	0.00
100	*493*	Octanenitrile	C8H15N	124-12-9	Test	-50.6	-48.37	2.23	-0.01
101	*494*	3,4,5,6-Tetrahydro-3,3,6,6-tetramethylpyridazine	C8H16N2	19403-24-8	Training	41.8	39.45	-2.35	0.01
102	*495*	Butanamide, 3-methyl-N-(2-methylpropylidene)	C8H17N	6898-75-5	Training	-91.2	-88.24	2.96	0.00
103	*496*	Azobutane	C8H18N2	2159-75-3	Training	19.3	17.43	-1.87	0.01
104	*497*	Dibutylamine	C8H19N	111-92-2	Training	-171.1	-166.53	4.57	0.00
105	*498*	Diisobutylamine	C8H19N	110-96-3	Training	-180.8	-185.55	-4.75	0.00
106	*499*	2-Butanamine, N-(1-methylpropyl)-	C8H19N	626-23-3	Training	-183.6	-180.5	3.1	0.00
107	*500*	isobutyl-n-butyl-amine	C8H19N	20810-06-4	Training	-175	-176.04	-1.04	0.00
108	*501*	benzene-1,3,5-tricarbonitrile	C9H3N3	10365-94-3	Training	509.6	506.31	-3.29	0.00
109	*502*	Isoquinoline	C9H7N	119-65-3	Training	204.61	204.61	0	0.00
110	*503*	Quinoline	C9H7N	91-22-5	Training	200.52	196.05	-4.47	0.00
111	*504*	5-Quinolinamine	C9H8N2	611-34-7	Training	210.6	216.12	5.52	0.00
112	*505*	6-Quinolinamine	C9H8N2	580-15-4	Training	206.1	197.19	-8.91	0.01
113	*506*	Quinoline, 1,2,3,4-tetrahydro-	C9H11N	635-46-1	Training	82	82	0	0.00
114	*507*	Quinoline, 5,6,7,8-tetrahydro-	C9H11N	10500-57-9	Training	71	76.3	5.3	0.01
115	*508*	N-Methyl methanimine	C2H5N	1761-67-7	Training	44	44	0	0.00
116	*509*	Acetaldimine	C2H5N	20729-41-3	Training	24	24	0	0.00
117	*510*	1-Norbornylisocyanide	C8H11N	103434-09-	Training	165.8	156.1	-9.7	0.01
118	*511*	Isocyanomethane	C2H3N	593-75-9	Training	163.5	163.32	-0.18	0.00
119	*512*	Ethyl isocyanide	C3H5N	624-79-3	Training	132.6	142.48	9.88	0.01

120	*513*	Azidocyclopentane	C5H9N3	33670-50-7	Training	220.8	230.34	9.54	0.01
121	*514*	Pyridinium dicyanomethylide	C8H5N3	27032-01-5	Training	523	523	0	0.00
122	*515*	1-Methylpyrrole	C5H7N	96-54-8	Training	103.1	109.6	6.5	0.01
123	*516*	Bicyclo[1,1,0]butane-1-carbonitrile	C5H5N	16955-35-4	Test	304.5	309.47	4.97	0.00
124	*517*	Butanenitrile	C4H7N	109-74-0	Training	31.2	34.99	3.79	0.02
125	*518*	Pentanenitrile	C5H9N	110-59-8	Test	11.1	14.15	3.05	0.04
126	*519*	Heptanenitrile	C7H13N	629-08-3	Training	-31	-27.53	3.47	-0.01
127	*520*	trans-3-Pentenenitrile	C5H7N	16529-66-1	Test	126	126.57	0.57	0.00
128	*521*	Acetonitrile, (dimethylamino)-	C4H8N2	926-64-7	Training	114.39	117.53	3.14	0.00
129	*522*	3-Aminopropionitrile	C3H6N2	151-18-8	Test	89.75	84.73	-5.02	0.01
130	*523*	Ethylamine	C2H7N	75-04-7	Test	-57.7	-53.93	3.77	-0.01
131	*524*	Aniline	C6H7N	62-53-3	Test	87.03	81.71	-5.32	0.01
132	*525*	2-Butynedinitrile	C4N2	1071-98-3	Training	533.46	535.26	1.8	0.00
133	*526*	Isobutylamine	C4H11N	78-81-9	Test	-98.62	-105.13	-6.51	-0.01
134	*527*	1-Octanamine	C8H19N	111-86-4	Test	-173.5	-178.98	-5.48	0.00
135	*528*	Quinazoline	C8H6N2	253-82-7	Test	243.1	254.43	11.33	0.01
136	*529*	Pyrazine, 2,3-dimethyl-	C6H8N2	5910-89-4	Test	126	114.96	-11.04	0.01
137	*530*	Pyrimidine	C4H4N2	289-95-2	Training	195.8	193.37	-2.43	0.00
138	*531*	Pyrazine	C4H4N2	290-37-9	Test	196.1	193.37	-2.73	0.00
1	*532*	Dinitromethane	CH2N2O4	625-76-3	Training	-58.9	-69.54	-10.64	-0.02
2	*533*	5-Nitroaminotetrazole	CH2N6O2	18588-16-4	Training	252	252	0	0.00
3	*534*	Methyl nitrate	CH3NO3	598-58-3	Training	-122	-116.72	5.28	-0.01
4	*535*	Nitroglycerin	C3H5N3O9	55-63-0	Training	-279.1	-277.09	2.01	0.00
5	*536*	1-Nitropropane	C3H7NO2	108-03-2	Training	-124.3	-113.66	10.64	-0.01
6	*537*	2-Nitropropane	C3H7NO2	79-46-9	Training	-138.9	-138.9	0	0.00
7	*538*	Alanine	C3H7NO2	56-41-7	Training	-414.7	-416.68	-1.98	0.00
8	*539*	Ethanediamide	C2H4N2O2	471-46-5	Training	-387.1	-389.33	-2.23	0.00
9	*540*	Acetamide	C2H5NO	60-35-5	Training	-238.33	-236.08	2.25	0.00
10	*541*	Acetaldoxime	C2H5NO	107-29-9	Training	-22.55	-23.45	-0.9	-0.01
11	*542*	Glycine	C2H5NO2	56-40-6	Training	-390.5	-384.26	6.24	0.00
12	*543*	Ethyl-nitrite-	C2H5NO2	109-95-5	Training	-108	-104.5	3.5	0.00
13	*544*	Urea, methyl-	C2H6N2O	598-50-5	Training	-235.68	-236.08	-0.4	0.00
14	*545*	N-Nitrosobis-(2,2,2-trinitroethyl)amine	C4H4N8O13	34882-73-0	Training	147	148.71	1.71	0.00

