SUBLIMATION ENTHALPIES OF ORGANIC COMPOUNDS: A VERY LARGE DATABASE WITH A MATCH TO CRYSTAL STRUCTURE DETERMINATIONS AND A COMPARISON WITH LATTICE ENERGIES

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Correction-RT: Vibrational energy corrections of sublimation enthalpies for comparison with lattice energies: invalid approximations

The lattice energy (LE, kJ mol^{-1}) for a one-component crystal is the difference in calculated internal energy between one mole of constituent molecules at infinite separation and one mole of the same constituents in the crystal. If infinite separation in the gas phase with zero interaction energy is taken as a reference, LE is by definition stabilizing and coincides with the thermodynamic internal intermolecular potential energy, U(interm,cry) = LE. Please note carefully that stabilizing/destabilizing refer to energies being < 0 or > 0, respectively, while attractive/repulsive refer to forces acting to decrease or increase separation, respectively.[ag]

Thermodynamic internal energy also has translational and rotational kinetic terms and vibrational terms. For the gas and liquid phases the complete expressions are:

U(tot,gas) = U(interm, gas) + E(kin, trasl) + E(kin, rot) + E(vib, intram)
U(tot,liq) = U(interm, liq) + E(kin, trasl) + E(kin, rot) + E(vib, intram)

where E(vib,intram) denotes the intramolecular vibrational energy. In the crystal full translational and full rotational energies are suppressed because there is no net motion of the center of mass and no net overall molecular rotation; these terms are replaced by potential end kinetic terms for translational and rotational librations (t-lib and r-lib):

U(tot,cry) = U(interm,cry)+E(t-lib,kin)+E(t-lib,pot)+E(r-lib,kin)+E(r-lib.pot)+E(vib,intram)

Let us first assume that E(vib,intram) is the same in all aggregation states (a far-fetched assumption except for very tightly bound molecules, benzene and little else) and can therefore be

neglected when taking energy differences. U(interm,gas) is assumed as zero for the very dilute (low-pressure) vapors of a solid at room temperature (semi-ideal gas assumption). In the harmonic equipartition regime each energy term is worth 3/2RT, therefore one gets:

U(tot,gas) = 3RT
U(tot,liq) = U(interm,liq) + 3RT
U(tot,cry) = U(interm,cry) + 6RT

Recalling now that H = U + PV and writing the phase transition functions one gets the following approximate expressions at constant pressure:

vaporization enthalpy:
$\Delta H(gas\text{-}liq) = \Delta U(gas\text{-}liq) + P\Delta V = \Delta U(gas\text{-}liq) + PV(gas) = \Delta U(gas\text{-}liq) + RT = -U(liq) + RT$
where the volume of the liquid is negligible against the volume of the (ideal) gas;
melting enthalpy:
$\Delta H(liq\text{-}cry) = \Delta U(liq\text{-}cry) + P\Delta V = \Delta U(liq\text{-}cry) = U(liq) - U(cry) - 3RT$
where the volume change on melting is negligible;
sublimation enthalpy
$\Delta H(gas\text{-}cry) = \Delta U(gas\text{-}cry) + P\Delta V = \Delta U(gas\text{-}cry) + RT = 3RT - U(cry) - 6RT + RT = -U(cry) - 2RT$
or SE = -LE - 2RT

Another way of seeing the matter is to assign a constant heat capacity of 3R to the gas and of 6R to the solid, and to perform the standard thermodynamic integration:

$\Delta Us(T) = \Delta Us(0) + \int_{(0\text{-}T)} \Delta Cv dT = \Delta Us(0) - 3R \int_{(0\text{-}T)} dT = \Delta Us(0) - 3RT$
$\Delta Hs = \Delta Us + \Delta(PV) = \Delta Us + PV = \Delta Us + RT = \Delta Us(0) - 2RT$

whereby the calculated LE is seen as the sublimation internal energy at 0 K. Here the assumption of constant Cv goes against one of the basic laws of thermodynamics, namely the convergence to zero of solid heat capacities at low temperature.

Table S1. 1655 reported sublimation enthalpies. First line: compound name; second line: brute formula, SE: assessed sublimation enthalpy, SEmin, max: range of experimental variation when not zero; T, temperature of the measurement, when zero, assumed at room T; Nmeas, number of accepted experimental measurements (0 = 1). Attached to each entry is the refcode for the 737 corresponding crystal structure determinations in the Cambridge Structural Database. Each refcode may correspond to more than one crystal structure determination for the same compound.

		SE	SEmin	SEmax	T	Nmeas	CSD refcode
1	cyanogen bromide						
C 1 Br 1 N 1		46.0	45.0	47.0	300.0	3	
2	carbon tetrabromide						CTBROM
C 1 Br 4		54.4	49.4	54.4	300.0	2	
3	cyanogen chloride						
C 1 Cl 1 N 1		36.0	0.0	0.0	230.0	1	
4	diFluorotrichloromethyl phosphine						
C 1 Cl 3 F 2 P 1		36.8	0.0	0.0	274.0	1	
5	carbon tetrachloride						CARBTC
C 1 Cl 4		41.0	38.0	43.0	220.0	3	
6	cyanogen Fluoride						
C 1 F 1 N 1		29.0	0.0	0.0	170.0	2	
7	carbonyl Fluoride						
C 1 F 2 O 1		23.0	0.0	0.0	145.0	1	
8	carbon tetrafluoride						TFMETH
C 1 F 4		16.0	14.0	17.0	80.0	5	
9	pentaFluoromethyl amine						
C 1 F 5 N 1		19.0	0.0	0.0	135.0	1	
10	cyanogen iodide						
C 1 I 1 N 1		59.0	58.0	60.0	350.0	4	
11	tetranitromethane						
C 1 N 4 O 8		47.0	0.0	0.0	270.0	1	
12	carbon monoxide						
C 1 O 1		8.1	8.0	8.2	61.5	2	
13	carbon dioxide						SACBAA
C 1 O 2		26.1	25.2	27.2	190.0	5	
14	triFluoromethane						
C 1 H 1 F 3		26.0	0.0	0.0	100.0	1	
15	iodoform						IODOFO
C 1 H 1 I 3		70.0	0.0	0.0	320.0	1	
16	hydrogen cyanide						
C 1 H 1 N 1		36.0	35.6	37.6	240.0	2	
17	trinitromethane						HEVRUV
C 1 H 1 N 3 O 6		48.0	47.0	55.0	300.0	2	
18	cyanamide						CYANAM
C 1 H 2 N 2		75.0	0.0	0.0	300.0	2	
19	tetrazole						TETZOL
C 1 H 2 N 4		88.0	88.0	98.0	350.0	3	
20	formic acid						FORMAC
C 1 H 2 O 2		61.0	60.0	62.0	260.0	4	
21	methyl chloride						CLMETH
C 1 H 3 Cl 1		32.0	0.0	0.0	150.0	1	
22	methyl iodide						
C 1 H 3 I 1		40.0	0.0	0.0	190.0	1	
23	formamide						FORMAM
C 1 H 3 N 1 O 1		72.0	0.0	0.0	300.0	3	
24	5-aminotetrazole						
C 1 H 3 N 5		113.0	0.0	0.0	400.0	1	
25	methane						
C 1 H 4		10.0	9.2	10.0	80.0	5	
26	urea						UREAXX
C 1 H 4 N 2 O 1		97.0	95.0	99.0	330.0	6	
27	thiourea						THIOUR
C 1 H 4 N 2 S 1		108.0	104.0	112.0	330.0	7	
28	nitroguanidine						NTRGUA
C 1 H 4 N 4 O 2		143.0	0.0	0.0	300.0	1	
29	N-methyl hydroxylamine						
C 1 H 5 N 1 O 1		57.0	0.0	0.0	290.0	1	
30	1-methyl-1-nitrosohydrazine						
C 1 H 5 N 3 O 1		80.0	0.0	0.0	300.0	1	
31	thiosemicarbazide						TSCRBZ
C 1 H 5 N 3 S 1		126.0	0.0	0.0	300.0	1	
32	thiocarbohydrazide						
C 1 H 6 N 4 S 1		152.0	0.0	0.0	300.0	1	
33	bromopentachloroethane						

