Contents of the supporting informations:

- Informations 1: descriptor statistics for series 1, 2 and 3
- Informations 2: Aqueous solubility validation data set (Klopman, G.; Wang, S.; Balthasar, D. M. Estimation of Aqueous Solubility of Organic Molecules by the Group Contribution Approach. Application to the Study of Biodegradation. *J. Chem. Inf. Comput.Sci*. **1992**, *32*, 474-482.).
- Octanol/water partition coefficient validation data set (Rekker, R.F; ter Laak, A. M. On the Reliability of Calculated Log P-values: Rekker, Hansch/Leo and Suzuki Approach *Quant. Struct.-Act. Relat.* **1993**, *12*, 152-157.).
- Correlation coefficients of the final descriptor sets for series 2 and 3

Aqueous solubility validation data set (Klopman, G.; Wang, S.; Balthasar, D. M. Estimation of Aqueous Solubility of Organic Molecules by the Group Contribution Approach. Application to the Study of Biodegradation. *J. Chem. Inf. Comput.Sci*. **1992**, *32*, 474-482.):

```
2,2´,4,5,5´-PCB
  -ISIS-          3D

 22 23  0  0  0  0  0  0  0  0  1 V2000
    2.3305    4.1669   -1.7231 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    1.0126    3.5841   -0.7551 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.1671    2.4363    0.0031 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.1213    1.9663    0.7766 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0839    2.6407    0.7963 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3953    2.0496    1.7682 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -1.2452    3.7977    0.0343 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1867    4.2698   -0.7385 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5376    4.5261    0.0511 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.7368    3.8240   -0.0462 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.9375    4.5066   -0.0297 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.4327    3.6331   -0.1509 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -4.9504    5.8873    0.0840 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.4627    6.7394    0.1054 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -3.7616    6.5895    0.1810 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5561    5.9157    0.1702 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0661    6.7972    0.2992 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    2.1076    1.9057   -0.0097 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.2472    1.0701    1.3659 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3048    5.1676   -1.3269 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.7278    2.7477   -0.1349 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.7768    7.6658    0.2694 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  2  3  2  0  0  0  0
  2  8  1  0  0  0  0
  3  4  1  0  0  0  0
  3 18  1  0  0  0  0
  4  5  2  0  0  0  0