15	*546*	N-Nitrobis-(2,2,2-trinitroethyl)amine	C4H4N8O14	19836-28-3	Training	89.6	88.24	-1.36	0.00
16	*547*	Morpholine, 4-nitro-	C4H8N2O3	4164-32-3	Test	-131	-127.29	3.71	0.00
17	*548*	Piperazine, 1,4-dinitro-	C4H8N4O4	4164-37-8	Test	58	68.22	10.22	0.02
18	*549*	2-Azetidinone	C3H5NO	930-21-2	Training	-96	-96	0	0.00
19	*550*	Cyclotetramethylenetetranitramine	C4H8N8O8	2691-41-0	Training	187.9	189.84	1.94	0.00
20	*551*	Propane, 2-methyl-2-nitro-	C4H9NO2	594-70-7	Training	-177.1	-178.21	-1.11	0.00
21	*552*	Acetamide, N-methyl-	C3H7NO	79-16-3	Training	-248	-248	0	0.00
22	*553*	2-Furancarboxaldehyde, 5-nitro-	C5H3NO4	698-63-5	Training	-147	-147	0	0.00
23	*554*	Pyridine, 4-nitro-, 1-oxide	C5H4N2O3	1124-33-0	Training	126	119.79	-6.21	0.01
24	*555*	Sarcosine	C3H7NO2	107-97-1	Training	-367.3	-371.55	-4.25	0.00
25	*556*	β-Alanine	C3H7NO2	107-95-9	Training	-424	-424	0	0.00
26	*557*	iso-Propyl nitrite	C3H7NO2	541-42-4	Training	-133	-134.85	-1.85	0.00
27	*558*	Propyl nitrite	C3H7NO2	543-67-9	Training	-119	-125.34	-6.34	-0.01
28	*559*	Urea, ethyl-	C3H8N2O	625-52-5	Training	-257.5	-256.92	0.58	0.00
29	*560*	Urea, N,N-dimethyl-	C3H8N2O	598-94-7	Training	-220	-225.31	-5.31	0.00
30	*561*	Proline	C5H9NO2	147-85-3	Training	-366.2	-366.2	0	0.00
31	*562*	Benzofurazan, 4-nitro-, 1-oxide	C6H3N3O4	18771-85-2	Training	299.9	303.8	3.9	0.00
32	*563*	Benzofuroxan	C6H4N2O2	480-96-6	Training	298.5	294.6	-3.9	0.00
33	*564*	Benzene, nitro-	C6H5NO2	98-95-3	Training	68.53	70.83	2.3	0.00
34	*565*	Phenol, 4-nitro-	C6H5NO3	100-02-7	Training	-114.7	-116.24	-1.54	0.00
35	*566*	3-Methylisoxazole	C4H5NO	30842-90-1	Training	35.6	30.13	-5.47	0.02
36	*567*	Acetic acid, cyano-, methyl ester	C4H5NO2	105-34-0	Training	-243.3	-249.37	-6.07	0.00
37	*568*	Cytosine	C4H5N3O	71-30-7	Training	-59	-60.69	-1.69	0.00
38	*569*	3-Isoxazolamine, 5-methyl-	C4H6N2O	1072-67-9	Training	20	19.86	-0.14	0.00
39	*570*	Furazan, dimethyl-	C4H6N2O	4975-21-7	Training	107	107	0	0.00
40	*571*	Oxazole, 4,5-dihydro-2-methyl-	C4H7NO	1120-64-5	Training	-130.5	-126.98	3.52	0.00
41	*572*	Piperazine, 1,4-dinitroso-	C4H8N4O2	140-79-4	Training	194	189.17	-4.83	0.00
42	*573*	4-Nitrocatechol	C6H5NO4	3316-09-4	Training	-290	-280.32	9.68	0.00
43	*574*	5-Nitro-2-furancarboxylic acid methyl ester	C6H5NO5	1874-23-3	Training	-367	-369.7	-2.7	0.00
44	*575*	Propanamide, 2-methyl-	C4H9NO	563-83-7	Training	-282.6	-287.27	-4.67	0.00
45	*576*	Butanamide	C4H9NO	541-35-5	Training	-279.17	-277.76	1.41	0.00
46	*577*	n-Butyl nitrite	C4H9NO2	544-16-1	Training	-146	-146.18	-0.18	0.00
47	*578*	4-Aminobutanoic acid	C4H9NO2	56-12-2	Training	-441	-440.18	0.82	0.00