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C 2 Br 1 Cl 5                    44.0   0.0   0.0 400.0  1
   34  1,2-dibromotetrachloroethane
C 2 Br 2 Cl 4                    55.0  53.0  57.0 380.0  2
   35  tetrabromoethylene                                    TBRETH
C 2 Br 4                         44.0   0.0   0.0 240.0  1
   36  hexachloroethane                                      HEXCET
C 2 Cl 6                         59.0   0.0   0.0 350.0  2
   37  hexafluoroethane
C 2  F 6                         26.0   0.0   0.0 100.0  1
   38  cyanogen                                              CYNGEN
C 2  N 2                         33.0  33.0  34.0 210.0  4
   39  hexanitroethane                                       QQQBRD
C 2  N 6  O 12                   71.0  71.0  71.0 300.0  3
   40  acetylene                                             ACETYL
C 2  H 2                         24.0  22.0  25.0 160.0  5
   41  triFluoroacetamide                                    TFACAM
C 2  H 2  F 3  N 1  O 1          79.0  78.0  81.0 300.0  2
   42  oxalic acid anhydrous.                                OXALAC
C 2  H 2  O 4                    95.0  91.0  99.0 310.0  7
   43  bromoacetic acid                                      BRMACA
C 2  H 3 Br 1  O 2               84.0   0.0   0.0 300.0  1
   44  chloroacetic acid                                     CLACET
C 2  H 3 Cl 1  O 2               82.0   0.0   0.0 300.0  1
   45  2-Fluoro-2,2-dinitroethanol
C 2  H 3  F 1  N 2  O 5          56.0   0.0   0.0   0.0  1
   46  iodoacetic acid
C 2  H 3  I 1  O 2               87.0   0.0   0.0 300.0  1
   47  oxalic acid,monoamide
C 2  H 3  N 1  O 3              108.0   0.0   0.0 320.0  2
   48  1,2,4-triazole                                        TRAZOL
C 2  H 3  N 3                    82.0  81.0  84.0 300.0  4
   49  1,1,1-trinitroethane                                  FINBIP
C 2  H 3  N 3  O 6               72.0   0.0   0.0 300.0  1
   50  ethylene                                              ETHLEN
C 2  H 4                         17.0  15.0  18.0 100.0  2
   51  1,2-dibromoethane
C 2  H 4 Br 2                    52.0  50.0  55.0 250.0  2
   52  1,2-diiodoethane                                      ZZZFHE
C 2  H 4  I 2                    66.0   0.0   0.0   0.0  1
   53  diformylhydrazine
C 2  H 4  N 2  O 2              101.0   0.0   0.0 390.0  1
   54  oxamide                                               OXAMID
C 2  H 4  N 2  O 2              115.0 113.0 117.0 330.0  3
   55  dithiooxamide                                         SSOXAM
C 2  H 4  N 2  S 2              104.0 104.0 105.0 330.0  3
   56  dicyandiamide                                         CYAMPD
C 2  H 4  N 4                   129.0   0.0   0.0 440.0  1
   57  1-methyltetrazole                                     TELPOP
C 2  H 4  N 4                    87.0   0.0   0.0 300.0  1
   58  5-methyltetrazole                                     FIZZOD
C 2  H 4  N 4                    94.0   0.0   0.0 350.0  1
   59  acetic acid                                           ACETAC
C 2  H 4  O 2                    68.0  67.0  70.0 220.0  2
   60  methyl hydrogen carbonate
C 2  H 4  O 2                    18.2 204.0 237.0 220.0  1
   61  acetamide                                             ACEMID
C 2  H 5  N 1  O 1               79.0  77.0  80.0 300.0  7
   62  methyl carbamate                                      FEPGEM
C 2  H 5  N 1  O 2               75.0   0.0   0.0 300.0  1
   63  thioacetamide                                         THACEM
C 2  H 5  N 1  S 1               83.0   0.0   0.0 300.0  2
   64  1-methyl-5-aminotetrazole
C 2  H 5  N 5                   116.0   0.0   0.0 400.0  1
   65  2-methyl-5-aminotetrazole                             AMMTAZ
C 2  H 5  N 5                    91.0   0.0   0.0 340.0  1
   66  ethane                                                ETHANE
C 2  H 6                         22.0  21.0  23.0  90.0  2
   67  chlorodimethyl phosphine
C 2  H 6 Cl 1  P 1               55.5   0.0   0.0 253.0  1
   68  N-methylurea                                          MEUREA
C 2  H 6  N 2  O 1               97.0  94.0  99.0 320.0  8
   69  N-methyl-N-nitromethanamine
C 2  H 6  N 2  O 2               70.0   0.0   0.0 320.0  1
   70  N-methylthiourea                                      BEXQOK
C 2  H 6  N 2  S 1              112.0 111.0 113.0 300.0  2
   71  dimethyl sulfone                                      DMSULO
C 2  H 6  O 2  S 1               77.0   0.0   0.0   0.0  1
   72  ethylenediamine                                       ETDIAM
C 2  H 8  N 2                    66.0   0.0   0.0 260.0  1
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   73  tricyanophosphine
C 3  N 3  P 1                  77.0  75.0  78.0 300.0  2
   74  cyanoacetylene                                        CAACTY
C 3  H 1  N 1                  42.0   0.0   0.0 260.0  1
   75  malononitrile                                         MALONT
C 3  H 2  N 2                  79.0   0.0   0.0 300.0  2
   76  imidazolidine-2,4,5-trione
C 3  H 2  N 2  O 3            118.0 115.0  19.0 298.0  2
   77  1,3-dithiol-2-one
C 3  H 2  O 1  S 2             74.0   0.0   0.0 300.0  1
   78  1,3-dithiole-2-thione
C 3  H 2  O 1  S 3             75.0   0.0   0.0 300.0  1
   79  1,3,5-triazine                                        TRIZIN
C 3  H 3  N 3                  57.0  54.0  58.0 300.0  3
   80  6-azauracil                                           AZURAC
C 3  H 3  N 3  O 2            141.0   0.0   0.0   0.0  1
   81  cyanuric acid                                         CYURAC
C 3  H 3  N 3  O 3            133.0   0.0   0.0 300.0  1
   82  1,1,1,2,2-pentanitropropane
C 3  H 3  N 5  O10             77.0   0.0   0.0 300.0  1
   83  imidazole                                             IMAZOL
C 3  H 4  N 2                  83.0  81.0  85.0 300.0  4
   84  pyrazole                                              PYRZOL
C 3  H 4  N 2                  73.0  72.0  74.0 300.0  4
   85  2-cyanoacetamide                                      CYANAC
C 3  H 4  N 2  O 1            100.0   0.0   0.0 340.0  1
   86  2-methyl-4-nitro-1,2,3-triazole
C 3  H 4  N 4  O 2             75.0   0.0   0.0 300.0  1
   87  1,3-dithiolan-2-one                                   IXANOK
C 3  H 4  O 1  S 2             80.0   0.0   0.0   0.0  1
   88  ethylene carbonate                                    ETHCAR
C 3  H 4  O 3                  77.0  73.0  79.0 300.0  3
   89  malonic acid                                          MALNAC
C 3  H 4  O 4                 109.0 105.0 111.0 310.0  3
   90  1,3-dithiolan-2-thione                                DTOLTO
C 3  H 4  S 3                  82.0   0.0   0.0 300.0  1
   91  acrylamide                                            ARCLAM
C 3  H 5  N 1  O 1             82.0   0.0   0.0 330.0  1
   92  2-azetidinone
C 3  H 5  N 1  O 1             78.0   0.0   0.0 300.0  1
   93  2-mercapto-2-oxazoline
C 3  H 5  N 1  O 1  S 1        105.0   0.0   0.0 319.0  1
   94  2-mercapto-2-thiazoline
C 3  H 5  N 1  S 2             100.0   0.0   0.0 300.0  1
   95  cyclopropane                                          QQQCIS
C 3  H 6                       29.0   0.0   0.0 135.0  1
   96  dimethyl triFluoromethyl phosphinesulfide
C 3  H 6  F 3  P 1  S 1         68.0   0.0   0.0 310.0  1
   97  2-imadazolidinone
C 3  H 6  N 2  O 1             97.0   0.0   0.0 300.0  1
   98  acetylurea                                            QQQGEM
C 3  H 6  N 2  O 2            103.0   0.0   0.0 300.0  1
   99  malonamide                                            MALOAM
C 3  H 6  N 2  O 2            126.0   0.0   0.0   0.0  1
  100  1,5-dimethyltetrazole
C 3  H 6  N 4                  86.0   0.0   0.0 320.0  1
  101  2,4,6-triamino-s-triazine,melamine.                   MELAMI
C 3  H 6  N 6                 122.0   0.0   0.0 450.0  2
  102  hexahydro-1,3,5-trinitro-1,3,5-triazine
C 3  H 6  N 6  O 6            132.5   0.0   0.0 320.0  2
  103  propionic acid                                        PRONAC
C 3  H 6  O 2                  73.5   0.0   0.0 230.0  2
  104  1,3,5-trioxane                                        TROXAN
C 3  H 6  O 3                  56.0   0.0   0.0 300.0  3
  105  1,3,5-trithiane                                       TRITAN
C 3  H 6  S 3                  94.0   0.0   0.0 300.0  2
  106  acetone oxime                                         ACEOXM
C 3  H 7  N 1  O 1             60.0   0.0   0.0 320.0  1
  107  propionamide                                          ZZZKAY
C 3  H 7  N 1  O 1             79.0   0.0   0.0 310.0  2
  108  N-methylacetamide                                     METACM
C 3  H 7  N 1  O 1             71.0   0.0   0.0 300.0  2
  109  ethyl carbamate                                       ECARBM
C 3  H 7  N 1  O 2             75.0  72.0  77.0 300.0  3
  110  propane                                               JAYDUI
C 3  H 8                       29.0   0.0   0.0  90.0  1
  111  N-ethylurea                                           YAQLAE
C 3  H 8  N 2  O 1             96.0  92.0 100.0 350.0  3
  112  1,1-dimethylurea                                      WIFKEB
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C 3  H 8  N 2  O 1              94.0  93.0  95.0 350.0  4
  113  1,3-dimethylurea                                      NIJHUJ
C 3  H 8  N 2  O 1              88.0  87.0  89.0 350.0  3
  114  1,3-dimethylthiourea
C 3  H 8  N 2  S 1             109.0 107.0 111.0 300.0  3
  115  1-ethylthiourea
C 3  H 8  N 2  S 1             119.0   0.0   0.0 300.0  2
  116  ethyl methyl sulfone
C 3  H 8  O 2  S 1              78.0   0.0   0.0   0.0  1
  117  trimethylphospine sulfide
C 3  H 9  P 1  S 1              70.3   0.0   0.0 380.0  1
  118  2,4,5,6-tetrachloropyrmidine
C 4 Cl 4  N 2                   83.0   0.0   0.0 298.0  1
  119  dicyanoacetylene                                      DCYANM
C 4  N 4                        44.0   0.0   0.0 270.0  1
  120  3,5-bis triFluoromethyl-1,2,4-triazole
C 4  H 1  F 6  N 3              75.0   0.0   0.0 300.0  1
  121  1,3-butadiyne
C 4  H 2                        36.0   0.0   0.0 210.0  2
  122  2,6-dichloropyrazine                                  DCPYAZ
C 4  H 2 Cl 2  N 2              70.0   0.0   0.0 298.0  1
  123  2,4-dichloropyrimidine                                BOTYIT
C 4  H 2 Cl 2  N 2              77.0   0.0   0.0 298.0  1
  124  fumaronitrile                                         BISJIW
C 4  H 2  N 2                   71.0  69.0  72.0 280.0  2
  125  4-cyanothiazole
C 4  H 2  N 2  S 1              74.0   0.0   0.0 300.0  1
  126  maleic anhydride                                      MLEICA
C 4  H 2  O 3                   86.0   0.0   0.0 320.0  1
  127  3,4-dihydroxy-3-cyclobutene-1,2-dione,squaric aci
C 4  H 2  O 4                  154.0   0.0   0.0 300.0  2
  128  5-fluorouracil                                        FURACL
C 4  H 3  F 1  N 2  O 2        133.0   0.0   0.0 298.0  2
  129  5-bromouracil                                         BRURAC
C 4  H 3 Br 1  N 2  O 2        149.0 148.0 151.0 300.0  2
  130  2-chloropyrimidine                                    CLPYMD
C 4  H 3 Cl 1  N 2              70.0   0.0   0.0 298.0  1
  131  5-chlorouracil                                        CLURAC
C 4  H 3 Cl 1  N 2  O 2        148.0   0.0   0.0 298.0  1
  132  6-chlorouracil
C 4  H 3 Cl 1  N 2  O 2        135.0   0.0   0.0 298.0  1
  133  5-iodouracil                                          IURACL
C 4  H 3  I 1  N 2  O 2        127.0   0.0   0.0 390.0  1
  134  2-nitrofuran
C 4  H 3  N 1  O 3              75.0   0.0   0.0   0.0  1
  135  5-bromocytosine                                       BRCYTS
C 4  H 4 Br 1  N 3  O 1        148.0   0.0   0.0 435.0  1
  136  3,3,4,4-tetrachlorotetrahydrothiophene-1,1-dioxid
C 4  H 4 Cl 4  O 2  S 1         89.0   0.0   0.0 325.0  2
  137  N-triFluoroacetylaminoacetic acid
C 4  H 4  F 3  N 1  O 3         99.0   0.0   0.0 290.0  1
  138  5-iodocytosine                                        ZILBIF
C 4  H 4  I 1  N 3  O 1        144.0   0.0   0.0 440.0  1
  139  pyrazine                                              PYRAZI
C 4  H 4  N 2                   56.0   0.0   0.0 300.0  2
  140  succinonitrile                                        QOPBED
C 4  H 4  N 2                   70.0   0.0   0.0 300.0  1
  141  2-thiouracil                                          TURCIL
C 4  H 4  N 2  O 1  S 1        129.0   0.0   0.0   0.0  1
  142  4-thiouracil
C 4  H 4  N 2  O 1  S 1        126.0   0.0   0.0   0.0  1
  143  pyrazine 1,4-dioxide                                  AHEMAB
C 4  H 4  N 2  O 2             117.0   0.0   0.0 300.0  1
  144  uracil                                                URACIL
C 4  H 4  N 2  O 2             131.0   0.0   0.0 298.0  7
  145  thiobarbituric acid                                   THBARB
C 4  H 4  N 2  O 2  S 1        110.0   0.0   0.0 430.0  1
  146  barbituric acid                                       BARBAC
C 4  H 4  N 2  O 3             118.0 111.0 123.0 420.0  3
  147  2,4-dithiouracil                                      DTURAC
C 4  H 4  N 2  S 2             120.0   0.0   0.0 420.0  1
  148  8-azaadenine
C 4  H 4  N 6                  128.0   0.0   0.0 440.0  1
  149  bis-2,2,2-trinitroethyl -N-NOamine
C 4  H 4  N 8  O 13             98.0   0.0   0.0 340.0  1
  150  bis-2,2,2-trinitroethyl -N-nitroamine
C 4  H 4  N 8  O 14            118.0   0.0   0.0 350.0  1
  151  cyclobutane-1,2-dione                                 NIKVUZ
C 4  H 4  O 2                   69.0   0.0   0.0 300.0  1
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  152  cyclobutane-1,3-dione
C 4  H 4  O 2                  74.0   0.0   0.0 300.0  1
  153  succinic  anhydride                                  SUCANH
C 4  H 4  O 3                  82.0   0.0   0.0 300.0  3
  154  cis-butenedioic acid maleic acid.                    MALIAC
C 4  H 4  O 4                 108.0 105.0 110.0 360.0  3
  155  trans-butenedioic  acid                             FUMAAC
C 4  H 4  O 4                 135.0   0.0   0.0 370.0  2
  156  diglycolic anhydride                                DLGYAH
C 4  H 4  O 4                  84.0   0.0   0.0 300.0  1
  157  thiophene
C 4  H 4  S 1                  48.0   0.0   0.0 210.0  2
  158  succinimide                                         SUCCIN
C 4  H 5  N 1  O 2             86.0  83.0  88.0 310.0  3
  159  cytosine                                            CYTSIN
C 4  H 5  N 3  O 1            168.0   0.0   0.0 365.0  1
  160  5-aminouracil
C 4  H 5  N 3  O 2            146.0   0.0   0.0   0.0  1
  161  6-azathymine                                        AZTHYM
C 4  H 5  N 3  O 2            113.0   0.0   0.0 380.0  1
  162  2-thiocytosine                                      THCYTO
C 4  H 5  N 3  S 1            158.0   0.0   0.0 433.0  1
  163  2-butyne
C 4  H 6                       37.4   0.0   0.0 220.0  1
  164  2-methylimidazole                                   FULPIM
C 4  H 6  N 2                  88.2   0.0   0.0 309.0  1
  165  3-amino-5-methylisoxazole
C 4  H 6  N 2  O 1             82.0   0.0   0.0   0.0  1
  166  2,5-piperazinedione                                 DIKPIP
C 4  H 6  N 2  O 2            104.0   0.0   0.0 428.0  1
  167  2,4-diamino-6-hydroxypyrimidine
C 4  H 6  N 4  O 1            148.0   0.0   0.0 450.0  1
  168  1,1,3,3-tetranitrobutane
C 4  H 6  N 4  O 8             88.0   0.0   0.0 298.0  1
  169  2,2,3,3-tetranitrobutane                            ZILNOX
C 4  H 6  N 4  O 8             78.0   0.0   0.0 298.0  1
  170  1,1,1,4-tetranitrobutane
C 4  H 6  N 4  O 8            100.0   0.0   0.0 298.0  1
  171  1,1,1,3-tetranitro-2-methylpropane
C 4  H 6  N 4  O 8             91.0   0.0   0.0 298.0  1
  172  dimethyl oxalate                                    DMEOXA
C 4  H 6  O 4                  75.6   0.0   0.0 283.0  1
  173  succinic acid                                       SUCACB
C 4  H 6  O 4                 122.0 120.0 123.0 300.0  4
  174  methylmalonic acid                                  MEMALA
C 4  H 6  O 4                 115.0 113.0 117.0 298.0  2
  175  1,3-dithian-2-thione                                PUVVUZ
C 4  H 6  S 3                  89.0  88.0  91.0 310.0  2
  176  cis  2-butenoic acid  amide
C 4  H 7  N 1  O 1             68.0   0.0   0.0 370.0  1
  177  trans 2-butenoic acid amide                         CROTAM
C 4  H 7  N 1  O 1             80.0   0.0   0.0 370.0  1
  178  diacetamide                                         DACETA
C 4  H 7  N 1  O 2             73.0   0.0   0.0 298.0  1
  179  cyclobutane                                         ZZZWEO
C 4  H 8                       36.0   0.0   0.0 145.0  1
  180  bis 2-chloroethylsulfide
C 4  H 8 Cl 2  S 1             83.0  81.0  85.0 280.0  2
  181  triChloroEthylphosphonic acid diMethylester
C 4  H 8 Cl 3  O 4  P 1       107.0   0.0   0.0 308.0  1
  182  tetrahydro-2-pyrimidone                             APYFEB
C 4  H 8  N 2  O 1            113.0   0.0   0.0 298.0  1
  183  1,2-diacetylhydrazine                               DIACHZ
C 4  H 8  N 2  O 2            103.0   0.0   0.0 352.0  1
  184  dimethylglyoxime
C 4  H 8  N 2  O 2             96.8   0.0   0.0 341.0  2
  185  N-acetylglycine amide                               JAHZEX
C 4  H 8  N 2  O 2            130.0 124.0 140.0 320.0  4
  186  1,4-diNOpiperazine                                  CUVJUY
C 4  H 8  N 4  O 2            101.0   0.0   0.0 343.0  1
  187  1,4-dinitropiperazine
C 4  H 8  N 4  O 4            111.0   0.0   0.0 343.0  1
  188  butanoic acid
C 4  H 8  O 2                  76.0   0.0   0.0 248.0  1
  189  1,4-dioxane                                         CUKCIU
C 4  H 8  O 2                  35.6   0.0   0.0 255.0  1
  190  1,3-dithiane sulfone
C 4  H 8  O 2  S 2            103.0 102.0 104.0 320.0  2
  191  1,4-dithiane sulfone
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C 4  H 8  O 2  S 2              99.3  98.7  99.9 322.5  2
  192  1,3-oxathiane sulfone
C 4  H 8  O 3  S 1              91.9   0.0   0.0 307.0  2
  193  1,4-oxathiane sulfone
C 4  H 8  O 3  S 1              91.8   0.0   0.0 306.0  2
  194  1,3,5,7-tetroxane                                  TOXOCN
C 4  H 8  O 4                   80.0   0.0   0.0 298.0  2
  195  1,3-dithiane
C 4  H 8  S 2                   72.0  70.0  73.0 300.0  2
  196  1,4-dithiane                                       DITHAN
C 4  H 8  S 2                   71.0  69.0  72.0 298.0  2
  197  2-iodo-2-methylpropane
C 4  H 9  I 1                   50.0   0.0   0.0 213.0  1
  198  butyramide                                         ZZZKDQ
C 4  H 9  N 1  O 1              85.0  82.0  87.0 310.7  7
  199  2-methylpropanamide                                IBURAM
C 4  H 9  N 1  O 1              86.1   0.0   0.0 294.0  1
  200  2-methyl-2-nitro-1-propanol
C 4  H 9  N 1  O 3              75.0  73.0  78.0 300.0  2
  201  2-methyl-2-nitro-1,3-propanediol                   MENPDL
C 4  H 9  N 1  O 4             100.0  98.0 102.0 340.0  2
  202  2-hydroxymethyl-2-nitro-1,3-propanediol
C 4  H 9  N 1  O 5             107.0   0.0   0.0 340.0  1
  203  1-2-ethenyloxy ethyl-1-nitrosohydrazine
C 4  H 9  N 3  O 2             112.0   0.0   0.0 298.0  1
  204  butane                                             DUCKOB
C 4  H10                        36.0   0.0   0.0 107.0  1
  205  piperazine                                         ITIZOA
C 4  H10  N 2                   72.1   0.0   0.0 300.0  2
  206  N-propylurea                                       KIKREC
C 4  H10  N 2  O 1             101.0   0.0   0.0 298.0  1
  207  N-isopropylurea
C 4  H10  N 2  O 1              98.0  97.0 100.0 350.0  3
  208  2-methyl-2-propanol  tBuOH                         VATSAK
C 4  H10  O 1                   51.3   0.0   0.0 275.0  1
  209  diethyl sulfone
C 4  H10  O 2  S 1              86.0   0.0   0.0   0.0  1
  210  diethanolamine                                     JAKKIP
C 4  H11  N 1  O 2             106.0   0.0   0.0 298.0  1
  211  2-amino-2-methyl-1,3-propanediol
C 4  H11  N 1  O 2             112.0 110.0 115.0 340.0  2
  212  bis dimethylphosphino amine
C 4  H13  N 1  P 2              62.0   0.0   0.0 305.0  1
  213  hexachlorocyclopentadiene
C 5 Cl 6                        74.0   0.0   0.0 283.0  1
  214  perFluorocyclopentane
C 5  F10                        32.1   0.0   0.0 266.0  1
  215  perFluoropentane
C 5  F12                        44.0   0.0   0.0 145.0  1
  216  tetracyanomethane                                  TCYMET
C 5  N 4                        61.0   0.0   0.0 298.0  1
  217  2,3,5-trichloropyridine                            GETVEH
C 5  H 2 Cl 3  N 1              74.0   0.0   0.0 298.0  1
  218  3,5-bis  triFluoromethyl pyrazole
C 5  H 2  F 6  N 2              69.0   0.0   0.0 266.0  1
  219  2,4,6-trinitropyridine
C 5  H 2  N 4  O 6             101.0   0.0   0.0 346.0  1
  220  2,4,6-trinitropyridine
C 5  H 2  N 4  O 7             106.0   0.0   0.0 390.0  1
  221  2,5-dibromopyridine                                VOQYUW
C 5  H 3 Br 2  N 1              82.0   0.0   0.0 298.0  1
  222  2,6-dibromopyridine
C 5  H 3 Br 2  N 1              86.0   0.0   0.0 298.0  1
  223  2,3-dichloropyridine                               AYONEI
C 5  H 3 Cl 2  N 1              74.0   0.0   0.0 298.0  1
  224  2,5-dichloropyridine
C 5  H 3 Cl 2  N 1              67.0   0.0   0.0 298.0  1
  225  2,6-dichloropyridine
C 5  H 3 Cl 2  N 1              72.0   0.0   0.0 298.0  1
  226  3,5-dichloropyridine
C 5  H 3 Cl 2  N 1              67.0   0.0   0.0 298.0  1
  227  5-  triFmethyl uracil                              UGUMUE
C 5  H 3  F 3  N 2  O 2        109.0 108.0 110.0 340.0  2
  228  5-nitro-2-furancarboxaldehyde
C 5  H 3  N 1  O 3              75.0   0.0   0.0   0.0  1
  229  1,2,4-triazolo 1,5-apyrimidine                     HAMGOT
C 5  H 4  N 4                   87.0   0.0   0.0 419.0  1
  230  hypoxanthine                                       GEBTUC
C 5  H 4  N 4  O 1             158.0   0.0   0.0 448.0  1
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  231  6-mercaptopurine                                                RAKSIG
C 5  H 4  N 4  S 1            149.0   0.0   0.0 435.0  1
  232  2-thiophene carboxylic acid                                     TPENAC
C 5  H 4  O 2  S 1             97.0   0.0   0.0 319.0  2
  233  2-furancarboxylic acid                                          FRANAC
C 5  H 4  O 3                  88.0   0.0   0.0 298.0  1
  234  3-furancarboxylic acid                                          HIFKUC
C 5  H 4  O 3                  87.1   0.0   0.0 298.0  1
  235  1-methyl-6-chlorouracil
C 5  H 5 Cl 1  N 2  O 2        108.0   0.0   0.0 441.0  1
  236  3-methyl-6-chlorouracil                                         ZUDTID
C 5  H 5 Cl 1  N 2  O 2        104.0   0.0   0.0 469.0  1
  237  1-methyl-5-Fluorouracil
C 5  H 5  F 1  N 2  O 2        125.0   0.0   0.0 498.0  1
  238  3-methyl-5-Fliorouracil                                         LAKJEM
C 5  H 5  F 1  N 2  O 2         79.5   0.0   0.0 476.0  1
  239  3  5 -triluoromethyl-5 3 -methylpyrazole                       TUHNEQ
C 5  H 5  F 3  N 2             78.0   0.0   0.0 298.0  1
  240  2-hydroxypyridine
C 5  H 5  N 1  O 1             87.0   0.0   0.0 298.0  1
  241  3-hydroxypyridine                                               BIRYIK
C 5  H 5  N 1  O 1             88.0   0.0   0.0 298.0  1
  242  4-hydroxypyridine
C 5  H 5  N 1  O 1            115.0 104.0 119.0 298.0  2
  243  pyridine N-oxide                                                PYRDNO
C 5  H 5  N 1  O 1             79.0   0.0   0.0 298.0  1
  244  2-hydroxypyridine N-oxide
C 5  H 5  N 1  O 2             89.0   0.0   0.0 298.0  1
  245  3-hydroxypyridine N-oxide                                       YELRUD
C 5  H 5  N 1  O 2            122.0   0.0   0.0 298.0  1
  246  pyrrole-2-carboxylic acid                                       XAGWIM
C 5  H 5  N 1  O 2            100.0   0.0   0.0 310.0  2
  247  N-methylmaleimide
C 5  H 5  N 1  O 2             73.0   0.0   0.0   0.0  1
  248  2,3-dihydroxypyridine
C 5  H 5  N 1  O 2            109.0   0.0   0.0   0.0  1
  249  pyrazine carboxamide                                            PYRZIN
C 5  H 5  N 3  O 1             87.9   0.0   0.0 368.0  1
  250  adenine                                                         KOBFUD
C 5  H 5  N 5                 118.0 109.0 127.0 440.5  5
  251  guanine                                                         KEMDOW
C 5  H 5  N 5  O 1            186.0   0.0   0.0 298.0  1
  252  1,1,1,3,5,5,5-heptanitropentane                                 CUVXOG
C 5  H 5  N 7  O 14           112.0   0.0   0.0 298.0  1
  253  dimethylmalononitrile
C 5  H 6  N 2                  62.0   0.0   0.0 298.0  1
  254  2-aminopyridine                                                 AMPYRD
C 5  H 6  N 2                  78.0   0.0   0.0 298.0  2
  255  3-aminopyridine                                                 AMIPYR
C 5  H 6  N 2                  83.0  81.0 840.0 298.0  2
  256  4-aminopyridine                                                 AMPYRE
C 5  H 6  N 2                  88.0   0.0   0.0 298.0  2
  257  2-thiophenecarboxylic acid hydrazide
C 5  H 6  N 2  O 1  S 1        113.0   0.0   0.0 298.0  1
  258  1-methyluracil                                                  METURA
C 5  H 6  N 2  O 2            119.0 113.0 122.0 410.0  2
  259  3-methyluracil                                                  WUDVAS
C 5  H 6  N 2  O 2            119.0   0.0   0.0 382.0  1
  260  5-methyluracil thymine.                                         THYMIN
C 5  H 6  N 2  O 2            133.0 131.0 134.0 298.0  2
  261  6-methyluracil                                                  CEWVOP
C 5  H 6  N 2  O 2            131.0   0.0   0.0 298.0  1
  262  2-furancarboxylic acid  hydrazide
C 5  H 6  N 2  O 2             99.0  98.1  99.0 307.5  2
  263  glutaric anhydride                                              LIJFUG
C 5  H 6  O 3                  86.0   0.0   0.0 298.0  1
  264  glutarimide                                                     GLUTIM
C 5  H 7  N 1  O 2             94.0   0.0   0.0 298.0  1
  265  N-methylsuccinimide                                             KOMYEQ
C 5  H 7  N 1  O 2             80.0   0.0   0.0 298.0  1
  266  dl -5-oxoproline
C 5  H 7  N 1  O 3            133.0   0.0   0.0 405.0  1
  267  1-methylcytosine                                                METCYT
C 5  H 7  N 3  O 1            151.0   0.0   0.0 500.0  1
  268  3-methylcytosine
C 5  H 7  N 3  O 1            151.0   0.0   0.0 500.0  1
  269  3,5-dimethyl-4-NOpyrazole                                       LETNAZ
C 5  H 7  N 3  O 1            103.0   0.0   0.0 298.0  1
  270  1-methyl-N-hydroxycytosine
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C 5  H 7  N 3  O 2            127.0   0.0   0.0   0.0  1
  271  pentarythritol tetraBRide
C 5  H 8 Br 4                  84.0   0.0   0.0 400.0  1
  272  5-amino-3,4-dimethylisoxazole
C 5  H 8  N 1  O 2             88.0   0.0   0.0   0.0  1
  273  2-ethylimidazole
C 5  H 8  N 2                  90.0   0.0   0.0 298.0  1
  274  2,3-diazabicyclo 2.2.1hept-2-ene
C 5  H 8  N 2                  52.0  44.0  55.0 298.0  2
  275  3,5-dimethylpyrazole                                DASXEA
C 5  H 8  N 2                  83.0   0.0   0.0 298.0  2
  276  1,3-dimethyluracil
C 5  H 8  N 2  O 2             97.0   0.0   0.0   0.0  1
  277  pentaerythritol tetranitrate                        PERYTN
C 5  H 8  N 4  O 12           155.3 152.0 156.0 320.0  3
  278  tetrahydro-4H-thiopyran-4-one                       OWEKEH
C 5  H 8  O 1  S 1             73.0   0.0   0.0 298.0  1
  279  methyl methacrylate
C 5  H 8  O 2                  60.7   0.0   0.0 205.0  1
  280  2,5-dihydro-2-methyl-thiophene-1,1-dioxide
C 5  H 8  O 2  S 1             61.0   0.0   0.0   0.0  1
  281  2,5-dihydro-3-methyl-thiophene-1,1-dioxide
C 5  H 8  O 2  S 1             64.0   0.0   0.0   0.0  1
  282  dimethyl malonate
C 5  H 8  O 4                 117.0   0.0   0.0 298.0  1
  283  glutaric acid                                       GLURAC
C 5  H 8  O 4                 130.2 120.6 134.0 320.0  3
  284  ethylmalonic acid                                   AMALOQ
C 5  H 8  O 4                 110.0 106.0 113.0 298.0  2
  285  cis 2-pentenoic acid amide
C 5  H 9  N 1  O 1            107.0   0.0   0.0 320.0  1
  286  2-ethyl-2-oxazoline
C 5  H 9  N 1  O 1             74.5   0.0   0.0 303.0  1
  287  cyclopentane                                        ZZZVYE
C 5  H10                       43.0   0.0   0.0 122.0  1
  288  trimethylacetic pivalic acid
C 5  H10  O 2                  62.0   0.0   0.0 298.0  1
  289  1,3,5,7,9-pentoxecane                               PTOXEC
C 5  H10  O 5                  88.0   0.0   0.0 298.0  1
  290  pentanamide                                         ZZZKJQ
C 5  H11  N 1  O 1             89.0   0.0   0.0 350.0  2
  291  2,2-dimethylpropanamide                             DIXTAF
C 5  H11  N 1  O 1             88.0   0.0   0.0 298.0  2
  292  butyl carbamate
C 5  H11  N 1  O 2             94.1   0.0   0.0 304.0  1
  293  pentane                                             PENTAN
C 5  H12                       42.0   0.0   0.0 143.0  1
  294  2,2-dimethylpropane
C 5  H12                       31.0  28.0  33.0 220.0  2
  295  1,1-diethylurea                                     XEWVEA
C 5  H12  N 2  O 1             96.0   0.0   0.0 310.0  2
  296  1,3-diethylurea
C 5  H12  N 2  O 1             95.1  92.0  97.0 330.0  3
  297  N-butylurea                                         YAQLEI
C 5  H12  N 2  O 1            104.0 101.0 106.0 320.0  3
  298  N-isobutylurea
C 5  H12  N 2  O 1            101.0   0.0   0.0 377.0  1
  299  N-sec-butylurea
C 5  H12  N 2  O 1            103.0 102.0 105.0 320.0  3
  300  N-tert-butylurea
C 5  H12  N 2  O 1            100.0  98.0 101.0 320.0  3
  301  1,3-diethylthiourea                                 ZEYBAG
C 5  H12  N 2  S 1            121.0   0.0   0.0 298.0  2
  302  tetramethylthiourea                                 OFIZEK
C 5  H12  N 2  S 1             84.0   0.0   0.0 298.0  4
  303  2,2-dimethyl-1,3-propanediol                        NEPGCL
C 5  H12  O 2                  87.0   0.0   0.0 320.0  2
  304  tert-butyl methylsulfone
C 5  H12  O 2  S 1             82.0   0.0   0.0   0.0  1
  305  2-hydroxymethyl-2-methyl-1,3-propanediol
C 5  H12  O 3                 109.0   0.0   0.0 311.0  1
  306  pentaerythritol                                     PERYTO
C 5  H12  O 4                 150.0 131.0 163.0 330.0  4
  307  xylitol                                             XYLTOL
C 5  H12  O 5                 161.0   0.0   0.0 298.0  1
  308  2,3,5,6-tetrachloro-1,4-benzoquinone                TCBENQ
C 6 Cl 4  O 2                  98.7   0.0   0.0 345.0  1
  309  pentachloronitrobenzene                             PCLNBZ
C 6 Cl 5  N 1  O 2             95.0   0.0   0.0 298.0  1
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  310  hexachlorobenzene                                                HCLBNZ
C 6 Cl 6                        97.0  77.0 105.0 298.0  9
  311  hexaFluorobenzene                                                HFBENZ
C 6  F 6                        49.0   0.0   0.0 260.0  2
  312  perFluorocyclohexane
C 6  F12                        36.0   0.0   0.0 298.0  2
  313  dicyanobutadiyne
C 6  N 2                        35.2  34.4  35.9 315.0  2
  314  tetracyanoethylene                                               TCYETY
C 6  N 4                        82.9  81.4  84.3 326.5  2
  315  benzotrifurazan
C 6  N 6  O 3                   95.8   0.0   0.0 318.0  1
  316  benzotrifuroxan                                                  BZOFOX
C 6  N 6  O 6                  172.0   0.0   0.0 398.0  1
  317  trichloro-1,4-benzoquinone
C 6  H 1 Cl 3  O 2              88.7   0.0   0.0 314.0  1
  318  1,2,4,5-tetrachloro-3-nitrobenzene
C 6  H 1 Cl 4  N 1  O 2         91.0   0.0   0.0 298.0  1
  319  pentachlorobenzene                                               PNCLBZ
C 6  H 1 Cl 5                   87.0   0.0   0.0 298.0  1
  320  pentachlorophenol                                                PCPHOL
C 6  H 1 Cl 5  O 1              91.6   0.0   0.0 376.0  1
  321  pentaFluorophenol                                                UCAYED
C 6  H 1  F 5  O 1              67.4   0.0   0.0 286.0  1
  322  1-chloro-2,4,6-trinitrobenzene                                   CLNOBE
C 6  H 2 Cl 1  N 3  O 6        103.0   0.0   0.0   0.0  2
  323  2,6-dichloro-1,4-benzoquinone                                    DCLBQN
C 6  H 2 Cl 2  O 2              70.0   0.0   0.0 298.0  1
  324  2,4,6-trichloro-1-nitrobenzene
C 6  H 2 Cl 3  N 1  O 2         87.0   0.0   0.0 298.0  1
  325  1,2,3,4-tetrachlorobenzene
C 6  H 2 Cl 4                   79.0   0.0   0.0 298.0  1
  326  1,2,3,5-tetrachlorobenzene                                       TCLBZN
C 6  H 2 Cl 4                   80.0   0.0   0.0 298.0  1
  327  1,2,4,5-tetrachlorobenzene                                       TCLBEN
C 6  H 2 Cl 4                   83.0   0.0   0.0 298.0  1
  328  tetrachlorohydroquinone                                          TCLHQU
C 6  H 2 Cl 4  O 2              89.0   0.0   0.0 320.0  2
  329  2,3-dicyanopyrazine
C 6  H 2  N 4                   89.0   0.0   0.0 298.0  0
  330  2,5-dibromonitrobenzene
C 6  H 3 Br 3  N 1  O 2         97.0   0.0   0.0 298.0  0
  331  2,4,6-tribromophenol
C 6  H 3 Br 3  O 1              97.0   0.0   0.0   0.0  0
  332  5-chlorobenzofurazan-1-oxide
C 6  H 3 Cl 1  N 2  O 2         81.0   0.0   0.0 298.0  0
  333  chlorobenzoquinone                                               CLBENQ
C 6  H 3 Cl 1  O 2              69.0   0.0   0.0 276.0  0
  334  2,4-dichloro-1-nitrobenzene                                      JIWQEM
C 6  H 3 Cl 2  N 1  O 2         88.0   0.0   0.0 298.0  0
  335  2,5-dichloro-1-nitrobenzene                                      ZZZEKW
C 6  H 3 Cl 2  N 1  O 2         87.0   0.0   0.0 298.0  0
  336  3,4-dichloro-1-nitrobenzene                                      CAGPUV
C 6  H 3 Cl 2  N 1  O 2         85.0  83.0  86.0 298.0  2
  337  3,5-dichloro-1-nitrobenzene                                      HIBWEU
C 6  H 3 Cl 2  N 1  O 2         83.0   0.0   0.0 298.0  0
  338  1,2,4-trichlorobenzene                                           KUBMAX
C 6  H 3 Cl 3                   62.0   0.0   0.0 298.0  0
  339  1,2,3-trichlorobenzene                                           TCBENZ
C 6  H 3 Cl 3                   74.0  72.0  75.0 298.0  2
  340  1,3,5-trichlorobenzene                                           TCHLBZ
C 6  H 3 Cl 3                   73.0   0.0   0.0 292.0  1
  341  2,4,6-trichlorophenol                                            SILGOK
C 6  H 3 Cl 3  O 1              82.3   0.0   0.0 320.0  1
  342  trichlorohydroquinone
C 6  H 3 Cl 3  O 2             101.0 101.0 101.0 321.0  2
  343  2,3,5,6-tetrachloroaniline
C 6  H 3 Cl 4  N 1              86.0   0.0   0.0 298.0  0
  344  4-nitrobenzofurazan-1-oxide
C 6  H 3  N 3  O 4              97.0   0.0   0.0 298.0  0
  345  1,3,5-trinitrobenzene
C 6  H 3  N 3  O 6             107.0   0.0   0.0 354.0  1
  346  2,4,6-trinitrophenol                                             PICRAC
C 6  H 3  N 3  O 7             105.0   0.0   0.0 360.0  2
  347  2,4,6-trinitroresorcinol
C 6  H 3  N 3  O 8             120.0   0.0   0.0 381.0  2
  348  1-bromo-4-chlorobenzene
C 6  H 4 Br 1 Cl 1              69.0   0.0   0.0 298.0  3
  349  1-bromo-4-iodobenzene
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C 6  H 4 Br 1  I 1              78.0   0.0   0.0 298.0  2
  350  2-bromo-1-nitrobenzene                                  YAQZUM
C 6  H 4 Br 1  N 1  O 2         85.0   0.0   0.0 298.0  0
  351  3-bromo-1-nitrobenzene                                  BRNIBZ
C 6  H 4 Br 1  N 1  O 2         87.0   0.0   0.0 298.0  0
  352  4-bromo-1-nitrobenzene                                  ULEBOD
C 6  H 4 Br 1  N 1  O 2         87.0   0.0   0.0 298.0  0
  353  1,4-dibromobenzene
C 6  H 4 Br 2                   74.0   0.0   0.0 298.0  4
  354  2,4,6-tribromoaniline                                   BRANIL
C 6  H 4 Br 3  N 1             100.0  97.0 101.0 298.0  2
  355  1-chloro-4-iodobenzene                                  FACPAA
C 6  H 4 Cl 1  F 1              72.0   0.0   0.0 298.0  2
  356  1-chloro-2-nitrobenzene                                 SETVIX
C 6  H 4 Cl 1  N 1  O 2         81.0   0.0   0.0 298.0  2
  357  1-chloro-3-nitrobenzene                                 CLNIBZ
C 6  H 4 Cl 1  N 1  O 2         82.0   0.0   0.0 298.0  2
  358  1-chloro-4-nitrobenzene
C 6  H 4 Cl 1  N 1  O 2         83.0   0.0   0.0 298.0  1
  359  2-chloro-4-nitrophenol
C 6  H 4 Cl 1  N 1  O 3         99.0   0.0   0.0 298.0  1
  360  4-chloro-2-nitrophenol                                  NTCPOL
C 6  H 4 Cl 1  N 1  O 3         88.0   0.0   0.0 298.0  1
  361  4-chloro-3-nitrophenol
C 6  H 4 Cl 1  N 1  O 3        111.0   0.0   0.0 298.0  1
  362  5-chloro-6-hydroxynicotinic
C 6  H 4 Cl 1  N 1  O 3        150.0   0.0   0.0 298.0  1
  363  2-chloro-4,6-dinitroaniline                             UCECAG
C 6  H 4 Cl 1  N 3  O 4        115.0   0.0   0.0 298.0  1
  364  4-chloro-2,6-dinitroaniline
C 6  H 4 Cl 1  N 3  O 4        105.0   0.0   0.0 298.0  1
  365  1,4-dichlorobenzene                                     DCLBEN
C 6  H 4 Cl 2                   65.0   0.0   0.0 298.0  5
  366  2,5-dichloro-4-nitrobenzenamine
C 6  H 4 Cl 2  N 2  O 2        114.0   0.0   0.0 298.0  1
  367  2,6-dichloro-4-nitroaniline                             CLNOAN
C 6  H 4 Cl 2  N 2  O 2        109.0   0.0   0.0 298.0  1
  368  4,5-dichloro-2-nitroaniline                             CARDOO
C 6  H 4 Cl 2  N 2  O 2        109.0   0.0   0.0 298.0  1
  369  2,3-dichlorophenol                                      DCPHOL
C 6  H 4 Cl 2  O 1              75.0  72.0  77.0 298.0  2
  370  2,4-dichlorophenol                                      DCPHOM
C 6  H 4 Cl 2  O 1              76.0  70.0  78.0 298.0  2
  371  2,5-dichlorophenol                                      DCLPOL
C 6  H 4 Cl 2  O 1              76.0  74.0  77.0 298.0  2
  372  2,6-dichlorophenol                                      DCLPHL
C 6  H 4 Cl 2  O 1              78.0  76.0  79.0 298.0  2
  373  3,4-dichlorophenol                                      DCLPHM
C 6  H 4 Cl 2  O 1              87.0  81.0  90.0 298.0  2
  374  3,5-dichlorophenol                                      DCLPHE
C 6  H 4 Cl 2  O 1              79.0  72.0  83.0 298.0  2
  375  2,6-dichlorohydroquinone
C 6  H 4 Cl 2  O 2              92.0   0.0   0.0 330.0  1
  376  2,3,4-trichloroaniline
C 6  H 4 Cl 3  N 1              92.0   0.0   0.0 298.0  1
  377  2,4,5-trichloroaniline
C 6  H 4 Cl 3  N 1              86.0   0.0   0.0 298.0  1
  378  2,4,6-trichloroaniline                                  TCANIL
C 6  H 4 Cl 3  N 1              85.0   0.0   0.0 298.0  1
  379  3,4,5-trichloroaniline
C 6  H 4 Cl 3  N 1              93.0   0.0   0.0 298.0  1
  380  2,3-diFluorophenol
C 6  H 4  F 2  O 1              68.0   0.0   0.0 298.0  1
  381  2,5-diFluorophenol
C 6  H 4  F 2  O 1              68.0   0.0   0.0 298.0  1
  382  2,6-diFluorophenol
C 6  H 4  F 2  O 1              78.0   0.0   0.0 298.0  1
  383  3,4-diFluorophenol
C 6  H 4  F 2  O 1              73.0   0.0   0.0 298.0  1
  384  3,5-diFluorophenol                                      LETFEV
C 6  H 4  F 2  O 1              73.0   0.0   0.0 298.0  1
  385  3-iodo-1-nitrobenzene                                   WURTOS
C 6  H 4  I 1  N 1  O 2         83.2   0.0   0.0 301.0  1
  386  1,4-diiodobenzene                                       ZZZPRO
C 6  H 4  I 2                   63.4   0.0   0.0 387.0  1
  387  2-cyanopyridine                                         MUBZOY
C 6  H 4  N 2                   71.0   0.0   0.0 298.0  1
  388  3-cyanopyridine                                         MUBZUE
C 6  H 4  N 2                   72.0   0.0   0.0 298.0  1
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  389  4-cyanopyridine                                                  CYAPYR
C 6  H 4  N 2                    75.0  73.0  76.0 298.0  2
  390  3-cyanopyridine noxide
C 6  H 4  N 2  O 1              101.0   0.0   0.0 369.0  1
  391  4-cyanopyridine Noxide                                           CYPYRO
C 6  H 4  N 2  O 1              104.0   0.0   0.0 369.0  1
  392  benzofurazan                                                     BEOXAZ
C 6  H 4  N 2  O 1               65.0   0.0   0.0   0.0  2
  393  benzofurazan Noxide
C 6  H 4  N 2  O 2               80.0   0.0   0.0   0.0  1
  394  1,2-dinitrobenzene                                               ZZZFYW
C 6  H 4  N 2  O 4               93.0  87.0  96.0   0.0  4
  395  1,3-dinitrobenzene                                               DNBENZ
C 6  H 4  N 2  O 4               85.0  81.0  87.0   0.0  3
  396  1,4-dinitrobenzene                                               DNITBZ
C 6  H 4  N 2  O 4               95.0   0.0   0.0   0.0  2
  397  2,3-dinitrophenol
C 6  H 4  N 2  O 5               96.6   0.0   0.0 323.0  1
  398  2,4-dinitrophenol                                                DNOPHL
C 6  H 4  N 2  O 5              104.0   0.0   0.0 313.0  1
  399  2,5-dinitrophenol
C 6  H 4  N 2  O 5               93.4   0.0   0.0 306.0  1
  400  2,6-dinitrophenol                                                DNPHOL
C 6  H 4  N 2  O 5              112.0   0.0   0.0 313.0  1
  401  3,4-dinitrophenol
C 6  H 4  N 2  O 5              123.0   0.0   0.0 356.0  1
  402  2,4,6-trinitroaniline                                            TNIOAN
C 6  H 4  N 4  O 6              125.0   0.0   0.0 310.0  2
  403  2,1,3-benzothiadiazole                                           BETHAZ
C 6  H 4  N 2  S 1               71.0   0.0   0.0 298.0  1
  404  1,4-benzoquinone                                                 BNZQUI
C 6  H 4  O 2                    68.8   0.0   0.0 298.0  3
  405  furan-2,5-dicarboxylic                                           FURDCA
C 6  H 4  O 5                   121.0   0.0   0.0 390.0  1
  406  tetrathiafulvene                                                 BDTOLE
C 6  H 4  S 4                    94.0  92.0  95.0 345.0  2
  407  4-bromophenol                                                    PBRPOL
C 6  H 5 Br 1  O 1               85.0  83.0  87.0 298.0  2
  408  2,4-dibromoaniline                                               CAJWEQ
C 6  H 5 Br 2  N 1               88.0   0.0   0.0 298.0  1
  409  2,5-dibromoaniline
C 6  H 5 Br 2  N 1               86.0   0.0   0.0 298.0  1
  410  2,6-dibromoaniline
C 6  H 5 Br 2  N 1               80.0   0.0   0.0 298.0  1
  411  2-chloro-4-nitroaniline                                          CLONAN
C 6  H 5 Cl 1  N 2  O 2         102.0   0.0   0.0 298.0  1
  412  2-chloro-5-nitroaniline                                          YOVCAO
C 6  H 5 Cl 1  N 2  O 2         100.0   0.0   0.0 298.0  1
  413  3-chlorophenol
C 6  H 5 Cl 1  O 1               77.0   0.0   0.0 298.0  1
  414  4-chlorophenol
C 6  H 5 Cl 1  O 1               77.0   0.0   0.0 298.0  1
  415  chlorohydroquinone
C 6  H 5 Cl 1  O 2              103.0   0.0   0.0 320.0  1
  416  2,3-dichloroaniline                                              WEMDAT
C 6  H 5 Cl 2  N 1               82.0   0.0   0.0 298.0  1
  417  2,4-dichloroaniline                                              WEMDIB
C 6  H 5 Cl 2  N 1               85.0   0.0   0.0 298.0  1
  418  2,5-dichloroaniline                                              DCHLAN
C 6  H 5 Cl 2  N 1               83.0   0.0   0.0 298.0  1
  419  2,6-dichloroaniline                                              WEMDEX
C 6  H 5 Cl 2  N 1               74.0   0.0   0.0 298.0  1
  420  4-Fluorophenol                                                   QQQBNG
C 6  H 5  F 1  O 1               74.0   0.0   0.0 298.0  1
  421  2-pyridinecarboxylic
C 6  H 5  N 1  O 2               96.0  93.0  98.0 298.0  2
  422  3-pyridinecarboxylic                                             NICOAC
C 6  H 5  N 1  O 2              124.0   0.0   0.0 298.0  2
  423  4-pyridinecarboxylic                                             ISNICA
C 6  H 5  N 1  O 2              113.0 111.0 114.0 298.0  2
  424  2-nitrophenol                                                    ONITPH
C 6  H 5  N 1  O 3               73.0   0.0   0.0 298.0  2
  425  3-nitrophenol
C 6  H 5  N 1  O 3               97.0  92.0 100.0 298.5  2
  426  4-nitrophenol                                                    NITPOL
C 6  H 5  N 1  O 3               95.0  91.0  99.0 298.0  2
  427  pyridine-2-carboxylic acidNoxide                                 PICANO
C 6  H 5  N 1  O 3               94.4   0.0   0.0 369.0  1
  428  pyridine-3-carboxylic acidNoxide                                 VATNUA
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C 6  H 5  N 1  O 3             152.0   0.0   0.0 298.0  1
  429  pyridine-4-carboxylic acidNoxide                          XUCPAO
C 6  H 5  N 1  O 3             136.0   0.0   0.0 369.0  1
  430  2-hydroxynicotinic
C 6  H 5  N 1  O 3             128.0   0.0   0.0 298.0  1
  431  4-hydroxynicotinic
C 6  H 5  N 1  O 3             148.0   0.0   0.0 298.0  1
  432  5-hydroxynicotinic
C 6  H 5  N 1  O 3             150.0   0.0   0.0 298.0  1
  433  6-hydroxynicotinic
C 6  H 5  N 1  O 3             146.0   0.0   0.0 298.0  1
  434  2-nitro-1,3-dihydroxybenzene                              TEMWUD
C 6  H 5  N 1  O 4              75.0   0.0   0.0 273.0  1
  435  4-nitrocatechol
C 6  H 5  N 1  O 4             121.0   0.0   0.0   0.0  1
  436  methyl 5-nitro-2-furancarboxylate
C 6  H 5  N 1  O 5             104.0   0.0   0.0   0.0  1
  437  1-H-benzotriazole                                         BZTRAZ
C 6  H 5  N 3                   98.0   0.0   0.0 298.0  3
  438  1,3-diamino-2,4,6-trinitrobenzene                         DATNBZ
C 6  H 5  N 5  O 6             145.0 144.0 147.0 298.0  2
  439  benzene                                                   BENZEN
C 6  H 6                        45.0  42.0  47.0 280.0 11
  440  2,4-hexadiyne
C 6  H 6                        47.0   0.0   0.0 307.0  1
  441  2-bromoaniline
C 6  H 6 Br 1  N 1              75.0   0.0   0.0 298.0  1
  442  4-bromoaniline                                            PBRANL
C 6  H 6 Br 1  N 1              79.0   0.0   0.0 298.0  1
  443  4-chloroaniline                                           CLANIC
C 6  H 6 Cl 1  N 1              86.0  81.0  91.0 298.0  2
  444  alfa-hexachlorocyclohexane                                AHCHEX
C 6  H 6 Cl 6                   94.0  93.0  95.0 310.0  2
  445  beta-hexachlorocyclohexane                                HCCYHB
C 6  H 6 Cl 6                  105.0 103.0 107.0 310.0  1
  446  gamma-hexachlorocyclohexane                               HCCYHG
C 6  H 6 Cl 6                   97.0  90.0 100.0 310.0  6
  447  delta-hexachlorocyclohexane
C 6  H 6 Cl 6                   97.0   0.0   0.0 310.0  2
  448  2-iodoaniline                                             RALTOO
C 6  H 6  I 1  N 1              81.0   0.0   0.0 298.0  1
  449  4-iodoaniline                                             EJAYET
C 6  H 6  I 1  N 1              85.0   0.0   0.0 298.0  1
  450  2-pyridinecarboxamide                                     PICAMD
C 6  H 6  N 2  O 1              93.0   0.0   0.0 320.0  2
  451  3-pyridinecarboxamide                                     NICOAM
C 6  H 6  N 2  O 1             120.0 112.0 121.0 298.0  2
  452  4-pyridinecarboxamide                                     EHOWIH
C 6  H 6  N 2  O 1             115.0 100.0 116.0 298.0  2
  453  2-nitroaniline                                            ONITAN
C 6  H 6  N 2  O 2              89.0   0.0   0.0 298.0  3
  454  3-nitroaniline                                            MNIANL
C 6  H 6  N 2  O 2              94.0  89.0  97.0 298.0  3
  455  4-nitroaniline                                            NANILI
C 6  H 6  N 2  O 2             101.0  99.0 103.0 298.0  8
  456  3-pyridinecarboxamide Noxid
C 6  H 6  N 2  O 2             119.0   0.0   0.0 298.0  1
  457  4-pyridinecarboxamide Noxide
C 6  H 6  N 2  O 2             125.0   0.0   0.0 298.0  1
  458  2-methyl-5-pyrazine carbox acid
C 6  H 6  N 2  O 2             101.0   0.0   0.0 298.0  1
  459  phthalhydrazide
C 6  H 6  N 2  O 2             140.0   0.0   0.0 298.0  1
  460  3-methyl-4-nitropyridine Noxide
C 6  H 6  N 2  O 3             107.0   0.0   0.0 298.0  1
  461  9-methylhypoxanthine
C 6  H 6  N 4  O 1              84.0   0.0   0.0 520.0  1
  462  2,4,6-trinitro-1,3,5-benzenetriamine                      TATNBZ
C 6  H 6  N 6  O 6             168.0   0.0   0.0 420.0  2
  463  phenol                                                    PHENOL
C 6  H 6  O 1                   69.0   0.0   0.0 298.0  4
  464  1,2-dihydroxybenzene                                      CATCOL
C 6  H 6  O 2                   85.0  81.0  88.0 298.0  2
  465  1,3-dihydroxybenzene                                      RESORA
C 6  H 6  O 2                   93.0  88.0  95.0 298.0  5
  466  1,4-dihydroxybenzene                                      HYQUIN
C 6  H 6  O 2                  100.0  94.0 104.0 320.0  6
  467  2-thiopheneacetic
C 6  H 6  O 2  S 1              97.5   0.0   0.0 300.0  1
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  468  3-thiopheneacetic
C 6  H 6  O 2  S 1            100.0   0.0   0.0 303.0  1
  469  5-methyl-2-thiophenecarboxylic
C 6  H 6  O 2  S 1            103.0   0.0   0.0 298.0  1
  470  1,2,3-trihydroxybenzene
C 6  H 6  O 3                 112.0 104.0 117.0 298.0  2
  471  1,2,4-trihydroxybenzene
C 6  H 6  O 3                 122.0 120.0 124.0 298.0  2
  472  1,3,5-trihydroxybenzene                                  PHGLOL
C 6  H 6  O 3                 134.0 132.0 136.0 298.0  2
  473  1,3-dimethyl-5-Furacil
C 6  H 7  F 1  N 2  O 2       119.0   0.0   0.0 350.0  1
  474  3-methylpyridine                                         ZZZKAO
C 6  H 7  N 1                  62.2   0.0   0.0 240.0  1
  475  4-methylpyridine                                         ZZZIVG
C 6  H 7  N 1                  62.7   0.0   0.0 226.0  1
  476  2-aminophenol                                            AMPHOM
C 6  H 7  N 1  O 1            101.0  97.0 104.0 298.0  2
  477  3-aminophenol                                            MAMPOL
C 6  H 7  N 1  O 1            104.0 102.0 105.0 298.0  2
  478  4-aminophenol                                            AMPHOL
C 6  H 7  N 1  O 1            108.0 104.0 111.0 300.0  3
  479  2-methyl-3-hydroxypyridine                               YELRIR
C 6  H 7  N 1  O 1             89.0   0.0   0.0 298.0  1
  480  2-methyl-4-hydroxypyridine
C 6  H 7  N 1  O 1            113.0   0.0   0.0 298.0  1
  481  2-methyl-5-hydroxypyridine
C 6  H 7  N 1  O 1             96.0   0.0   0.0 298.0  1
  482  2-methyl-6-hydroxypyridine
C 6  H 7  N 1  O 1             92.0   0.0   0.0 298.0  1
  483  2-methylpyridine Noxide                                  RAJGUG
C 6  H 7  N 1  O 1             89.0  78.0  93.0 298.0  2
  484  3-methylpyridine Noxide
C 6  H 7  N 1  O 1             82.0   0.0   0.0 298.0  1
  485  4-methylpyridine Noxide                                  ZZZVCO
C 6  H 7  N 1  O 1             83.0  79.0  85.0 298.0  2
  486  2-acetylpyrrole                                          RICFEP
C 6  H 7  N 1  O 1             81.0   0.0   0.0 298.0  1
  487  3-acetylpyrrole
C 6  H 7  N 1  O 1             95.0   0.0   0.0 298.0  1
  488  1-methyl-2-pyrrolecarboxylic
C 6  H 7  N 1  O 2             96.0   0.0   0.0 298.0  1
  489  benzenesulfonamide                                       YIFZAP
C 6  H 7  N 1  O 2  S 1       115.0   0.0   0.0 298.0  1
  490  sulfanilic acid                                          AFAZEM
C 6  H 7  N 1  O 3  S 1        67.0   0.0   0.0   0.0  1
  491  4-  methylthio pyridine
C 6  H 7  N 1  S 1             75.0   0.0   0.0 365.0  1
  492  2-hydrazino-1-nitrobenzene
C 6  H 7  N 3  O 2            125.0   0.0   0.0   0.0  1
  493  1-methyladenine
C 6  H 7  N 5                 138.0   0.0   0.0   0.0  1
  494  2-methyladenine
C 6  H 7  N 5                 122.0   0.0   0.0   0.0  1
  495  3-methyladenine
C 6  H 7  N 5                 117.0   0.0   0.0   0.0  1
  496  N-methyladenine
C 6  H 7  N 5                 123.0   0.0   0.0   0.0  1
  497  8-methyladenine
C 6  H 7  N 5                 103.0   0.0   0.0   0.0  1
  498  9-methyladenine                                          MEADEN
C 6  H 7  N 5                 122.0   0.0   0.0 400.0  1
  499  1,2-diaminobenzene                                       BAGFIY
C 6  H 8  N 2                  86.0   0.0   0.0 298.0  1
  500  1,3-diaminobenzene
C 6  H 8  N 2                  90.0   0.0   0.0 298.0  1
  501  1,4-diaminobenzene                                       PENDAM
C 6  H 8  N 2                  92.0   0.0   0.0 298.0  1
  502  1,3-dimethyluracil                                       DMURAC
C 6  H 8  N 2  O 2            110.0  96.0 116.0 310.0  3
  503  1-methylthymine                                          METHYM
C 6  H 8  N 2  O 2            124.0   0.0   0.0 398.0  1
  504  1,3-cyclohexanedione                                     FACRIK
C 6  H 8  O 2                  90.0   0.0   0.0 298.0  1
  505  1,4-cyclohexanedione                                     CYHEXO
C 6  H 8  O 2                  84.0   0.0   0.0 298.0  1
  506  dimethyl fumarate                                        ZZZDRQ
C 6  H 8  O 4                  85.0   0.0   0.0   0.0  1
  507  cyclobutane-1,1-dicarboxylic                             CBUTAC
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C 6  H 8  O 4                  112.0   0.0   0.0   0.0  1
  508  cyclobutane-1,2-dicarboxylic
C 6  H 8  O 4                  120.0   0.0   0.0   0.0  1
  509  1,3,5-trimethyl-4-NOpyrazole                          RIVBED
C 6  H 9  N 3  O 1              88.0   0.0   0.0 298.0  1
  510  1,5-dimethylcytosine
C 6  H 9  N 3  O 1             133.0   0.0   0.0 410.0  1
  511  1,N-dimethylcytosine
C 6  H 9  N 3  O 1             122.0   0.0   0.0 410.0  1
  512  1-methyl- N 4-methoxycytosine
C 6  H 9  N 3  O 2             107.0   0.0   0.0 320.0  2
  513  1,5-dimethyl-N-hydroxcytosine                          DMXCYT
C 6  H 9  N 3  O 2             115.0   0.0   0.0 370.0  1
  514  trimethyl isocyanurate
C 6  H 9  N 3  O 3              88.0   0.0   0.0 298.0  1
  515  trimethyl cyanurate
C 6  H 9  N 3  O 3              90.0   0.0   0.0 298.0  2
  516  1-methylcyclopentanol
C 6  H10  O 1                   71.0  67.0  74.0 298.0  2
  517  4-methyl-2,6,7-trioxabicyclo 2.2.2octane
C 6  H10  O 3                   67.0   0.0   0.0 298.0  1
  518  cis-1,3,5,7-tetraoxadecalin                            POKKAB
C 6  H10  O 4                   95.0   0.0   0.0 298.0  1
  519  trans-1,3,5,7-tetraoxadecalin                          GOCWEA
C 6  H10  O 4                   82.0   0.0   0.0 298.0  1
  520  adipic acid                                            ADIPAC
C 6  H10  O 4                  144.1 140.0 146.0 320.0  2
  521  cyclohexanone oxime                                    ZZZVPO
C 6  H11  N 1  O 1              77.0  74.0  79.0 320.0  2
  522  epsilon-caprolactam                                    CAPLAC
C 6  H11  N 1  O 1              85.0  83.0  87.0 310.0  3
  523  cis 2hexenoic acid amide
C 6  H11  N 1  O 1              80.0   0.0   0.0 328.0  1
  524  1-aminocyclopentanecarboxylic
C 6  H11  N 1  O 2             123.0   0.0   0.0 456.0  2
  525  2-piperidinethione
C 6  H11  N 1  S 1              81.2   0.0   0.0 367.0  1
  526  2,3,3-trinitro-2-methylpentane                         JORCAU
C 6  H11  N 3  O 6              91.0   0.0   0.0 298.0  1
  527  N-2,2-dinitropropyl2,2dinitro1propanamine
C 6  H11  N 5  O 8             105.0   0.0   0.0   0.0  1
  528  cyclohexane                                            CYCHEX
C 6  H12                        37.0   0.0   0.0 250.0  4
  529  1,4-diazabicyclo 2.2.2octane
C 6  H12  N 2                   53.0  52.3  54.0 330.0  2
  530  3,3,4,4-tetramethyl- 1-1,2-diazetine
C 6  H12  N 2                   62.0   0.0   0.0 298.0  1
  531  1-piperidinecarboxamide
C 6  H12  N 2  O 1             100.0   0.0   0.0 298.0  1
  532  3-piperidinecarboxamide
C 6  H12  N 2  O 1             113.0   0.0   0.0 298.0  1
  533  4-piperdinecarboxamide
C 6  H12  N 2  O 1             124.0   0.0   0.0 298.0  1
  534  2,3-dinitro-2,3-dimethylbutane                         BECJEY
C 6  H12  N 2  O 4              90.0  75.0  94.0   0.0  4
  535  1,3,5,7-tetraazatricyclo 3.3.1.13,7decane              HXMTAM
C 6  H12  N 4                   77.0  75.0  80.0 298.0  5
  536  cis 1,2cyclohexanediol
C 6  H12  O 2                   88.0   0.0   0.0 343.0  1
  537  trans 1,2-cyclohexane diol
C 6  H12  O 2                   86.0   0.0   0.0 343.0  1
  538  myo-inositol
C 6  H12  O 6                  175.0 161.0 181.0 298.0  3
  539  tert-butylacetamide                                    APUYIU
C 6  H13  N 1  O 1              78.0   0.0   0.0 298.0  1
  540  hexanamide
C 6  H13  N 1  O 1              99.0  85.0  99.0 298.0  2
  541  2-piperidinemethanol
C 6  H13  N 1  O 1              93.0   0.0   0.0 298.0  1
  542  3-piperidinemethanol
C 6  H13  N 1  O 1              96.0   0.0   0.0 298.0  1
  543  4-piperidinemethanol
C 6  H13  N 1  O 1              98.0   0.0   0.0 298.0  1
  544  dl-2-aminohexanoic
C 6  H13  N 1  O 2             114.0   0.0   0.0 452.0  1
  545  hexane                                                 HEXANE
C 6  H14                        51.0   0.0   0.0 178.0  1
  546  trans-cyclohexyl-1,4-diamine
C 6  H14  N 2                  105.0   0.0   0.0 298.0  1
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  547  1,6-hexanediol                                                FECCOF
C 6  H14  O 2                  110.0 109.0 112.0 298.0  2
  548  tert-butyl ethyl sulfone
C 6  H14  O 2  S 1              87.0   0.0   0.0   0.0  1
  549  N,N-bis  2-hydroxyethyl ethylenediamine
C 6  H16  N 2  O 2             143.0   0.0   0.0 373.0  1
  550  perfluoromethylcyclohexane
C 7  F14                        52.0   0.0   0.0 234.0  1
  551  perfluorooheptane
C 7  F16                        58.0   0.0   0.0   0.0  1
  552  pentafluorobenzoic acid                                       PFBZAC
C 7  H 1  F 5  O 2              91.6   0.0   0.0 347.0  1
  553  2-nitrobenzonitrile
C 7  H 4  N 2  O 2              88.0   0.0   0.0 298.0  1
  554  3-nitrobenzonitrile
C 7  H 4  N 2  O 2              93.0   0.0   0.0 298.0  1
  555  4-nitrobenzonitrile                                           PNBZNT
C 7  H 4  N 2  O 2              91.0   0.0   0.0 298.0  1
  556  2,4-dinitrobenzoic acid                                       BIPJUF
C 7  H 4  N 2  O 6             135.0   0.0   0.0 298.0  1
  557  3,4-dinitrobenzoic acid                                       YADKOF
C 7  H 4  N 2  O 6             129.0   0.0   0.0 298.0  1
  558  4,5-benzo-1,2-dithiole-3-thione
C 7  H 4  S 3                  107.0   0.0   0.0 298.0  1
  559  4,5-benzo-1,3-dithiole-2-thione
C 7  H 4  S 3                  119.0   0.0   0.0 298.0  1
  560  2-bromobenzoic acid                                           BRBZAC
C 7  H 5 Br 1  O 2             109.0  95.0 111.0 298.0  3
  561  3-bromobenzoic acid                                           MBBNZA
C 7  H 5 Br 1  O 2             105.0  99.0 106.0 298.0  3
  562  4-bromobenzoic acid                                           BRBZAP
C 7  H 5 Br 1  O 2             107.0 103.0 110.0 298.0  3
  563  2-chlorobenzoic acid                                          CLBZAC
C 7  H 5 Cl 1  O 2             110.0 106.0 116.0 298.0  3
  564  3-chlorobenzoic acid                                          MCBZAC
C 7  H 5 Cl 1  O 2             104.0 101.0 106.0 298.0  4
  565  4-chlorobenzoic acid                                          CLBZAP
C 7  H 5 Cl 1  O 2             105.0 103.0 107.0 298.0  3
  566  2-fluorobenzoic acid                                          FBENZA
C 7  H 5  F 1  O 2              94.0   0.0   0.0 298.0  1
  567  3-fluorobenzoic acid                                          COVJIG
C 7  H 5  F 1  O 2              94.3   0.0   0.0 298.0  1
  568  4-fluorobenzoic acid                                          PFBZAD
C 7  H 5  F 1  O 2              93.0   0.0   0.0 298.0  1
  569  trifluoromethylbenzene                                        XOGJAG
C 7  H 5  F 3                   55.0   0.0   0.0 227.0  1
  570  2-iodobenzoic acid                                            OIBZAC
C 7  H 5  I 1  O 2             111.0  93.0 113.0 298.0  3
  571  3-iodobenzoic acid                                            ZZZOAE
C 7  H 5  I 1  O 2             109.0  97.0 111.0 298.0  2
  572  4-iodobenzoic acid                                            BENMOW
C 7  H 5  I 1  O 2             110.0  99.0 111.0 298.0  2
  573  benzoxazole
C 7  H 5  N 1  O 1              70.0   0.0   0.0 298.0  1
  574  2-benzoxazolinone                                             BZOXZO
C 7  H 5  N 1  O 2              98.0   0.0   0.0 298.0  1
  575  1,1-dioxo-1,2-benzisothiazol-3  2H -one
C 7  H 5  N 1  O 3  S 1        113.0   0.0   0.0 298.0  1
  576  2-nitrobenzoic acid                                           NBZOAO
C 7  H 5  N 1  O 4             119.0   0.0   0.0 298.0  1
  577  3-nitrobenzoic acid                                           MNBZAC
C 7  H 5  N 1  O 4             110.0   0.0   0.0 298.0  1
  578  4-nitrobenzoic acid                                           NBZOAC
C 7  H 5  N 1  O 4             120.0   0.0   0.0 298.0  1
  579  pyridine-2,5-dicarboxylic
C 7  H 5  N 1  O 4             164.0   0.0   0.0 298.0  1
  580  pyridine-2,6-dicarboxylic                                     AFEBUI
C 7  H 5  N 1  O 4             137.0   0.0   0.0 298.0  1
  581  3-  5-nitro-2-furyl -2-propenal
C 7  H 5  N 1  O 4              98.0   0.0   0.0   0.0  1
  582  5-nitro-1,3-benzodioxole
C 7  H 5  N 1  O 4              97.0   0.0   0.0 298.0  1
  583  benzothiazole
C 7  H 5  N 1  S 1              73.0   0.0   0.0 298.0  1
  584  2,4,6-trinitrotoluene                                         ZZZMUC
C 7  H 5  N 3  O 6             110.0  92.0 118.0 298.0  7
  585  2,4,6-trinitroanisole
C 7  H 5  N 3  O 7             133.0   0.0   0.0 330.0  2
  586  3-hydroxy-2,4,6-trinitrotoluene
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C 7  H 5  N 3  O 7             108.0 103.0 111.0 298.0  3
  587  2,4,6-N-tetranitro-N-methylaniline                      MTNANL
C 7  H 5  N 5  O 8             133.0   0.0   0.0 298.0  2
  588  1-  chloromethyl -2-nitrobenzene                       UCOVAL
C 7  H 6 Cl 1  N 1  O 2         96.0   0.0   0.0   0.0  1
  589  2,3-dichloroanisole
C 7  H 6 Cl 2  O 1              84.0   0.0   0.0 298.0  1
  590  3,5-dichloroanisole
C 7  H 6 Cl 2  O 1              79.0   0.0   0.0 298.0  1
  591  benzimidazole                                           BZDMAZ
C 7  H 6  N 2                  100.0  90.0 102.0 298.0  3
  592  indazole
C 7  H 6  N 2                   92.0  88.0  97.0 298.0  3
  593  1,3-dihydro-2H-benzimidazol-2-one
C 7  H 6  N 2  O 1             127.0   0.0   0.0 298.0  1
  594  1,2-dihydro-3H-indazol-3-one
C 7  H 6  N 2  O 1             127.0   0.0   0.0 298.0  1
  595  5-methoxybenzofurazan
C 7  H 6  N 2  O 2              89.0   0.0   0.0 298.0  1
  596  5-methylbenzofurazan-1-oxide                           MBZFZO
C 7  H 6  N 2  O 2              92.0   0.0   0.0 298.0  1
  597  5-methoxybenzofurazan-1-oxide
C 7  H 6  N 2  O 3              96.0   0.0   0.0 298.0  1
  598  1,1-dinitrophenylmethane
C 7  H 6  N 2  O 4              76.0   0.0   0.0 310.0  1
  599  2,3-dinitrotoluene                                      FIHLOY
C 7  H 6  N 2  O 4              97.0   0.0   0.0 293.0  1
  600  2,4-dinitrotoluene                                      ZZZGVU
C 7  H 6  N 2  O 4              99.0  96.0 100.0 300.0  4
  601  2,6-dinitrotoluene                                      ZZZQSC
C 7  H 6  N 2  O 4              99.0  98.0 100.0 298.0  2
  602  3,4-dinitrotoluene                                      FIHLUE
C 7  H 6  N 2  O 4              99.6   0.0   0.0 293.0  1
  603  dinitromethyl benzene
C 7  H 6  N 2  O 4              76.0   0.0   0.0 320.0  1
  604  3,5-dinitro-o-cresol
C 7  H 6  N 2  O 5             103.0   0.0   0.0 298.0  1
  605  benzoic acid                                            BENZAC
C 7  H 6  O 2                   91.0  88.0  93.0 298.0 10
  606  3-hydroxybenzaldehyde                                   XAYCIJ
C 7  H 6  O 2                  100.0   0.0   0.0 298.0  2
  607  4-hydroxybenzaldehyde                                   PHBALD
C 7  H 6  O 2                  101.0 100.0 103.0 298.0  3
  608  tropolone                                               TROPOL
C 7  H 6  O 2                   84.0   0.0   0.0 298.0  2
  609  3-  2-furyl -2-propenal
C 7  H 6  O 2                   76.0   0.0   0.0   0.0  1
  610  2-furanacrylic acid
C 7  H 6  O 3                  103.0   0.0   0.0 298.0  1
  611  3-furanacrylic acid
C 7  H 6  O 3                  105.0   0.0   0.0 298.0  1
  612  2-hydroxybenzoic acid                                   SALIAC
C 7  H 6  O 3                   97.0  93.0  99.0 298.0  7
  613  3-hydroxybenzoic acid                                   BIDLOP
C 7  H 6  O 3                  123.0 118.0 125.0 298.0  2
  614  4-hydroxybenzoic acid                                   JOZZIH
C 7  H 6  O 3                  115.0 114.0 117.0 298.0  3
  615  5-hydroxy-1,3-benzodioxole
C 7  H 6  O 3                   92.0   0.0   0.0 298.0  1
  616  5-acetyl-2-thiophenecarboxylic
C 7  H 6  O 3  S 1             124.0   0.0   0.0 298.0  1
  617  2,3-dihydroxybenzoic acid                               CACDAM
C 7  H 6  O 4                  111.0   0.0   0.0 298.0  1
  618  2,4-dihydroxybenzoic acid                               ZZZEEU
C 7  H 6  O 4                  125.0   0.0   0.0 298.0  1
  619  2,5-dihydroxybenzoic acid                               BESKAL
C 7  H 6  O 4                  130.0   0.0   0.0 298.0  1
  620  2,6-dihydroxybenzoic acid                               LEZJAB
C 7  H 6  O 4                  109.0   0.0   0.0 298.0  1
  621  3,4-dihydroxybenzoic acid                               WUYNUA
C 7  H 6  O 4                  135.0   0.0   0.0 298.0  1
  622  3,5-dihydroxybenzoic acid                               WUYPOW
C 7  H 6  O 4                  143.0   0.0   0.0 298.0  1
  623  3,4,5-trihydroxybenzoic acid                            IJUMEG
C 7  H 6  O 5                   75.0   0.0   0.0 406.0  1
  624  2-aminotropone
C 7  H 7  N 1  O 1              71.0   0.0   0.0 298.0  1
  625  benzamide                                               BZAMID
C 7  H 7  N 1  O 1             100.0  97.0 102.0 310.0  2
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  626  formanilide
C 7  H 7  N 1  O 1              78.0   0.0   0.0 308.0  1
  627  4-nitrotoluene                                          NITOLU
C 7  H 7  N 1  O 2              77.0  75.0  79.0 298.0  2
  628  2-aminobenzoic acid                                     AMBACO
C 7  H 7  N 1  O 2             110.0 105.0 112.0 298.0  2
  629  3-aminobenzoic acid                                     AMBNZA
C 7  H 7  N 1  O 2             128.0   0.0   0.0 298.0  1
  630  4-aminobenzoic acid                                     AMBNAC
C 7  H 7  N 1  O 2             116.0   0.0   0.0 298.0  1
  631  2-hydroxybenzamide                                      SALMID
C 7  H 7  N 1  O 2             101.0  99.0 102.0 298.0  2
  632  4-hydroxybenzamide                                      VIDMAX
C 7  H 7  N 1  O 2             125.0 118.0 130.0 298.0  2
  633  2-methoxy-4-nitrophenol
C 7  H 7  N 1  O 4              99.0   0.0   0.0 298.0  1
  634  2-methoxy-5-nitrophenol
C 7  H 7  N 1  O 4             106.0   0.0   0.0 298.0  1
  635  4-methoxy-2-nitrophenol
C 7  H 7  N 1  O 4              91.0   0.0   0.0 298.0  1
  636  thiobenzamide                                           ZORSEG
C 7  H 7  N 1  S 1             100.0  97.0 103.0 298.0  2
  637  toluene                                                 TOLUEN
C 7  H 8                        43.0   0.0   0.0 298.0  1
  638  1-amino-7-imino-1,3,5-cycloheptatriene
C 7  H 8  N 2                   49.4   0.0   0.0 303.0  1
  639  monophenylurea                                          PHUREA
C 7  H 8  N 2  O 1             136.0   0.0   0.0 406.0  1
  640  2-pyridyl)acetamide
C 7  H 8  N 2  O 1             104.0   0.0   0.0 298.0  1
  641  9-Ethylhypoxanthine
C 7  H 8  N 4  O 1             108.0   0.0   0.0   0.0  1
  642  1,9-dimethylhypoxanthine
C 7  H 8  N 4  O 1              75.0   0.0   0.0   0.0  1
  643  1,3-dimethylxanthine theophylline
C 7  H 8  N 4  O 2             140.0 135.0 144.0 298.0  3
  644  2-hydroxytoluene                                        OCRSOL
C 7  H 8  O 1                   75.4  74.8  76.0 288.0  3
  645  3-hydroxytoluene                                        MCRSOL
C 7  H 8  O 1                   60.0  56.0  62.0 298.0  2
  646  4-hydroxytoluene                                        CRESOL
C 7  H 8  O 1                   74.0   0.0   0.0 298.0  2
  647  3-methyl-1,2-dihydroxybenzene
C 7  H 8  O 2                   93.0   0.0   0.0 298.0  1
  648  2,4-dihydroxytoluene
C 7  H 8  O 2                  107.0   0.0   0.0 298.0  1
  649  2,6-dihydroxytoluene                                    NUQKER
C 7  H 8  O 2                   99.0   0.0   0.0 298.0  1
  650  3,4-dihydroxytoluene
C 7  H 8  O 2                   95.0   0.0   0.0 298.0  1
  651  3,5-dihydroxytoluene                                    EWAMAR
C 7  H 8  O 2                  103.0   0.0   0.0 298.0  1
  652  2-methyl-1,4-dihydroxybenzene
C 7  H 8  O 2                  105.0 100.0 105.0 298.0  2
  653  4-methoxyphenol
C 7  H 8  O 2                   92.0  89.0  94.0 298.0  2
  654  MEphenylsulfone                                         MPSUFO
C 7  H 8  O 2  S 1              92.0   0.0   0.0   0.0  1
  655  4,5-tetramethylene-1,3-dithiole-2-thione
C 7  H 8  S 3                  102.3   0.0   0.0 298.0  1
  656  4,5-tetramethylene-1,2-dithiole-3-thione
C 7  H 8  S 3                  105.0   0.0   0.0 298.0  1
  657  p-toluidine                                             TOLDIN
C 7  H 9  N 1                   78.0  76.0  79.0 298.0  2
  658  3,5-dimethylpyridine Noxide
C 7  H 9  N 1  O 1             100.0   0.0   0.0 298.0  1
  659  8,9-dimethyladenine
C 7  H 9  N 5                  105.0   0.0   0.0 350.0  1
  660  2,9-dimethyladenine
C 7  H 9  N 5                  123.0   0.0   0.0 350.0  1
  661  N,N-dimethyladenine                                     DMADEN
C 7  H 9  N 5                  116.0   0.0   0.0 350.0  1
  662  N,9-dimethyladenine
C 7  H 9  N 5                  116.0   0.0   0.0 350.0  1
  663  bicyclo 2.2.1hept-2-ene
C 7  H10                        37.0  34.0  39.0 298.0  4
  664  tricyclo 2.2.1.02,6heptane
C 7  H10                        39.0   0.0   0.0 298.0  2
  665   alfatert-butylmalononitrile
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C 7  H10  N 2                   60.0   0.0   0.0 298.0  1
  666  1,3-dimethylthymine
C 7  H10  N 2  O 2             109.0   0.0   0.0 338.0  1
  667  1,3,5-trimethyluracil
C 7  H10  N 2  O 2             103.0   0.0   0.0 326.0  1
  668  1,3,6-trimethyluracil                                  LIMLOI
C 7  H10  N 2  O 2             106.0   0.0   0.0 320.0  1
  669  7-norbornanone
C 7  H10  O 1                   47.0   0.0   0.0 298.0  1
  670  2-norbornanone
C 7  H10  O 1                   49.0   0.0   0.0 298.0  1
  671  2-oxabicyclo 2.2.2 octan-3-one
C 7  H10  O 2                   70.0   0.0   0.0   0.0  1
  672  2,4,10-trioxaadamantane
C 7  H10  O 3                   74.0   0.0   0.0 298.0  1
  673  trimethylsuccinic anhydride
C 7  H10  O 3                   74.0   0.0   0.0   0.0  1
  674  4,5-tetramethylene-1,3-dithiolan-2-thione
C 7  H10  S 3                  104.0   0.0   0.0 298.0  1
  675  1,N,N-trimethylcytosine
C 7  H11  N 3  O 1             111.0   0.0   0.0   0.0  1
  676  1,5,N-trimethylcytosine
C 7  H11  N 3  O 1             108.0   0.0   0.0 414.0  1
  677  1,5-dimethyl-N-methoxycytosine
C 7  H11  N 3  O 2              96.0   0.0   0.0 335.0  0
  678  1,1,1,4,4-pentanitro-2,2-dimethylpentane
C 7  H11  N 5  O10             104.0   0.0   0.0 298.0  0
  679  bicyclo 2.2.1heptane norbornane                        QQQAPG
C 7  H12                        40.1   0.0   0.0 298.0  7
  680  2-chloro-4,6-bis  ETamino -s-triazine
C 7  H12 Cl 1  N 5             130.0   0.0   0.0 338.0  1
  681  1,4-dimethyl-2,6,7-trioxabicyclo 2.2.2octane
C 7  H12  O 3                   75.0   0.0   0.0 298.0  0
  682  heptanedioic acid                                      PIMELA
C 7  H12  O 4                  140.0   0.0   0.0 298.0  1
  683  butylmalonic ACID
C 7  H12  O 4                  125.0   0.0   0.0 298.0  0
  684  1-azabicyclooctane
C 7  H13  N 1                   51.0   0.0   0.0 298.0  2
  685  trans-6-heptenoic
C 7  H13  N 1  O 1              97.2   0.0   0.0 378.0  1
  686  cycloheptane
C 7  H14                        54.0   0.0   0.0 134.0  0
  687  3,3,5,5-tetramethyl-1-pyrazoline
C 7  H14  N 2                   62.0   0.0   0.0 298.0  0
  688  N-acetylLvalinamide                                    JEXNAB
C 7  H14  N 2  O 2             133.0   0.0   0.0 298.0  2
  689  2-methyl-2  methylthio propanal,
C 7  H14  N 2  O 2  S 1         80.0   0.0   0.0 311.0  1
  690  1-methylcyclohexanol
C 7  H14  O 1                   76.0   0.0   0.0 291.0  0
  691  heptane                                                HEPTAN
C 7  H16                        58.0   0.0   0.0 183.0  0
  692  1,3-propylthiourea
C 7  H16  N 2  S 1             134.0   0.0   0.0 298.0  2
  693  2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile
C 8 Cl 4  N 2                  109.0   0.0   0.0 391.0  1
  694  perfluorooctanoic
C 8  H 1  F15  O 2              88.9   0.0   0.0 308.0  1
  695  2,3,6,7-tetrachloroquinoxaline
C 8  H 2 Cl 4  N 2             108.0   0.0   0.0 298.0  2
  696  2,3-dichloroquinoxaline
C 8  H 4 Cl 2  N 2              92.4   0.0   0.0 298.0  2
  697  1,2-dicyanobenzene                                     YUYPUD
C 8  H 4  N 2                   87.0   0.0   0.0 298.0  0
  698  1,3-dicyanobenzene                                     OBIZEE
C 8  H 4  N 2                   90.0   0.0   0.0 298.0  0
  699  1,4-dicyanobenzene                                     TEPNIT
C 8  H 4  N 2                   90.0   0.0   0.0 298.0  2
  700  1,4-dicyanobenzene diN-oxid
C 8  H 4  N 2  O 2              73.0   0.0   0.0 298.0  0
  701  benzocyclobutenedione                                  BZCBUO
C 8  H 4  O 2                   89.5   0.0   0.0 336.0  1
  702  phthalic anhydride                                     PHTHAO
C 8  H 4  O 3                   88.0  84.4  88.4 330.0  3
  703  1,1,1-triF-4-2-thienyl-4-mercapto-3-buten-2-one
C 8  H 5  F 3  O 1  S 2         95.0   0.0   0.0 298.0  0
  704  1,1,1-triF-4-  2-thienyl -4-OH-3-buten-2-one
C 8  H 5  F 3  O 2  S 1         86.0   0.0   0.0 298.0  0
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  705  4,4,4-trifluoro-1-  2-furanyl -butane-1,3-dione
C 8  H 5  F 3  O 3              70.0   0.0   0.0 298.0  0
  706  benzoylnitrile
C 8  H 5  N 1  O 1              78.7   0.0   0.0 298.0  1
  707  phthalimide                                          PHALIM
C 8  H 5  N 1  O 2             106.0   0.0   0.0 298.0  1
  708  1H-indole-2,3-dione
C 8  H 5  N 1  O 2             119.0   0.0   0.0 298.0  0
  709  5-cyano-1,3-benzodioxole
C 8  H 5  N 1  O 2              91.0   0.0   0.0 298.0  0
  710  2-cyanobenzoic acid
C 8  H 5  N 1  O 2             115.0   0.0   0.0 298.0  0
  711  3-cyanobenzoic acid
C 8  H 5  N 1  O 2             116.0   0.0   0.0 298.0  0
  712  4-cyanobenzoic acid                                  TAGNAR
C 8  H 5  N 1  O 2             113.0   0.0   0.0 298.0  0
  713  isatoic anhydride
C 8  H 5  N 1  O 3             116.0   0.0   0.0 298.0  0
  714  2H-1,3-benzoxazine-2,4  3H -dione                   BOXAZD
C 8  H 5  N 1  O 3             114.0   0.0   0.0 298.0  0
  715  pyridinium dicyanomethyl ide                         PYRCYN
C 8  H 5  N 3                  125.0 125.0 125.0 411.5  2
  716  2-nitrobenzeneacetyl chloride
C 8  H 6 Cl 1  N 1  O 3        104.0   0.0   0.0 311.0  0
  717  3-nitrobenzeneacetyl chloride
C 8  H 6 Cl 1  N 1  O 3        109.0   0.0   0.0 314.0  0
  718  2,4-dichlorophenoxy acetic                           CPXACA
C 8  H 6 Cl 2  O 3             120.0 115.0 125.0 298.0  3
  719  phthalazine                                          DAZNAP
C 8  H 6  N 2                   82.0   0.0   0.0 298.0  2
  720  quinoxaline  1,4                                    HEYJOK
C 8  H 6  N 2                   68.0   0.0   0.0 298.0  2
  721  quinazoline
C 8  H 6  N 2                   77.0   0.0   0.0 298.0  2
  722  2-hydroxyquinoxaline                                 HQOXAL
C 8  H 6  N 2  O 1             124.0 119.0 126.0 391.0  2
  723  1-(2H)-phthalazinone                                 WIGYIV
C 8  H 6  N 2  O 1             107.0   0.0   0.0 298.0  1
  724  2,3-dihydroxyquinoxaline
C 8  H 6  N 2  O 2             156.0   0.0   0.0 298.0  0
  725  quinoxaline-1,4-dioxide
C 8  H 6  N 2  O 2             112.0   0.0   0.0   0.0  0
  726  3-aminophthalimide
C 8  H 6  N 2  O 2             108.0   0.0   0.0 401.0  1
  727  4-aminophthalimide                                   MODYAG
C 8  H 6  N 2  O 2             135.0   0.0   0.0 459.0  1
  728  5-nitroindole
C 8  H 6  N 2  O 2             110.0   0.0   0.0 298.0  1
  729  monobenzo-1,3 ,4,6 -tetraazapentalene
C 8  H 6  N 4                   74.9   0.0   0.0 348.0  1
  730  monobenzo-1,3 ,6,6 -tetraazapentalene
C 8  H 6  N 4                   63.6   0.0   0.0 353.0  1
  731  piperonal
C 8  H 6  O 3                   90.8   0.0   0.0 323.0  1
  732  phthalic acid                                        PHTHAC
C 8  H 6  O 4                  130.0   0.0   0.0 298.0  0
  733  isophthalic acid                                     BENZDC
C 8  H 6  O 4                  142.0   0.0   0.0 298.0  2
  734  terephthalic acid                                    TEPHTH
C 8  H 6  O 4                  146.0   0.0   0.0 298.0  2
  735  1,3-benzodioxole-5-carboxylic
C 8  H 6  O 4                  117.0   0.0   0.0 298.0  1
  736  benzo (b)thiophene
C 8  H 6  S 1                   66.0   0.0   0.0 298.0  0
  737  2,2  -bithiophene                                    DTENYL
C 8  H 6  S 2                   85.6   0.0   0.0 298.0  1
  738  3,3  -bithiophene
C 8  H 6  S 2                   88.9   0.0   0.0 298.0  1
  739  2-chloroacetophenone
C 8  H 7 Cl 1  O 1              90.7   0.0   0.0 293.0  1
  740  indole                                               INDOLE
C 8  H 7  N 1                   76.0  70.0  78.0 298.0  5
  741  2H-1,4-benzoxazin-3  4H -one
C 8  H 7  N 1  O 2             106.0   0.0   0.0 298.0  0
  742  3-nitroacetophenone
C 8  H 7  N 1  O 3             110.0   0.0   0.0 208.0  0
  743  2,3-dihydro-6-nitro-1,4-benzodioxin
C 8  H 7  N 1  O 4             101.0   0.0   0.0 298.0  0
  744  2-methyl-3-nitrobenzoic acid
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C 8  H 7  N 1  O 4            120.0   0.0   0.0 298.0  0
  745  2-methyl-6-nitrobenzoic acid
C 8  H 7  N 1  O 4            120.0   0.0   0.0 298.0  0
  746  3-methyl-2-nitrobenzoic acid                          JONPUZ
C 8  H 7  N 1  O 4            124.0   0.0   0.0 298.0  0
  747  3-methyl-4-nitrobenzoic acid                          TOYGIZ
C 8  H 7  N 1  O 4            119.0   0.0   0.0 298.0  0
  748  4-methyl-3-nitrobenzoic acid
C 8  H 7  N 1  O 4            119.0   0.0   0.0 298.0  0
  749  2-methyl-3-nitrobenzoic acid
C 8  H 7  N 1  O 4            119.0   0.0   0.0 298.0  0
  750  3-methoxy-2-nitrobenzoic acid
C 8  H 7  N 1  O 5            142.0   0.0   0.0 298.0  0
  751  4-methoxy-3-nitrobenzoic acid
C 8  H 7  N 1  O 5            131.0   0.0   0.0 298.0  0
  752  3-methoxy-4-nitrobenzoic acid
C 8  H 7  N 1  O 5            131.0   0.0   0.0 298.0  1
  753  3,6-diaminophthalimide
C 8  H 7  N 3  O 2             98.5   0.0   0.0 485.0  1
  754  2,2,2-trinitro-1-phenylethane
C 8  H 7  N 3  O 6             84.1   0.0   0.0 301.0  1
  755  3-methyl-2,4,6-trinitrotoluene
C 8  H 7  N 3  O 6            129.0   0.0   0.0 365.0  1
  756  2,4,6-trinitrophenetole                               TNPHNT
C 8  H 7  N 3  O 7            121.0   0.0   0.0 340.0  1
  757  cubane                                                CUBANE
C 8  H 8                       55.0   0.0   0.0 298.0  1
  758  cyclooctatetraene
C 8  H 8                       54.0   0.0   0.0   0.0  0
  759  4-bromoacetanilide
C 8  H 8 Br 1  N 1  O 1       110.0   0.0   0.0 298.0  0
  760  2-amino-5-methoxybenzoic acid
C 8  H 8  N 1  O 3            119.0 116.0 119.0 298.0  2
  761  3-amino-4-methoxybenzoic acid
C 8  H 8  N 1  O 3            131.0 127.0 130.0 298.0  2
  762  3-amino-5-methoxybenzoic acid
C 8  H 8  N 1  O 3            136.0 132.0 136.0 298.0  2
  763  4-amino-3-methoxybenzoic acid
C 8  H 8  N 1  O 3            132.0 128.0 132.0 298.0  2
  764  5-nitroindoline
C 8  H 8  N 2  O 2            109.0   0.0   0.0 298.0  1
  765  1,2-benzenedicarboxamide
C 8  H 8  N 2  O 2             57.0   0.0   0.0   0.0  0
  766  1,3-benzenedicarboxamide
C 8  H 8  N 2  O 2             54.0   0.0   0.0   0.0  0
  767  1,4-benzenedicarboxamide                              TRPHAM
C 8  H 8  N 2  O 2             57.3   0.0   0.0 436.0  1
  768  4-hydroxyacetophenone                                 HACTPH
C 8  H 8  O 2                  96.0   0.0   0.0 335.0  1
  769  2,5dimethyl1,4benzoquinone                            DMEBQU
C 8  H 8  O 2                  77.0   0.0   0.0 283.0  0
  770  o-toluic acid                                         OTOLIC
C 8  H 8  O 2                  96.0   0.0   0.0 298.0  0
  771  m-toluic acid                                         ZZZKWI
C 8  H 8  O 2                  97.0   0.0   0.0 298.0  0
  772  p-toluic acid                                         PTOLIC
C 8  H 8  O 2                  99.0   0.0   0.0 298.0  2
  773  phenyl vinyl sulfone
C 8  H 8  O 2  S 1             82.0   0.0   0.0   0.0  0
  774  4-hydroxybenzoic acid methyl ester
C 8  H 8  O 3                  98.0   0.0   0.0 298.0  1
  775  2-hydroxy-3-methoxybenzaldehyde                       OVANIL
C 8  H 8  O 3                  54.1   0.0   0.0 293.0  1
  776  4-hydroxy-3-methoxybenzaldehyde                       YUHTEA
C 8  H 8  O 3                  88.7   0.0   0.0 323.0  1
  777  2-methoxybenzoic acid                                 FUFBOX
C 8  H 8  O 3                 107.0 101.0 111.0 298.0  3
  778  3-methoxybenzoic acid                                 EFINEO
C 8  H 8  O 3                 114.0 108.0 115.0 330.0  2
  779  4-methoxybenzoic acid                                 ANISIC
C 8  H 8  O 3                 111.0   0.0   0.0 298.0  2
  780  1,3-benzodioxole-5-methanol
C 8  H 8  O 3                 103.0   0.0   0.0 298.0  2
  781  acetanilide                                           ACANIL
C 8  H 9  N 1  O 1             83.0  81.0  87.0 298.0  2
  782  2-phenylacetamide
C 8  H 9  N 1  O 1             96.0   0.0   0.0 340.0  0
  783  4-aminoacetophenone                                   AMACPH
C 8  H 9  N 1  O 1             92.7   0.0   0.0 326.0  1
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  784  N-methylbenzamide                                                MBNZAM
C 8  H 9  N 1  O 1              83.0  75.0  86.0 310.0  2
  785  methyl-2-aminobenzoate
C 8  H 9  N 1  O 2              78.4   0.0   0.0 293.0  1
  786  2-amino-3-methylbenzoic acid                                     AMEBAC
C 8  H 9  N 1  O 2             107.0   0.0   0.0 298.0  1
  787  2-amino-5-methylbenzoic acid
C 8  H 9  N 1  O 2             111.0   0.0   0.0 298.0  1
  788  2-amino-6-methylbenzoic acid
C 8  H 9  N 1  O 2             116.0   0.0   0.0 298.0  1
  789  3-amino-2-methylbenzoic acid
C 8  H 9  N 1  O 2             127.0   0.0   0.0 298.0  1
  790  3-amino-4-methylbenzoic acid
C 8  H 9  N 1  O 2             119.0   0.0   0.0 298.0  1
  791  4-amino-3-methylbenzoic acid
C 8  H 9  N 1  O 2             122.0   0.0   0.0 298.0  1
  792  1,2-dimethylbenzene
C 8  H10                        60.0   0.0   0.0 248.0  0
  793  1,4-dimethylbenzene                                              ZZZITY
C 8  H10                        60.0   0.0   0.0 267.0  2
  794  4-N,N-dimethylaminoNObenzene
C 8  H10  N 2  O 1              82.0   0.0   0.0 298.0  1
  795  3-nitro-N,N-dimethylaniline                                      MNTDMA
C 8  H10  N 2  O 2              93.0   0.0   0.0 298.0  0
  796  N,N-dimethyl-4-nitroaniline                                      DIMNAN
C 8  H10  N 2  O 2             102.0   0.0   0.0 298.0  2
  797  2,3-dimethylphenol                                               DIMPHE
C 8  H10  O 1                   84.0   0.0   0.0 303.0  1
  798  2,5-dimethylphenol                                               DMPHOL
C 8  H10  O 1                   85.0   0.0   0.0 303.0  1
  799  2,6-dimethylphenol                                               DMEPOL
C 8  H10  O 1                   75.6   0.0   0.0 295.0  1
  800  3,4-dimethylphenol                                               DPHNOL
C 8  H10  O 1                   85.7   0.0   0.0 303.0  1
  801  3,5-dimethylphenol
C 8  H10  O 1                   83.0   0.0   0.0 298.0  0
  802  2-ETphenol
C 8  H10  O 1                   80.0   0.0   0.0 298.0  0
  803  2,5-dimethylhydroquinone
C 8  H10  O 2                  101.0   0.0   0.0 330.0  0
  804  1,4-dimethoxybenzene                                             MOXBEN
C 8  H10  O 2                   84.0   0.0   0.0 298.0  0
  805  2,6-dimethoxyphenol
C 8  H10  O 3                   98.0   0.0   0.0 298.0  0
  806  3,5-dimethoxyphenol
C 8  H10  O 3                  101.0   0.0   0.0 298.0  0
  807  1-norbornylisocyanide
C 8  H11  N 1                   61.0   0.0   0.0 298.0  0
  808  8-Ethyl-9-methyladenine                                          VAYJIO
C 8  H11  N 5                  115.0   0.0   0.0 368.0  1
  809  6,8,9-trimethyladenine
C 8  H11  N 5                   98.6   0.0   0.0 338.0  1
  810  N,N,9-trimethyladenine
C 8  H11  N 5                  101.0   0.0   0.0 334.0  1
  811  bicyclo 2.2.2octene
C 8  H12                        44.0   0.0   0.0   0.0  0
  812  tetramethylsuccinonitrile                                        BISJAO
C 8  H12  N 2                   81.0   0.0   0.0   0.0  0
  813  tetramethylpyrazine                                              MPYRAZ
C 8  H12  N 2                   95.0   0.0   0.0 298.0  0
  814  1-cyanoacetyl piperidine
C 8  H12  N 2  O 1             104.0   0.0   0.0 298.0  0
  815  1,3-dimethyl-5-ETuracil
C 8  H12  N 2  O 2             105.0  98.7 110.0 312.5  2
  816  4,4-dimethyl-1,3-cyclohexanedione
C 8  H12  O 2                   99.0   0.0   0.0 298.0  0
  817  5,5-dimethyl-1,3-cyclohexanedione                                DIMEDO
C 8  H12  O 2                  100.0   0.0   0.0 298.0  0
  818  2,2,4,4-tetramethyl-1,3-cyclobutanedione                         DMKETD
C 8  H12  O 2                   71.0  70.0  72.0   0.0  3
  819  5,5  -diEthylbarbituric
C 8  H13  N 2  O 3             117.0   0.0   0.0 298.0  1
  820  bicyclo 2.2.2 octane
C 8  H14                        48.0   0.0   0.0 298.0  3
  821  3,4-dimethylhexadiene
C 8  H14                        53.0   0.0   0.0   0.0  0
  822  2 Cl-4-ETamino-6-isopropylamino-1,3,5-triazine
C 8  H14 Cl 1  N 5             114.0   0.0   0.0 338.0  2
  823  1,4-dimethyl-2,3-diazabicyclo 2.2.2 octane
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C 8  H14  N 2                   72.0   0.0   0.0 298.0  0
  824  3-oxabicyclo 3.2.2nonane
C 8  H14  O 1                   53.0   0.0   0.0   0.0  0
  825  octanedioic                                       SUBRAC
C 8  H14  O 4                  148.0   0.0   0.0 298.0  1
  826  3-azabicyclo 3.2.2nonane                          ZBCNON
C 8  H15  N 1                   58.0   0.0   0.0 298.0  0
  827  trans 2octenoic acid amide
C 8  H15  N 1  O 1              73.5   0.0   0.0 383.0  1
  828  2-methoxy-4,6-bis Ethylamino -1,3,5-triazine
C 8  H15  N 5  O 1              98.2   0.0   0.0 338.0  1
  829  2-methylthio-4,6-bis Ethylamino -1,3,5-triazine
C 8  H15  N 5  S 1             101.0   0.0   0.0 339.0  1
  830  2-methylthio-4-methylamino-6-isopropyl-1,3,5-tria
C 8  H15  N 5  S 1             101.0   0.0   0.0 340.0  1
  831  cyclooctane
C 8  H16                        59.0   0.0   0.0 166.0  0
  832  octanoic                                          ISENUP
C 8  H16  O 2                  113.0   0.0   0.0 298.0  0
  833  octanamide
C 8  H17  N 1  O 1              110.0   0.0   0.0 350.0  1
  834  octane                                            OCTANE
C 8  H18                        68.0   0.0   0.0 216.0  0
  835  2,2,3,3-tetramethylbutane
C 8  H18                        43.0   0.0   0.0 298.0  3
  836  1,4-bis-  2-hydroxyEthyl piperazine
C 8  H18  N 2  O 2             130.0   0.0   0.0 298.0  0
  837  1-octanol                                         ZZZVYK
C 8  H18  O 1                  100.0   0.0   0.0 298.0  0
  838  1,8-octanediol                                    QATVEM
C 8  H18  O 2                  139.0   0.0   0.0 298.0  0
  839  di-n-butyl sulfone
C 8  H18  O 2  S 1             100.0   0.0   0.0   0.0  0
  840  di-tert-butyl sulfone
C 8  H18  O 2  S 1              94.0   0.0   0.0   0.0  0
  841  7-bromo-5-chloro-8-hydroxyquinoline
C 9  H 5 Br 1 Cl 1  N 1  O 1   113.0   0.0   0.0 298.0  1
  842  5,7-dibromo-8-hydroxyquinoline
C 9  H 5 Br 2  N 1  O 1        117.0   0.0   0.0 298.0  1
  843  5-chloro-7-iodo-8-hydroxyquinoline
C 9  H 5 Cl 1  I 1  N 1  O 1   115.0   0.0   0.0 298.0  1
  844  5-iodo-7-chloro-8-hydroxyquinoline
C 9  H 5 Cl 1  I 1  N 1  O 1   131.0   0.0   0.0 400.0  1
  845  4,7-dichloroquinoline
C 9  H 5 Cl 2  N 1              90.0   0.0   0.0 298.0  1
  846  5,7-dichloro-8-hydroxyquinoline
C 9  H 5 Cl 2  N 1  O 1        109.0   0.0   0.0 298.0  1
  847  5,7-diiodo-8-hydroxyquinoline
C 9  H 5  I 2  N 1  O 1        127.0   0.0   0.0 298.0  1
  848  2-chloroquinoline                                 CHLQUI
C 9  H 6 Cl 1  N 1              84.0   0.0   0.0 298.0  1
  849  4-chloroquinoline
C 9  H 6 Cl 1  N 1              79.0   0.0   0.0 298.0  1
  850  6-chloroquinoline                                 CLQUIN
C 9  H 6 Cl 1  N 1              81.0   0.0   0.0 298.0  1
  851  5-chloro-8-hydroxyquinoline                       FAMDIG
C 9  H 6 Cl 1  N 1  O 1        112.0 111.0 114.0 298.0  2
  852  N-chloromethylphthalimide
C 9  H 6 Cl 1  N 1  O 2        104.0   0.0   0.0 298.0  1
  853  5-iodo-8-hydroxyquinoline
C 9  H 6  I 1  N 1  O 1        118.0   0.0   0.0 378.0  1
  854  5-nitroquinoline
C 9  H 6  N 2  O 2              93.7   0.0   0.0 298.0  2
  855  6-nitroquinoline
C 9  H 6  N 2  O 2             104.0   0.0   0.0 298.0  2
  856  8-nitroquinoline                                  UPAJIF
C 9  H 6  N 2  O 2             107.0   0.0   0.0 298.0  2
  857  5-nitro-8-hydroxyquinoline
C 9  H 6  N 2  O 3             111.0   0.0   0.0 298.0  1
  858  3-amino-2-quinoxalinecarbonitrile
C 9  H 6  N 4  O 2             140.0   0.0   0.0 298.0  1
  859  coumarin                                          COUMAR
C 9  H 6  O 2                   92.2  86.0  95.0 300.0  3
  860  chromone
C 9  H 6  O 2                   84.0  81.0  87.0 298.0  2
  861  1,3-indandione                                    INDDON
C 9  H 6  O 2                   97.0   0.0   0.0 298.0  1
  862  1,3,5-benzenetricarboxylic acid
C 9  H 6  O 6                  159.0   0.0   0.0 573.0  1
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863 5-phenyl-1,2-dithiole-3-thione FABPON
C 9 H 6 S 3 123.0 0.0 0.0 298.0 1
864 2-hydroxyquinoline
C 9 H 7 N 1 O 1 119.0 0.0 0.0 298.0 1
865 4-hydroxyquinoline
C 9 H 7 N 1 O 1 135.0 0.0 0.0 298.0 1
866 8-hydroxyquinoline HXQUIN
C 9 H 7 N 1 O 1 99.0 90.0 109.0 298.0 2
867 1-hydroxyisoquinoline
C 9 H 7 N 1 O 1 114.0 0.0 0.0 298.0 1
868 5-hydroxyisoquinoline
C 9 H 7 N 1 O 1 110.0 0.0 0.0 298.0 1
869 □-cyanoacetophenone
C 9 H 7 N 1 O 1 97.0 93.0 100.0 300.0 2
870 1,5-dihydroxyisoquinoline
C 9 H 7 N 1 O 2 124.0 0.0 0.0 0.0 1
871 N-methylphthalimide
C 9 H 7 N 1 O 2 91.0 0.0 0.0 298.0 1
872 1-methyl-1H-indole-2,3-dione ZZZPRC
C 9 H 7 N 1 O 2 106.0 0.0 0.0 298.0 1
873 5-amino-6-nitroquinoline
C 9 H 7 N 3 O 2 136.0 0.0 0.0 298.0 1
874 2-2,4-dichlorophenoxy propanoic acid
C 9 H 8 Cl 2 O 3 122.0 116.0 13.0 298.0 2
875 3-aminoquinoline SECQEY
C 9 H 8 N 2 104.0 0.0 0.0 298.0 1
876 5-aminoquinoline
C 9 H 8 N 2 104.0 0.0 0.0 298.0 1
877 6-aminoquinoline
C 9 H 8 N 2 106.0 0.0 0.0 298.0 1
878 8-aminoquinoline NONMEI
C 9 H 8 N 2 93.0 0.0 0.0 298.0 1
879 2-methyl-3-hydroxyquinoxaline
C 9 H 8 N 2 O 1 121.0 120.0 123.0 298.0 2
880 2-methylquinoxaline-1,4-dioxide
C 9 H 8 N 2 O 2 107.0 0.0 0.0 298.0 1
881 3-methylaminophthalimide
C 9 H 8 N 2 O 2 105.0 0.0 0.0 417.0 1
882 1-indanone
C 9 H 8 O 1 82.0 79.0 84.0 298.0 2
883 2-indanone
C 9 H 8 O 1 78.0 0.0 0.0 298.0 1
884 trans cinnamic acid CINMAC
C 9 H 8 O 2 107.0 0.0 0.0 298.0 1
885 chromanone
C 9 H 8 O 2 85.0 0.0 0.0 298.0 1
886 3-isochromanone
C 9 H 8 O 2 97.0 0.0 0.0 298.0 1
887 phenyl propadienyl sulfone
C 9 H 8 O 2 S 1 105.0 0.0 0.0 0.0 1
888 phenyl prop-1-ynyl sulfone
C 9 H 8 O 2 S 1 95.0 0.0 0.0 0.0 1
889 phenyl prop-2-ynyl sulfone
C 9 H 8 O 2 S 1 105.0 0.0 0.0 0.0 1
890 endo-5-norbornene-2,3-dicarboxylic anhydride NBORAN
C 9 H 8 O 3 97.0 0.0 0.0 298.0 1
891 5-oxoET-1,3-benzodioxole
C 9 H 8 O 3 104.0 0.0 0.0 298.0 1
892 2,3-dihydro-1,4-benzodioxin-6-carboxaldehyde
C 9 H 8 O 3 98.0 0.0 0.0 298.0 1
893 3,4-dihydroxycinnamic acid caffeic acid FESNOG
C 9 H 8 O 4 170.0 0.0 0.0 411.0 1
894 monomethyl terephthalate
C 9 H 8 O 4 124.0 121.0 130.0 298.0 3
895 monomethyl phthalate
C 9 H 8 O 4 118.0 0.0 0.0 298.0 1
896 monomethyl isophthalate
C 9 H 8 O 4 126.0 0.0 0.0 298.0 1
897 1,3-benzodioxole-5-acetic acid
C 9 H 8 O 4 123.0 0.0 0.0 298.0 1
898 dl 1,4benzodioxan-2-carboxylic acid
C 9 H 8 O 4 118.0 0.0 0.0 298.0 1
899 2-methylindole
C 9 H 9 N 1 89.0 0.0 0.0 0.0 1
900 3-methylindole
C 9 H 9 N 1 87.0 83.0 90.0 298.0 2
901 2,6-dimethylbenzonitrile JIBDON
C 9 H 9 N 1 84.0 0.0 0.0 298.0 1
902 4-acetomidobenzaldehyde