  4 19  1  0  0  0  0
```

```
  5  6  1  0  0  0  0
  5  7  1  0  0  0  0
  7  8  2  0  0  0  0
  7  9  1  0  0  0  0
  8 20  1  0  0  0  0
  9 10  2  0  0  0  0
  9 16  1  0  0  0  0
 10 11  1  0  0  0  0
 10 21  1  0  0  0  0
 11 12  1  0  0  0  0
 11 13  2  0  0  0  0
 13 14  1  0  0  0  0
 13 15  1  0  0  0  0
 15 16  2  0  0  0  0
 15 22  1  0  0  0  0
 16 17  1  0  0  0  0
M  END
> <logS_expected>
-7.89

> <CAS number>
37680-73-2

> <Kuehne_logS>
-7.47

> <Klopman_logS>
-7.90

> <Huuskonen_logS>
-7.21

> <Tetko_logS>
-7.57

> <Gasteiger_logS>
-7.85

$$$$
benzocaine
  -ISIS-            3D

 23 23  0  0  0  0  0  0  0  0  1 V2000
    0.0021   -0.0041    0.0020 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0144    1.2110    0.0087 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.1434    1.9006    0.0013 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.4105    1.1918   -0.0146 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.5598    2.2018   -0.0201 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3006    1.9305    0.0187 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5031    1.2163    0.0205 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6980    1.8888    0.0298 C   0  0  0  0  0  0  0  0  0  0  0  0
```

```
   -3.7151    3.2810    0.0374 C  0  0  0  0  0  0  0  0  0  0  0  0
   -4.9282    3.9596    0.0473 N  0  0  0  0  0  0  0  0  0  0  0  0
   -2.5197    3.9951    0.0356 C  0  0  0  0  0  0  0  0  0  0  0  0
   -1.3214    3.3288    0.0322 C  0  0  0  0  0  0  0  0  0  0  0  0
    2.4852    0.5612    0.8714 H  0  0  0  0  0  0  0  0  0  0  0  0
    2.4682    0.5708   -0.9085 H  0  0  0  0  0  0  0  0  0  0  0  0
    4.5110    1.6697   -0.0320 H  0  0  0  0  0  0  0  0  0  0  0  0
    3.4851    2.8323   -0.9060 H  0  0  0  0  0  0  0  0  0  0  0  0
    3.5021    2.8228    0.8738 H  0  0  0  0  0  0  0  0  0  0  0  0
   -2.4906    0.1364    0.0143 H  0  0  0  0  0  0  0  0  0  0  0  0
   -4.6269    1.3379    0.0309 H  0  0  0  0  0  0  0  0  0  0  0  0
   -5.7616    3.4633    0.0488 H  0  0  0  0  0  0  0  0  0  0  0  0
   -4.9414    4.9295    0.0526 H  0  0  0  0  0  0  0  0  0  0  0  0
   -2.5365    5.0749    0.0415 H  0  0  0  0  0  0  0  0  0  0  0  0
   -0.3945    3.8832    0.0356 H  0  0  0  0  0  0  0  0  0  0  0  0
  1  2  2  0  0  0  0
  2  3  1  0  0  0  0
  2  6  1  0  0  0  0
  3  4  1  0  0  0  0
  4  5  1  0  0  0  0
  4 13  1  0  0  0  0
  4 14  1  0  0  0  0
  5 15  1  0  0  0  0
  5 16  1  0  0  0  0
  5 17  1  0  0  0  0
  6  7  2  0  0  0  0
  6 12  1  0  0  0  0
  7  8  1  0  0  0  0
  7 18  1  0  0  0  0
  8  9  2  0  0  0  0
  8 19  1  0  0  0  0
  9 10  1  0  0  0  0
  9 11  1  0  0  0  0
 10 20  1  0  0  0  0
 10 21  1  0  0  0  0
 11 12  2  0  0  0  0
 11 22  1  0  0  0  0
 12 23  1  0  0  0  0
M  END
> <logS_expected>
-2.32

> <CAS number>
94-09-7

> <Kuehne_logS>
NaN

> <Klopman_logS>
-1.71
```