48	*579*	Isobutyl nitrite	C4H9NO2	542-56-3	Training	-151	-155.69	-4.69	0.00
49	*580*	t-Butyl nitrite	C4H9NO2	540-80-7	Training	-172	-163.48	8.52	-0.01
50	*581*	sec-Butyl nitrite	C4H9NO2	924-43-6	Training	-153	-155.4	-2.4	0.00
51	*582*	isopropylurea	C4H10N2O	691-60-1	Training	-289.8	-287.27	2.53	0.00
52	*583*	Diethylhydroxylamine	C4H11NO	3710-84-7	Training	-121.77	-121.77	0	0.00
53	*584*	Diethanolamine	C4H11NO2	111-42-2	Training	-397.1	-397.34	-0.24	0.00
54	*585*	N-Nitroso-bis-(2,2-dinitropropyl)amine	C6H10N6O9	28464-26-8	Training	-81.5	-74.35	7.15	-0.01
55	*586*	4-Pyridinol	C5H5NO	626-64-2	Training	-30.3	-40.74	-10.44	-0.05
56	*587*	N-Nitrobis-(2,2-dinitropropyl)amine	C6H10N6O10	28464-24-6	Training	-133	-134.83	-1.83	0.00
57	*588*	3-Pyridinol	C5H5NO	109-00-2	Training	-43.7	-40.28	3.42	-0.01
58	*589*	Isoxazole, 3,5-dimethyl-	C5H7NO	300-87-8	Training	-18	-22.05	-4.05	-0.03
59	*590*	2,5-Pyrrolidinedione, 1-methyl-	C5H7NO2	1121-07-9	Training	-389.7	-402.42	-12.72	0.00
60	*591*	5-Amino-3,4-dimethyl-isoxazole	C5H8N2O	19947-75-2	Training	5.2	5.16	-0.04	0.00
61	*592*	Oxazole, 2-ethyl-4,5-dihydro-	C5H9NO	10431-98-8	Training	-148.9	-152.42	-3.52	0.00
62	*593*	α-Methoxyisobutyronitrile	C5H9NO	76474-09-4	Training	-125.4	-130.69	-5.29	-0.01
63	*594*	Methyl N,N-dimethylalaninate	C6H13NO2	130515-23-	Training	-394.4	-404.22	-9.82	0.00
64	*595*	Trinitrotoluene	C7H5N3O6	118-96-7	Training	24.1	19.61	-4.49	0.02
65	*596*	Propanamide, 2,2-dimethyl-	C5H11NO	754-10-9	Training	-313.1	-315.9	-2.8	0.00
66	*597*	Propanamide, N,N-dimethyl-	C5H11NO	758-96-3	Training	-250.2	-249.74	0.46	0.00
67	*598*	2-Propanone, 1-(dimethylamino)-	C5H11NO	15364-56-4	Training	-180.1	-179.16	0.94	0.00
68	*599*	Glycine, N,N-dimethyl-, methyl ester	C5H11NO2	7148--06-3	Training	-370.4	-376.84	-6.44	0.00
69	*600*	5-Aminovaleric acid	C5H11NO2	660-88-8	Training	-460.2	-461.02	-0.82	0.00
70	*601*	2-methylbutan-2-yl nitrite	C5H11NO2	5156-41-2	Training	-192	-188.57	3.43	0.00
71	*602*	Urea, tetramethyl-	C5H12N2O	632-22-4	Training	-205.6	-205.6	0	0.00
72	*603*	Urea, N,N-diethyl-	C5H12N2O	634-95-7	Training	-272.3	-266.99	5.31	0.00
73	*604*	Urea, (1,1-dimethylethyl)-	C5H12N2O	1118-12-3	Training	-314	-315.9	-1.9	0.00
74	*605*	Urea, N,N-diethyl-	C5H12N2O	623-76-7	Training	-282.9	-284.57	-1.67	0.00
75	*606*	sec-butylurea	C5H12N2O	689-11-2	Training	-307	-307.82	-0.82	0.00
76	*607*	5-nitrofuran-2-acrylaldehyde	C7H5NO4	1874-22-2	Training	-65	-56.23	8.77	-0.02
77	*608*	Benzofurazan	C6H4N2O	273-09-6	Training	300.2	296.86	-3.34	0.00
78	*609*	1,2,3-Benzoxadiazole	C6H4N2O	273-59-6	Training	300.7	300.7	0	0.00
79	*610*	Benzofurazan, 5-methyl-, 1-oxide	C7H6N2O2	19164-41-1	Training	267.4	275.19	7.79	0.00
80	*611*	5-Methoxybenzofurazan, 1-oxide	C7H6N2O3	7791-49-3	Training	148.3	148.87	0.57	0.00

81	*612*	1-Methyl-2,4-dinitrobenzene	C7H6N2O4	121-14-2	Training	33.2	35.84	2.64	0.01
82	*613*	Niacin	C6H5NO2	59-67-6	Training	-221.5	-228.23	-6.73	0.00
83	*614*	(Dinitromethyl)benzene	C7H6N2O4	611-38-1	Training	35	30.3	-4.7	0.02
84	*615*	(Nitromethyl)benzene	C7H7NO2	622-42-4	Training	30.7	40.11	9.41	0.04
85	*616*	Benzene, 1-methyl-4-nitro-	C7H7NO2	99-99-0	Test	30.9	32.48	1.58	0.01
86	*617*	Terephthalonitrile N,N-dioxide	C8H4N2O2	3729-34-8	Training	410.5	408.52	-1.98	0.00
87	*618*	Benzoic acid, 4-nitro-, methyl ester	C8H7NO4	619-50-1	Training	-287	-285.8	1.2	0.00
88	*619*	2,2,2-Trinitro-1-phenylethane	C8H7N3O6	38677-56-4	Training	65.7	64.99	-0.71	0.00
89	*620*	Phenol, 3-amino-	C6H7NO	591-27-5	Training	-98.6	-107.02	-8.42	-0.01
90	*621*	Phenol, o-amino-	C6H7NO	95-55-6	Test	-104.4	-94.75	9.65	-0.01
91	*622*	2(1H)-Pyridone, 6-methyl-	C6H7NO	3279-76-3	Training	-120.3	-117.31	2.99	0.00
92	*623*	3-Pyridinol, 6-methyl-	C6H7NO	1121-78-4	Training	-69.8	-81.21	-11.41	-0.02
93	*624*	3-Pyridinol, 2-methyl-	C6H7NO	1121-25-1	Training	-84.5	-82.46	2.04	0.00
94	*625*	2-Methyl-4-hydroxypyridine	C6H7NO	18615-86-6	Training	-71.7	-78.26	-6.56	-0.01
95	*626*	Benzenamine, N,N-dimethyl-4-nitro-	C8H10N2O2	100-23-2	Training	62.8	69.96	7.16	0.02
96	*627*	Benzenamine, N,N-dimethyl-3-nitro-	C8H10N2O2	619-31-8	Training	72.6	68.31	-4.29	0.01
97	*628*	Isoxazole, trimethyl-	C6H9NO	10557-82-1	Training	-20	-15.55	4.45	-0.03
98	*629*	Ethyl 2-cyanopropionate	C6H9NO2	1572-99-2	Training	-311.96	-305.89	6.07	0.00
99	*630*	Triacetamide	C6H9NO3	641-06-5	Training	-550.1	-550.1	0	0.00
100	*631*	Nitroxoline	C9H6N2O3	4008-48-4	Training	-1.7	0.87	2.57	-0.20
101	*632*	1,2-Cyclohexanedione dioxime	C6H10N2O2	492-99-9	Training	-69.66	-69.66	0	0.00
102	*633*	2-Methylquinoxaline-1,4-dioxide	C9H8N2O2	6639-86-7	Training	169.9	169.9	0	0.00
103	*634*	2-(Diacetoxymethyl)-5-nitrofuran	C9H9NO7	92-55-7	Training	-772	-773.1	-1.1	0.00
104	*635*	Caprolactam	C6H11NO	105-60-2	Training	-239.6	-238.15	1.45	0.00
105	*636*	Benzamide, N,N-dimethyl-4-nitro-	C9H10N2O3	7291-01-2	Training	-86	-86.61	-0.61	0.00
106	*637*	Acetamide, N,N-diethyl-	C6H13NO	685-91-6	Training	-287.2	-287.2	0	0.00
107	*638*	N,N-Dimethylbutyramide	C6H13NO	760-79-2	Training	-270.9	-270.58	0.32	0.00
108	*639*	Aminocaproic acid	C6H13NO2	60-32-2	Training	-482.4	-479.21	3.19	0.00
109	*640*	Glycine, N,N-dimethyl-, ethyl ester	C6H13NO2	33229-89-9	Training	-407.1	-397.69	9.41	0.00
110	*641*	Triethanolamine	C6H15NO3	102-71-6	Training	-558.3	-554.47	3.83	0.00
111	*642*	1-Piperidinyloxy, 4-hydroxy-2,2,6,6-tetramethyl-	C9H18NO2	2226-96-2	Training	-291.2	-299.56	-8.36	0.00
112	*643*	Benzoxazole	C7H5NO	273-53-0	Training	45.14	45.14	0	0.00
113	*644*	Benzene, isocyanato-	C7H5NO	103-71-9	Training	-14.5	-9.35	5.15	-0.05