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C 9  H 9  N 1  O 2              99.0   0.0   0.0 337.0  1
  903  dimethylpyreidine-2,6-dicarboxylate
C 9  H 9  N 1  O 4             114.0   0.0   0.0 298.0  1
  904  2,4,6-trinitromesitylene                                HEXTIN
C 9  H 9  N 3  O 6             104.0   0.0   0.0 350.0  1
  905  3-(3,4-dichlorophenyl -1,1-dimethylurea
C 9  H10 Cl 2  N 2  O 1        134.0   0.0   0.0 298.0  1
  906  1-phenyl-3-pyrazolidinone
C 9  H10  N 2  O 1              84.0   0.0   0.0 338.0  1
  907  (E) -3-phenyl-2-propen-1-ol
C 9  H10  O 1                  110.0   0.0   0.0 298.0  1
  908  chroman
C 9  H10  O 1                   57.0   0.0   0.0 298.0  1
  909  isochroman
C 9  H10  O 1                   57.0   0.0   0.0 298.0  1
  910  methyl-p-toluate
C 9  H10  O 2                   83.0   0.0   0.0 298.0  1
  911  4-acetylanisole
C 9  H10  O 2                   94.0   0.0   0.0 308.0  1
  912  3-phenylpropionic acid
C 9  H10  O 2                  102.0   0.0   0.0 298.0  1
  913  3-methylphenyl acetate
C 9  H10  O 2                   60.7   0.0   0.0 296.0  1
  914  2-ethylbenzoic acid
C 9  H10  O 2                  101.0   0.0   0.0 298.0  1
  915  3-ethylbenzoic acid
C 9  H10  O 2                   99.0   0.0   0.0 298.0  1
  916  4-ethylbenzoic acid
C 9  H10  O 2                   98.0   0.0   0.0 298.0  1
  917  2,3-dimethylbenzoic acid                                DMBZAC
C 9  H10  O 2                  105.0   0.0   0.0 298.0  1
  918  2,4-dimethylbenzoic acid                                WIZJUL
C 9  H10  O 2                  104.0   0.0   0.0 298.0  1
  919  2,5-dimethylbenzoic acid
C 9  H10  O 2                  105.0   0.0   0.0 298.0  1
  920  2,6-dimethylbenzoic acid                                DMBNZA
C 9  H10  O 2                   99.0   0.0   0.0 298.0  1
  921  3,4-dimethylbenzoic acid
C 9  H10  O 2                  106.0   0.0   0.0 298.0  1
  922  3,5-dimethylbenzoic acid
C 9  H10  O 2                  102.0   0.0   0.0 298.0  1
  923  p-tolyl vinyl sulfone
C 9  H10  O 2  S 1              82.0   0.0   0.0   0.0  1
  924  3-ethoxy-4-hydroxybenzadehyde
C 9  H10  O 3                  101.0   0.0   0.0 311.0  1
  925  4-ethoxybenzoic acid                                    PEXBZA
C 9  H10  O 3                  123.0   0.0   0.0 298.0  1
  926  1,4-benzodioxan-2-hydroxymethyl
C 9  H10  O 3                  107.0   0.0   0.0 298.0  1
  927  2,3-dimethoxybenzoic acid                               OVERAT
C 9  H10  O 4                  117.0   0.0   0.0 298.0  1
  928  2,4-dimethoxybenzoic acid                               ISUQUI
C 9  H10  O 4                  123.0   0.0   0.0 298.0  1
  929  2,6-dimethoxybenzoic acid                               DMOXBA
C 9  H10  O 4                  122.0   0.0   0.0 298.0  1
  930  3,4-dimethoxybenzoic acid                               DMXBZA
C 9  H10  O 4                  130.0   0.0   0.0 298.0  1
  931  2,5-dimethoxybenzoic acid                               ISURAP
C 9  H10  O 4                  116.0   0.0   0.0 298.0  1
  932  3,5-dimethoxybenzoic acid                               HEKMOZ
C 9  H10  O 4                  127.0   0.0   0.0 298.0  1
  933  2-  diacetoxymethyl furan
C 9  H10  O 5                  110.0   0.0   0.0   0.0  1
  934  3-  4-chlorophenyl -1,1-dimethylurea
C 9  H11 Cl 1  N 2  O 1        114.0   0.0   0.0 341.0  1
  935  N-  2-methylphenyl acetamide                           REZRIY
C 9  H11  N 1  O 1              97.0   0.0   0.0 328.0  1
  936  N-  4-methylphenyl acetamide                           ACTOLD
C 9  H11  N 1  O 1              99.0   0.0   0.0 341.0  1
  937  N,N-dimethylbenzamide                                  ODOTOQ
C 9  H11  N 1  O 1              93.0  90.0  95.0 298.0  2
  938  2,4,6-trimethylnitrobenzene
C 9  H11  N 1  O 2              79.0   0.0   0.0 298.0  1
  939  3-ethoxyphenylurea
C 9  H12  N 2  O 2              75.0   0.0   0.0   0.0  1
  940  4-ethoxyphenylurea
C 9  H12  N 2  O 2              84.0   0.0   0.0   0.0  1
  941  2,3,6-trimethylphenol
C 9  H12  O 1                   88.0   0.0   0.0 298.0  1
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  942  2,4,6-trimethylphenol                                          XAXSIY
C 9  H12  O 1                  90.0  83.0  95.0 298.0  2
  943  a-a-dimethylbenzyl alcohol
C 9  H12  O 1                  83.0   0.0   0.0 298.0  0
  944  3-isopropyl-1,2-dihydroxybenzene
C 9  H12  O 2                  98.0   0.0   0.0 298.0  0
  945  1,2,3-trimethoxybenzene
C 9  H12  O 3                  98.0   0.0   0.0 298.0  0
  946  1,3,5-trimethoxybenzene                                        TMOXBZ
C 9  H12  O 3                 100.0   0.0   0.0 298.0  0
  947  3,3-tetramethyleneglutaric acid anhydride
C 9  H12  O 3                  96.0   0.0   0.0 298.0  0
  948  3,3-tetramethyleneglutarimide
C 9  H13  N 1  O 2             107.0   0.0   0.0 298.0  0
  949  6,9-dimethyl-8-ethyladenine
C 9  H13  N 5                  94.1   0.0   0.0 348.0  1
  950  8-propyl-9-methyladenine
C 9  H13  N 5                 124.0   0.0   0.0 367.0  0
  951  bicyclo 3.2.2non-6-ene
C 9  H14                       48.0   0.0   0.0 298.0  0
  952  bicyclo 3.3.1non-2-ene
C 9  H14                       48.0   0.0   0.0 298.0  0
  953  bicyclo 4.2.1non-3-ene
C 9  H14                       50.0   0.0   0.0 298.0  0
  954  1,3-dimethyl-5-propyluracil
C 9  H14  N 2  O 2             111.0   0.0   0.0 322.0  1
  955  1,3-dimethyl-5-isopropyluracil
C 9  H14  N 2  O 2             103.0   0.0   0.0 322.0  1
  956  1,3-diethylthymine
C 9  H14  N 2  O 2              93.0  90.0  95.0 316.0  2
  957  3-oxononanedioic
C 9  H14  O 5                  118.0   0.0   0.0   0.0  0
  958  bicyclo 3.3.1nonane
C 9  H16                       51.0   0.0   0.0 298.0  0
  959  2-methyl-2-piperidinopropionitrile                             DMPIPA
C 9  H16  N 2                  80.0   0.0   0.0 298.0  0
  960  nonanedioic acid azelaic                                       AZELAC
C 9  H16  O 4                  160.0   0.0   0.0 298.0  1
  961  2,2,6,6-tetramethyl-4-oxopiperidine
C 9  H17  N 1  O 1              61.0   0.0   0.0   0.0  0
  962  trans2-nonenoic acid amide
C 9  H17  N 1  O 1             111.0   0.0   0.0 388.0  1
  963  2,2,6,6-tetramethyl-1-hydroxy-4-oxopiperidine
C 9  H17  N 1  O 2              80.0   0.0   0.0 308.0  1
  964  2,2,6,6-tetramethyl-4-hydroxypiperidine-1-oxyl
C 9  H18  N 1  O 2             101.0   0.0   0.0 306.0  1
  965  N,N-diethyl-N  -isobutanoylthiourea
C 9  H18  N 2  O 1  S 1        121.0   0.0   0.0 298.0  0
  966  di-tert-butylcarbonate
C 9  H18  O 3                   65.0   0.0   0.0 298.0  0
  967  nonanamide
C 9  H19  N 1  O 1             114.0   0.0   0.0 362.0  1
  968  2,2,6,6-tetramethyl-1,4-dihydroxypiperidine
C 9  H19  N 1  O 2             100.0   0.0   0.0 333.0  1
  969  nonane                                                         QQQFAY
C 9  H20                        75.0   0.0   0.0 219.0  0
  970  1,3-dibutylurea
C 9  H20  N 2  O 1              90.0   0.0   0.0 350.0  0
  971  1,3-butylthiourea                                              UPACIY
C 9  H20  N 2  S 1             140.0 137.0 141.0 298.0  2
  972  1,9-nonanediol
C 9  H20  O 2                  149.0   0.0   0.0   0.0  0
  973  octafluoronaphthalene
C10  F 8                        79.4   0.0   0.0 308.0  1
  974  1,2,4,5-benzenetetracarboxylic acid anhydride                  PYMDAN
C10  H 2  O 6                  122.0   0.0   0.0 298.0  0
  975  1-4-bromophenyl -1H-pyrrole-2,5-dione
C10  H 6 Br 1  N 1  O 2        105.0   0.0   0.0 360.0  1
  976  1,4-dibromonaphthalene                                         DBRNAQ
C10  H 6 Br 2                   90.8   0.0   0.0 310.0  1
  977  dimethyltetrachloroterephthalane
C10  H 6 Cl 4  O 4             104.0   0.0   0.0 391.0  1
  978  2-cyanoquinoline                                               SUZXOB
C10  H 6  N 2                   94.0   0.0   0.0 298.0  1
  979  3-cyanoquinoline
C10  H 6  N 2                   93.0   0.0   0.0 298.0  1
  980  1-  3-nitrophenyl -1H-pyrrole-2,5-dione
C10  H 6  N 2  O 4             115.0   0.0   0.0 360.0  1
  981  1-  4-nitrophenyl -1H-pyrrole-2,5-dione
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C10  H 6  N 2  O 4             117.0   0.0   0.0 360.0  1
  982  1,4-naphthoquinone                                    NAPHQU
C10  H 6  O 2                   91.0   0.0   0.0 298.0  2
  983  2-bromonaphthalene
C10  H 7 Br 1                   81.0   0.0   0.0 298.0  0
  984  benzoyltrifluoroacetone
C10  H 7  F 3  O 2              87.0   0.0   0.0 298.0  0
  985  2-iodonaphthalene
C10  H 7  I 1                   91.0   0.0   0.0   0.0  0
  986  1-nitronaphthalene
C10  H 7  N 1  O 2             102.0  95.0 107.0 298.0  3
  987  1-nitroso-2-naphthol
C10  H 7  N 1  O 2              87.0   0.0   0.0   0.0  0
  988  4-nitroso-1-naphthol
C10  H 7  N 1  O 2              87.0   0.0   0.0   0.0  0
  989  1-phenyl-1H-pyrrole-2,5-dione
C10  H 7  N 1  O 2              98.0   0.0   0.0 360.0  0
  990  azulene
C10  H 8                        83.0  76.0  95.0 300.0  0
  991  naphthalene                                           NAPHTA
C10  H 8                        73.0  71.0  76.0 298.0 20
  992  N-  2-bromoethyl phthalimide
C10  H 8 Br 1  N 1  O 2        109.0   0.0   0.0 298.0  0
  993  2,3-bis  bromomethyl quinoxaline
C10  H 8 Br 2  N 2             114.0   0.0   0.0 298.0  1
  994  N-  2-chloroethyl phthalimide
C10  H 8 Cl 1  N 1  O 2         98.0   0.0   0.0 298.0  0
  995  indole-3-acetic
C10  H 8  N 1  O 2              64.0   0.0   0.0 368.0  1
  996  2,2  -bipyridine                                      BIPYRL
C10  H 8  N 2                   80.0  75.0  82.0 298.0  3
  997  2,4  -bipyridine
C10  H 8  N 2                   88.0   0.0   0.0 298.0  0
  998  4,4  -bipyridine                                      HIQWEJ
C10  H 8  N 2                  106.0   0.0   0.0 298.0  0
  999  8-nitroquinaldine
C10  H 8  N 2  O 2             111.0   0.0   0.0 298.0  1
 1000  3-acetamidophthalimide
C10  H 8  N 2  O 3             108.0   0.0   0.0 443.0  1
 1001  1-naphthol                                            NAPHOL
C10  H 8  O 1                   90.0  84.3  93.3 298.0  4
 1002  2-naphthol                                            NAPHOB
C10  H 8  O 1                   90.0  78.7  97.8 298.0  5
 1003  1,6-oxido 10annulene
C10  H 8  O 1                   80.0   0.0   0.0   0.0  0
 1004  1,4-naphthohydroquinone                               NPHHQU
C10  H 8  O 2                  119.0   0.0   0.0 381.0  0
 1005  1,2-dihydroxynaphthalene
C10  H 8  O 2                  104.0   0.0   0.0 298.0  0
 1006  1,3-dihydroxynaphthalene                              HEGFAB
C10  H 8  O 2                  116.0   0.0   0.0 298.0  0
 1007  2,3-dihydroxynaphthalene                              VOGSEP
C10  H 8  O 2                  110.0   0.0   0.0 298.0  1
 1008  1-naphthylamine
C10  H 9  N 1                   90.0   0.0   0.0 298.0  2
 1009  2-naphthylamine
C10  H 9  N 1                   88.0   0.0   0.0 298.0  1
 1010   beta-cyanopropiophenone
C10  H 9  N 1  O 1             108.0   0.0   0.0 326.0  0
 1011  2-methyl-8-hydroxyquinoline                           YIRKOA
C10  H 9  N 1  O 1              90.0   0.0   0.0 298.0  3
 1012  2-methyl-4-hydroxyquinoline
C10  H 9  N 1  O 1             139.0   0.0   0.0 298.0  0
 1013  4-methyl-2-hydroxyquinoline
C10  H 9  N 1  O 1             128.0   0.0   0.0 298.0  0
 1014  N-ethylphthalimide
C10  H 9  N 1  O 2              91.0   0.0   0.0 298.0  0
 1015  6-methoxyquinoline N-oxide
C10  H 9  N 1  O 2             118.0   0.0   0.0 298.0  0
 1016  pentacyclo dec-9-ene  basketene
C10  H10                        55.0   0.0   0.0 298.0  0
 1017  1,4-dihydronaphthalene
C10  H10                        64.0   0.0   0.0 298.0  0
 1018  bullvalene                                            BULVAL
C10  H10                        72.0   0.0   0.0 298.0  0
 1019  1,5-diaminonaphthalene
C10  H10  N 2                  120.0 120.0 122.0 298.0  2
 1020  1,8-diaminonaphthalene                                JISVEM
C10  H10  N 2                   97.0  94.0  99.0 298.0  2
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 1021  2,3-dimethylquinoxaline                                        KEYNOR
C10  H10  N 2                   87.7   0.0   0.0 298.0  2
 1022  4-aminoquinaldine
C10  H10  N 2                  115.0   0.0   0.0 298.0  0
 1023  1-benzylimidazole                                              EYIRIN
C10  H10  N 2                  102.0   0.0   0.0 298.0  0
 1024  3-dimethylaminophthalimide
C10  H10  N 2  O 2              91.0   0.0   0.0 407.0  0
 1025  2,3-dimethylquinoxaline 1,4dioxide                             VAKJUM
C10  H10  N 2  O 2             124.0   0.0   0.0 298.0  0
 1026  1-phenyl-1,3-butanedione
C10  H10  O 2                   90.0  84.0  91.0 298.0  2
 1027  5-hydroxy- -tetralone
C10  H10  O 2                  119.0   0.0   0.0 298.0  0
 1028  6-hydroxy- -tetralone
C10  H10  O 2                  118.0   0.0   0.0 298.0  0
 1029  p-tolyl propadienylsulfone
C10  H10  O 2  S 1             113.0   0.0   0.0   0.0  0
 1030  p-tolyl prop-1-ynyl sulfone
C10  H10  O 2  S 1             103.0   0.0   0.0   0.0  0
 1031  p-tolyl prop-2-ynyl sulfone
C10  H10  O 2  S 1             107.0   0.0   0.0   0.0  0
 1032  cis-2-methoxycinnamic
C10  H10  O 3                  122.0   0.0   0.0 298.0  0
 1033  trans-2-methoxycinnamic                                        ZZZFLM
C10  H10  O 3                  129.0   0.0   0.0 298.0  0
 1034  trans-3-methoxycinnamic                                        ZZZNRU
C10  H10  O 3                  124.0   0.0   0.0 298.0  0
 1035  trans-4-methoxycinnamic                                        MXCINN
C10  H10  O 3                  134.0   0.0   0.0 298.0  0
 1036  6-acetylbenzodioxan
C10  H10  O 3                  103.0   0.0   0.0 298.0  0
 1037  dimethylthyl terephthalate                                     DMTPAL
C10  H10  O 4                  105.0   0.0   0.0 302.0  2
 1038  dimethyl isophthalate                                          GOHRUS
C10  H10  O 4                  100.0   0.0   0.0 300.0  2
 1039  4-hydroxy-3-methoxycinnamic
C10  H10  O 4                  132.0   0.0   0.0 380.0  1
 1040  2,4,6-trimethylbenzonitrile
C10  H11  N 1                   83.0   0.0   0.0 298.0  0
 1041  2,4,6-trimethylbenzonitrile Noxide
C10  H11  N 1  O 1              86.0   0.0   0.0 300.0  2
 1042  3-amino-1-phenyl-but-2-enone                                   PICGAJ
C10  H11  N 1  O 1             109.0   0.0   0.0 298.0  0
 1043  N-phenyldiacetamide
C10  H11  N 1  O 2              90.0   0.0   0.0 298.0  0
 1044  N-benzoylthiocarbamic Oethylester
C10  H11  N 1  O 2  S 1        112.0   0.0   0.0 298.0  0
 1045  2,4,6-trimethoxybenzonitrile
C10  H11  N 1  O 3             113.0   0.0   0.0 298.0  0
 1046  2,4,6-trimethoxybenzonitrile Noxide
C10  H11  N 1  O 4              92.0   0.0   0.0 298.0  0
 1047  3,5-dimethyl-1-phenyl-4-nitrosopyrazole
C10  H11  N 3  O 1              90.0   0.0   0.0 298.0  0
 1048  3-dimethylamino-6-aminophthalimide
C10  H11  N 3  O 2             108.0   0.0   0.0 447.0  1
 1049  cyclodeca-1,2,6,7-tetraene
C10  H12                        73.0   0.0   0.0 298.0  0
 1050  2-propylbenzimidazole
C10  H12  N 2                  109.0   0.0   0.0 298.0  1
 1051  2-isopropylbenzimidazole
C10  H12  N 2                  110.0   0.0   0.0 298.0  0
 1052  4-methoxy- -methylstyrene
C10  H12  O 1                   81.0   0.0   0.0 298.0  0
 1053  2-phenyl-2-methyl-1,3-dioxolane
C10  H12  O 2                   81.9   0.0   0.0 309.0  1
 1054  2,3,6-trimethylbenzoic
C10  H12  O 2                  104.0   0.0   0.0 298.0  0
 1055  2,4,6-trimethylbenzoic                                         TMBZAC
C10  H12  O 2                  104.0   0.0   0.0 298.0  0
 1056  2,3,4-trimethylbenzoic
C10  H12  O 2                  109.0   0.0   0.0 298.0  0
 1057  2,3,5-trimethylbenzoic
C10  H12  O 2                  107.0   0.0   0.0 298.0  0
 1058  2,4,5-trimethylbenzoic                                         RUVQAA
C10  H12  O 2                  110.0   0.0   0.0 298.0  0
 1059  3,4,5-trimethylbenzoic                                         TMEBZA
C10  H12  O 2                  111.0   0.0   0.0 298.0  0
 1060  4-propylbenzoic
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C10  H12  O 2                  109.0   0.0   0.0 298.0  1
 1061  2-isopropylbenzoic
C10  H12  O 2                  101.0   0.0   0.0 298.0  0
 1062  3-isopropylbenzoic
C10  H12  O 2                  104.0   0.0   0.0 298.0  0
 1063  4-isopropylbenzoic
C10  H12  O 2                   99.0   0.0   0.0 298.0  0
 1064  4-phenylbutyric                                    ZZZNCU
C10  H12  O 2                  113.0   0.0   0.0 298.0  0
 1065  2,3,5,6-tetramethyl-1,4-benzoquinone
C10  H12  O 2                   93.0   0.0   0.0 298.0  0
 1066  p-tolyl transpropenylsulfone
C10  H12  O 2  S 1              84.0   0.0   0.0   0.0  0
 1067  p-tolyl propenylsulfone                            PRYLTS
C10  H12  O 2  S 1              96.0   0.0   0.0   0.0  0
 1068  p-tolyl isopropenylsulfone
C10  H12  O 2  S 1              89.0   0.0   0.0   0.0  0
 1069  propyl 4-hydroxybenzoate                           DUPKAB
C10  H12  O 3                  123.0   0.0   0.0 298.0  1
 1070  3-  2-methoxyphenyl propionic
C10  H12  O 3                  118.0   0.0   0.0 298.0  0
 1071  3-  4-methoxyphenyl propionic
C10  H12  O 3                  124.0   0.0   0.0 298.0  0
 1072  3,4,5-trimethoxybenzoic                            LIJKOF
C10  H12  O 5                  131.0   0.0   0.0 298.0  0
 1073  4-ethoxyacetanilide phenacetin
C10  H13  N 1  O 2             115.0   0.0   0.0 320.0  1
 1074  N-theonylthiocarbamic-O-butylester
C10  H13  N 1  O 2  S 2        147.0   0.0   0.0 298.0  0
 1075  1,2,4,5-tetramethylbenzene                         DURENE
C10  H14                        73.0  71.0  75.0 300.0  4
 1076  4-diethylaminonitrosobenzene
C10  H14  N 2  O 1             108.0   0.0   0.0 298.0  0
 1077  N,N-diethyl-N'-furoylthiourea
C10  H14  N 2  O 2  S 1        132.0   0.0   0.0 298.0  0
 1078  2,2-dinitroadamantane                              CAXNIY
C10  H14  N 2  O 4              96.4   0.0   0.0 298.0  1
 1079  3-tert-butylphenol
C10  H14  O 1                   87.0   0.0   0.0 298.0  3
 1080  4-tert-butylphenol
C10  H14  O 1                   87.0  84.0  89.0 298.0  3
 1081  2-isopropyl-5-methylphenol thymol                  IPMEPL
C10  H14  O 1                   91.0   0.0   0.0 300.0  3
 1082  2-adamantanone
C10  H14  O 1                   66.3   0.0   0.0 307.0  1
 1083  1,2-dihydroxy-4-tert-butylbenzene
C10  H14  O 2                   99.0   0.0   0.0 298.0  2
 1084  2-tert-butyl-1,4-dihydroxybenzene
C10  H14  O 2                  104.0   0.0   0.0 298.0  1
 1085  6-methyl-3-isopropyl-1,2-dihydroxybenzene
C10  H14  O 2                   97.0   0.0   0.0 298.0  0
 1086  1-bromoadamantane                                  DOKXIL
C10  H15 Br 1                   72.0   0.0   0.0 300.0  2
 1087  2-chloroadamantane                                 GUYBAF
C10  H15 Cl 1                   62.0   0.0   0.0 298.0  0
 1088  dl carvoxime                                       CARVOX
C10  H15  N 1  O 1             101.0   0.0   0.0 334.0  1
 1089  d-carvoxime
C10  H15  N 1  O 1              90.8   0.0   0.0 334.0  1
 1090  1-nitroadamantane
C10  H15  N 1  O 2              63.6   0.0   0.0 339.0  1
 1091  2-nitroadamantane
C10  H15  N 1  O 2              58.0   0.0   0.0 350.0  1
 1092  6,9-dimethyl-8-propyladenine
C10  H15  N 5                  129.0   0.0   0.0 347.0  1
 1093  8-butyl-9-methyladenine
C10  H15  N 5                  135.0   0.0   0.0 366.0  1
 1094  tricyclo 4.3.1.03,8decane
C10  H16                        64.9   0.0   0.0 300.0  1
 1095  tricyclo 5.2.1.02,6decane
C10  H16                        52.9   0.0   0.0 298.0  1
 1096  tricyclo 5.2.1.04,10ecane
C10  H16                        57.0   0.0   0.0 307.0  0
 1097  bicyclo 3.3.2decane
C10  H16                        58.0   0.0   0.0 298.0  0
 1098  adamantane
C10  H16                        60.0  53.6  62.0 300.8 17
 1099  2,2-dimethyl-3-methylenebicyclo 2.2.1heptane camp
C10  H16                        47.0   0.0   0.0   0.0  0
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 1100  methyl1,1,1trimethylpropylpropanedinitrile
C10  H16  N 2                   62.0   0.0   0.0 298.0  0
 1101  dl camphor
C10  H16  O 1                   53.0  51.5  54.0 300.0  4
 1102  3-bornanone
C10  H16  O 1                   54.0   0.0   0.0 300.0  0
 1103  1-adamantanol                                          ADAMOL
C10  H16  O 1                   87.0   0.0   0.0 300.0  3
 1104  adamantan-2-ol                                         SEYDEF
C10  H16  O 1                   88.0   0.0   0.0 300.0  2
 1105  cis-8-methyl-2-hydrindanone
C10  H16  O 1                   61.0   0.0   0.0 298.0  0
 1106  thiocamphor                                            MOYGUC
C10  H16  S 1                   62.2   0.0   0.0 298.0  1
 1107  1,3,5,7-tetramethyl-2,4,6,8-tetrathiaadamantane        QQQFHJ
C10  H16  S 4                  117.0   0.0   0.0 298.0  0
 1108  1-aminoadamantane
C10  H17  N 1                   62.0   0.0   0.0 298.0  0
 1109  cis decahydronaphthalene
C10  H18                        63.0   0.0   0.0 298.0  0
 1110  trans decahydronaphthalene
C10  H18                        64.0   0.0   0.0 298.0  0
 1111  dl borneol
C10  H18  O 1                   69.0   0.0   0.0 365.0  0
 1112  dl alpha-terpineol
C10  H18  O 1                   80.0   0.0   0.0 298.0  0
 1113  alphaterpineol
C10  H18  O 1                   80.3   0.0   0.0 306.0  1
 1114  dl -isoborneol
C10  H18  O 1                   41.0   0.0   0.0 288.0  0
 1115  sebacic acid                                           SEBAAC
C10  H18  O 4                  181.0   0.0   0.0 389.3  1
 1116  N,N-diethyl-N  -isovaleroylthiourea
C10  H20  N 2  O 1  S 1         122.0   0.0   0.0 298.0  0
 1117  N,N-diethyl-N  -pivaloylthiourea
C10  H20  N 2  O 1  S 1         115.0   0.0   0.0 298.0  0
 1118  citronellol
C10  H20  O 1                    66.0   0.0   0.0 308.0  0
 1119  l-menthol                                              BAVLOZ
C10  H20  O 1                    95.8   0.0   0.0 289.0  1
 1120  dl menthol
C10  H20  O 1                    78.6   0.0   0.0 289.0  1
 1121  cyclodecanol                                           PEMYUB
C10  H20  O 1                   100.0   0.0   0.0 288.0  0
 1122  decanoic acid                                          ISEPEB
C10  H20  O 2                   125.0 119.0 130.0 298.0  2
 1123  peroxydecanoic
C10  H20  O 3                   117.0   0.0   0.0 298.0  1
 1124  decanamide
C10  H21  N 1  O 1              125.0   0.0   0.0 362.0  1
 1125  decane                                                 QQQFBG
C10  H22                         82.0   0.0   0.0 298.0  0
 1126  1-decanol
C10  H22  O 1                   114.0   0.0   0.0 298.0  2
 1127  1,10-decanediol                                        WESTIX
C10  H22  O 2                   156.0   0.0   0.0 298.0  0
 1128  1,4,8,11-tetraazacyclotetradecane                      FOFDIN
C10  H24  N 4                   134.0   0.0   0.0 362.0  1
 1129  bicyclo 2.2.1hept-5-ene-2,2,3,3-tetracarbonitril
C11  H 6  N 4                   117.2   0.0   0.0 408.0  0
 1130  1-bromo-2-naphthoic acid
C11  H 7 Br 1  O 2              109.0   0.0   0.0 371.0  1
 1131  1-naphthoic acid                                       NAPOAC
C11  H 8  O 2                   115.0 110.0 118.0 320.0  3
 1132  2-naphthoic acid                                       NAPHAC
C11  H 8  O 2                   118.0 114.0 119.0 320.0  3
 1133  4-phenylpyridine
C11  H 9  N 1                    81.0   0.0   0.0 298.0  0
 1134  2-methylnaphthalene
C11  H10                         64.0   0.0   0.0   0.0  0
 1135  N-3-bromopropyl phthalimide
C11  H10 Br 1  N 1  O 2         116.0   0.0   0.0 298.0  0
 1136  1-naphthalenemethanol
C11  H10  O 1                   102.0   0.0   0.0 298.0  0
 1137  2-naphthalenemethanol
C11  H10  O 1                   106.0   0.0   0.0 298.0  0
 1138  pentacyclo 5.4.02,603,1005,9undecane-8,11-dione        FOBPAO
C11  H10  O 2                    93.0   0.0   0.0 298.0  0
 1139  2,6-dimethylquinoline                                  PILFOG
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C11  H11  N 1                    85.0   0.0   0.0 298.0  0
 1140  2,7-dimethylquinoline
C11  H11  N 1                    88.0   0.0   0.0 298.0  0
 1141  N-propylphthalimide
C11  H11  N 1  O 2               98.0   0.0   0.0 298.0  0
 1142  4- 4-nitrophenyl aminopent-3-ene-2-one                PICFOW
C11  H12  N 2  O 3              122.0   0.0   0.0 298.0  0
 1143  1-phenyl-4,7-dioxaspiro 2.4 heptane
C11  H12  O 2                    91.0   0.0   0.0 298.0  0
 1144  3,4-dihyro-5-methoxy-1 2H -naphthalenone
C11  H12  O 2                    98.0   0.0   0.0 298.0  0
 1145  3,4-dihyro-6-methoxy-1 2H -naphthalenone
C11  H12  O 2                   105.0   0.0   0.0 298.0  0
 1146  3,4-dihyro-7-methoxy-1 2H -naphthalenone
C11  H12  O 2                   103.0   0.0   0.0 298.0  0
 1147  trans-2,3-dimethoxycinnamic
C11  H12  O 4                   141.0   0.0   0.0 386.0  1
 1148  trans-2,4-dimethoxycinnamic
C11  H12  O 4                   149.0   0.0   0.0 398.0  1
 1149  trans-2,5-dimethoxycinnamic
C11  H12  O 4                   138.0   0.0   0.0 384.0  1
 1150  trans-3,4-dimethoxycinnamic                           CEMJOT
C11  H12  O 4                   149.0   0.0   0.0 397.0  1
 1151  trans-3,5-dimethoxycinnamic
C11  H12  O 4                   141.0   0.0   0.0 391.0  1
 1152  pentacyclo 5.4.02,603,1005,9undecane
C11  H14                         54.9   0.0   0.0 298.0  2
 1153  4-nitrobenzylidene t-Bu amine
C11  H14  N 2  O 2               91.0   0.0   0.0 298.0  0
 1154  2-cyano-2-nitroadamantane
C11  H14  N 2  O 2               70.0   0.0   0.0 338.0  1
 1155  4-nitrobenzylidene t-Bu amine Noxide
C11  H14  N 2  O 3              117.0   0.0   0.0 298.0  0
 1156  3-nitro-3-4nitrophenyl pentane
C11  H14  N 2  O 4              111.0   0.0   0.0 298.0  0
 1157  2-tert-butylbenzoic acid
C11  H14  O 2                    99.8   0.0   0.0 314.0  1
 1158  3-tert-butylbenzoic acid
C11  H14  O 2                   103.0   0.0   0.0 327.0  1
 1159  4-tert-butylbenzoic acid                              BONLOF
C11  H14  O 2                   103.0   0.0   0.0 334.0  1
 1160  4-butylbenzoic acid
C11  H14  O 2                   110.0   0.0   0.0 298.0  1
 1161  2,3,4,5-tetramethylbenzoic acid
C11  H14  O 2                   116.0   0.0   0.0 298.0  1
 1162  2,3,4,6-tetramethylbenzoic acid
C11  H14  O 2                   110.5   0.0   0.0 298.0  1
 1163  2,3,5,6-tetramethylbenzoic acid
C11  H14  O 2                   106.0   0.0   0.0 298.0  1
 1164  3,5-diethylbenzoic acid
C11  H14  O 2                   104.0   0.0   0.0 334.0  1
 1165  p-tolyl but-1-enyl sulfone
C11  H14  O 2  S 1              106.0   0.0   0.0   0.0  0
 1166  p-tolyl but 2-enyl sulfone
C11  H14  O 2  S 1              108.0   0.0   0.0   0.0  0
 1167  p-tolyl but 3-enyl sulfone
C11  H14  O 2  S 1              113.0   0.0   0.0   0.0  0
 1168  p-tolyl-isobutenyl sulfone
C11  H14  O 2  S 1              102.0   0.0   0.0   0.0  0
 1169  p-tolyl 2methylprop-2-enyl sulfone
C11  H14  O 2  S 1              107.0   0.0   0.0   0.0  0
 1170  butyl 4-hydroxybenzoate                               UDOMIL
C11  H14  O 3                   108.0   0.0   0.0 298.0  1
 1171  4-n-butoxybenzoic acid                                BUXBZA
C11  H14  O 3                   129.0   0.0   0.0 298.0  0
 1172  3- 3,4-dimethoxyphenyl propionic
C11  H14  O 4                   144.0   0.0   0.0 298.0  0
 1173  1-adamantyl-1-carbonitrile
C11  H15  N 1                    67.0   0.0   0.0 298.0  0
 1174  benzylidene t-Bu amine Noxide                         FEXBOZ
C11  H15  N 1  O 1               87.0   0.0   0.0 298.0  0
 1175  pentamethylbenzene                                    COPMUR
C11  H16                         75.0  72.0  77.0 298.0  2
 1176  2-tert-butyl-4-methylphenol                           PAGMEQ
C11  H16  O 1                    81.0  77.4  82.9 298.0  2
 1177  2-tert-butyl-5-methylphenol
C11  H16  O 1                    80.0   0.0   0.0 298.0  0
 1178  4-tert-pentylphenol
C11  H16  O 1                    88.0   0.0   0.0 298.0  0
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 1179  1-adamantyl carboxamide
C11  H17  N 1  O 1             108.0   0.0   0.0 298.0  1
 1180  1-methyladamantane
C11  H18                        67.0   0.0   0.0 298.0  2
 1181  2-methyladamantane
C11  H18                        67.0   0.0   0.0 298.0  2
 1182  2-methyl-2-adamantanol
C11  H18  O 1                   91.0   0.0   0.0 298.0  1
 1183  bicyclo 3.3.3undecane
C11  H20                        64.0   0.0   0.0 298.0  0
 1184  undecanedioic acid                                    UNDEAC
C11  H20  O 4                  162.0   0.0   0.0 298.0  1
 1185  undecanoic  acid                                      ZZZNYY
    C11  H22  O 2                  121.0   0.0   0.0 298.0
 1186  N-methyl  decanamide
C11  H23  N 1  O 1             103.0   0.0   0.0 314.0  0
 1187  undecane
C11  H24                        92.0   0.0   0.0 236.0  0
 1188  octachlorodibenzofuran
C12 Cl 8  O 1                  145.0 141.0 149.0 440.0  2
 1189  octachlorodibenzo b,e  1,4 dioxin                     OCDBDO
C12 Cl 8  O 2                  147.0 145.0 149.0 480.5  2
 1190  decachlorobiphenyl                                    DCLBPH
C12 Cl10                       122.0   0.0   0.0 343.0  1
 1191  decafluorobiphenyl                                    DECFDP
C12  F10                        87.0   0.0   0.0 300.0  2
 1192  1,2,3,4,6,7,9-heptachlorodibenzo b,e  1,4 dioxin
C12  H 1 Cl 7  O 2             144.0   0.0   0.0 436.0  1
 1193  1,2,3,4,6,9-hexachlorodibenzo b,e  1,4 dioxin
C12  H 2 Cl 6  O 2             128.0   0.0   0.0 428.0  1
 1194  2,2',3,3',5,5',6,6'-octachlorobiphenyl
C12  H 2 Cl 8                  101.0   0.0   0.0 318.0  1
 1195  1,2,4,7,8-pentachlorodibenzo b,e  1,4 dioxin
C12  H 3 Cl 5  O 2             125.0   0.0   0.0 416.0  1
 1196  1,2,3,4,8-pentachlorodibenzofuran
C12  H 3 Cl 7  O 1             125.0   0.0   0.0 401.0  1
 1197  1,2,3,4-tetrachlorodibenzofuran
C12  H 4 Cl 4  O 1             118.0   0.0   0.0 363.0  1
 1198  2,3,7,8-tetrachlorodibenzofuran                       TCBZFU
C12  H 4 Cl 4  O 1             124.0   0.0   0.0 323.0  0
 1199  1,2,3,4-tetrachlorodibenzo b,e  1,4 dioxin           FELSEU
C12  H 4 Cl 4  O 2             111.0   0.0   0.0 391.0  1
 1200  1,2,6,7-tetrachlorodibenzo b,e  1,4 dioxin
C12  H 4 Cl 4  O 2             120.0   0.0   0.0 403.0  1
 1201  1,3,6,8-tetrachlorodibenzo b,e  1,4 dioxin
C12  H 4 Cl 4  O 2             118.0   0.0   0.0 393.0  1
 1202  1,3,7,9-tetrachlorodibenzo b,e  1,4 dioxin
C12  H 4 Cl 4  O 2             123.0   0.0   0.0 396.0  1
 1203  2,3,7,8-tetrachlorodibenzo b,e  1,4 dioxin           TCBZDX
C12  H 4 Cl 4  O 2             124.0   0.0   0.0 578.0  0
 1204  2,2',4,4',6,6'-hexachlorobiphenyl                     HCLBPH
C12  H 4 Cl 6                  103.0   0.0   0.0 283.0  1
 1205  7,7,8,8-tetracyanoquinodimethane                      TCYQME
C12  H 4  N 4                  118.0 105.0 126.0 430.0  6
 1206  2,4,6-dibenzofuran
C12  H 5 Cl 3  O 1             109.0   0.0   0.0 355.0  0
 1207  1,2,3-trichlorodibenzo b,e  1,4 dioxin
C12  H 5 Cl 3  O 2             117.0   0.0   0.0 375.0  0
 1208  1,2,4-trichlorodibenzo b,e  1,4 dioxin
C12  H 5 Cl 3  O 2             121.0   0.0   0.0 365.0  0
 1209  1,3,7-trichlorodibenzo b,e  1,4 dioxin
C12  H 5 Cl 3  O 2             116.0   0.0   0.0 342.0  1
 1210  1,7,8-trichlorodibenzo b,e  1,4 dioxin
C12  H 5 Cl 3  O 2             114.0   0.0   0.0 373.0  0
 1211  2,2',4,5,5'-pentachlorobiphenyl
C12  H 5 Cl 5                   92.7   0.0   0.0 308.0  1
 1212  2,8-dichlorodibenzofuran
C12  H 6 Cl 2  O 1             110.0   0.0   0.0 360.0  0
 1213  3,6-dichlorodibenzofuran
C12  H 6 Cl 2  O 1             110.0   0.0   0.0 340.0  1
 1214  1,6-dichlorodibenzo b,e  1,4 dioxin
C12  H 6 Cl 2  O 2             114.0   0.0   0.0 365.0  0
 1215  2,3-dichlorodibenzo b,e  1,4 dioxin
C12  H 6 Cl 2  O 2             108.0   0.0   0.0 300.0  4
 1216  2,7-dichlorodibenzo b,e  1,4 dioxin                   DCBZDX
C12  H 6 Cl 2  O 2             110.0 106.0 114.0 360.0  2
 1217  2,8-dichlorodibenzo b,e  1,4 dioxin                   DCBDOX
C12  H 6 Cl 2  O 2             109.0   0.0   0.0 334.0  0
 1218  2,2',5,5'-tetrachlorobiphenyl                         TEKQIJ
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C12  H 6 Cl 4                  100.0  95.0 102.0 330.0  2
 1219  2,3,4,5-tetrachlorobiphenyl
C12  H 6 Cl 4                   88.7   0.0   0.0 323.0  1
 1220  2,3',4,4'-tetrachlorobiphenyl
C12  H 6 Cl 4                  106.0   0.0   0.0 353.0  0
 1221  3,3',4,4'-tetrachlorobiphenyl                        FUHDAN
C12  H 6 Cl 4                  122.0   0.0   0.0 393.0  0
 1222  1-chlorodibenzo b,e  1,4 dioxin
C12  H 7 Cl 1  O 2              98.0  95.0 100.0 300.0  4
 1223  2-chlorodibenzo b,e  1,4 dioxin                      SESHED
C12  H 7 Cl 1  O 2              98.0   0.0   0.0 298.0  4
 1224  2,2',5-trichlorobiphenyl
C12  H 7 Cl 3                   94.0   0.0   0.0 308.0  0
 1225  2,4,4' -trichlorobiphenyl
C12  H 7 Cl 3                   97.0   0.0   0.0 320.0  0
 1226  2',3,4-trichlorobiphenyl
C12  H 7 Cl 3                   98.0   0.0   0.0 320.0  0
 1227  acenaphthylene
C12  H 8                        73.0   0.0   0.0 298.0  4
 1228  biphenylene                                          BIPHNE
C12  H 8                        85.0  83.0  87.0 298.0  3
 1229  2,2' -dichlorobiphenyl                               DCLBIP
C12  H 8 Cl 2                   96.0   0.0   0.0 298.0  0
 1230  4,4' -dichlorobiphenyl                               DCLBIQ
C12  H 8 Cl 2                  104.0   0.0   0.0 298.0  0
 1231  2,2' -difluorobiphenyl                               PUGPIQ
C12  H 8  F 2                   95.1   0.0   0.0 310.0  1
 1232  4,4' -difluorobiphenyl                               ZZZAOS
C12  H 8  F 2                   95.0   0.0   0.0 300.0  2
 1233  1,10-phenanthroline                                  OPENAN
C12  H 8  N 2                   98.0   0.0   0.0   0.0  0
 1234  phenazine                                            PHENAZ
C12  H 8  N 2                   96.0  91.0 100.0 298.0  7
 1235  phenazine-N-oxide
C12  H 8  N 2  O 1             100.0   0.0   0.0 298.0  0
 1236  4,4' -dinitrobiphenyl                                DNTDPH
C12  H 8  N 2  O 4             105.0   0.0   0.0 420.0  0
 1237  bicyclo 2.2.2 oct-5-ene-2,2,3,3-tetracarbonitril
C12  H 8  N 4                  110.0   0.0   0.0 433.0  0
 1238  dibenzo-1,3a,4,6a-tetraazapentalene                  TAZPEN
C12  H 8  N 4                   70.0   0.0   0.0 400.0  0
 1239  dibenzofuran                                         DBZFUR
C12  H 8  O 1                   84.0  77.0  86.0 300.0  7
 1240  dibenzo b,e  1,4 dioxin                              BZDIOX
C12  H 8  O 2                   92.0  89.0  94.0 300.0  5
 1241  dibenzothiophene                                     DBZTHP
C12  H 8  S 1                   96.0  91.0  98.0 300.0  4
 1242  thianthrene                                          THIANT
C12  H 8  S 2                   99.0   0.0   0.0 350.0  3
 1243  5-bromoacenaphthene
C12  H 9 Br 1                   87.0   0.0   0.0 298.0  0
 1244  4-chlorobiphenyl
C12  H 9 Cl 1                   80.0  74.0  86.0 300.0  2
 1245  carbazole                                            CRBZOL
C12  H 9  N 1                  101.0  98.0 103.0 298.0  2
 1246  10H-phenoxazine
C12  H 9  N 1  O 1              96.0   0.0   0.0 298.0  0
 1247  phenothiazine                                        PHESAZ
C12  H 9  N 1  S 1             115.0   0.0   0.0 298.0  1
 1248  4-nitroazobenzene
C12  H 9  N 3  O 2             110.0   0.0   0.0   0.0  0
 1249  4-hydroxy-4  -nitroazobenzene
C12  H 9  N 3  O 3             143.0 140.0 146.0 431.0  3
 1250  acenaphthene                                         ACENAP
C12  H10                        85.0  82.0  86.0 300.0  6
 1251  biphenyl                                             BIPHEN
C12  H10                        82.0   0.0   0.0 298.0  6
 1252  cis-azobenzene                                       AZBENC
C12  H10  N 2                   93.0   0.0   0.0 300.0  2
 1253  trans-azobenzene                                     AZOBEN
C12  H10  N 2                   96.0  94.0  96.0 300.0  6
 1254  trans-diphenyldiazene  Noxide
C12  H10  N 2  O 1              99.0   0.0   0.0 298.0  0
 1255  N-  2-nitrophenyl -N-phenylamine
C12  H10  N 2  O 2             104.0 101.0 108.0 340.0  3
 1256  N-  4-nitrophenyl -N-phenylamine
C12  H10  N 2  O 2             127.0 121.0 130.0 350.0  3
 1257  4-amino-4  -nitroazobenzene
C12  H10  N 4  O 2             138.0 134.0 140.0 410.0  7
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 1258  2-acetylnaphthalene
C12  H10  O 1                  88.0   0.0   0.0 305.0  0
 1259  diphenyl ether                                          RAFFIO
C12  H10  O 1                  82.0   0.0   0.0   0.0  0
 1260  2-hydroxybiphenyl
C12  H10  O 1                  87.0  83.0  89.0 300.0  2
 1261  4-hydroxybiphenyl                                       BOPSAA
C12  H10  O 1                 110.0   0.0   0.0 298.0  0
 1262  2,2' -dihydroxybiphenyl                                 NUTSUQ
C12  H10  O 2                 114.0   0.0   0.0 298.0  0
 1263  4,4' -dihydroxybiphenyl                                 DOHDPH
C12  H10  O 2                 143.0   0.0   0.0 298.0  0
 1264  alpha naphthyl  acetate                                 PARPEE
C12  H10  O 2                  95.0   0.0   0.0 298.0  1
 1265  beta -naphthyl acetate
C12  H10  O 2                  96.3   0.0   0.0 298.0  1
 1266  1-naphthaleneacetic                                     NAPACA
C12  H10  O 2                 112.0   0.0   0.0 298.0  1
 1267  2-naphthaleneacetic                                     PEYGEF
C12  H10  O 2                 124.0   0.0   0.0 298.0  0
 1268  diphenyl sulfone                                        DPSULO
C12  H10  O 2  S 1            106.0   0.0   0.0   0.0  0
 1269  diphenyl disulfone                                      DPDSON
C12  H10  O 4  S 2            162.0   0.0   0.0   0.0  0
 1270  diphenyl sulfide
C12  H10  S 1                  95.0   0.0   0.0   0.0  0
 1271  diphenylamine                                           QQQBVP
C12  H11  N 1                 105.0  97.0 110.0 300.0  4
 1272  N-acetyl-1-naphthylamine
C12  H11  N 1  O 1             94.0   0.0   0.0 349.0  1
 1273  4-aminoazobenzene
C12  H11  N 3                 110.0   0.0   0.0 364.0  1
 1274  1,8-dimethylnaphthalene                                 DMNAPH
C12  H12                       81.0  78.0  83.0 310.0  3
 1275  2,3-dimethylnaphthalene
C12  H12                       83.0   0.0   0.0 310.0  2
 1276  2,6-dimethylnaphthalene                                 DMNPTL
C12  H12                       83.0   0.0   0.0 300.0  2
 1277  2,7-dimethylnaphthalene
C12  H12                       84.0   0.0   0.0 350.0  3
 1278  4,4' -dimethyl-2-2'bipyridyl                            NAMKAN
C12  H12  N 2                 100.0   0.0   0.0 298.0  0
 1279  4,4' -diaminodiphenyl oxide
C12  H12  N 2  O 1             63.0   0.0   0.0   0.0  0
 1280  1,4-dimethylcubane dicarboxylate                        HEGSAN
C12  H12  O 4                 117.0   0.0   0.0 298.0  0
 1281  1,3,5-benzenetricarboxylic acid triMeester              DUJTIM
C12  H12  O 6                 118.0   0.0   0.0 298.0  2
 1282  1,1-diacetoxy-1-phenylethane
C12  H14  O 4                  94.0   0.0   0.0 318.0  1
 1283  2,4,6-trinitro-1,3-dimethyl-5-tert-butylbenzene         DOHCOS
C12  H15  N 3  O 6            100.0   0.0   0.0 330.0  1
 1284  tetraspiro 2.0.2.0.2.0.2.0 dodecane 4rotane             SCPCBU
C12  H16                       75.0   0.0   0.0 318.0  1
 1285  N-benzoyl-N' ,N' -diethylurea
C12  H16  N 2  O 2            132.0   0.0   0.0 298.0  0
 1286  pentamethylbenzoic                                      TUSQIH
C12  H16  O 2                 113.0   0.0   0.0 298.0  1
 1287  1-nitro-2,6-diisopropylbenzene
C12  H17  N 1  O 2             81.0   0.0   0.0 298.0  0
 1288  hexamethylbenzene                                       HMBENZ
C12  H18                       84.0  81.0  86.0 298.0  7
 1289  1-adamantyl methylchetone
C12  H18  O 1                  84.2   0.0   0.0 298.0  1
 1290  1-adamantyl-1-carboxylic acid Meester                   KUKLIN
C12  H18  O 2                  82.0   0.0   0.0 298.0  1
 1291  1,3-dimethyladamantane
C12  H20                       68.0   0.0   0.0 298.0  0
 1292  2,2-dimethyladamantane
C12  H20                       74.0   0.0   0.0 298.0  1
 1293  trans 2cyclohexylcyclohexanol
C12  H22  O 1                  99.0   0.0   0.0 320.0  1
 1294  cyclododecanone
C12  H22  O 1                  83.0   0.0   0.0 298.0  0
 1295  dodecanedioic  acid                                     DECDAC
C12  H22  O 4                 160.0 153.0 169.0 350.0  2
 1296  cyclododecane
C12  H24                       76.0   0.0   0.0 298.0  2
 1297  dodecanoic  acid                                        LAURAC
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C12  H24  O 2                  140.0 133.0 147.0 298.0  3
 1298  dodecanamide
C12  H25  N 1  O 1             153.0   0.0   0.0 385.0  1
 1299  dodecane
C12  H26                       101.0   0.0   0.0 298.0  2
 1300  1-dodecanol
C12  H26  O 1                  130.0   0.0   0.0 298.0  1
 1301  1,2,4,5,7,8-hexachloroxanthene
C13  H 4 Cl 6  O 1             147.0   0.0   0.0 401.0  0
 1302  benz g isoquinoline-5,10-dione
C13  H 7  N 1  O 2             108.0 108.0 117.0 358.0  3
 1303  5- 2,4-difluorophenyl salicylic acid
C13  H 8  F 2  O 3             119.0   0.0   0.0 382.0  1
 1304  9-fluorenone                                          FLURON
C13  H 8  O 1                   91.0  88.0  94.0 298.0  2
 1305  thioxanthone
C13  H 8  O 1  S 1             115.0   0.0   0.0 298.0  0
 1306  xanthone
C13  H 8  O 2                  101.0  99.0 103.0 298.0  2
 1307  2-chlorobenzophenone                                  BIMVEZ
C13  H 9 Cl 1  O 1             100.0   0.0   0.0 298.0  1
 1308  3-chlorobenzophenone
C13  H 9 Cl 1  O 1             110.0   0.0   0.0 298.0  1
 1309  4-chlorobenzophenone
C13  H 9 Cl 1  O 1             108.0   0.0   0.0 298.0  1
 1310  5-chloro-2-hydroxybenzophenone                        OLOHIG
C13  H 9 Cl 1  O 2              92.0   0.0   0.0 308.0  1
 1311  3,4,4'-trichlorocarbanilide
C13  H 9 Cl 3  N 2  O 1        182.0   0.0   0.0 298.0  0
 1312  acridine
C13  H 9  N 1                   93.0  90.0  95.0 298.0  8
 1313  3,4-benzoquinoline
C13  H 9  N 1                   98.0  95.0 100.0 298.0  3
 1314  5,6-benzoquinoline
C13  H 9  N 1                  100.0  83.0 106.0 298.0  2
 1315  7,8-benzoquinoline
C13  H 9  N 1                   92.0  81.0 100.0 300.0  3
 1316  acridone                                              HIBXOF
C13  H 9  N 1  O 1             135.0   0.0   0.0 298.0  2
 1317  N-methyl-1,8-naphthalimide
C13  H 9  N 1  O 2             110.0   0.0   0.0 298.0  1
 1318  2-nitrofluorene
C13  H 9  N 1  O 2             114.0   0.0   0.0 367.0  1
 1319  fluorene                                              FLUREN
C13  H10                        85.0  80.0  88.0 300.0 10
 1320  9-aminoacridine
C13  H10  N 2                  115.0   0.0   0.0 520.0  0
 1321  2-phenylbenzimidazole
C13  H10  N 2                  123.0   0.0   0.0 298.0  0
 1322  1,5-diphenyltetrazole                                 MOYLAP
C13  H10  N 4                  122.0   0.0   0.0 355.0  0
 1323  2,5-diphenyltetrazole                                 QOZYIP
C13  H10  N 4                  120.0   0.0   0.0 343.0  0
 1324  benzophenone                                          BPHENO
C13  H10  O 1                   93.0  91.0  95.0 300.0 13
 1325  xanthene                                              CONYAH
C13  H10  O 1                   92.5   0.0   0.0 329.0  1
 1326  2-biphenylcarboxylic acid                             NOZVIH
C13  H10  O 2                  121.0   0.0   0.0 298.0  0
 1327  4-biphenylcarboxylic acid                             BOPSEE
C13  H10  O 2                  128.0   0.0   0.0 298.0  0
 1328  phenyl benzoate                                       PHBENZ
C13  H10  O 2                   98.0  96.0  99.0 298.0  2
 1329  2,4-dihydroxybenzophenone                             DHXBZP
C13  H10  O 3                  134.0   0.0   0.0 327.0  0
 1330  phenyl salicylate                                     QQQAXJ
C13  H10  O 3                  109.0   0.0   0.0 298.0  1
 1331  diphenyl carbonate                                    ZZZPCA
C13  H10  O 3                   90.0   0.0   0.0 298.0  0
 1332  2,2' ,4,4 '-tetrahydroxybenzophenone                  BADVIL
C13  H10  O 5                  143.0 143.0 179.0 378.0  2
 1333  thioxanthene                                          TOXANT
C13  H10  S 1                  101.0   0.0   0.0 298.0  1
 1334  4-methyldibenzothiophene
C13  H10  S 1                   90.0   0.0   0.0 298.0  0
 1335  N-phenyl-benzaldehyde imine
C13  H11  N 1                   97.0   0.0   0.0 298.0  2
 1336  9-methylcarbazole
C13  H11  N 1                   96.0   0.0   0.0 298.0  1
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 1337  benzanilide
C13  H11  N 1  O 1             125.0  99.0 125.0 298.0  2
 1338  N-phenylanthranilic acid
C13  H11  N 1  O 2             126.0   0.0   0.0 298.0  1
 1339  4-methylbiphenyl
C13  H12                        80.0   0.0   0.0 298.0  0
 1340  diphenylmethane                                          ZZZMKS
C13  H12                        86.0  72.0  89.0 298.0  6
 1341  1,3-diphenylurea                                         DPUREA
C13  H12  N 2  O 1             152.0   0.0   0.0   0.0  0
 1342  4'-nitro-2-methylaminoazobenzene
C13  H12  N 4  O 2             135.0   0.0   0.0   0.0  0
 1343  diphenylmethanol                                         YUHHUE
C13  H12  O 1                  106.0   0.0   0.0 298.0  1
 1344  4-benzylphenol                                           INEGAK
C13  H12  O 1                   97.4   0.0   0.0 324.0  1
 1345  2-biphenylmethanol
C13  H12  O 1                  107.0   0.0   0.0 298.0  0
 1346  4-biphenylmethanol
C13  H12  O 1                  107.0   0.0   0.0 298.0  0
 1347  3-acetyl-2-methyl-5-phenylthiophene
C13  H12  O 1  S 1             108.0   0.0   0.0 298.0  1
 1348  phenyl benzyl sulfide
C13  H12  S 1                   98.0   0.0   0.0 298.0  0
 1349  N-benzylaniline                                          UREJOR
C13  H13  N 1                  103.0   0.0   0.0 303.0  1
 1350  2,2' -diaminodiphenylmethane
C13  H14  N 2                  111.0   0.0   0.0 358.0  1
 1351  morpholine cinnamate
C13  H17  N 1  O 3             118.0   0.0   0.0 313.0  1
 1352  N,N-dimethyl-1-adamantylcarboxamide
C13  H21  N 1  O 1              98.0   0.0   0.0 298.0  1
 1353  1,3,5-trimethyladamantane
C13  H22                        78.0   0.0   0.0 298.0  1
 1354  7-tridecanone
C13  H26  O 1                  104.0   0.0   0.0 290.0  0
 1355  methyl laurate
C13  H26  O 2                  122.0   0.0   0.0 267.0  1
 1356  peroxytridecanoic
C13  H26  O 3                  143.0   0.0   0.0 298.0  0
 1357  N-methyl dodecanamide
C13  H27  N 1  O 1             117.0   0.0   0.0 330.0  0
 1358  tridecane
C13  H28                        91.0   0.0   0.0 298.0  0
 1359  tri-tert-butylmethane
C13  H28                        58.0  55.0  61.0 298.0  3
 1360  1-amino-4-nitro-5,8-dichloroanthraquinone
C14  H 6 Cl 2  N 2  O 4        158.2   0.0   0.0   0.0  1
 1361  1,4-dinitroanthraquinone
C14  H 6  N 2  O 6             131.0   0.0   0.0   0.0  0
 1362  1,2-bis  2,4,6-trinitrophenyl ethylene
C14  H 6  N 6  O 12            179.0   0.0   0.0 457.0  2
 1363  1-nitroanthraquinone
C14  H 7  N 1  O 4             139.0   0.0   0.0 400.0  2
 1364  paracylene
C14  H 8                        83.0   0.0   0.0 330.0  2
 1365  1,5-dibromoanthracene
C14  H 8 Br 2                  116.0   0.0   0.0 383.0  1
 1366  9,10-dibromoanthracene                                   DBANTH
C14  H 8 Br 2                  114.0   0.0   0.0 375.0  1
 1367  9,10-dichloroanthracene                                  DCLANT
C14  H 8 Cl 2                  113.0   0.0   0.0 346.0  1
 1368  9,10-anthraquinone                                       ANTQUO
C14  H 8  O 2                  111.0 108.0 113.0 298.2  5
 1369  9,10-phenanthraquinone                                   ZZZIYE
C14  H 8  O 2                  108.0   0.0   0.0 298.0  0
 1370  1-hydroxy-9,10-anthraquinone
C14  H 8  O 3                  113.0   0.0   0.0 358.0  1
 1371  9-hydroxy-1,4-anthraquinone
C14  H 8  O 3                  110.0   0.0   0.0 350.0  2
 1372  2,2  -biphenyldicarboxylic  anhydride
C14  H 8  O 3                  121.0   0.0   0.0 298.0  0
 1373  1,2-dihydroxyanthraquinone
C14  H 8  O 4                  123.0   0.0   0.0 400.0  3
 1374  1,4-dihydroxy-9,10-anthraquinone                         DHXANT
C14  H 8  O 4                  113.0 103.0 122.0 400.0  4
 1375  1,5-dihydroxyanthraquinone                               DHANTQ
C14  H 8  O 4                  118.0   0.0   0.0 298.0  0
 1376  1,8-dihydroxyanthraquinone                               DHANQU
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C14  H 8  O 4                  110.0   0.0   0.0 298.0  0
 1377  2,6-dihydroxyanthraquinone
C14  H 8  O 4                  170.0   0.0   0.0 498.0  0
 1378  1,4,5,8-tetrahydroxyanthraquinone
C14  H 8  O 6                  152.0   0.0   0.0 438.0  0
 1379  9-bromoanthracene                                    QQQFDS
C14  H 9 Br 1                  101.0   0.0   0.0 350.0  0
 1380  2-chloroanthracene
C14  H 9 Cl 1                   99.3   0.0   0.0 351.0  1
 1381  1,1,1-trichloro-2,2-bis  4-chlorophenyl ethane      CPTCET
C14  H 9 Cl 5                  118.0 110.0 120.0 300.0  6
 1382  1-aminoanthraquinone
C14  H 9  N 1  O 2             120.0 113.9 126.0 400.0  3
 1383  2-aminoanthraquinone
C14  H 9  N 1  O 2             140.0 137.0 144.0   0.0  2
 1384  9-nitroanthracene                                    NTRANT
C14  H 9  N 1  O 2             114.0   0.0   0.0 330.0  2
 1385  anthracene                                          ANTCEN
C14  H10                        97.0  92.0 105.0 300.0 15
 1386  phenanthrene                                        PHENAN
C14  H10                        92.0  87.0  95.0 298.0 10
 1387  diphenylacetylene                                   DPHACT
C14  H10                        93.0  89.0  95.0 298.0  4
 1388  1,1,2,2-tetrafluoro-1,2-diphenylethane
C14  H10  F 4                  102.0   0.0   0.0 298.0  0
 1389  anthrone
C14  H10  O 1                  105.0   0.0   0.0 298.0  2
 1390  2-fluorenecarboxaldehyde                            SAZQIT
C14  H10  O 1                  100.0   0.0   0.0 347.0  1
 1391  benzil                                              BENZIL
C14  H10  O 2                   98.4   0.0   0.0 330.0  1
 1392  9-fluorenecarboxylic acid
C14  H10  O 2                  110.0   0.0   0.0 384.0  1
 1393  benzoic anhydride
C14  H10  O 3                   96.0   0.0   0.0 298.0  2
 1394  benzoyl peroxide                                    DBEZPO
C14  H10  O 4                   95.0  90.0  95.0 298.0  2
 1395  diphenyl  oxalate                                   HEKTUM
C14  H10  O 4                  103.0   0.0   0.0   0.0  0
 1396  2,2  -biphenyldicarboxylic  acid                    ZZZUCY
C14  H10  O 4                  152.0   0.0   0.0 298.0  1
 1397  4,4  -biphenyldicarboxylic acid
C14  H10  O 4                  196.0   0.0   0.0 298.0  0
 1398  2-2,6-dichlorophenyl amino benzoic acid
C14  H11 Cl 2  N 1  O 2        116.0   0.0   0.0 298.0  1
 1399  2  -fluoro-2-hydroxy-4-methoxybenzophenone
C14  H11  F 1  O 3             109.0   0.0   0.0 313.0  1
 1400  1,1,2-trifluoro-1,2-diphenylethane
C14  H11  F 3                   93.0   0.0   0.0 298.0  0
 1401  10-methylacridin-9  10H -one                        NMACRO
C14  H11  N 1  O 1             105.0   0.0   0.0   0.0  0
 1402  2-cyanophenyl benzyl sulfide
C14  H11  N 1  S 1             118.0   0.0   0.0 298.0  0
 1403  1-methylfluorene                                    TOKKIN
C14  H12                        91.2   0.0   0.0 301.0  1
 1404  9-methylfluorene                                    BISDOY
C14  H12                        83.3   0.0   0.0 298.0  2
 1405  9,10-dihydroanthracene                              DITBOX
C14  H12                        93.0   0.0   0.0 298.0  3
 1406  trans-stilbene                                      TSTILB
C14  H12                       102.0 100.0 104.0 298.0  5
 1407  1,1-difluoro-1,2-diphenylethane
C14  H12  F 2                   95.0   0.0   0.0 298.0  0
 1408  dibenzylideneazine                                  BZAZIN
C14  H12  N 2                   93.0   0.0   0.0 293.0  0
 1409  2-benzylbenzimidazole                               LAXGAT
C14  H12  N 2                  136.0   0.0   0.0 298.0  1
 1410  desoxybenzoin
C14  H12  O 1                   99.0   0.0   0.0   0.0  0
 1411  2-hydroxy-4-methoxybenzophenone
C14  H12  O 3                  119.0   0.0   0.0 298.0  1
 1412  N-ethylcarbazole                                    ETCABZ
C14  H13  N 1                   99.0   0.0   0.0 298.0  1
 1413  N,N-diphenylacetamide                               DPACTM
C14  H13  N 1  O 1             123.0   0.0   0.0 360.0  1
 1414  2,2  -dimethylbiphenyl
C14  H14                        66.0   0.0   0.0 298.0  1
 1415  3,3  -dimethylbiphenyl
C14  H14                        72.0   0.0   0.0 298.0  1
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 1416  4,4  -dimethylbiphenyl                                        BTOLYL
C14  H14                     95.0   0.0   0.0 298.0  0
 1417  1,2-diphenylethane                                           DIBENZ
C14  H14                     92.0   0.0   0.0 298.0  4
 1418  p-azoxyanisole
C14  H14  N 2  O 1           135.0   0.0   0.0 298.0  0
 1419  3-nitro-4  -  N,N-dimethylamino -azobenzene
C14  H14  N 4  O 2           133.0   0.0   0.0 400.0  1
 1420  4-nitro-4  -  N,N-dimethylamino -azobenzene
C14  H14  N 4  O 2           134.5   0.0   0.0 420.0  1
 1421  1,1-diphenylethanol                                          CINVEA
C14  H14  O 1                105.0   0.0   0.0 298.0  0
 1422  4-methoxyphenyl benzyl sulfide
C14  H14  O 1  S 1           113.0   0.0   0.0 298.0  0
 1423  dibenzyl sulfone                                             TUXFIC
C14  H14  O 2  S 1           125.0   0.0   0.0   0.0  0
 1424  di-p-tolyl sulfone                                           QIBQOH
C14  H14  O 2  S 1           110.0   0.0   0.0   0.0  0
 1425  6-methoxy-alfa -methyl-2-naphthaleneacetic acid              COYRUD
C14  H14  O 3                128.0   0.0   0.0 360.0  1
 1426  1,2,4,5-tetramethoxycarbonylbenzene
C14  H14  O 8                140.0   0.0   0.0 298.0  2
 1427  dibenzyl sulfide                                             ZZZSRY
C14  H14  S 1                 93.0   0.0   0.0   0.0  0
 1428  4-(N,N-dimethylamino azobenzene                              VUFZUR
C14  H15  N 3                118.0 116.0 120.0 360.0  2
 1429  2,3 -dimethyl-4-aminoazobenzene
C14  H15  N 3                113.0   0.0   0.0   0.0  0
 1430  1,4,5,8-tetramethylnaphthalene                               CEKREP
C14  H16                     100.0   0.0   0.0 298.0  0
 1431  1,5-N,N,N'N'-tetramethyldiaminonaphthalene
C14  H18  N 2                 98.6   0.0   0.0 298.0  1
 1432  1,8-N,N,N'N'-tetramethyldiaminonaphthalene                   DMANAP
C14  H18  N 2                 94.7   0.0   0.0 298.0  1
 1433  diamantanone
C14  H18  O 1                103.0   0.0   0.0 320.0  0
 1434  1,8-cyclotetradecadiyne                                      RIQVOC
C14  H20                     94.0   0.0   0.0 298.0  1
 1435  1,2,3,4,5,6,7,8-octahydroanthracene
C14  H20                     82.3   0.0   0.0 298.0  1
 1436  diadamantane
C14  H20                     96.0   0.0   0.0 319.0  1
 1437  diamantan-1-ol                                               WEJMAA
C14  H20  O 1                118.0   0.0   0.0 334.0  1
 1438  diamantan-3-ol
C14  H20  O 1                116.0   0.0   0.0 339.0  1
 1439  diamantan-4-ol
C14  H20  O 1                117.0   0.0   0.0 338.0  1
 1440  4-heptylbenzoic acid                                         ZIKWOF
C14  H20  O 2                130.0   0.0   0.0 298.0  1
 1441  1,4-di-tert-butylbenzene                                     BUTBNZ
C14  H22                      83.0   0.0   0.0 298.0  2
 1442  2,4-di-tert-butylphenol
C14  H22  O 1                 90.0  87.0  93.0 298.0  2
 1443  2,6-di-tert-butylphenol                                      LERFET
C14  H22  O 1                 83.0   0.0   0.0 298.0  2
 1444  3,5-di-tert-butylphenol
C14  H22  O 1                 98.0   0.0   0.0 298.0  0
 1445  4-tert-octylphenol ?
C14  H22  O 1                 98.0   0.0   0.0 298.0  1
 1446  3,5-di-tert-butyl-1,2-dihydroxybenzene
C14  H22  O 2                103.0   0.0   0.0 298.0  2
 1447  2,5-di-tert-butyl-1,4-dihydroxybenzene                       HESKOF
C14  H22  O 2                122.0   0.0   0.0 298.0  1
 1448  dicyclohexyl peroxydicarbonate                               SEGROL
C14  H22  O 6                100.0   0.0   0.0 303.0  1
 1449  1,3,5,7-tetramethyladamantane
C14  H24                      83.0   0.0   0.0 298.0  2
 1450  cyclotetradecanone
C14  H26  O 1                 81.0   0.0   0.0   0.0  0
 1451  cyclotetradecane                                             CYTDEC
C14  H28                      98.0  89.3 134.0 298.0  3
 1452  2-tetradecanone
C14  H28  O 1                131.0   0.0   0.0 298.0  0
 1453  tetradecanoic acid                                           ZZZOEG
C14  H28  O 2                140.0 140.0 169.0 318.0  2
 1454  peroxytetradecanoic
C14  H28  O 3                156.0   0.0   0.0 298.0  1
 1455  tetradecanamide
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C14  H29  N 1  O 1             167.0   0.0   0.0 352.0  0
 1456  tetradecane
C14  H30                       118.0   0.0   0.0 298.0  0
 1457  diphenylcyclopropenone
C15  H10  O 1                  130.0 120.0 140.0 350.0  2
 1458  9-anthraldehyde                                    ANTHAL
C15  H10  O 1                  100.0   0.0   0.0 346.0  1
 1459  2-anthracenecarboxylic
C15  H10  O 2                  134.0   0.0   0.0 411.0  1
 1460  9-anthracenecarboxylic                             QQQFDJ
C15  H10  O 2                  120.0   0.0   0.0 403.0  1
 1461  2-phenyl-4H-1-benzopyran-4-one flavone             WADRAV
C15  H10  O 2                  108.0   0.0   0.0 298.0  0
 1462  1-methoxy-9,10-anthraquinone
C15  H10  O 3                  120.0 107.0 128.0   0.0  2
 1463  2-methoxy-9,10-anthraquinone
C15  H10  O 3                  123.0 118.0 125.0   0.0  2
 1464  9-methoxy-1,4-anthraquinone
C15  H10  O 3                  132.0   0.0   0.0 298.0  1
 1465  2-hydroxy-3'trifluoromethyl-4-methoxybenzophenon
C15  H11  F 3  O 3             103.0   0.0   0.0 318.0  1
 1466  2-hydroxy-4'trifluoromethyl-4-methoxybenzophenon
C15  H11  F 3  O 3              91.0   0.0   0.0 323.0  1
 1467  2-phenylquinoline
C15  H11  N 1                  105.0   0.0   0.0 298.0  1
 1468  1-methylamino-9,10-anthraquinone
C15  H11  N 1  O 2             119.0 113.0 123.0 384.0  4
 1469  1-amino-2-methyl-9,10-anthraquinone
C15  H11  N 1  O 2             124.0   0.0   0.0 374.0  1
 1470  9-methylanthracene                                 MANTHR
C15  H12                       101.0  99.0 102.0 298.0  2
 1471  dibenzosuberone
C15  H12  O 1                  109.0   0.0   0.0 298.0  0
 1472  dibenzoylmethane                                   DBEZLM
C15  H12  O 2                  115.0   0.0   0.0 298.0  2
 1473  2,10-dimethylacridin-9(10H)one
C15  H13  N 1  O 1             119.0   0.0   0.0   0.0  0
 1474  10-ehylacridin-9(10H)-one                          EACDRO
C15  H13  N 1  O 1             117.0   0.0   0.0   0.0  0
 1475  N-benzoyl-N-methylbenzamide
C15  H13  N 1  O 2             120.0   0.0   0.0 298.0  1
 1476  1,3-diphenylacetone                                WUXDOJ
C15  H14  O 1                   89.0   0.0   0.0   0.0  0
 1477  3,4-dimethylbenzophenone
C15  H14  O 1                  108.0   0.0   0.0 298.0  0
 1478  2,2-diphenyl-1,3-dioxolane
C15  H14  O 2                  100.0   0.0   0.0 298.0  0
 1479  dimethoxydiphenylmethane
C15  H16  O 2                  104.0   0.0   0.0 298.0  0
 1480  1-methyldiamantane
C15  H22                        81.0   0.0   0.0   0.0  0
 1481  3-methyldiamantane
C15  H22                       103.0   0.0   0.0 316.0  1
 1482  4-methyldiamantane
C15  H22                        79.0   0.0   0.0 322.0  1
 1483  3,5-di-tert-butylbenzoic acid                      DTBUBZ
C15  H22  O 2                  108.0   0.0   0.0 348.0  1
 1484  3,5-di-tert-butyl-2-hydroxybenzaldehyde
C15  H22  O 2                   96.0   0.0   0.0 298.0  1
 1485  4-octylbenzoic acid
C15  H22  O 2                  135.0   0.0   0.0 298.0  0
 1486  4-octyloxybenzoic  acid                           ZZZZCB
C15  H22  O 3                  163.0   0.0   0.0 298.0  0
 1487  3,5-di-tert-butylsalicylic acid
C15  H22  O 3                   84.0   0.0   0.0   0.0  0
 1488  1,3-di-tert-butyl-5-methylbenzene
C15  H24                        82.1   0.0   0.0 298.0  1
 1489  2,6-di-tert-butyl-4-methylphenol                   MBPHOL
C15  H24  O 1                   90.0  88.0  92.0 298.0  3
 1490  pentadecane
C15  H32                       108.0   0.0   0.0 298.0  0
 1491  1-bromopyrene                                      MEGTOI
C16  H 9 Br 1                   99.2   0.0   0.0 345.0  1
 1492  1-nitropyrene
C16  H 9  N 1  O 2             125.0   0.0   0.0 394.0  1
 1493  fuoranthene                                        FLUANT
C16  H10                       101.0  98.0 103.0 310.0  4
 1494  pyrene                                             PYRENE
C16  H10                       100.0  97.9 104.0 350.0  8
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 1495  2-phenylnaphthalene
C16  H12                    108.0   0.0   9.0 298.0  1
 1496  3,6-diphenyl-1,2-dithiin
C16  H12  S 2                183.0   0.0   0.0 298.0  0
 1497  N-phenyl-1-naphthylamine
C16  H13  N 1                 96.5   0.0   0.0 323.0  1
 1498  N-phenyl-2-naphthylamine
C16  H13  N 1                115.0   0.0   0.0 348.0  1
 1499  9-acetamidoanthracene
C16  H13  N 1  O 1           134.0   0.0   0.0 461.0  1
 1500  4,5,9,10-tetrahydropyrene
C16  H14                      90.4   0.0   0.0 398.0  1
 1501  9,10-dimethylanthracene                                DMANTR
C16  H14                     114.0   0.0   0.0 330.0  2
 1502  2-ethylanthracene
C16  H14                     108.0   0.0   0.0 298.0  1
 1503  2,7-dimethylphenanthrene
C16  H14                     107.0   0.0   0.0   0.0  0
 1504  4,5-dimethylphenanthrene                               FEWWEJ
C16  H14                     105.0   0.0   0.0   0.0  1
 1505  9,10-dimethylphenanthrene                              KEDJOS
C16  H14                     120.0   0.0   0.0   0.0  0
 1506  1,4-diphenylbutadiene
C16  H14                      87.0   0.0   0.0   0.0  0
 1507  3-4-biphenylylcarbonyl propionic acid fenbufen         SAFNIW
C16  H14  O 3                154.0   0.0   0.0 298.0  1
 1508  3-anilino-1-phenylbut-2-enone
C16  H15  N 1  O 1           127.0   0.0   0.0 298.0  0
 1509  1,2,3,6,7,8-hexahydropyrene                            TICJEU
C16  H16                      92.3   0.0   0.0 398.0  1
 1510  (2,2)paracyclophane                                    DXYLEN
C16  H16                      95.0   0.0   0.0 350.0  3
 1511  (2,2)metacyclophane                                    METCYP
C16  H16                      92.0   0.0   0.0 298.0  0
 1512  (2,2)parametacyclophane
C16  H16                      88.0   0.0   0.0 298.0  0
 1513  1,1-bis-  4-methylphenyl ethene
C16  H16                     101.0   0.0   0.0 298.0  1
 1514  N,N-bissalicylaldehydoEthylenediimine                  ESALIM
C16  H16  N 2  O 2           141.0   0.0   0.0 298.0  1
 1515  pentamethoxycarbonylbenzene
C16  H16  O10                165.0   0.0   0.0 298.0  2
 1516  1,3-diphenylbutane
C16  H18                      73.6   0.0   0.0 298.0  1
 1517  2,3-diphenylbutane
C16  H18                      96.7   0.0   0.0 321.0  1
 1518  4-tert-butylbiphenyl
C16  H18                      98.0   0.0   0.0 298.0  0
 1519  p-azoxyphenetole
C16  H18  N 2  O 3           127.0   0.0   0.0 298.0  0
 1520  tricyclo 8.2.2.2(4,7) hexadecane
C16  H28                      90.0  85.0  92.0 298.0  2
 1521  tetracyclopropylsuccinonitrile
C16  H30  N 2                110.0   0.0   0.0   0.0  0
 1522  cyclohexadecanone
C16  H30  O 1                 82.0   0.0   0.0   0.0  0
 1523  hexadecanedioic acid
C16  H30  O 4                155.0   0.0   0.0 298.0  0
 1524  cyclohexadecane
C16  H32                      82.0   0.0   0.0   0.0  0
 1525  hexadecanoic acid                                      YEFWEM
C16  H32  O 2                154.0   0.0   0.0 327.0  1
 1526  hexadecanamide
C16  H33  N 1  O 1           181.0   0.0   0.0 371.0  1
 1527  hexadecane                                             QQQFBP
C16  H34                     135.0   0.0   0.0 298.0  2
 1528  1-hexadecanol
C16  H34  O 1                170.0   0.0   0.0 298.0  0
 1529  benzanthrone
C17  H10  O 1                126.0   0.0   0.0 298.0  4
 1530  1,2-benzoFluorene
C17  H12                     105.0   0.0   0.0 383.0  1
 1531  2,3-benzofluorene
C17  H12                     115.0 111.0 119.0 377.0  2
 1532  diphenylmethylene diacetate
C17  H16  O 4                122.0   0.0   0.0 368.0  1
 1533  salicyclic acid 4(t-Btuphenyl)ester
C17  H18  O 3                137.0   0.0   0.0 308.0  1
 1534  2-hydroxy-4,4'-diethoxybenzophenone
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C17  H18  O 4                  135.0   0.0   0.0 298.0  0
 1535  diethoxydiphenylmethane
C17  H20  O 2                   97.0   0.0   0.0 298.0  0
 1536  cocaine                                            COCAIN
C17  H21  N 1  O 4              113.0 113.0 127.0 304.0  2
 1537  cycloheptadecanone
C17  H32  O 1                   76.0   0.0   0.0   0.0  0
 1538  cycloheptadecane
C17  H34                        66.0   0.0   0.0   0.0  0
 1539  heptadecane
C17  H36                       129.0 125.0 131.0 298.0  2
 1540  1-heptadecanol
C17  H36  O 1                  179.0   0.0   0.0   0.0  0
 1541  1,2-benzanthra-9,10-quinone                        ZZZJWM
C18  H10  O 2                   83.0   0.0   0.0   0.0  0
 1542  5,12-tetracenequinone
C18  H10  O 2                  109.0   0.0   0.0   0.0  0
 1543  6,11-dihydroxy-5,12-naphthacenedione
C18  H10  O 4                  144.0   0.0   0.0 436.0  1
 1544  naphthacene  (tetracene) linear fit                 TETCEN
C18  H12                       139.0   0.0   0.0 298.0  7
 1545  benz a anthracene  linear fit                      BEANTR
C18  H12                       118.0   0.0   0.0 298.0  7
 1546  triphenylene linear fit                            TRIPHE
C18  H12                       127.0   0.0   0.0 298.0  5
 1547  chrysene linear fit                                CRYSEN
C18  H12                       131.0   0.0   0.0 384.5  4
 1548  benzo c phenanthrene                               BZPHAN
C18  H12                       106.0   0.0   0.0   0.0  0
 1549  2,2  -biquinoline                                  BIQUOL
C18  H12  N 2                  135.0   0.0   0.0 298.0  1
 1550  2-phenylindeno 2,1-b pyran
C18  H12  O 1                  132.0   0.0   0.0 409.0  1
 1551  o-terphenyl                                        TERPHO
C18  H14                       101.0  97.0 103.0 298.0  2
 1552  m-terphenyl                                        ZZZMTW
C18  H14                       119.0   0.0   0.0 298.0  3
 1553  p-terphenyl                                        TERPHE
C18  H14                       122.0 113.0 126.0 298.0  3
 1554  5,12-dihydrotetracene                              REGXUY
C18  H14                       121.0   0.0   0.0 298.0  1
 1555  diphenylfulvene                                    RIWTAS
C18  H14                       105.0   0.0   0.0   0.0  0
 1556  2,6-diphenylphenol                                 DPPHOL
C18  H14  O 1                  119.0   0.0   0.0 298.0  1
 1557  triphenylamine                                     ZZZJCQ
C18  H15  N 1                   87.9   0.0   0.0 337.0  1
 1558  9-diacetylaminoanthracene
C18  H15  N 1  O 2              106.0   0.0   0.0   0.0  0
 1559  dihydrodibenzotetra-aza-annulene
C18  H16  N 4                   82.0   0.0   0.0 513.0  0
 1560  9-butylanthracene
C18  H18                       108.0   0.0   0.0 303.0  0
 1561  2,4,5,7-tetraMethylphenanthrene                    FUFQIG
C18  H18                       114.0   0.0   0.0   0.0  0
 1562  3,4,5,6-tetramethylthylphenanthrene                FEWWIN
C18  H18                       134.0   0.0   0.0   0.0  0
 1563  3-diphenylmethylthyl-2,4-pentanedione
C18  H18  O 2                  112.0   0.0   0.0 366.0  1
 1564  N-benzyl-pivalophenone imine
C18  H21  N 1                  110.0   0.0   0.0 298.0  0
 1565  2,3-diMEthyl-2,3-diphenylbutane
C18  H22                        96.7   0.0   0.0 321.0  1
 1566  2,4,6-tri-tert-butylnitrosobenzene
C18  H29  N 1  O 1              91.0   0.0   0.0 298.0  0
 1567  2,4,6-tri-tert-butylnitrobenzene
C18  H29  N 1  O 2              96.0   0.0   0.0 298.0  0
 1568  hexaethylbenzene                                   ZZZEMS
C18  H30                        95.0   0.0   0.0 340.0  0
 1569  1,3,5-tri-tert-butylbenzene                        TTBUBZ
C18  H30                        81.0   0.0   0.0 298.0  2
 1570  2,4,6-tri-tert-butylphenol
C18  H30  O 1                   86.0  84.0  88.0 298.0  4
 1571  4-diacetylbenzene diethyl ketal
C18  H30  O 4                  112.0   0.0   0.0 317.0  1
 1572  2,4,6-tri-tert-butylaniline
C18  H31  N 1                   93.0   0.0   0.0 298.0  0
 1573  cyclooctadecanone
C18  H34  O 1                   77.0   0.0   0.0   0.0  0
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 1574  octadecanoic acid stearic                                      STARAC
C18  H36  O 2                166.0   0.0   0.0 336.0  1
 1575  octadecanamide
C18  H37  N 1  O 1             195.0   0.0   0.0 373.0  1
 1576  octadecane                                                     NOCTDC
C18  H38                     153.0   0.0   0.0 298.0  2
 1577  1,1,2,2-tetra-tert-butylethane
C18  H38                      74.0   0.0   0.0 298.0  0
 1578  1-octadecanol
C18  H38  O 1                191.0   0.0   0.0 298.0  0
 1579  10-phenylacridin-9  10H -one                                   PHACRD
C19  H13  N 1  O 1             128.0   0.0   0.0   0.0  0
 1580  N-phenyl  benzophenone imine                                   DPMYAN
C19  H15  N 1                120.0   0.0   0.0 298.0  1
 1581  triphenylazidomethane                                          PIPHAX
C19  H15  N 3                120.0   0.0   0.0 349.0  1
 1582  triphenylmethane                                               TPHMET
C19  H16                     111.0 105.0 114.0 298.0  5
 1583  triphenylmethanol
C19  H16  O 1                122.0   0.0   0.0 298.0  2
 1584  3-diphenylMEthyl-3-MEthyl-2,4-pentanedione
C19  H20  O 2                114.0   0.0   0.0 298.0  0
 1585  tricyclohexylmethane                                           LEPRON
C19  H34                     117.0   0.0   0.0 311.0  1
 1586  cyclononadecanone
C19  H36  O 1                 82.0   0.0   0.0   0.0  0
 1587  nonadecanoic acid                                              CEVWAC
C19  H38  O 2                199.0   0.0   0.0   0.0  1
 1588  nonadecane
C19  H40                     144.0   0.0   0.0 298.0  0
 1589  corannulene                                                    CORANN
C20  H10                     120.0   0.0   0.0 298.0  1
 1590  perylene linear fit 5                                          PERLEN
C20  H12                     140.0   0.0   0.0 298.0  5
 1591  benzo a pyrene                                                 BNPYRE
C20  H12                     120.0   0.0   0.0 370.0  2
 1592  benzo e pyrene                                                 CEQGEL
C20  H12                     118.0   0.0   0.0 380.0  2
 1593  9-phenylanthracene                                             QURDOY
C20  H14                     118.0 115.0 119.0 380.0  3
 1594  binaphthalene
C20  H14                     138.0   0.0   0.0 383.0  1
 1595  1-anilino-4-aminoanthraquinone
C20  H14  N 2  O 2             135.0   0.0   0.0 520.0  1
 1596  dibenzoyl resorcinol
C20  H14  O 4                165.0   0.0   0.0 361.0  1
 1597  1,1,1-triFluoro-2,2,2-triphenylethane
C20  H15  F 3                112.0   0.0   0.0 298.0  0
 1598  triphenylethylhylene
C20  H16                     112.0   0.0   0.0 298.0  1
 1599  7,12-diMEthylbenz a anthracene
C20  H16                     135.0   0.0   0.0 380.0  0
 1600  5,6-diMEthylchrysene                                           ZEGKAX
C20  H16                     135.0   0.0   0.0 400.0  0
 1601  1,1,1-triphenylethane                                          TRPETN
C20  H18                     109.0   0.0   0.0 298.0  2
 1602  1,1,2-triphenylethane
C20  H18                      92.0   0.0  92.2 298.0  2
 1603  pagodane                                                       VABNAN
C20  H20                      90.2   0.0   0.0 446.0  1
 1604  1,1,1-tris methoxycarbonyl -2,2-diphenylethane
C20  H20  O 6                136.0   0.0   0.0 298.0  0
 1605  3-diphenylmethyl-3-ethyl-2,4-pentanedione
C20  H22  O 2                122.0   0.0   0.0 368.0  1
 1606  dibenzo-18-crown-6                                             ROFYIV
C20  H24  O 6                179.0   0.0   0.0 298.0  0
 1607  4,4  -di-tert-butylbiphenyl
C20  H26                     107.0   0.0   0.0 298.0  0
 1608  hexacyclopropylethane                                          CIDBUM
C20  H30                     109.0   0.0   0.0   0.0  0
 1609  1,1  -biadamantane                                            BADAMN
C20  H30                     114.0   0.0   0.0 298.0  0
 1610  eicosanedioic acid
C20  H38  O 4                170.0   0.0   0.0 298.0  0
 1611  eicosanoic acid
C20  H40  O 2                200.0   0.0   0.0 342.0  1
 1612  eicosane                                                       QQQCIM
C20  H42                     177.0 173.0 180.0 320.0  2
 1613  1-eicosanol
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C20  H42  O 1                  223.0   0.0   0.0 298.0  0
 1614  1,1-diFluoro-3,3,3-triphenylpropane
C21  H18  F 2                  113.0   0.0   0.0 298.0  0
 1615  1-fluoro-3,3,3-triphenylpropane
C21  H19  F 1                  129.0   0.0   0.0 298.0  0
 1616  2-fluoro-1,2,3-triphenylpropane
C21  H19  F 1                  133.0   0.0   0.0 298.0  0
 1617  diacetylmorphine heroin                              DACMOR
C21  H23  N 1  O 5             144.0   0.0   0.0 332.0  1
 1618  l,1 -diadamantyl ketone                              PUSDIQ
C21  H30  O 1                  109.0   0.0   0.0 298.0  1
 1619  heneicosane
C21  H44                       142.0   0.0   0.0 298.0  0
 1620  anthanthrone dibenzochrysene6,12dione                ANTHON
C22  H10  O 2                  152.0   0.0   0.0 500.0  1
 1621  benzo ghi perylene                                   BNPERY
C22  H12                       132.0 126.0 135.0 442.0  4
 1622  6,13-pentacenequinone                                PENTQU
C22  H12  O 2                  116.0   0.0   0.0 298.0  0
 1623  dibenz a,c anthracene
C22  H14                       160.0   0.0   0.0 298.0  1
 1624  dibenz a,h anthracene                                DBNTHR
C22  H14                       163.0   0.0   0.0 298.0  1
 1625  pentacene                                            PENCEN
C22  H14                       184.0   0.0   0.0 298.0  1
 1626  picene                                               ZZZOYC
C22  H14                       140.0   0.0   0.0 430.5  2
 1627  2-(biphen-4-yl) naphthalene
C22  H16                       140.0   0.0   0.0 298.0  1
 1628  N,N  -bis  2-methoxyphenyl terephthalamide
C22  H20  N 2  O 4             197.0   0.0   0.0   0.0  1
 1629  N,N  -bis  3-methoxyphenyl terephthalamide
C22  H20  N 2  O 4             209.0   0.0   0.0   0.0  1
 1630  N,N  -bis  4-methoxyphenyl terephthalamide
C22  H20  N 2  O 4             228.0   0.0   0.0   0.0  0
 1631  1,4-bis  N-butylamino -9,10-anthraquinone            CAMJOP
C22  H26  N 2  O 2             116.0   0.0   0.0 394.0  1
 1632  1,4-bis  N-isobutylamino -9,10-anthraquinone
C22  H26  N 2  O 2              96.4   0.0   0.0 378.0  1
 1633  docosane
C22  H46                       173.0   0.0   0.0 391.0  0
 1634  1-docosanol
C22  H46  O 1                  239.0   0.0   0.0 298.0  1
 1635  finasteride                                          WOLXOK
C23  H36  N 2  O 2             144.0   0.0   0.0 470.0  1
 1636  coronene  linear fit                                 CORONE
C24  H12                       152.0   0.0   0.0 298.0  6
 1637  2,2,5,25 5 ,5,2,5,2 -sexithiophene                   ZAQZUM
C24  H14  S 6                  211.0   0.0   0.0 560.0  1
 1638  1,2,3-triphenylbenzene
C24  H18                       134.0   0.0   0.0 298.0  1
 1639  1,3,5-triphenylbenzene                               TPHBEN
C24  H18                       150.0   0.0   0.0 298.0  5
 1640  tetracosane
C24  H50                       162.0   0.0   0.0 298.0  0
 1641  tetraphenylmethane                                   TEPHME
C25  H20                       146.0 140.0 151.0 298.0  2
 1642  pentacosane
C25  H52                       174.0   0.0   0.0 298.0  0
 1643  9,10-diphenylanthracene                              DPANTR
C26  H18                       150.3 137.0 156.0 429.3  3
 1644  tetraphenylethene
C26  H20                       133.0   0.0   0.0 298.0  1
 1645  1,1,2,2-tetraphenylethane
C26  H22                       137.0   0.0   0.0 298.0  1
 1646  1,1,1,2-tetraphenylethane                            TPHETN
C26  H22                       133.0   0.0   0.0 298.0  1
 1647  hexacosane
C26  H54                       177.0   0.0   0.0 298.0  0
 1648  cholesterol
C27  H46  O 1                  142.0   0.0   0.0 400.0  1
 1649  ergosterol
C28  H44  O 1                  147.0   0.0   0.0 365.0  1
 1650  octacosane
C28  H58                       209.0   0.0   0.0 298.0  1
 1651  pyranthrene
C30  H16                       195.0   0.0   0.0 595.0  0
 1652  ovalene                                              OVALEN
C32  H14                       212.0   0.0   0.0 600.0  0
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 1653  dibenzanthrone  violanthrone                                DIBANT
C34  H16  O 2                  207.0 203.0 209.0 531.0  2
 1654  isodibenzanthrone isoviolanthrone                          IDBANT
C34  H16  O 2                  219.0 215.0 221.0 538.0  1
 1655  violanthrene                                               CORXAI
C34  H18                       224.0   0.0   0.0 590.0  1
```

Table S2. Chemical composition of the 1655-data sample. Number of molecules in which each atomic species is present, and number of compounds in selected chemical classes. Compounds belonging to more than one class were assigned according to the most prominent functionality..

atomic species	number of molecules		chemical class	number of entries
H	1611		amines, amides, -aza compounds	365
C	1655		hydrocarbons	192
N	783		DNA bases and uracils	74
O	1113		acids	104
S	120		alcohols	68
P	7		nitro	129
F	58			
Cl	174			
Br	46			
I	21			

Table S3. Attempted fitting of SE data (kJ mol^{-1}) from different sources against temperature.

compound	npts[a]	nout[b]	T range[c]	ΔCp[d]	SE_0[e]	SE(298) or range[f]
coronene	6	1	383-473	-0.071	173	152
p-terphenyl	4	0	298-397	-0.050	138	123
hexachlorobenzene	10	3	278-480	-0.082	124	100
4-nitroaniline	8	2	298-362	-0.041	113	101
acridine	9	0	298-430	-0.051	108	93
tetracyanoquinodimethane	5	0	413-500	-0.223	214	147
benzoic acid	36	3	298-400	-0.035	101	91
	39	12	298-400	-	-	88-91
benzene	12	0	193-298	-0.014	49	44
	12	5	261-298	-	-	44-46
anthracene	31	3	298-450	-0.011	102	99
	31	3		-	-	92-103
	31	14		-	-	95-100
acenaphthene	8	0	298-366	-0.030	94	85

[a] Number of available data. [b] Number of outliers excluded. [c] Temperature range of data. [d]Slope of the least-squares line. [e]Intercept of the fitting line. [f] SE(298) from fit, or range without fit.

Table S4. First line: sequence number as in Table S1, CSD refcode, compound name
Second line: sublimation enthalpy, Pixel lattice energy, Dabsolute, D%;
AA-CLP lattice energy, Dabsolute, D%. kJ/mol units.

2	CTBROM06	carbon tetrabromide						
	54.5				55.0	-0.5	-0.9	
5	CARBTC	carbon tetrachloride						
	37.9				56.1	-18.2	-48.0	
8	TFMETH02	carbon tetrafluoride						
	7.3	10.6	-3.3	-45.2	17.7	-10.4	-142.7	
13	SACBAA02	carbon dioxide						
	21.8	22.3	-0.5	-2.2	29.5	-7.7	-35.2	
15	IODOFO	iodoform						
	70.9	65.9	5.0	7.1	60.8	10.1	14.3	
18	CYANAM01	cyanamide						
	75.1	79.2	-4.1	-5.5	64.9	10.2	13.6	
19	TETZOL02	tetrazole						
	90.1	88.2	1.9	2.1	74.4	15.7	17.4	
20	FORMAC01	formic acid						
	59.5	53.7	5.8	9.7	53.5	6.0	10.1	
23	FORMAM02	formamide						
	72.1	71.9	0.2	0.2	63.8	8.3	11.5	
26	UREAXX25	urea						
	98.3	103.8	-5.6	-5.7	99.8	-1.5	-1.5	
27	THIOUR16	thiourea						
	109.3	122.9	-13.6	-12.4	69.2	40.1	36.7	
28	NTRGUA01	nitroguanidine						
	143.1	155.9	-12.8	-8.9	136.4	6.7	4.7	
31	TSCRBZ22	thiosemicarbazide						
	126.1	152.9	-26.9	-21.3	83.9	42.1	33.4	
36	HEXCET05	hexachloroethane						
	61.1	70.4	-9.3	-15.2	73.6	-12.5	-20.5	
38	CYNGEN	cyanogen						
	29.5	33.9	-4.4	-14.9	49.4	-19.9	-67.5	
39	QQQBRD02	hexanitroethane						
	71.1				101.7	-30.6	-43.0	
40	ACETYL	acetylene						
	18.5	21.0	-2.5	-13.5	16.0	2.5	13.5	
41	TFACAM	triFluoroacetamide						
	79.1	72.9	6.2	7.9	71.6	7.5	9.5	
42	OXALAC08	oxalic acid anhydrous.						
	95.5	106.9	-11.4	-11.9	117.6	-22.1	-23.1	
43	BRMACA01	bromoacetic acid						
	84.1	72.4	11.7	13.9	67.6	16.5	19.6	
44	CLACET07	chloroacetic acid						
	82.1	81.1	1.0	1.2	75.8	6.3	7.6	
48	TRAZOL04	1,2,4-triazole						
	82.1	89.0	-6.9	-8.4	74.0	8.1	9.9	
49	FINBIP	1,1,1-trinitroethane						
	72.1	70.6	1.5	2.0	69.5	2.6	3.6	
52	ZZZFHE01	1,2-diiodoethane						
	66.0	57.5	8.5	13.0	50.8	15.3	23.1	
55	SSOXAM02	dithiooxamide						
	105.3	110.8	-5.5	-5.3	80.1	25.2	23.9	
56	CYAMPD11	dicyandiamide						
	134.7	158.0	-23.3	-17.3	127.1	7.6	5.6	
57	TELPOP	1-methyltetrazole						
	87.1	88.6	-1.5	-1.8	65.8	21.3	24.4	
58	FIZZOD	5-methyltetrazole						
	96.1	86.7	9.4	9.8	88.3	7.8	8.1	
59	ACETAC03	acetic acid						
	64.9	60.0	4.8	7.4	64.9	-0.1	-0.1	
61	ACEMID05	acetamide						
	79.1	74.6	4.5	5.7	73.3	5.7	7.2	
62	FEPGEM	methyl carbamate						
	75.1	75.3	-0.2	-0.2	85.4	-10.4	-13.8	
63	THACEM01	thioacetamide						
	83.1	87.6	-4.5	-5.4	55.0	28.1	33.8	
65	AMMTAZ01	2-methyl-5-aminotetrazole						
	92.7	106.1	-13.4	-14.5	96.1	-3.4	-3.7	
68	MEUREA01	N-methylurea						
	97.9	106.3	-8.4	-8.6	91.7	6.2	6.3	
70	BEXQOK01	N-methylthiourea						
	112.1	121.0	-8.9	-8.0	68.9	43.2	38.5	
71	DMSULO04	dimethyl sulfone						
	77.0	96.9	-19.9	-25.9	80.4	-3.4	-4.4	
72	ETDIAM12	ethylenediamine						