114	*645*	4-Hydroxy-5-methyl-1H-pyrrole-3-carboxylic acid ethyl ester	C8H11NO3	65713-63-5	Training	-611.9	-609.2	2.7	0.00
115	*646*	Benzofurazan, 5-methoxy-	C7H6N2O2	4413-48-3	Training	147.1	142.09	-5.01	0.00
116	*647*	Benzonitrile,2,4,6-trimethoxy-N-oxide	C10H11NO4	2904-59-8	Training	-228.2	-224.24	3.96	0.00
117	*648*	Benzamide	C7H7NO	27208-38-4	Training	-100.9	-100.86	0.04	0.00
118	*649*	Tricyclo[3,3,1,1(3,7)]decane, 2-nitro-	C10H15NO2	54564-31-7	Training	-179.8	-180.9	-1.1	0.00
119	*650*	(E)-4-(p-Nitroanilino)-3-penten-2-one	C11H12N2O3	20771-72-6	Training	-98.9	-92.65	6.25	-0.01
120	*651*	4-aminobenzoic acid	C7H7NO2	150-13-0	Test	-293.9	-293.32	0.58	0.00
121	*652*	Benzoic acid, 3-amino-	C7H7NO2	99-05-8	Test	-289.3	-294.97	-5.67	0.00
122	*653*	5-Nitro-2-acetoxy-2,5-dihydrofurfural diacetate	C11H13NO9	75631-81-1	Training	-1285	-1283.9	1.1	0.00
123	*654*	2-Methoxy-3,3-dimethylbutanenitrile	C7H13NO	162047-91-	Training	-164.7	-168.36	-3.66	0.00
124	*655*	2-Methoxy-2-methylpentanenitrile	C7H13NO	162047-90-	Training	-169.28	-172.37	-3.09	0.00
125	*656*	Diethylaminoacetone	C7H15NO	1620-14-0	Training	-233.3	-233.84	-0.54	0.00
126	*657*	p-Nitrobenzylidene tert-butylamine	C11H14N2O2	718-36-5	Training	49.4	46.44	-2.96	0.01
127	*658*	Terephthalamide	C8H8N2O2	3010-82-0	Training	-292	-292.18	-0.18	0.00
128	*659*	Isophthalamide	C8H8N2O2	1740-57-4	Training	-294	-293.84	0.16	0.00
129	*660*	Formamide, N-methyl-N-phenyl-	C8H9NO	93-61-8	Training	-75.6	-75.6	0	0.00
130	*661*	Benzene, 1,3-dimethyl-2-nitroso-	C8H9NO	19519-71-2	Training	139.8	147.29	7.49	0.01
131	*662*	N-Phenylglycine	C8H9NO2	103-01-5	Training	-268.7	-271.9	-3.2	0.00
132	*663*	2-Phenylglycine	C8H9NO2	69-91-0	Training	-280.5	-280.5	0	0.00
133	*664*	Benzenamine, N,N-dimethyl-4-nitroso-	C8H10N2O	138-89-6	Training	185	190.88	5.88	0.00
134	*665*	N-Formylimidazole diethyl acetal	C8H14N2O2	61278-81-7	Training	-255.3	-250.12	5.18	0.00
135	*666*	octan-2-one oxime	C8H17NO	7207-49-0	Training	-180.8	-178.23	2.57	0.00
136	*667*	Octanone-4-oxime	C8H17NO	7207-51-4	Training	-181.1	-178.23	2.87	0.00
137	*668*	Octanone-3-oxime	C8H17NO	7207-50-3	Training	-172.8	-178.23	-5.43	0.00
138	*669*	Octanaloxime	C8H17NO	929-55-5	Training	-149.4	-148.5	0.9	0.00
139	*670*	8-Aminocaprylic acid	C8H17NO2	1002-57-9	Training	-524	-527.47	-3.47	0.00
140	*671*	trans-Di-tert-butylhyponitrite	C8H18N2O2	82554-97-0	Training	-189	-189	0	0.00
141	*672*	Isoxazole, 3-phenyl-	C9H7NO	1006-65-1	Training	139	133.36	-5.64	0.01
142	*673*	1H-Isoindole-1,3(2H)-dione, 2-methyl-	C9H7NO2	550-44-7	Training	-233.9	-232.83	1.07	0.00
143	*674*	Alpha-methoxybenzyl cyanide	C9H9N2O	87732-38-5	Training	26.5	29.08	2.58	0.01
144	*675*	Acetylimidazole diethyl acetal	C9H16N2O2	111456-84-	Training	-296.8	-297.46	-0.66	0.00
145	*676*	Urea, N,N-bis(1,1-dimethylethyl)-	C9H20N2O	5336-24-3	Training	-404.2	-402.53	1.67	0.00
146	*677*	Ethyl-m-phenylenediisocyanate	C10H8N2O2	64711-83-7	Training	-135	-137.57	-2.57	0.00