```
     64.5   87.4  -23.0  -35.6   74.1   -9.7  -15.0
 74  CAACTY    cyanoacetylene
     40.5   38.9    1.6    4.0   30.0   10.5   26.0
 75  MALONT    malononitrile
     79.1   62.9   16.2   20.5   79.8   -0.7   -0.9
 79  TRIZIN01  1,3,5-triazine
     57.1   59.6   -2.5   -4.4   64.7   -7.6  -13.3
 80  AZURAC10  6-azauracil
    141.0  101.9   39.1   27.8  103.1   37.9   26.9
 81  CYURAC13  cyanuric acid
    133.1  129.3    3.7    2.8  126.1    6.9    5.2
 83  IMAZOL13  imidazole
     83.1   88.0   -4.9   -5.9   70.3   12.8   15.4
 84  PYRZOL38  pyrazole
     73.1   77.3   -4.2   -5.7   61.0   12.1   16.6
 85  CYANAC    2-cyanoacetamide
    101.7  107.0   -5.3   -5.2  122.4  -20.7  -20.3
 87  IXANOK    1,3-dithiolan-2-one
     80.0   63.2   16.8   21.0   77.4    2.6    3.2
 88  ETHCAR    ethylene carbonate
     77.1   65.5   11.6   15.1   65.8   11.3   14.7
 89  MALNAC16  malonic acid
    109.5  101.0    8.5    7.7  120.3  -10.8   -9.9
 90  DTOLTO    1,3-dithiolan-2-thione
     82.1   70.2   11.9   14.5   77.6    4.5    5.5
 91  ARCLAM01  acrylamide
     83.3   79.8    3.5    4.2   73.3    9.9   11.9
 95  QQQCIS01  cyclopropane
     22.5   23.5   -1.0   -4.4   28.0   -5.5  -24.4
 98  QQQGEM01  acetylurea
    103.1  109.3   -6.2   -6.0  118.4  -15.4  -14.9
 99  MALOAM02  malonamide
    126.0  140.9  -14.9  -11.8  140.2  -14.2  -11.3
101  MELAMI02  2,4,6-triamino-s-triazine,melamine.
    128.1  164.3  -36.2  -28.3  193.2  -65.1  -50.8
103  PRONAC    propionic acid
     70.8   66.9    3.9    5.5   75.4   -4.6   -6.5
104  TROXAN    1,3,5-trioxane
     56.1   63.0   -6.9  -12.3   70.8  -14.7  -26.2
105  TRITAN10  1,3,5-trithiane
     94.1   89.2    4.9    5.2   71.8   22.3   23.7
107  ZZZKAY02  propionamide
     79.5   83.5   -4.1   -5.1   89.5  -10.1  -12.7
109  ECARBM01  ethyl carbamate
     75.1   77.5   -2.4   -3.2   88.2  -13.1  -17.5
110  JAYDUI    propane
     20.7   24.9   -4.2  -20.5   32.4  -11.7  -56.8
111  YAQLAE    N-ethylurea
     98.1  109.2  -11.1  -11.3  102.8   -4.7   -4.8
112  WIFKEB02  1,1-dimethylurea
     96.1  101.1   -5.0   -5.2   89.1    7.0    7.3
113  NIJHUJ04  1,3-dimethylurea
     90.1   94.1   -4.0   -4.5   84.1    6.0    6.6
119  DCYANM    dicyanoacetylene
     42.9   39.7    3.2    7.4   62.7  -19.8  -46.2
122  DCPYAZ01  2,6-dichloropyrazine
     70.0   73.0   -3.0   -4.3   70.4   -0.4   -0.6
123  BOTYIT    2,4-dichloropyrimidine
     77.0   81.3   -4.3   -5.5   78.7   -1.7   -2.2
124  BISJIW    fumaronitrile
     70.3   67.3    3.0    4.3   67.9    2.4    3.4
126  MLEICA01  maleic anhydride
     86.9   62.2   24.7   28.4   85.9    1.0    1.1
128  FURACL03  5-fluorouracil
    133.0  113.9   19.1   14.3  102.3   30.7   23.1
130  CLPYMD    2-chloropyrimidine
     70.0   78.2   -8.2  -11.7   70.5   -0.5   -0.7
133  IURACL14  5-iodouracil
    130.7  101.4   29.3   22.4  113.4   17.3   13.2
135  BRCYTS    5-bromocytosine
    153.5  139.9   13.6    8.9  115.0   38.5   25.1
138  ZILBIF    5-iodocytosine
    149.7                      91.3   58.4   39.0
139  PYRAZI01  pyrazine
     56.1   62.5   -6.4  -11.4   48.8    7.3   13.1
140  QOPBED    succinonitrile
     70.1   70.6   -0.5   -0.8   94.1  -24.0  -34.3
141  TURCIL03  2-thiouracil
    129.0  125.0    4.0    3.1   83.3   45.7   35.4
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143 AHEMAB pyrazine 1,4-dioxide
117.1 101.6 15.4 13.2 33.2 83.9 71.7
144 URACIL uracil
131.0 114.1 16.9 12.9 98.9 32.1 24.5
145 THBARB01 thiobarbituric acid
115.3 107.4 7.8 6.8 116.8 -1.6 -1.4
146 BARBAC01 barbituric acid
122.9 106.5 16.4 13.3 127.1 -4.2 -3.5
147 DTURAC01 2,4-dithiouracil
124.9 126.4 -1.5 -1.2 79.8 45.1 36.1
151 NIKVUZ cyclobutane-1,2-dione
69.1 52.5 16.6 24.0 79.2 -10.1 -14.7
153 SUCANH15 succinic anhydride
82.1 76.4 5.7 6.9 101.5 -19.4 -23.7
154 MALIAC13 cis-butenedioic acid maleic acid.
110.5 107.3 3.2 2.9 109.3 1.2 1.0
155 FUMAAC01 trans-butenedioic acid
137.9 124.1 13.8 10.0 121.8 16.1 11.7
156 DLGYAH diglycolic anhydride
84.1 77.9 6.2 7.4 97.2 -13.1 -15.6
158 SUCCIN09 succinimide
86.5 83.4 3.1 3.5 89.0 -2.5 -2.9
159 CYTSIN01 cytosine
170.7 144.9 25.8 15.1 126.3 44.4 26.0
161 AZTHYM10 6-azathymine
116.3 99.4 16.9 14.5 99.1 17.2 14.8
162 THCYTO10 2-thiocytosine
163.4 120.9 42.5 26.0
164 FULPIM 2-methylimidazole
88.6 87.9 0.7 0.8 82.4 6.2 7.0
166 DIKPIP03 2,5-piperazinedione
109.2 123.4 -14.3 -13.0 112.6 -3.4 -3.1
169 ZILNOX 2,2,3,3-tetranitrobutane
78.0 97.3 -19.3 -24.7 113.2 -35.2 -45.1
172 DMEOXA06 dimethyl oxalate
75.0 70.9 4.1 5.4 78.0 -3.0 -4.0
173 SUCACB18 succinic acid
122.1 112.8 9.3 7.6 126.5 -4.4 -3.6
174 MEMALA01 methylmalonic acid
115.0 109.3 5.7 4.9 123.2 -8.2 -7.1
175 PUVVUZ 1,3-dithian-2-thione
89.5 78.9 10.6 11.8 83.0 6.5 7.2
177 CROTAM trans 2-butenoic acid amide
82.9 84.8 -1.9 -2.3 82.2 0.7 0.9
178 DACETA diacetamide
73.0 80.3 -7.3 -10.0 104.2 -31.2 -42.7
179 ZZZWEO02 cyclobutane
29.9 28.5 1.4 4.7 33.4 -3.5 -11.7
182 APYFEB01 tetrahydro-2-pyrimidone
113.0 107.6 5.4 4.8 85.3 27.7 24.5
183 DIACHZ 1,2-diacetylhydrazine
105.2 106.9 -1.7 -1.6 95.0 10.2 9.7
185 JAHZEX10 N-acetylglycine amide
130.9 135.0 -4.1 -3.1 131.5 -0.6 -0.5
186 CUVJUY 1,4-diNOpiperazine
102.8 88.9 13.9 13.6 101.9 0.9 0.9
194 TOXOCN 1,3,5,7-tetroxane
80.0 79.3 0.7 0.9 96.6 -16.6 -20.7
196 DITHAN03 1,4-dithiane
71.0 70.6 0.4 0.5 62.9 8.1 11.4
198 ZZZKDQ01 butyramide
85.5 87.9 -2.4 -2.8 84.8 0.7 0.8
199 IBURAM 2-methylpropanamide
85.9 82.2 3.8 4.4 80.3 5.7 6.6
201 MENPDL 2-methyl-2-nitro-1,3-propanediol
101.7 105.0 -3.3 -3.2 152.3 -50.6 -49.8
204 DUCKOB03 butane
28.4 30.0 -1.7 -5.9 37.3 -9.0 -31.6
205 ITIZOA piperazine
72.2 76.7 -4.5 -6.3 67.4 4.8 6.6
206 KIKREC N-propylurea
101.0 121.2 -20.2 -20.0 110.1 -9.1 -9.0
208 VATSAK02 2-methyl-2-propanol tBuOH
50.4 80.7 -30.3 -60.2
210 JAKKIP diethanolamine
106.0 124.3 -18.3 -17.3 120.1 -14.1 -13.3
216 TCYMET tetracyanomethane
61.0 80.7 -19.7 -32.2 133.4 -72.4 -118.6
217 GETVEH 2,3,5-trichloropyridine