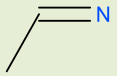
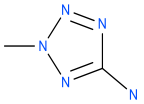
147	*678*	Isoxazole, 3-methyl-5-phenyl-	C10H9NO	1008-75-9	Training	103	108.47	5.47	0.01
148	*679*	β-Cyanopropiophenone	C10H9NO	5343-98-6	Test	30	33.61	3.61	0.02
149	*680*	2,4,6-Trimethoxybenzonitrile	C10H11NO3	2571-54-2	Training	-244.6	-247.52	-2.92	0.00
150	*681*	N,N,4-Trimethyl benzamide	C10H13NO	14062-78-3	Training	-113	-105.34	7.66	-0.01
151	*682*	N,N-Dimethyl 4-methoxybenzamide	C10H13NO2	7291-00-1	Training	-224.6	-231.65	-7.05	0.00
152	*683*	2-Buten-1-one, 3-(methylamino)-1-phenyl-	C11H13NO	14091-93-1	Training	-53.7	-48.07	5.63	-0.01
153	*684*	1-Adamantanecarboxamide	C11H17NO	5511-18-2	Training	-319	-318.85	0.15	0.00
154	*685*	N,N-Dimethylnonamide	C11H23NO	6225-08-7	Training	-374	-374.78	-0.78	0.00
155	*686*	Phenoxazine	C12H9NO	135-67-1	Training	94	94	0	0.00
156	*687*	Phenol, 2-[(phenylimino)methyl]-, N-oxide	C13H11NO2	20357-59-9	Training	53.9	53.9	0	0.00
157	*688*	2-Propanol, 1-phenoxy-3-(phenylamino)-	C15H17NO2	16112-55-3	Training	-185	-184.52	0.48	0.00
158	*689*	DL-2,3-Dimethoxy-2,3-diphenylsuccinonitrile	C18H16N2O2	61502-57-6	Training	175	173.71	-1.29	0.00
159	*690*	m-Terephthalanisidide	C22H20N2O4	6957-81-9	Training	-340	-332.62	7.38	0.00
160	*691*	N,N-Bis-(p-methoxyphenyl)terephthalamide	C22H20N2O4	7144-15-2	Training	-320	-329.3	-9.3	0.00
161	*692*	N,N-Bis(o-methoxyphenyl)terephthalamide	C22H20N2O4	36360-34-6	Training	-310	-308.07	1.93	0.00
162	*693*	1-Butanone, 3,3-(1,2-ethanediyldinitrilo)bis[1-phenyl-	C22H24N2O2	16087-30-2	Training	-104.5	-104.5	0	0.00
163	*694*	Benzenamine, N,N-bis(2-hydroxy-3-phenoxypropyl)-	C24H27NO4	434039	Training	-436.8	-435.87	0.93	0.00
164	*695*	Cyanoketene	C3HNO	4452-08-8	Training	100	100	0	0.00
165	*696*	N,N-Dimethylamino-2,4-pentadiene-5-al	C7H11NO	4688-60-2	Training	-29.1	-28.86	0.24	0.00
166	*697*	N,N-Dimethylamino-2,4,6-heptatriene-7al	C9H13NO	13044-92-3	Training	21.6	21.36	-0.24	0.00
167	*698*	4,4-methylenedicyclohexyl diisocyanate	C15H22N2O2	5124-30-1	Training	-311	-311	0	0.00
168	*699*	2-Propanamine, 2-methyl-N-(phenylmethylene)-, N-oxide	C11H15NO	3376-24-7	Training	30.9	30.27	-0.63	0.00
169	*700*	o-Nitrosonitrobenzene dimer	C12H8N4O6	56079-22-2	Training	313	311.48	-1.52	0.00
170	*701*	Azoxybenzene	C12H10N2O	495-48-7	Training	342	337.81	-4.19	0.00
171	*702*	Nitrosobenzene dimer	C12H10N2O2	35506-28-6	Training	328	329.52	1.52	0.00
172	*703*	4-Isopropylbenzylidene t-butylamine N-oxide	C14H21NO	121678-88-	Training	-50.9	-49.81	1.09	0.00
173	*704*	Diazene, bis(4-ethoxyphenyl)-, 1-oxide	C16H18N2O3	4792-83-0	Training	-37.4	-33.21	4.19	-0.01
174	*705*	Phenazine, 5-oxide	C12H8N2O	304-81-4	Training	297.3	297.3	0	0.00
175	*706*	N-Tert-butyl-alpha-(4-nitrophenyl)nitrone	C11H14N2O3	3585-88-4	Training	11.1	10.64	-0.46	0.01
176	*707*	2,4,6-Trimethylbenzonitrile, N-oxide	C10H11NO	2904-57-6	Training	137	137	0	0.00
177	*708*	Di-t-butyldiazene N-oxide	C8H18N2O	16649-52-8	Training	-107.6	-107.49	0.11	0.00
178	*709*	Di-t-butyldiazene N-oxide	C8H18N2O	54168-23-9	Training	-107.6	-107.49	0.11	0.00
179	*710*	Quindoxin	C8H6N2O2	2423-66-7	Training	227.1	227.19	0.09	0.00