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     74.0   81.6   -7.6  -10.3   79.0   -5.0   -6.8
221  VOQYUW    2,5-dibromopyridine
     82.0   74.5    7.5    9.1   67.4   14.6   17.8
227  UGUMUE    5-  triFmethyl uracil
    110.7  115.7   -5.0   -4.5  109.0    1.7    1.6
229  HAMGOT    1,2,4-triazolo 1,5-apyrimidine
     91.8   94.8   -3.0   -3.2   92.3   -0.5   -0.5
230  GEBTUC01  hypoxanthine
    164.0  153.9   10.1    6.1  139.7   24.3   14.8
231  RAKSIG    6-mercaptopurine
    154.5  167.6  -13.1   -8.5  140.5   14.0    9.1
232  TPENAC02  2-thiophene carboxylic acid
     97.8   91.8    6.1    6.2   90.5    7.4    7.5
233  FRANAC03  2-furancarboxylic acid
     88.0   83.8    4.2    4.8   85.1    2.9    3.3
234  HIFKUC    3-furancarboxylic acid
     87.1   89.0   -1.9   -2.1   82.0    5.1    5.9
236  ZUDTID    3-methyl-6-chlorouracil
    110.8  110.2    0.7    0.6  104.9    5.9    5.3
238  LAKJEM    3-methyl-5-Fliorouracil
     86.6   99.0  -12.3  -14.2   92.4   -5.7   -6.6
239  TUHNEQ    3  5 -triluoromethyl-5 3 -methylpyrazole
     78.0                        72.9    5.1    6.5
241  BIRYIK11  3-hydroxypyridine
     88.0   92.0   -4.0   -4.6   84.8    3.3    3.7
243  PYRDNO11  pyridine N-oxide
     79.0   83.6   -4.6   -5.8   69.1    9.9   12.6
246  XAGWIM02  pyrrole-2-carboxylic acid
    100.5   97.3    3.2    3.1   96.1    4.4    4.3
249  PYRZIN23  pyrazine carboxamide
     90.7  101.7  -11.0  -12.1   91.4   -0.7   -0.8
250  KOBFUD    adenine
    123.7                       140.3  -16.6  -13.5
251  KEMDOW    guanine
    186.0  203.2  -17.2   -9.3  204.6  -18.6  -10.0
252  CUVXOG    1,1,1,3,5,5,5-heptanitropentane
    112.0                       162.3  -50.3  -44.9
254  AMPYRD    2-aminopyridine
     78.0   83.5   -5.5   -7.0   82.4   -4.4   -5.6
255  AMIPYR    3-aminopyridine
     83.0   90.5   -7.5   -9.0   76.5    6.5    7.9
256  AMPYRE01  4-aminopyridine
     88.0   96.9   -8.9  -10.1   88.0
258  METURA01  1-methyluracil
    123.5  100.6   22.9   18.6   94.1   29.4   23.8
259  WUDVAS    3-methyluracil
    122.4   96.2   26.2   21.4  104.6   17.8   14.5
260  THYMIN01  5-methyluracil thymine.
    133.0  114.8   18.2   13.7  100.7   32.3   24.3
261  CEWVOP02  6-methyluracil
    131.0  120.5   10.5    8.0  120.6   10.4    8.0
263  LIJFUG    glutaric anhydride
     86.0   81.6    4.4    5.1  100.8  -14.8  -17.2
264  GLUTIM    glutarimide
     94.0   84.5    9.5   10.1  101.4   -7.4   -7.8
265  KOMYEQ01  N-methylsuccinimide
     80.0   72.7    7.3    9.2   93.8  -13.8  -17.2
267  METCYT01  1-methylcytosine
    159.1  137.7   21.4   13.5  138.2   20.9   13.1
269  LETNAZ01  3,5-dimethyl-4-NOpyrazole
    103.0  105.4   -2.4   -2.3   96.9    6.1    5.9
277  PERYTN13  pentaerythritol tetranitrate
    156.2                       139.4   16.8   10.8
278  OWEKEH    tetrahydro-4H-thiopyran-4-one
     73.0   68.9    4.1    5.5   79.3   -6.3   -8.6
283  GLURAC13  glutaric acid
    131.1  127.0    4.1    3.1  140.2   -9.1   -7.0
287  ZZZVYE01  cyclopentane
     36.0   35.2    0.8    2.3   43.4   -7.4  -20.6
289  PTOXEC    1,3,5,7,9-pentoxecane
     88.0   87.6    0.4    0.5   89.8   -1.8   -2.0
290  ZZZKJQ01  pentanamide
     91.1   96.5   -5.4   -6.0   96.2   -5.1   -5.6
291  DIXTAF01  2,2-dimethylpropanamide
     88.0   86.8    1.3    1.4   88.8   -0.8   -0.9
293  PENTAN01  pentane
     35.8   39.4   -3.6  -10.1   48.1  -12.3  -34.4
297  YAQLEI    N-butylurea
    104.9  118.8  -13.9  -13.2  117.0  -12.2  -11.6
```

302 OFIZEK tetramethylthiourea
84.0 82.4 1.6 1.9 78.5 5.5 6.5
303 NEPGCL02 2,2-dimethyl-1,3-propanediol
87.9 90.5 -2.6 -2.9 104.6 -16.7 -19.0
306 PERYTO13 pentaerythritol
151.3 149.4 1.9 1.3 185.7 -34.4 -22.7
307 XYLTOL03 xylitol
161.0 263.6 -102.6 -63.8
308 TCBENQ18 2,3,5,6-tetrachloro-1,4-benzoquinone
100.6 89.0 11.6 11.5 132.7 -32.1 -32.0
310 HCLBNZ14 hexachlorobenzene
97.0 96.4 0.6 0.6 93.4 3.6 3.7
314 TCYETY11 tetracyanoethylene
84.0 74.8 9.3 11.0 141.8 -57.7 -68.7
316 BZOFOX benzotrifuroxan
176.0 160.2 15.8 9.0
319 PNCLBZ pentachlorobenzene
87.0 91.5 -4.5 -5.1 85.3 1.7 2.0
320 PCPHOL01 pentachlorophenol
94.7 112.4 -17.7 -18.7 115.6 -20.9 -22.1
321 UCAYED01 pentaFluorophenol
66.9 69.9 -3.0 -4.5 90.4 -23.5 -35.1
322 CLNOBE02 1-chloro-2,4,6-trinitrobenzene
103.0 108.4 -5.4 -5.2 118.2 -15.2 -14.7
323 DCLBQN01 2,6-dichloro-1,4-benzoquinone
70.0 70.2 -0.2 -0.2 93.5 -23.5 -33.5
326 TCLBZN 1,2,3,5-tetrachlorobenzene
80.0 82.8 -2.8 -3.5 80.2 -0.2 -0.2
327 TCLBEN03 1,2,4,5-tetrachlorobenzene
83.0 91.1 -8.1 -9.8 85.9 -2.9 -3.5
333 CLBENQ chlorobenzoquinone
68.1 71.1 -2.9 -4.3 81.6 -13.4 -19.7
334 JIWQEM 2,4-dichloro-1-nitrobenzene
88.0 82.9 5.1 5.8
335 ZZZEKW02 2,5-dichloro-1-nitrobenzene
87.0 85.3 1.7 1.9 75.6 11.4 13.1
336 CAGPUV01 3,4-dichloro-1-nitrobenzene
85.0 84.0 1.0 1.2 77.5 7.5 8.8
337 HIBWEU 3,5-dichloro-1-nitrobenzene
83.0 81.5 1.5 1.8 81.6 1.4 1.7
339 TCBENZ01 1,2,3-trichlorobenzene
74.0 79.3 -5.3 -7.2 75.1 -1.1 -1.4
340 TCHLBZ03 1,3,5-trichlorobenzene
72.8 79.0 -6.3 -8.6 75.2 -2.5 -3.4
341 SILGOK 2,4,6-trichlorophenol
83.2 92.5 -9.3 -11.2 92.0 -8.8 -10.6
346 PICRAC13 2,4,6-trinitrophenol
107.5 142.1 -34.6 -32.2
350 YAQZUM 2-bromo-1-nitrobenzene
85.0 79.6 5.4 6.3 72.8 12.2 14.3
351 BRNIBZ 3-bromo-1-nitrobenzene
87.0 86.8 0.2 0.3 76.4 10.6 12.2
352 ULEBOD 4-bromo-1-nitrobenzene
87.0 82.2 4.8 5.5 76.2 10.8 12.4
354 BRANIL 2,4,6-tribromoaniline
100.0 89.7 10.3 10.3 95.3 4.7 4.7
355 FACPAA01 1-chloro-4-iodobenzene
72.0 58.0 14.0 19.4
356 SETVIX 1-chloro-2-nitrobenzene
81.0 78.4 2.6 3.2 74.0 7.0 8.6
357 CLNIBZ01 1-chloro-3-nitrobenzene
82.0 84.1 -2.1 -2.5 76.0 6.0 7.4
360 NTCPOL01 4-chloro-2-nitrophenol
88.0 85.1 2.9 3.3 89.7 -1.7 -1.9
363 UCECAG02 2-chloro-4,6-dinitroaniline
115.0 100.7 14.3 12.4 117.1 -2.1 -1.8
365 DCLBEN03 1,4-dichlorobenzene
65.0 74.9 -9.9 -15.3 69.1 -4.1 -6.3
367 CLNOAN 2,6-dichloro-4-nitroaniline
109.0 102.4 6.6 6.1 108.2 0.8 0.8
368 CARDOO 4,5-dichloro-2-nitroaniline
109.0 105.0 4.0 3.7 105.6 3.4 3.1
373 DCLPHM01 3,4-dichlorophenol
87.0 99.3 -12.3 -14.2 103.6 -16.6 -19.1
378 TCANIL02 2,4,6-trichloroaniline
85.0 89.5 -4.5 -5.3
384 LETFEV 3,5-diFluorophenol
73.0 75.7 -2.7 -3.7 94.0 -21.0 -28.7
385 WURTOS 3-iodo-1-nitrobenzene

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     83.3   63.8   19.6   23.5   76.1    7.3    8.7
386  ZZZPRO08  1,4-diiodobenzene
     67.0   62.7    4.3    6.4   81.7  -14.7  -21.9
387  MUBZOY    2-cyanopyridine
     71.0   74.7   -3.7   -5.2   75.8   -4.8   -6.8
388  MUBZUE    3-cyanopyridine
     72.0   69.1    2.9    4.0   72.9   -0.9   -1.3
389  CYAPYR    4-cyanopyridine
     75.0   74.0    1.0    1.4   67.6    7.4    9.9
391  CYPYRO01  4-cyanopyridine Noxide
    106.8   91.3   15.6   14.6   84.9   22.0   20.6
392  BEOXAZ    benzofurazan
     65.0   60.2    4.8    7.4   62.7    2.3    3.6
394  ZZZFYW02  1,2-dinitrobenzene
     93.0   95.1   -2.1   -2.3   91.7    1.3    1.4
395  DNBENZ15  1,3-dinitrobenzene
     85.0   86.4   -1.4   -1.7   86.6   -1.6   -1.9
396  DNITBZ11  1,4-dinitrobenzene
     95.0   94.4    0.6    0.7   89.2    5.8    6.1
398  DNOPHL02  2,4-dinitrophenol
    104.6   93.3   11.3   10.9  111.8   -7.3   -6.9
400  DNPHOL02  2,6-dinitrophenol
    112.6   96.1   16.5   14.6  116.8   -4.2   -3.7
402  TNIOAN02  2,4,6-trinitroaniline
    125.5  117.3    8.2    6.5  139.8  -14.3  -11.4
403  BETHAZ01  2,1,3-benzothiadiazole
     71.0   75.4   -4.4   -6.3  111.8  -40.8  -57.5
404  BNZQUI03  1,4-benzoquinone
     68.8   59.7    9.2   13.3   66.2    2.7    3.9
405  FURDCA    furan-2,5-dicarboxylic
    124.7  124.7                 128.3   -3.6   -2.9
406  BDTOLE11  tetrathiafulvene
     95.9   83.0   12.9   13.4   98.4   -2.5   -2.6
407  PBRPOL    4-bromophenol
     85.0   87.1   -2.1   -2.4   92.3   -7.3   -8.6
408  CAJWEQ01  2,4-dibromoaniline
     88.0   84.8    3.2    3.7   82.2    5.8    6.6
412  YOVCAO    2-chloro-5-nitroaniline
    100.0  104.4   -4.4   -4.4  104.3   -4.3   -4.3
416  WEMDAT    2,3-dichloroaniline
     82.0   89.7   -7.7   -9.4   80.7    1.3    1.6
417  WEMDIB    2,4-dichloroaniline
     85.0   95.2  -10.2  -12.0   83.8    1.2    1.4
418  DCHLAN01  2,5-dichloroaniline
     83.0   95.4  -12.4  -15.0   85.4   -2.4   -2.9
419  WEMDEX    2,6-dichloroaniline
     74.0   85.3  -11.3  -15.2   79.1   -5.1   -6.9
420  QQQBNG01  4-Fluorophenol
     74.0   76.5   -2.5   -3.4   80.3   -6.3   -8.5
422  NICOAC02  3-pyridinecarboxylic
    124.0  107.4   16.6   13.4   91.7   32.3   26.1
423  ISNICA    4-pyridinecarboxylic
    113.0  111.1    1.9    1.7   90.4   22.6   20.0
424  ONITPH    2-nitrophenol
     73.0   71.8    1.2    1.7   87.0  -14.0  -19.1
426  NITPOL08  4-nitrophenol
     95.0   97.1   -2.1   -2.2   90.7    4.3    4.5
427  PICANO04  pyridine-2-carboxylic acidNoxide
     97.2   92.9    4.4    4.5   95.7    1.6    1.6
434  TEMWUD    2-nitro-1,3-dihydroxybenzene
     74.0   73.1    0.9    1.3   93.2  -19.2  -25.9
437  BZTRAZ01  1-H-benzotriazole
     98.0                        86.4   11.6   11.9
438  DATNBZ01  1,3-diamino-2,4,6-trinitrobenzene
    145.0  128.4   16.6   11.5  168.6  -23.6  -16.2
439  BENZEN18  benzene
     44.3   46.2   -1.9   -4.4   46.7   -2.4   -5.5
442  PBRANL01  4-bromoaniline
     79.0   88.6   -9.6  -12.1   73.4    5.6    7.2
443  CLANIC06  4-chloroaniline
     86.0   96.6  -10.6  -12.3   78.5    7.5    8.7
444  AHCHEX01  alfa-hexachlorocyclohexane
     94.5  106.1  -11.6  -12.3   90.4    4.1    4.4
445  HCCYHB    beta-hexachlorocyclohexane
    105.5  120.7  -15.2  -14.4  105.6   -0.1   -0.1
446  HCCYHG02  gamma-hexachlorocyclohexane
     97.5  102.5   -5.0   -5.1   91.9    5.6    5.8
448  RALTOO    2-iodoaniline
     81.0   68.3   12.7   15.7   73.6    7.4    9.1
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449 EJAYET 4-iodoaniline
85.0 78.4 6.6 7.8 78.7 6.3 7.5
450 PICAMD06 2-pyridinecarboxamide
93.9 97.2 -3.3 -3.5 99.0 -5.1 -5.4
451 NICOAM06 3-pyridinecarboxamide
120.0 112.6 7.4 6.2 97.4 22.6 18.8
452 EHOWIH 4-pyridinecarboxamide
115.0 110.1 4.9 4.3 104.5 10.5 9.2
453 ONITAN03 2-nitroaniline
89.0 95.9 -6.9 -7.8
454 MNIANL10 3-nitroaniline
94.0 105.1 -11.1 -11.8 89.8 4.2 4.5
455 NANILI31 4-nitroaniline
101.0 104.2 -3.2 -3.1 103.6 -2.6 -2.6
462 TATNBZ 2,4,6-trinitro-1,3,5-benzenetriamine
172.9 207.7 -34.8 -20.1
463 PHENOL03 phenol
69.0 82.9 -13.9 -20.2
464 CATCOL16 1,2-dihydroxybenzene
85.0 100.9 -15.9 -18.7 115.7 -30.7 -36.1
465 RESORA03 1,3-dihydroxybenzene
93.0 100.9 -7.9 -8.5 123.9 -30.9 -33.2
466 HYQUIN08 1,4-dihydroxybenzene
100.9 106.2 -5.3 -5.2 121.8 -20.9 -20.7
472 PHGLOL01 1,3,5-trihydroxybenzene
134.0 141.1 -7.1 -5.3 171.8 -37.8 -28.2
474 ZZZKAO01 3-methylpyridine
59.9 61.3 -1.4 -2.4 62.5 -2.6 -4.4
475 ZZZIVG02 4-methylpyridine
59.8 63.4 -3.6 -6.0 62.6 -2.8 -4.7
476 AMPHOM02 2-aminophenol
101.0 114.6 -13.6 -13.4 99.3 1.7 1.7
477 MAMPOL 3-aminophenol
104.0 107.6 -3.6 -3.4 104.9 -0.9 -0.8
478 AMPHOL01 4-aminophenol
108.1 124.2 -16.1 -14.9 111.2 -3.1 -2.9
479 YELRIR 2-methyl-3-hydroxypyridine
89.0 94.6 -5.6 -6.3 92.4 -3.4 -3.8
483 RAJGUG 2-methylpyridine Noxide
89.0 78.0 11.0 12.3 68.2 20.8 23.3
485 ZZZVCO04 4-methylpyridine Noxide
83.0 80.4 2.6 3.2 24.6 58.4 70.4
486 RICFEP01 2-acetylpyrrole
81.0 78.8 2.3 2.8 84.0 -3.0 -3.8
489 YIFZAP benzenesulfonamide
115.0 129.0 -14.0 -12.1 104.4 10.6 9.2
498 MEADEN05 9-methyladenine
126.1 135.4 -9.3 -7.4 139.0 -12.9 -10.3
502 DMURAC 1,3-dimethyluracil
110.5 91.7 18.8 17.0 100.6 9.9 9.0
503 METHYM04 1-methylthymine
128.0 102.0 26.0 20.3 70.2 57.8 45.1
504 FACRIK05 1,3-cyclohexanedione
90.0 89.8 0.2 0.2 119.0 -29.0 -32.2
505 CYHEXO01 1,4-cyclohexanedione
84.0 73.1 10.9 13.0 94.4 -10.4 -12.3
506 ZZZDRQ01 dimethyl fumarate
85.0 80.7 4.3 5.0 89.5 -4.5 -5.3
507 CBUTAC cyclobutane-1,1-dicarboxylic
112.0 112.2 -0.2 -0.2 118.3 -6.3 -5.6
518 POKKAB cis-1,3,5,7-tetraoxadecalin
95.0 96.3 -1.3 -1.3 107.9 -12.9 -13.6
519 GOCWEA trans-1,3,5,7-tetraoxadecalin
82.0 79.6 2.4 2.9 78.4 3.6 4.4
520 ADIPAC20 adipic acid
145.0 125.7 19.3 13.3 134.1 10.9 7.5
522 CAPLAC epsilon-caprolactam
85.5 81.7 3.8 4.5 80.1 5.4 6.3
526 JORCAU 2,3,3-trinitro-2-methylpentane
91.0 113.6 -22.6 -24.8
528 CYCHEX cyclohexane
35.1 40.5 -5.4 -15.4 50.2 -15.1 -43.0
534 BECJEY 2,3-dinitro-2,3-dimethylbutane
90.0 93.7 -3.7 -4.1 106.7 -16.7 -18.5
535 HXMTAM23 1,3,5,7-tetraazatricyclo 3.3.1.13,7decane
77.0 85.4 -8.4 -10.9 71.1 5.9 7.7
545 HEXANE01 hexane
46.2 45.7 0.5 1.0 57.0 -10.8 -23.4
547 FECCOF01 1,6-hexanediol

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    110.0  117.4   -7.4   -6.7  137.0  -27.0  -24.6
552  PFBZAC01  pentafluorobenzoic acid
     93.6   75.7   17.8   19.1   87.6    5.9    6.3
555  PNBZNT    4-nitrobenzonitrile
     91.0   84.2    6.8    7.5   90.1    0.9    1.0
556  BIPJUF    2,4-dinitrobenzoic acid
    135.0  126.3    8.7    6.5  120.0   15.0   11.1
560  BRBZAC01  2-bromobenzoic acid
    109.0  103.1    5.9    5.4   97.3   11.7   10.7
562  BRBZAP01  4-bromobenzoic acid
    107.0  100.2    6.8    6.3   92.1   14.9   13.9
563  CLBZAC02  2-chlorobenzoic acid
    110.0   99.1   10.9    9.9   96.2   13.8   12.5
564  MCBZAC02  3-chlorobenzoic acid
    104.0   98.1    5.9    5.7   98.6    5.4    5.2
565  CLBZAP13  4-chlorobenzoic acid
    105.0  101.4    3.6    3.4   96.4    8.6    8.2
566  FBENZA02  2-fluorobenzoic acid
     94.0   90.4    3.6    3.8   94.7   -0.7   -0.8
567  COVJIG01  3-fluorobenzoic acid
     94.3   90.1    4.2    4.4   87.3    7.0    7.4
568  PFBZAD15  4-fluorobenzoic acid
     93.0   77.7   15.3   16.4   84.8    8.2    8.8
569  XOGJAG    trifluoromethylbenzene
     52.2   50.2    2.0    3.9   56.5   -4.3   -8.2
570  OIBZAC01  2-iodobenzoic acid
    111.0   77.9   33.1   29.8   97.6   13.4   12.0
572  BENMOW07  4-iodobenzoic acid
    110.0   82.8   27.3   24.8   91.3   18.8   17.0
574  BZOXZO    2-benzoxazolinone
     98.0   90.0    8.0    8.2   90.0    8.0    8.2
576  NBZOAO04  2-nitrobenzoic acid
    119.0  114.2    4.8    4.0  110.1    8.9    7.5
577  MNBZAC04  3-nitrobenzoic acid
    110.0                      105.4    4.6    4.2
578  NBZOAC12  4-nitrobenzoic acid
    120.0  114.6    5.4    4.5  107.9   12.1   10.1
584  ZZZMUC09  2,4,6-trinitrotoluene
    110.0                      120.4  -10.4   -9.5
587  MTNANL    2,4,6-N-tetranitro-N-methylaniline
    133.0                      148.3  -15.3  -11.5
588  UCOVAL    1-  chloromethyl -2-nitrobenzene
     96.0   95.4    0.6    0.6   86.8    9.2    9.6
591  BZDMAZ04  benzimidazole
    100.0  100.6   -0.6   -0.6   96.7    3.3    3.3
599  FIHLOY    2,3-dinitrotoluene
     96.8                       79.8   17.1   17.6
600  ZZZGVU01  2,4-dinitrotoluene
     99.1                       95.9    3.2    3.2
601  ZZZQSC02  2,6-dinitrotoluene
     99.0   91.2    7.8    7.9   90.6    8.4    8.5
602  FIHLUE    3,4-dinitrotoluene
     99.4                       97.1    2.3    2.4
605  BENZAC20  benzoic acid
     91.0   93.1   -2.1   -2.3   84.1    6.9    7.6
606  XAYCIJ    3-hydroxybenzaldehyde
    100.0   82.8   17.2   17.2  111.7  -11.7  -11.7
607  PHBALD11  4-hydroxybenzaldehyde
    101.0   85.1   15.9   15.8  107.0   -6.0   -5.9
608  TROPOL10  tropolone
     84.0   71.1   12.9   15.4   92.2   -8.2   -9.7
612  SALIAC19  2-hydroxybenzoic acid
     97.0   92.1    4.9    5.0  105.2   -8.2   -8.5
613  BIDLOP02  3-hydroxybenzoic acid
    123.0  115.3    7.7    6.2  127.4   -4.4   -3.6
617  CACDAM01  2,3-dihydroxybenzoic acid
    111.0  109.6    1.4    1.3  133.7  -22.7  -20.5
618  ZZZEEU04  2,4-dihydroxybenzoic acid
    125.0  121.6    3.4    2.7  146.1  -21.1  -16.9
619  BESKAL    2,5-dihydroxybenzoic acid
    130.0  123.2    6.8    5.3  153.2  -23.2  -17.8
620  LEZJAB01  2,6-dihydroxybenzoic acid
    109.0  119.8  -10.8   -9.9  130.6  -21.6  -19.8
625  BZAMID12  benzamide
    100.5   99.1    1.4    1.4   97.3    3.2    3.2
627  NITOLU01  4-nitrotoluene
     77.0   72.5    4.5    5.8   78.6   -1.6   -2.1
628  AMBACO08  2-aminobenzoic acid
    110.0   99.8   10.2    9.3   99.5   10.5    9.6
```