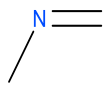
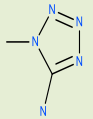
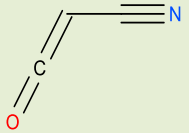
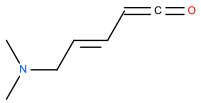
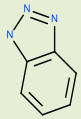
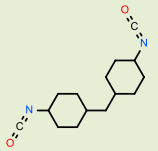
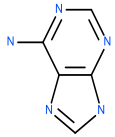
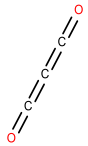
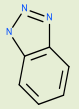
180	*711*	Tetramethylene furoxan	C6H8N2O2	2209-36-1	Training	95.31	104.13	8.82	0.01
181	*712*	Diazene, dipropyl-, 1-oxide	C6H14N2O	17697-55-1	Training	-31	-31.21	-0.21	0.00
182	*713*	6,7-Diazatricyclo[3,2,2,0(2,4)]non-6-ene, oxide	C7H10N2O	25926-99-2	Training	226.1	236.37	10.27	0.01
183	*714*	Dimethylfurazan monoxide	C4H6N2O2	2518-42-5	Training	102	102	0	0.00
184	*715*	4,5-Bis(nitratomethyl)furoxan	C4H4N4O8	57449-44-2	Training	21	14.34	-6.66	0.04
185	*716*	(E)-Azodioxymethane	C2H6N2O2	37765-15-4	Training	65.9	65.9	0	0.00
186	*717*	4,5-Dihydro-3-nitro-isoxazole-2-oxide	C3H4N2O4	4122-45-6	Training	20	17.85	-2.15	0.01
187	*718*	4,5-Furazandimethanol dinitrate	C4H4N4O7	57449-43-1	Training	11	12.01	1.01	0.01
188	*719*	2-Methyl-3-acetyl-quinoxaline 1,4-dioxide	C11H10N2O3	13297-17-1	Training	33.1	34.68	1.58	0.01
189	*720*	2-Methyl-3-carbomethoxyquinoxaline-1,4-dioxide	C11H10N2O4	40016-70-4	Training	-148.7	-147.27	1.43	0.00
190	*721*	1,1-Dinitroethylazide	C2H3N5O4	56522-42-0	Training	253	243.46	-9.54	0.01
191	*722*	2,3-Diazabicyclo[2,2,1]hept-2-ene,2-oxide	C5H8N2O	22509-00-8	Training	127.8	118.26	-9.54	0.01
192	*723*	Benzene, 1-azido-4-nitro-	C6H4N4O2	1516-60-5	Training	389.7	389.7	0	0.00
193	*724*	2,3-Diazabicyclo[2,2,2]oct-2-ene,2-oxide	C6H10N2O	25926-96-9	Training	92.4	93.69	1.29	0.00
194	*725*	Pyridazine, 3,4,5,6-tetrahydro-3,3,6,6-tetramethyl-1-oxide	C8H16N2O	54143-34-9	Training	-26.5	-28.52	-2.02	-0.01
195	*726*	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-trimethyl-	C6H9N3O3	827-16-7	Training	-590.5	-583.54	6.96	0.00
196	*727*	2,4(1H,3H)-Pyrimidinedione, 1,3-dimethyl-	C6H8N2O2	874-14-6	Training	-313.6	-319.94	-6.34	0.00
197	*728*	Formamide	CH3NO	75-12-7	Training	-186	-178.01	7.99	-0.01
198	*729*	Urea	CH4N2O	57-13-6	Training	-235.5	-243.45	-7.95	0.00
199	*730*	Benzene, 1,3,5-trimethyl-2-nitro-	C9H11NO2	603-71-4	Training	-26.8	-23.95	2.85	-0.01
200	*731*	anthranilic acid	C7H7NO2	118-92-3	Test	-296.2	-282.7	13.5	-0.01
201	*732*	p-Nitroaniline	C6H6N2O2	100-01-6	Test	55.2	62.08	6.88	0.02
202	*733*	Propanediamide	C3H6N2O2	108-13-4	Training	-416.4	-410.17	6.23	0.00
203	*734*	Propanamide	C3H7NO	79-05-0	Training	-258.94	-256.92	2.02	0.00
204	*735*	Octanamide	C8H17NO	629-01-6	Training	-362.7	-361.12	1.58	0.00
205	*736*	4-Quinolinol, 2-methyl-	C10H9NO	607-67-0	Test	-23.3	-23.73	-0.43	0.00
206	*737*	m-Nitroaniline	C6H6N2O2	99-09-2	Test	62.5	60.42	-2.08	0.00
207	*738*	Phenol, 3-nitro-	C6H5NO3	554-84-7	Training	-109.3	-117.9	-8.6	-0.01
208	*739*	2-Pyrrolidinone	C4H7NO	616-45-5	Training	-197.4	-189.11	8.29	-0.01
209	*740*	2,2,6,6-Tetramethyl-4-piperidinone	C9H17NO	826-36-8	Test	-273.4	-268.93	4.47	0.00
210	*741*	Isoxazole, 5-methyl-	C4H5NO	5765-44-6	Training	34.1	35.35	1.25	0.00
211	*742*	4-Quinolinol	C9H7NO	611-36-9	Test	20.8	15.48	-5.32	0.03
212	*743*	2-(Diethylamino)-1-phenylethanone	C12H17NO	4061-29-4	Training	-96.2	-98.03	-1.83	0.00

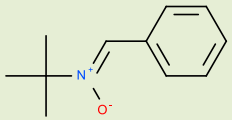
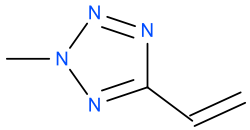
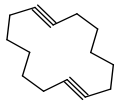
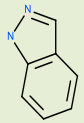
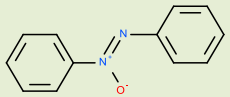
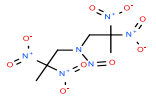
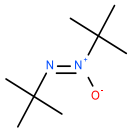
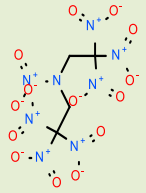
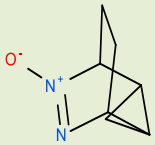
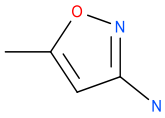
213	*744*	Ethanone, 2-(dimethylamino)-1-phenyl-	C10H13NO	3319-03-7	Training	-46.3	-43.35	2.95	-0.01
214	*745*	Diethylpropion	C13H19NO	90-84-6	Training	-124.1	-128.09	-3.99	0.00
215	*746*	Benzeneacetonitrile, α-oxo-	C8H5NO	613-90-1	Training	117.5	110.29	-7.21	0.01
216	*747*	1,3,5-tri(tert-butyl)-2-nitrosobenzene	C18H29NO	24973-59-9	Training	-117.4	-119.54	-2.14	0.00
217	*748*	Metamfepramone	C11H15NO	15351-09-4	Training	-69.9	-73.41	-3.51	-0.01
218	*749*	2,4,6-Trimethylnitrosobenzene	C9H11NO	1196-12-9	Training	107.4	96.97	-10.43	0.01
219	*750*	4,5-Dihydro-3-nitro-isoxazole	C3H4N2O3	1121-14-8	Test	39	40.62	1.62	0.01

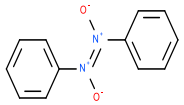
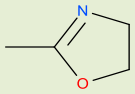
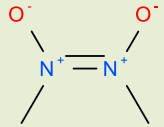
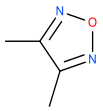
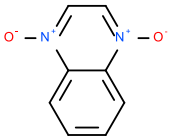
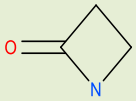
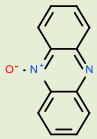
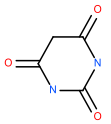
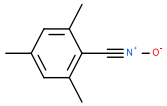
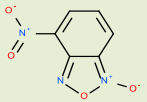
Table S6. Groups Contribution values of the new fragments with illustrative examples.