630 AMBNAC12 4-aminobenzoic acid
116.0 125.7 -9.7 -8.4 105.2 10.8 9.3
631 SALMID02 2-hydroxybenzamide
101.0 105.3 -4.3 -4.3 110.3 -9.3 -9.3
632 VIDMAX 4-hydroxybenzamide
125.0 127.3 -2.3 -1.8 141.3 -16.3 -13.1
636 ZORSEG thiobenzamide
100.0 80.4 19.6 19.6
637 TOLUEN03 toluene
43.0 49.2 -6.2 -14.5 52.9 -9.9 -23.1
639 PHUREA02 monophenylurea
140.3 131.0 9.3 6.6 126.1 14.2 10.1
646 CRESOL01 4-hydroxytoluene
74.0 71.9 2.1 2.8 79.6 -5.6 -7.5
649 NUQKER 2,6-dihydroxytoluene
99.0 126.6 -27.6 -27.9
651 EWAMAR 3,5-dihydroxytoluene
103.0 107.1 -4.1 -4.0 124.4 -21.4 -20.8
654 MPSUFO01 MEphenylsulfone
92.0 104.4 -12.4 -13.4 85.8 6.2 6.8
661 DMADEN11 N,N-dimethyladenine
118.1 117.9 0.2 0.1 117.4 0.7 0.6
668 LIMLOI 1,3,6-trimethyluracil
106.9 91.1 15.8 14.8 109.7 -2.8 -2.6
679 QQQAPG02 bicyclo 2.2.1heptane norbornane
40.1 42.8 -2.7 -6.8 49.9 -9.8 -24.5
682 PIMELA15 heptanedioic acid
140.0 135.9 4.1 2.9 151.5 -11.5 -8.2
688 JEXNAB N-acetylLvalinamide
133.0 129.0 4.0 3.0 128.8 4.2 3.2
691 HEPTAN02 heptane
53.4 51.1 2.3 4.3 64.0 -10.6 -19.9
697 YUYPUD02 1,2-dicyanobenzene
87.0 79.8 7.2 8.3 92.8 -5.8 -6.7
698 OBIZEE 1,3-dicyanobenzene
90.0 79.2 10.8 12.0 93.8 -3.8 -4.2
699 TEPNIT11 1,4-dicyanobenzene
90.0 80.8 9.2 10.3 94.3 -4.3 -4.7
701 BZCBUO benzocyclobutenedione
91.0 72.2 18.8 20.7 90.2 0.8 0.9
702 PHTHAO phthalic anhydride
89.3 74.9 14.4 16.1 95.0 -5.7 -6.4
707 PHALIM04 phthalimide
106.0 88.2 17.8 16.8 89.6 16.4 15.5
714 BOXAZD 2H-1,3-benzoxazine-2,4 3H -dione
114.0 97.1 16.9 14.9 103.9 10.1 8.9
715 PYRCYN06 pyridinium dicyanomethyl ide
129.5 101.8 27.8 21.4 106.9 22.7 17.5
718 CPXACA01 2,4-dichlorophenoxy acetic
120.0 124.3 -4.3 -3.6 117.9 2.1 1.7
719 DAZNAP phthalazine
82.0 92.4 -10.4 -12.6 86.1 -4.1 -5.0
720 HEYJOK01 quinoxaline 1,4
68.0 72.9 -4.9 -7.2 73.6 -5.6 -8.3
722 HQOXAL01 2-hydroxyquinoxaline
127.7 102.8 24.9 19.5 94.6 33.2 26.0
723 WIGYIV 1-(2H)-phthalazinone
107.0 103.5 3.5 3.3 90.7 16.3 15.3
727 MODYAG01 4-aminophthalimide
141.4 114.8 26.6 18.8 133.0 8.4 6.0
732 PHTHAC06 phthalic acid
130.0 137.8 -7.8 -6.0 135.5 -5.5 -4.2
733 BENZDC11 isophthalic acid
142.0 122.4 19.6 13.8 130.0 12.0 8.4
734 TEPHTH14 terephthalic acid
146.0 135.6 10.4 7.1 129.1 16.9 11.6
737 DTENYL02 2,2 -bithiophene
85.6 76.8 8.8 10.3 106.0 -20.4 -23.9
746 JONPUZ 3-methyl-2-nitrobenzoic acid
124.0 108.0 16.0 12.9 114.3 9.7 7.8
756 TNPHNT 2,4,6-trinitrophenetole
122.7 114.5 8.2 6.7 130.1 -7.4 -6.0
757 CUBANE cubane
55.0 41.7 13.3 24.2 49.4 5.6 10.2
768 HACTPH16 4-hydroxyacetophenone
97.5 89.2 8.3 8.5 120.7 -23.2 -23.8
769 DMEBQU01 2,5dimethyl1,4benzoquinone
76.4 71.0 5.4 7.1 94.0 -17.6 -23.0
770 OTOLIC02 o-toluic acid