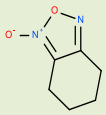
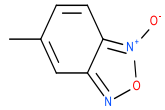
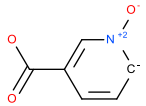
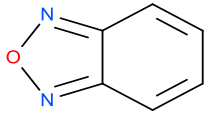
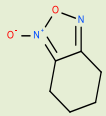
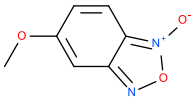
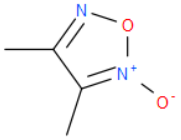
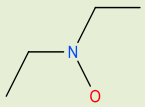
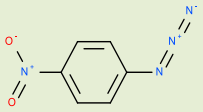
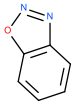
***Occ**: occurrences; **Par**: parameters.*

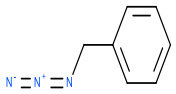
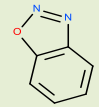
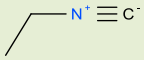
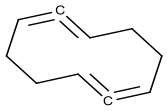
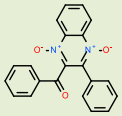
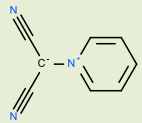
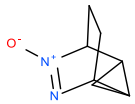
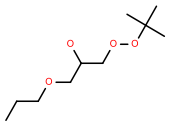
N°	Groups	Occ.	Par.	Examples	N°	Groups	Occ	Par	Examples
1	**NH=CH**	1	65.41		**44**	**(N=C-N)**	6	27.7	

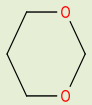
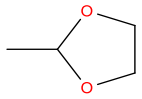
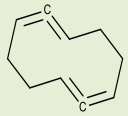
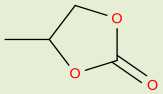
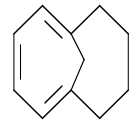
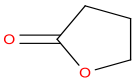
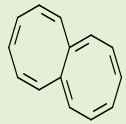
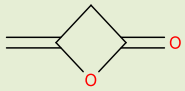
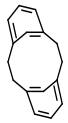
2	**N=CH2**	1	85.41		**45**	**NHn-(C=N)**	5	53.87	
3	**O=C=CH**	3	-53.08		**46**	**(C=N-C)**	1	102.39	
4	**>N-**	2	86.25		**47**	**(N=N-N)**	1	19.68	
5	**(-N=C=O)**	1	-40.17		**48**	**(-AC-N=C-N-AC)**	1	32.38	
6	**O=C=C=C=O**	1	-93.64		**49**	**(-AC-N=N-N-AC)**	1	20.25	

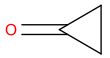
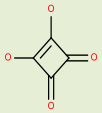
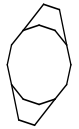
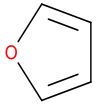
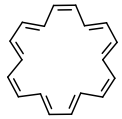
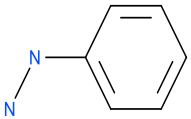
7	**aC-C=[N+][O-]**	3	75.41		**50**	**(N-C=N-N)**	2	30.54	
8	**-C≡C-cyc**	1	233.58		**51**	**(ac-C=N-N-ac-)**	1	39.48	
9	**aC-N=[N+][O-].**	2	182.71		**52**	**C-(NO2)2**	3	-70.42	
10	**N=[N+][O-].**	3	134.98		**53**	**C-(NO2)3**	3	-52.57	
11	**(N=[N+])cycl [O-].**	4	98.36		**54**	**(C=N-O)**	12	169.64	

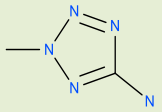
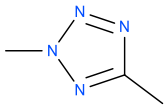
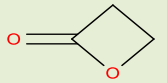
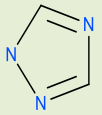
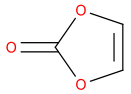
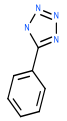
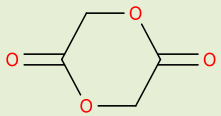
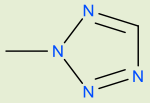
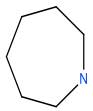
12	**aC-[O-][N+]=[N+][O-].**	2	174.42		**55**	**(N=C-O)**	3	91.13	
13	**[O-][N+]=[N+][O-].**	1	148.73		**56**	**(-C=N-O-N=O-)**	1	3.51	
14	**(aC=[N+]-[O])aromatic**	5	-7.58		**57**	**(C-CO-)cyc**	1	-47.27	
15	**aFC=[N+]-[O]**	1	35.27		**58**	**(-N-CO-)n cycl**	8	-28.21	
16	**aC-C#[N+]-[O-]**	1	155.69		**59**	**(N-O-)cyc**	8	149.22	

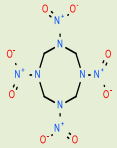
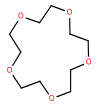
17	**(C=[N+]([O-])-O cyc**	4	85.74		**60**	**(N-)cyc-O**	5	212.98	
18	**([C-]-[N+2]-[0-])cyc**	1	28		**61**	**(-N-O-N-)**	6	-12.81	
19	**(C=[N+])cyc-[O-]**	4	86.22		**62**	**(aC-N-O-N-aC)**	4	9.04	
20	**(C=[N+])cyc-[O-]$_c$-CH$_3$**	1	-26.4		**63**	**N-OH**	1	85.81	
21	**aC-NNN**	1	333.24		**64**	**(-N=N-O-)**	1	77.11	

22	**NNN**	2	290.81		**65**	**(aC-N=N-O-aC)**	1	76.78	
23	**(-[N+]#[C-]**	3	204.73		**66**	**(AC-N=C-O-AC)**	1	-18.86	
24	**(C=C=C)**	1	192.14		**67**	**(aC=[N+]-[O])aromatic**	4	24.01	
25	**N#C-[C-]-C#N**	1	225.97		**68**	**Carboaliphatic 3**	20	117.17	
26	**O-O-**	2	175.72		**69**	**Carboaliphatic 4**	12	162.78	

27	**(-O-CH2-O-)cyc**	3	-7.5		**70**	**Carboaliphatic 5**	48	50.36	
28	**(-O-CHn-O-)cyc n=0,1**	3	-5.17		**71**	**Carboaliphatic 6**	60	26.82	
29	**(O-CO-O-)cyc**	2	-54.95		**72**	**Carboaliphatic 7**	4	37.65	
30	**(O-CO-C-)cyc**	2	-10.87		**73**	**Carboaliphatic 8**	6	78.13	
31	**(CO-O-CO-)cyc**	2	-49.11		**74**	**Carboaliphatic 10**	3	64.47	