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     96.0   94.1    1.9    1.9   93.6    2.4    2.4
772  PTOLIC01  p-toluic acid
     99.0   88.5   10.5   10.6   91.1    7.9    8.0
776  YUHTEA    4-hydroxy-3-methoxybenzaldehyde
     89.7                        95.6   -5.9   -6.5
777  FUFBOX    2-methoxybenzoic acid
    107.0  106.1    0.9    0.9  107.1   -0.1   -0.1
779  ANISIC04  4-methoxybenzoic acid
    111.0   99.7   11.3   10.2  102.7    8.3    7.5
781  ACANIL06  acetanilide
     83.0   95.6  -12.6  -15.2  106.8  -23.8  -28.7
783  AMACPH01  4-aminoacetophenone
     93.8   97.8   -4.0   -4.3  111.3  -17.4  -18.6
784  MBNZAM10  N-methylbenzamide
     83.5   93.5  -10.0  -12.0   88.3   -4.8   -5.7
786  AMEBAC    2-amino-3-methylbenzoic acid
    107.0  100.2    6.8    6.4  115.5   -8.5   -7.9
793  ZZZITY02  1,4-dimethylbenzene
     58.8   63.8   -5.0   -8.5   73.3  -14.5  -24.7
795  MNTDMA01  3-nitro-N,N-dimethylaniline
     93.0   88.3    4.8    5.1   96.2   -3.2   -3.4
796  DIMNAN01  N,N-dimethyl-4-nitroaniline
    102.0   97.0    5.0    4.9  111.6   -9.6   -9.4
797  DIMPHE12  2,3-dimethylphenol
     84.2   87.1   -2.9   -3.4  102.4  -18.3  -21.7
798  DMPHOL11  2,5-dimethylphenol
     85.2   82.4    2.8    3.2   90.4   -5.3   -6.2
799  DMEPOL10  2,6-dimethylphenol
     75.5   78.8   -3.3   -4.3   89.2  -13.7  -18.1
800  DPHNOL10  3,4-dimethylphenol
     85.9                        96.9  -11.1  -12.9
804  MOXBEN01  1,4-dimethoxybenzene
     84.0   76.9    7.1    8.4   82.9    1.1    1.3
808  VAYJIO    8-Ethyl-9-methyladenine
    117.8  133.0  -15.2  -12.9  131.3  -13.5  -11.4
812  BISJAO02  tetramethylsuccinonitrile
     81.0   77.7    3.3    4.1   95.8  -14.8  -18.3
813  MPYRAZ02  tetramethylpyrazine
     95.0   77.3   17.7   18.6  100.4   -5.4   -5.7
817  DIMEDO02  5,5-dimethyl-1,3-cyclohexanedione
    100.0   91.3    8.7    8.7  119.8  -19.8  -19.8
818  DMKETD02  2,2,4,4-tetramethyl-1,3-cyclobutanedione
     71.0   60.9   10.1   14.3   81.0  -10.0  -14.0
825  SUBRAC12  octanedioic
    148.0  135.0   13.0    8.8  148.7   -0.7   -0.5
826  ZBCNON    3-azabicyclo 3.2.2nonane
     58.0   57.9    0.1    0.2   60.5   -2.5   -4.3
832  ISENUP    octanoic
    113.0   97.6   15.4   13.6  107.5    5.5    4.8
834  OCTANE01  octane
     64.7                        72.1   -7.4  -11.4
837  ZZZVYK01  1-octanol
    100.0   90.8    9.2    9.2  113.7  -13.7  -13.7
838  QATVEM    1,8-octanediol
    139.0  129.5    9.5    6.8  154.4  -15.4  -11.1
848  CHLQUI10  2-chloroquinoline
     84.0   91.2   -7.2   -8.5   93.8   -9.8  -11.6
850  CLQUIN    6-chloroquinoline
     81.0   86.5   -5.5   -6.8   83.6   -2.6   -3.2
851  FAMDIG    5-chloro-8-hydroxyquinoline
    112.0  102.3    9.7    8.7  104.5    7.5    6.7
856  UPAJIF    8-nitroquinoline
    107.0  105.0    2.0    1.9  100.5    6.5    6.1
859  COUMAR02  coumarin
     92.3   80.4   11.9   12.9   93.2   -0.9   -1.0
861  INDDON    1,3-indandione
     97.0   76.6   20.4   21.1   91.7    5.3    5.5
863  FABPON11  5-phenyl-1,2-dithiole-3-thione
    123.0   97.6   25.4   20.6  125.3   -2.3   -1.9
866  HXQUIN11  8-hydroxyquinoline
     99.0   92.1    6.9    6.9   98.8    0.2    0.2
872  ZZZPRC03  1-methyl-1H-indole-2,3-dione
    106.0   81.1   24.9   23.5   99.8    6.2    5.9
875  SECQEY    3-aminoquinoline
    104.0  109.3   -5.3   -5.1   99.4    4.6    4.4
878  NONMEI    8-aminoquinoline
     93.0   99.3   -6.3   -6.7   95.9   -2.9   -3.1
884  CINMAC    trans cinnamic acid
    107.0  103.8    3.2    3.0   95.8   11.2   10.5
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 890  NBORAN02  endo-5-norbornene-2,3-dicarboxylic anhydride
      97.0   84.2   12.8   13.2  101.3   -4.3   -4.4
 893  FESNOG02  3,4-dihydroxycinnamic acid caffeic acid
     174.5  166.9    7.6    4.4  192.4  -17.9  -10.2
 901  JIBDON    2,6-dimethylbenzonitrile
      84.0   72.0   12.0   14.3   83.6    0.4    0.5
 904  HEXTIN01  2,4,6-trinitromesitylene
     106.1                      105.4    0.7    0.7
 917  DMBZAC01  2,3-dimethylbenzoic acid
     105.0   97.6    7.4    7.1   99.0    6.0    5.7
 918  WIZJUL    2,4-dimethylbenzoic acid
     104.0   93.3   10.8   10.3  104.1   -0.1   -0.1
 920  DMBNZA11  2,6-dimethylbenzoic acid
      99.0   97.0    2.0    2.0   98.3    0.7    0.7
 925  PEXBZA    4-ethoxybenzoic acid
     123.0  112.0   11.0    9.0  111.9   11.1    9.0
 927  OVERAT01  2,3-dimethoxybenzoic acid
     117.0  117.8   -0.8   -0.7  119.0   -2.0   -1.7
 928  ISUQUI    2,4-dimethoxybenzoic acid
     123.0  112.4   10.6    8.6  117.4    5.6    4.5
 929  DMOXBA01  2,6-dimethoxybenzoic acid
     122.0  133.5  -11.5   -9.4  132.4  -10.4   -8.5
 930  DMXBZA01  3,4-dimethoxybenzoic acid
     130.0  109.3   20.8   16.0  115.2   14.8   11.4
 931  ISURAP    2,5-dimethoxybenzoic acid
     116.0   99.5   16.5   14.2  116.3   -0.3   -0.3
 932  HEKMOZ    3,5-dimethoxybenzoic acid
     127.0  115.2   11.8    9.3  120.0    7.0    5.5
 935  REZRIY    N-  2-methylphenyl acetamide
      98.2   98.3   -0.1   -0.1  105.8   -7.6   -7.7
 937  ODOTOQ    N,N-dimethylbenzamide
      93.0   84.2    8.8    9.4   84.2    8.8    9.4
 942  XAXSIY    2,4,6-trimethylphenol
      90.0   85.9    4.1    4.5   98.4   -8.4   -9.4
 946  TMOXBZ10  1,3,5-trimethoxybenzene
     100.0   87.2   12.8   12.8   92.2    7.8    7.8
 959  DMPIPA    2-methyl-2-piperidinopropionitrile
      80.0   75.1    4.9    6.2   89.3   -9.3  -11.6
 960  AZELAC05  nonanedioic acid azelaic
     160.0                      162.0   -2.0   -1.2
 969  QQQFAY01  nonane
      71.8                       81.1   -9.3  -12.9
 971  UPACIY    1,3-butylthiourea
     140.0                      114.3   25.7   18.3
 974  PYMDAN    1,2,4,5-benzenetetracarboxylic acid anhydride
     122.0   94.0   28.0   23.0  147.9  -25.9  -21.2
 976  DBRNAQ01  1,4-dibromonaphthalene
      91.3                       92.3   -1.0   -1.1
 978  SUZXOB    2-cyanoquinoline
      94.0   88.3    5.7    6.0  101.6   -7.6   -8.1
 982  NAPHQU01  1,4-naphthoquinone
      91.0   79.1   11.9   13.1   94.0   -3.0   -3.3
 991  NAPHTA10  naphthalene
      73.0   74.9   -1.9   -2.6   77.0   -4.0   -5.5
 996  BIPYRL04  2,2  -bipyridine
      80.0   87.8   -7.8   -9.7   94.8  -14.8  -18.6
 998  HIQWEJ01  4,4  -bipyridine
     106.0                       88.5   17.5   16.5
1001  NAPHOL01  1-naphthol
      90.0   97.1   -7.1   -7.9  105.8  -15.8  -17.6
1002  NAPHOB03  2-naphthol
      90.0   85.3    4.7    5.2   93.3   -3.3   -3.7
1004  NPHHQU10  1,4-naphthohydroquinone
     122.3  123.4   -1.1   -0.9  146.0  -23.7  -19.3
1006  HEGFAB    1,3-dihydroxynaphthalene
     116.0  128.3  -12.3  -10.6  143.8  -27.8  -24.0
1007  VOGSEP    2,3-dihydroxynaphthalene
     110.0                      122.5  -12.5  -11.3
1011  YIRKOA    2-methyl-8-hydroxyquinoline
      90.0                      106.3  -16.3  -18.1
1018  BULVAL03  bullvalene
      72.0   65.1    6.9    9.6   70.0    2.0    2.7
1020  JISVEM    1,8-diaminonaphthalene
      97.0  106.6   -9.6   -9.9  103.6   -6.6   -6.8
1021  KEYNOR    2,3-dimethylquinoxaline
      87.7   84.5    3.2    3.7  102.1  -14.4  -16.4
1023  EYIRIN    1-benzylimidazole
     102.0  105.5   -3.5   -3.5  100.8    1.2    1.2
1025  VAKJUM    2,3-dimethylquinoxaline 1,4dioxide
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     124.0  103.6   20.4   16.5  107.7   16.3   13.2
1033  ZZZFLM01  trans-2-methoxycinnamic
     129.0  112.3   16.8   13.0  115.8   13.3   10.3
1034  ZZZNRU02  trans-3-methoxycinnamic
     124.0  110.8   13.3   10.7  114.9    9.1    7.3
1035  MXCINN02  trans-4-methoxycinnamic
     134.0  116.5   17.5   13.1  112.4   21.6   16.1
1037  DMTPAL    dimethylthyl terephthalate
     105.2   93.3   11.9   11.3  109.1   -3.9   -3.7
1038  GOHRUS    dimethyl isophthalate
     100.1                      104.8   -4.7   -4.7
1042  PICGAJ    3-amino-1-phenyl-but-2-enone
     109.0  111.3   -2.3   -2.1  125.6  -16.6  -15.2
1055  TMBZAC01  2,4,6-trimethylbenzoic
     104.0   96.1    7.9    7.6  106.0   -2.0   -1.9
1058  RUVQAA    2,4,5-trimethylbenzoic
     110.0  100.5    9.5    8.7  104.6    5.4    4.9
1059  TMEBZA    3,4,5-trimethylbenzoic
     111.0  101.5    9.5    8.6  102.8    8.2    7.4
1064  ZZZNCU01  4-phenylbutyric
     113.0  104.1    8.9    7.8  115.8   -2.8   -2.5
1067  PRYLTS    p-tolyl propenylsulfone
      96.0  113.3  -17.3  -18.0  109.3  -13.3  -13.8
1069  DUPKAB    propyl 4-hydroxybenzoate
     123.0                      126.5   -3.5   -2.8
1072  LIJKOF    3,4,5-trimethoxybenzoic
     131.0                      121.9    9.1    6.9
1075  DURENE    1,2,4,5-tetramethylbenzene
      73.1   67.1    6.0    8.2   79.8   -6.7   -9.2
1078  CAXNIY    2,2-dinitroadamantane
      96.4                       93.2    3.2    3.4
1081  IPMEPL    2-isopropyl-5-methylphenol thymol
      91.1   85.0    6.1    6.7   99.9   -8.8   -9.7
1086  DOKXIL    1-bromoadamantane
      72.1   70.4    1.7    2.3   72.2   -0.1   -0.2
1087  GUYBAF    2-chloroadamantane
      62.0   67.8   -5.8   -9.4   67.6   -5.6   -9.1
1088  CARVOX01  dl carvoxime
     102.4                      105.6   -3.1   -3.1
1103  ADAMOL01  1-adamantanol
      87.1   83.0    4.1    4.7  102.1  -15.0  -17.3
1104  SEYDEF    adamantan-2-ol
      88.1                       98.7  -10.6  -12.0
1106  MOYGUC01  thiocamphor
      62.2   63.9   -1.7   -2.8   71.3   -9.1  -14.7
1107  QQQFHJ01  1,3,5,7-tetramethyl-2,4,6,8-tetrathiaadamantane
     117.0                      89.5   27.5   23.5
1115  SEBAAC06  sebacic acid
     184.7                      164.6   20.1   10.9
1119  BAVLOZ    l-menthol
      95.4                      102.5   -7.1   -7.4
1121  PEMYUB    cyclodecanol
      99.6                       83.0   16.6   16.7
1122  ISEPEB    decanoic acid
     125.0                      119.9    5.1    4.1
1125  QQQFBG01  decane
      82.0                       89.9   -7.9   -9.7
1127  WESTIX01  1,10-decanediol
     156.0                      168.7  -12.7   -8.1
1128  FOFDIN    1,4,8,11-tetraazacyclotetradecane
     136.6                      118.4   18.1   13.3
1131  NAPOAC01  1-naphthoic acid
     115.9  105.3   10.6    9.2  107.7    8.2    7.1
1132  NAPHAC02  2-naphthoic acid
     118.9  111.4    7.5    6.3  107.5   11.4    9.6
1138  FOBPAO    pentacyclo 5.4.02,603,1005,9undecane-8,11-dione
      93.0                       89.2    3.8    4.1
1139  PILFOG    2,6-dimethylquinoline
      85.0   83.3    1.7    1.9   92.3   -7.3   -8.6
1142  PICFOW    4- 4-nitrophenyl aminopent-3-ene-2-one
     122.0                      139.1  -17.1  -14.0
1150  CEMJOT02  trans-3,4-dimethoxycinnamic
     153.0                      131.6   21.4   14.0
1159  BONLOF    4-tert-butylbenzoic acid
     104.4                      109.6   -5.1   -4.9
1174  FEXBOZ    benzylidene t-Bu amine Noxide
      87.0   91.5   -4.5   -5.1  104.6  -17.6  -20.2
1175  COPMUR    pentamethylbenzene
      75.0   70.4    4.6    6.1   85.9  -10.9  -14.6
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1176 PAGMEQ 2-tert-butyl-4-methylphenol
81.0 89.3 -8.3 -10.3
1184 UNDEAC10 undecanedioic acid
162.0 172.6 -10.6 -6.5
1185 ZZZNYY01 undecanoic acid
121.0 119.6 1.4 1.1
1189 OCDBDO10 octachlorodibenzo b,e 1,4 dioxin
154.3 145.7 8.6 5.6 152.5 1.8 1.2
1190 DCLBPH decachlorobiphenyl
123.8 132.4 -8.6 -6.9 142.7 -18.9 -15.2
1191 DECFDP01 decafluorobiphenyl
87.1 75.4 11.7 13.4 98.2 -11.1 -12.7
1198 TCBZFU 2,3,7,8-tetrachlorodibenzofuran
125.0 117.7 7.3 5.9 122.0 3.0 2.4
1199 FELSEU 1,2,3,4-tetrachlorodibenzo b,e 1,4 dioxin
114.7 115.9 -1.2 -1.0 130.2 -15.4 -13.5
1203 TCBZDX20 2,3,7,8-tetrachlorodibenzo b,e 1,4 dioxin
135.2 132.5 2.7 2.0
1204 HCLBPH 2,2',4,4',6,6'-hexachlorobiphenyl
102.4 100.1 2.3 2.3 110.0 -7.6 -7.4
1205 TCYQME03 7,7,8,8-tetracyanoquinodimethane
123.3 116.3 7.0 5.6 146.0 -22.7 -18.4
1216 DCBZDX20 2,7-dichlorodibenzo b,e 1,4 dioxin
112.5 111.5 1.0 0.9 124.0 -11.5 -10.2
1217 DCBDOX10 2,8-dichlorodibenzo b,e 1,4 dioxin
110.4 101.5 9.0 8.1 112.9 -2.4 -2.2
1218 TEKQIJ 2,2',5,5'-tetrachlorobiphenyl
101.3 112.3 -11.0 -10.9 112.7 -11.4 -11.2
1221 FUHDAN01 3,3',4,4'-tetrachlorobiphenyl
125.8 133.4 -7.6 -6.1 123.4 2.4 1.9
1223 SESHED 2-chlorodibenzo b,e 1,4 dioxin
98.0 95.7 2.3 2.4 107.1 -9.1 -9.3
1229 DCLBIP 2,2' -dichlorobiphenyl
96.0 95.0 1.0 1.1 89.1 6.9 7.2
1230 DCLBIQ10 4,4' -dichlorobiphenyl
104.0 99.2 4.8 4.6
1231 PUGPIQ 2,2' -difluorobiphenyl
95.6 90.1 5.5 5.7 90.6 5.0 5.2
1232 ZZZAOS02 4,4' -difluorobiphenyl
95.1 83.8 11.3 11.9 90.4 4.7 5.0
1233 OPENAN 1,10-phenanthroline
98.0 109.8 -11.8 -12.0
1234 PHENAZ11 phenazine
96.0 92.8 3.2 3.3 101.0 -5.0 -5.3
1236 DNTDPH 4,4' -dinitrobiphenyl
109.9 120.8 -10.9 -9.9
1239 DBZFUR02 dibenzofuran
84.1 79.9 4.2 5.0 88.2 -4.1 -4.9
1240 BZDIOX01 dibenzo b,e 1,4 dioxin
92.1 85.4 6.7 7.3 98.4 -6.3 -6.8
1241 DBZTHP dibenzothiophene
96.1 90.6 5.5 5.7 103.4 -7.3 -7.6
1242 THIANT03 thianthrene
101.1 96.6 4.5 4.5 100.2 0.9 0.9
1245 CRBZOL03 carbazole
101.0 111.1 -10.1 -10.0 103.6 -2.6 -2.5
1247 PHESAZ01 phenothiazine
115.0 102.2 12.8 11.2 106.2 8.8 7.7
1250 ACENAP03 acenaphthene
85.1 89.7 -4.6 -5.4
1251 BIPHEN04 biphenyl
82.0 83.9 -1.9 -2.3 89.1 -7.1 -8.6
1252 AZBENC01 cis-azobenzene
93.1 93.1 88.0 5.1 5.5
1253 AZOBEN01 trans-azobenzene
96.1 100.8 -4.7 -4.9
1259 RAFFIO01 diphenyl ether
82.0 86.1 -4.1 -5.0 91.1 -9.1 -11.1
1261 BOPSAA10 4-hydroxybiphenyl
110.0 118.1 -8.1 -7.3 129.6 -19.6 -17.8
1262 NUTSUQ 2,2' -dihydroxybiphenyl
114.0 121.3 -7.3 -6.4 130.7 -16.7 -14.6
1263 DOHDPH02 4,4' -dihydroxybiphenyl
143.0 152.5 -9.5 -6.6 172.1 -29.1 -20.3
1264 PARPEE alpha naphthyl acetate
95.0 94.3 0.7 0.7 102.4 -7.4 -7.8
1266 NAPACA12 1-naphthaleneacetic
112.0 114.3 -2.3 -2.1 118.9 -6.9 -6.2
1267 PEYGEF01 2-naphthaleneacetic

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     124.0  124.7   -0.7   -0.5  130.5   -6.5   -5.2
1268  DPSULO    diphenyl sulfone
     106.0  111.7   -5.7   -5.3  102.9    3.1    3.0
1269  DPDSON    diphenyl disulfone
     162.0                       122.4   39.6   24.5
1271  QQQBVP02  diphenylamine
     105.1                       101.2    3.9    3.7
1274  DMNAPH    1,8-dimethylnaphthalene
      81.5   80.9    0.6    0.7   88.3   -6.8   -8.3
1276  DMNPTL02  2,6-dimethylnaphthalene
      83.1   85.4   -2.4   -2.9   91.0   -8.0   -9.6
1278  NAMKAN01  4,4' -dimethyl-2-2'bipyridyl
     100.0   98.9    1.1    1.1  118.5  -18.5  -18.5
1280  HEGSAN01  1,4-dimethylcubane dicarboxylate
     117.0   92.5   24.5   21.0   90.9   26.1   22.3
1281  DUJTIM    1,3,5-benzenetricarboxylic acid triMeester
     118.0                       170.4  -52.4  -44.4
1283  DOHCOS    2,4,6-trinitro-1,3-dimethyl-5-tert-butylbenzene
     101.3                       122.1  -20.8  -20.5
1288  HMBENZ17  hexamethylbenzene
      84.0   74.4    9.6   11.4   90.9   -6.9   -8.3
1290  KUKLIN    1-adamantyl-1-carboxylic acid Meester
      82.0   78.3    3.7    4.5   90.4   -8.4  -10.3
1295  DECDAC02  dodecanedioic  acid
     162.1                       180.3  -18.2  -11.2
1297  LAURAC04  dodecanoic  acid
     140.0                       133.3    6.7    4.8
1304  FLURON    9-fluorenone
      91.0   80.2   10.8   11.9   88.3    2.7    3.0
1307  BIMVEZ    2-chlorobenzophenone
     100.0   99.2    0.8    0.8   95.8    4.2    4.2
1310  OLOHIG    5-chloro-2-hydroxybenzophenone
      92.4  107.3  -14.9  -16.1  125.7  -33.3  -36.1
1316  HIBXOF    acridone
     135.0  121.4   13.6   10.1  138.7   -3.7   -2.7
1319  FLUREN01  fluorene
      85.1   81.0    4.1    4.8   87.4   -2.3   -2.7
1322  MOYLAP    1,5-diphenyltetrazole
     124.3                       126.9   -2.6   -2.1
1324  BPHENO10  benzophenone
      93.1   87.4    5.7    6.1   95.6   -2.5   -2.7
1325  CONYAH    xanthene
      93.7   86.6    7.1    7.6   97.6   -3.9   -4.1
1326  NOZVIH    2-biphenylcarboxylic acid
     121.0                       110.7   10.3    8.5
1328  PHBENZ01  phenyl benzoate
      98.0   97.7    0.3    0.3  106.8   -8.8   -8.9
1329  DHXBZP10  2,4-dihydroxybenzophenone
     135.2                       146.9  -11.7   -8.7
1330  QQQAXJ02  phenyl salicylate
     109.0                       125.9  -16.9  -15.6
1331  ZZZPCA02  diphenyl carbonate
      90.0  103.7  -13.7  -15.2  119.6  -29.6  -32.9
1332  BADVIL10  2,2' ,4,4 '-tetrahydroxybenzophenone
     146.2                       201.7  -55.5  -37.9
1333  TOXANT    thioxanthene
     101.0   93.2    7.8    7.8  102.2   -1.2   -1.2
1340  ZZZMKS01  diphenylmethane
      86.0   87.4   -1.4   -1.6   92.4   -6.4   -7.4
1341  DPUREA02  1,3-diphenylurea
     152.0                       145.8    6.2    4.0
1343  YUHHUE    diphenylmethanol
     106.0                       126.0  -20.0  -18.8
1344  INEGAK    4-benzylphenol
      98.4                       124.9  -26.5  -26.9
1349  UREJOR    N-benzylaniline
     103.2                       103.7   -0.5   -0.5
1366  DBANTH11  9,10-dibromoanthracene
     117.1                       116.5    0.6    0.5
1367  DCLANT10  9,10-dichloroanthracene
     114.9  121.3   -6.4   -5.5  120.6   -5.7   -4.9
1368  ANTQUO08  9,10-anthraquinone
     111.0   98.0   13.0   11.7  112.5   -1.5   -1.3
1369  ZZZIYE01  9,10-phenanthraquinone
     108.0                       119.0  -11.0  -10.2
1374  DHXANT10  1,4-dihydroxy-9,10-anthraquinone
     117.1  101.4   15.7   13.4  140.6  -23.5  -20.1
1375  DHANTQ02  1,5-dihydroxyanthraquinone
     118.0                       153.7  -35.7  -30.2
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1376 DHANQU03 1,8-dihydroxyanthraquinone
110.0 133.3 -23.3 -21.1
1379 QQQFDS02 9-bromoanthracene
103.1 108.4 -5.3 -5.2 107.2 -4.1 -4.0
1381 CPTCET10 1,1,1-trichloro-2,2-bis 4-chlorophenyl ethane
118.1 124.0 -5.9 -5.0
1384 NTRANT01 9-nitroanthracene
115.3 113.9 1.4 1.2 115.4 -0.1 -0.1
1385 ANTCEN14 anthracene
97.1 105.0 -7.9 -8.1 106.8 -9.7 -10.0
1386 PHENAN08 phenanthrene
92.0 97.2 -5.2 -5.6 99.7 -7.7 -8.3
1387 DPHACT03 diphenylacetylene
93.0 94.2 -1.2 -1.3
1390 SAZQIT 2-fluorenecarboxaldehyde
102.0 97.2 4.8 4.7 106.3 -4.3 -4.2
1391 BENZIL02 benzil
99.7 95.8 3.9 3.9
1394 DBEZPO02 benzoyl peroxide
95.0 116.9 -21.9 -23.1
1395 HEKTUM diphenyl oxalate
103.0 138.8 -35.8 -34.7
1396 ZZZUCY01 2,2 -biphenyldicarboxylic acid
152.0 142.4 9.6 6.3
1401 NMACRO11 10-methylacridin-9 10H -one
105.0 113.6 -8.6 -8.2 123.4 -18.4 -17.5
1403 TOKKIN 1-methylfluorene
91.3 83.7 7.7 8.4 91.4 -0.1 -0.1
1404 BISDOY 9-methylfluorene
83.3 83.5 -0.2 -0.3 92.2 -8.9 -10.7
1405 DITBOX01 9,10-dihydroanthracene
93.0 86.0 7.0 7.6 93.9 -0.9 -0.9
1406 TSTILB16 trans-stilbene
102.0 101.2 0.8 0.8
1408 BZAZIN12 dibenzylideneazine
92.8 108.5 -15.7 -17.0 110.3 -17.5 -18.9
1409 LAXGAT02 2-benzylbenzimidazole
136.0 134.8 1.2 0.9
1412 ETCABZ10 N-ethylcarbazole
99.0 102.1 -3.1 -3.1
1413 DPACTM N,N-diphenylacetamide
125.5 111.8 13.7 10.9
1416 BTOLYL01 4,4 -dimethylbiphenyl
95.0 94.7 0.3 0.3
1417 DIBENZ12 1,2-diphenylethane
92.0 90.6 1.4 1.5
1421 CINVEA10 1,1-diphenylethanol
105.0 121.2 -16.2 -15.4
1423 TUXFIC02 dibenzyl sulfone
125.0 153.7 -28.7 -23.0 138.7 -13.7 -11.0
1424 QIBQOH di-p-tolyl sulfone
110.0 113.8 -3.8 -3.4
1425 COYRUD13 6-methoxy-alfa -methyl-2-naphthaleneacetic acid
130.5 133.5 -3.0 -2.3 144.3 -13.8 -10.6
1427 ZZZSRY01 dibenzyl sulfide
93.0 104.4 -11.4 -12.3
1428 VUFZUR01 4-(N,N-dimethylamino azobenzene
120.5 118.7 1.8 1.5 128.7 -8.2 -6.8
1430 CEKREP 1,4,5,8-tetramethylnaphthalene
100.0 103.7 -3.7 -3.7
1432 DMANAP10 1,8-N,N,N'N'-tetramethyldiaminonaphthalene
94.7 88.5 6.2 6.6 101.7 -7.0 -7.4
1434 RIQVOC 1,8-cyclotetradecadiyne
94.0 104.7 -10.7 -11.3
1437 WEJMAA diamantan-1-ol
119.4 95.8 23.6 19.8 116.3 3.2 2.7
1440 ZIKWOF 4-heptylbenzoic acid
130.0 124.6 5.4 4.2
1441 BUTBNZ01 1,4-di-tert-butylbenzene
83.0 99.4 -16.4 -19.8
1443 LERFET01 2,6-di-tert-butylphenol
83.0 84.2 -1.2 -1.5 111.6 -28.6 -34.5
1447 HESKOF 2,5-di-tert-butyl-1,4-dihydroxybenzene
122.0 123.7 -1.7 -1.4 147.3 -25.3 -20.7
1448 SEGROL dicyclohexyl peroxydicarbonate
100.2 129.6 -29.4 -29.3
1451 CYTDEC cyclotetradecane
98.0 100.4 -2.4 -2.4
1453 ZZZOEG02 tetradecanoic acid

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     140.8                        156.1  -15.3  -10.9
1458  ANTHAL    9-anthraldehyde
     101.9   99.6    2.3    2.3  111.7   -9.8   -9.6
1460  QQQFDJ01  9-anthracenecarboxylic
     124.2  138.9  -14.7  -11.8  135.7  -11.5   -9.2
1461  WADRAV    2-phenyl-4H-1-benzopyran-4-one flavone
     108.0                        121.3  -13.3  -12.3
1470  MANTHR14  9-methylanthracene
     101.0  101.3   -0.3   -0.3  103.2   -2.2   -2.2
1472  DBEZLM01  dibenzoylmethane
     115.0  106.2    8.8    7.7  128.9  -13.9  -12.1
1474  EACDRO01  10-ehylacridin-9(10H)-one
     117.0  104.5   12.5   10.7  129.2  -12.2  -10.4
1476  WUXDOJ    1,3-diphenylacetone
      89.0  107.3  -18.3  -20.5  125.3  -36.3  -40.8
1483  DTBUBZ01  3,5-di-tert-butylbenzoic acid
     110.0                        125.3  -15.3  -13.9
1486  ZZZZCB02  4-octyloxybenzoic  acid
     163.0                        149.5   13.5    8.3
1489  MBPHOL14  2,6-di-tert-butyl-4-methylphenol
      90.0                        113.7  -23.7  -26.4
1491  MEGTOI    1-bromopyrene
     101.1                        120.5  -19.4  -19.2
1493  FLUANT03  fuoranthene
     101.5                         98.6    2.9    2.9
1494  PYRENE02  pyrene
     102.1  108.2   -6.1   -6.0  103.8   -1.7   -1.7
1501  DMANTR01  9,10-dimethylanthracene
     115.3                        116.4   -1.1   -1.0
1504  FEWWEJ    4,5-dimethylphenanthrene
     105.0                        106.9   -1.9   -1.8
1505  KEDJOS    9,10-dimethylphenanthrene
     120.0                        110.3    9.7    8.1
1507  SAFNIW    3-4-biphenylylcarbonyl propionic acid fenbufen
     154.0                        168.6  -14.6   -9.5
1509  TICJEU    1,2,3,6,7,8-hexahydropyrene
      96.3                        108.8  -12.5  -12.9
1510  DXYLEN24  (2,2)paracyclophane
      97.1                         95.3    1.8    1.9
1511  METCYP    (2,2)metacyclophane
      92.0                         96.6   -4.6   -4.9
1514  ESALIM    N,N-bissalicylaldehydoEthylenediimine
     141.0                        129.9   11.1    7.9
1525  YEFWEM    hexadecanoic acid
     155.2                        165.6  -10.4   -6.7
1527  QQQFBP01  hexadecane
     135.0                        135.4   -0.4   -0.3
1536  COCAIN10  cocaine
     113.2                        134.2  -20.9  -18.5
1541  ZZZJWM01  1,2-benzanthra-9,10-quinone
      83.0                        130.4  -47.4  -57.1
1544  TETCEN01  naphthacene  (tetracene) linear fit
     139.0                        142.5   -3.5   -2.5
1546  TRIPHE11  triphenylene linear fit
     127.0                        119.9    7.1    5.6
1547  CRYSEN02  chrysene linear fit
     134.5                        138.1   -3.6   -2.7
1548  BZPHAN01  benzo c phenanthrene
     106.0  118.5  -12.5  -11.8  120.3  -14.3  -13.5
1549  BIQUOL01  2,2  -biquinoline
     135.0                        141.1   -6.1   -4.5
1551  TERPHO11  o-terphenyl
     101.0                        104.8   -3.8   -3.7
1552  ZZZMTW01  m-terphenyl
     119.0                        121.2   -2.2   -1.9
1553  TERPHE03  p-terphenyl
     122.0                        131.9   -9.9   -8.1
1554  REGXUY    5,12-dihydrotetracene
     121.0                        124.9   -3.9   -3.2
1555  RIWTAS02  diphenylfulvene
     105.0                        107.8   -2.8   -2.7
1556  DPPHOL    2,6-diphenylphenol
     119.0                        130.8  -11.8   -9.9
1557  ZZZJCQ01  triphenylamine
      89.5                        112.5  -23.0  -25.7
1561  FUFQIG    2,4,5,7-tetraMethylphenanthrene
     114.0                        117.8   -3.8   -3.4
1562  FEWWIN    3,4,5,6-tetramethylthylphenanthrene
     134.0                        106.1   27.9   20.8
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1568 ZZZEMS01 hexaethylbenzene
96.7 111.7 -15.0 -15.5
1574 STARAC05 octadecanoic acid stearic
167.5 192.5 -24.9 -14.9
1576 NOCTDC octadecane
153.0 150.4 2.6 1.7
1579 PHACRD 10-phenylacridin-9 10H -one
128.0 132.9 -4.9 -3.8
1580 DPMYAN N-phenyl benzophenone imine
120.0 130.0 -10.0 -8.4
1581 PIPHAX triphenylazidomethane
122.0 134.5 -12.4 -10.2
1582 TPHMET01 triphenylmethane
111.0 114.5 -3.5 -3.2
1585 LEPRON01 tricyclohexylmethane
117.5 113.9 3.6 3.1
1587 CEVWAC nonadecanoic acid
199.0 194.3 4.8 2.4
1589 CORANN11 corannulene
120.0 129.8 -9.8 -8.1
1590 PERLEN04 perylene linear fit 5
140.0 129.8 10.2 7.3
1591 BNPYRE11 benzo a pyrene
122.9 131.6 -8.7 -7.1
1592 CEQGEL benzo e pyrene
121.3 131.1 -9.8 -8.1
1593 QURDOY 9-phenylanthracene
121.3 118.9 2.3 1.9
1600 ZEGKAX10 5,6-diMEthylchrysene
139.1 131.6 7.5 5.4
1601 TRPETN 1,1,1-triphenylethane
109.0 112.7 -3.7 -3.4
1603 VABNAN pagodane
96.1 96.7 -0.6 -0.6
1606 ROFYIV dibenzo-18-crown-6
179.0 166.4 12.6 7.0
1608 CIDBUM hexacyclopropylethane
109.0 104.0 5.0 4.6
1609 BADAMN10 1,1 -biadamantane
114.0 113.7 0.3 0.3
1612 QQQCIM01 eicosane
177.9 165.2 12.7 7.1
1617 DACMOR01 diacetylmorphine heroin
145.4 161.4 -16.0 -11.0
1620 ANTHON10 anthanthrone dibenzochrysene6,12dione
160.1 171.0 -10.9 -6.8
1621 BNPERY02 benzo ghi perylene
137.8 144.0 -6.2 -4.5
1622 PENTQU 6,13-pentacenequinone
116.0 165.0 -49.0 -42.2
1624 DBNTHR02 dibenz a,h anthracene
163.0 154.1 8.9 5.5
1625 PENCEN02 pentacene
184.0 174.8 9.2 5.0
1626 ZZZOYC01 picene
145.3 157.3 -12.0 -8.2
1631 CAMJOP 1,4-bis N-butylamino -9,10-anthraquinone
119.8 188.3 -68.4 -57.1
1635 WOLXOK02 finasteride
150.9 169.8 -18.9 -12.5
1636 CORONE02 coronene linear fit
152.0 156.2 -4.2 -2.7
1637 ZAQZUM01 2,2,5,25 5 ,5,2,5,2 -sexithiophene
221.5 273.3 -51.8 -23.4
1639 TPHBEN02 1,3,5-triphenylbenzene
150.0 138.9 11.1 7.4
1641 TEPHME12 tetraphenylmethane
146.0 139.8 6.3 4.3
1643 DPANTR01 9,10-diphenylanthracene
155.6 146.9 8.6 5.5
1646 TPHETN 1,1,1,2-tetraphenylethane
133.0 137.7 -4.7 -3.5
1652 OVALEN01 ovalene
224.1 208.7 15.4 6.9
1653 DIBANT dibenzanthrone violanthrone
216.3 225.5 -9.1 -4.2
1654 IDBANT isodibenzanthrone isoviolanthrone
228.6 241.9 -13.3 -5.8
1655 CORXAI10 violanthrene

235.7 214.4 21.3 9.0

Figure S1. Plot of AA-CLP calculated lattice energies vs. experimental sublimation enthalpies.