32	**(C-CO-C-)cyc**	1	105.01		**75**	**Carboaliphatic 11**	2	109.76	
33	**(-CO-CO-)**	1	-137.29		**76**	**Carboaliphatic 12**	3	138.27	
34	**(-C=C-O-)**	2	22.98		**77**	**Carboaliphatic 14**	3	78.25	
35	**(-C=C-O-C=C-)**	1	-83.64		**78**	**Carboaliphatic 18**	1	-249.97	
36	**N-N ALIPHATC**	2	129.79		**79**	**Carboaliphatic 17**	1	40.54	

37	**(N-N)cycl**	3	81.68		**80**	**Hetero ring 3**	4	137.26
38	**(N-N-N)cycl**	3	40.87		**81**	**Hetero ring 4**	6	125.68 
39	**(C=N-N-C=N**	1	137.44		**82**	**Hetero ring 5**	68	36.68 
40	**(N=N-N-C=N)**	6	157.26		**83**	**Hetero ring 6**	22	58.81 
41	**(N=N-N-N=C)**	1	162.88		**84**	**Hetero ring 7**	2	33.95 

42	**(N=C-C=N)**	1	132.56		**85**	**Hetero ring 8**	2	78.39	
43	**(C=N-N)**	4	55.6		**86**	**Hetero ring 15**	1	154.5	

Appendix E. Prediction results of standard enthalpies of formation in gaseous stat using DFT method.

- ***No***: number of the compounds.
- ***Name***: name of the compounds.
- ***Formula***: The chemical formula of the compound.
- ***EXP***: Experimental values.
- ***CAS***: The CAS number of the compounds, (Chemical Abstracts Service).
- ***GAUSSIAN***: Calculated formation enthalpy using DFT (ab-initio reference state).
- ***CAL-DFT***: Calculated formation enthalpy using DFT (kJ/mol).
- ***AAD-DFT***: Mean absolute error for the DFT method.
- ***CAL-N-M***: Calculated formation enthalpy using the new group contribution method (kJ/mol).
- ***AAD-NM***: Mean absolute error for the new group contribution method (kJ/mol).

Table S7. Prediction results of standard enthalpies of formation in gaseous stat using DFT method.

N0	***Names***	***Formula***	***CAS N°***	***kJ/mol***	***UA***	***kJ/mol***			
				EXP	***GAUSSIAN***	***CAL-DFT***	***AAD-DFT***	***CAL-N-M***	***AAD-NM***
1	Cyclopropane	C3H6	75-19-4	53,3	-117,81	73,11	19,81	47,69	5,61
2	Cyclobutene	C4H6	822-35-5	157	-155,89	157,44	0,44	175,35	18,35
3	Methylenecyclopropane	C4H6	6142-73-0	201	-155,88	182,55	18,45	126,62	74,38
4	Cyclopropylacetylene	C5H6	6746-94-7	292	-193,95	303,64	11,64	283,6	8,4
5	Bicyclo[2,1,0]pentane	C5H8	185-94-4	158	-195,17	156,57	1,43	176,41	18,41
6	1,1-Dimethylcyclopropane	C5H10	1630-94-0	-8,2	-196,4	-9,75	1,55	-5,81	2,39
7	1,3-Cyclopentadiene	C5H6	542-92-7	139	-194,01	135,91	3,09	144,98	5,98
8	Cyclopropane,ethenyl-	C5H8	693-86-7	127	-195,18	122,78	4,22	128,16	1,16
9	Methylenecyclobutane	C5H8	1120-56-5	121,5	-195,19	115,54	5,96	149,07	27,57
10	Bicyclo[3,1,0]hexane	C6H10	285-58-5	39	-234,49	55,96	16,96	40,83	1,83
11	1,1'-Bicyclopropyl	C6H10	5685-46-1	130	-234,46	135,86	5,86	134,96	4,96
12	Cyclopentane, methylene-	C6H10	1528-30-9	10,2	-234,5	13,77	3,57	13,49	3,29
13	Bicyclo[2,2,0]hexane	C6H10	186-04-9	125	-234,46	127,27	2,27	198,86	73,86
14	4-Methylcyclopentene	C6H10	1759-81-5	15	-234,5	12,13	2,87	13,46	1,54
15	Cyclohexane, methyl-	C7H14	108-87-2	-154,8	-275	-136,22	18,58	-138,45	16,35
16	Cyclohexane, ethyl-	C8H16	1678-91-7	-172,6	-314,29	-161,88	10,72	-172,12	0,48
17	Cyclohexane, propyl-	C9H18	1678-92-8	-192,4	-353,58	-171,89	20,51	-192,96	0,56
18	Bicyclo[3,3,2]decane	C10H18	283-50-1	-106	-391,65	-63,62	42,38	-144,04	38,04
19	Benzobicyclo[2,2,0]hexa-2,5-diene	C10H8	20847-82-9	399	-385,63	438,76	39,76	425,75	26,75
20	Azulene	C10H8	275-51-4	308	-385,7	269,24	19,86	363,88	55,88
21	Bicyclo[6,2,0]decapentaene	C10H8	20455-01-0	514,2	-385,61	486,74	27,46	516,78	2,58
22	Bullvalene	C10H10	1005-51-2	334,1	-386,83	364,71	30,61	263,37	70,73
23	cis-Decahydronaphthalene	C10H18	493-01-6	-169,2	-391,68	-142,86	26,34	-165,7	3,5
24	1,2,6,7-Cyclodecatetraene	C10H12	3451-55-6	356,1	-387,99	355,86	0,24	356,11	0,01
25	3,4-Dimethylenebicyclo[4,2,0]octa-1,5-diene	C10H10	136846-72-5	359	-386,83	353,65	5,35	354,02	4,98
26	1,2,3,4-Tetrahydronaphthalene	C10H12	119-64-2	30	-388,12	21,62	8,38	9,54	20,46
27	Benzene, (methylenecyclopropyl)-	C10H10	29817-09-2	292	-386,86	282,76	9,24	204,96	87,04
28	Tricyclo[6,2,0,03,6]deca-1(8),2,6-triene	C10H10	1610-51-1	310	-386,85	292,91	17,09	303,56	6,44
29	Cyclohexane, pentyl-	C11H22	4292-92-6	-233,8	-432,14	-194,88	38,92	-234,64	0,84
30	Heptylcyclohexane	C13H26	5617-41-4	*-275*	-510,73	-261,97	13,03	-276,32	1,32