> <Huuskonen_logS>
-1.79

> <Tetko_logS>
-1.63

> <Gasteiger_logS>
-2.19

$$$$
acetylsalicylic_acid
  -ISIS-   3D

 21 21 0 0 0 0 0 0 0 0 1 V2000
    0.0594   0.0331   -0.5150 O   0 0 0 0 0 0 0 0 0 0 0 0
    0.0093   1.2111   -0.2509 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.1396   1.8914   0.0013 O   0 0 0 0 0 0 0 0 0 0 0 0
    2.3228   1.2326   0.0889 C   0 0 0 0 0 0 0 0 0 0 0 0
    3.5227   1.9505   0.1871 C   0 0 0 0 0 0 0 0 0 0 0 0
    4.7346   1.2608   0.2772 C   0 0 0 0 0 0 0 0 0 0 0 0
    4.7431   -0.1171   0.2690 C   0 0 0 0 0 0 0 0 0 0 0 0
    3.5549   -0.8228   0.1714 C   0 0 0 0 0 0 0 0 0 0 0 0
    3.5062   3.4249   0.1947 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.4504   4.0211   0.1158 O   0 0 0 0 0 0 0 0 0 0 0 0
    4.6619   4.1112   0.2892 O   0 0 0 0 0 0 0 0 0 0 0 0
    2.3498   -0.1538   0.0875 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.3208   1.9185   -0.2108 C   0 0 0 0 0 0 0 0 0 0 0 0
    5.6633   1.8069   0.3527 H   0 0 0 0 0 0 0 0 0 0 0 0
    5.6803   -0.6493   0.3387 H   0 0 0 0 0 0 0 0 0 0 0 0
    3.5710   -1.9027   0.1651 H   0 0 0 0 0 0 0 0 0 0 0 0
    4.6511   5.0781   0.2942 H   0 0 0 0 0 0 0 0 0 0 0 0
    1.4274   -0.7110   0.0166 H   0 0 0 0 0 0 0 0 0 0 0 0
   -2.1159   1.2106   -0.4447 H   0 0 0 0 0 0 0 0 0 0 0 0
   -1.4829   2.3312   0.7849 H   0 0 0 0 0 0 0 0 0 0 0 0
   -1.3254   2.7253   -0.9437 H   0 0 0 0 0 0 0 0 0 0 0 0
  1 2 2 0 0 0 0
  2 3 1 0 0 0 0
  2 13 1 0 0 0 0
  3 4 1 0 0 0 0
  4 5 2 0 0 0 0
  4 12 1 0 0 0 0
  5 6 1 0 0 0 0
  5 9 1 0 0 0 0
  6 7 2 0 0 0 0
  6 14 1 0 0 0 0
  7 8 1 0 0 0 0
  7 15 1 0 0 0 0
  8 12 2 0 0 0 0
  8 16 1 0 0 0 0
  9 10 2 0 0 0 0
  9 11 1 0 0 0 0

```
 11 17  1  0  0  0  0
 12 18  1  0  0  0  0
 13 19  1  0  0  0  0
 13 20  1  0  0  0  0
 13 21  1  0  0  0  0
M  END
>  <logS_expected>
-1.72

>  <CAS number>
50-78-2

>  <Kuehne_logS>
-1.93

>  <Klopman_logS>
-1.52

>  <Huuskonen_logS>
-1.69

>  <Tetko_logS>
-1.81

>  <Gasteiger_logS>
-1.87

$$$$
theophylline
  -ISIS-            3D

 21 22  0  0  0  0  0  0  0  0  1 V2000
   -0.0178    1.4608    0.0101 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0021   -0.0041    0.0020 N   0  0  0  0  0  0  0  0  0  0  0  0
    0.0222   -0.6726    1.1671 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0230   -0.0409    2.2061 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.0410   -2.0159    1.2245 N   0  0  0  0  0  0  0  0  0  0  0  0
    0.0620   -2.6843    2.5280 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0404   -2.7703    0.0738 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0568   -4.1036   -0.1896 N   0  0  0  0  0  0  0  0  0  0  0  0
    0.0465   -4.2560   -1.5456 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0247   -3.0857   -2.1152 N   0  0  0  0  0  0  0  0  0  0  0  0
    0.0200   -2.1272   -1.1580 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0057   -0.6637   -1.1766 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0289   -0.0548   -2.2305 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.0048    1.8381    0.0023 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5450    1.8219   -0.8730 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5280    1.8123    0.9069 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9603   -2.8641    2.8606 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5881   -3.6349    2.4405 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5739   -2.0512    3.2528 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
    0.0732   -4.8173    0.4671 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.0553   -5.2021   -2.0663 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1 14  1  0  0  0  0
  1 15  1  0  0  0  0
  1 16  1  0  0  0  0
  2  3  1  0  0  0  0
  2 12  1  0  0  0  0
  3  4  2  0  0  0  0
  3  5  1  0  0  0  0
  5  6  1  0  0  0  0
  5  7  1  0  0  0  0
  6 17  1  0  0  0  0
  6 18  1  0  0  0  0
  6 19  1  0  0  0  0
  7  8  1  0  0  0  0
  7 11  2  0  0  0  0
  8  9  1  0  0  0  0
  8 20  1  0  0  0  0
  9 10  2  0  0  0  0
  9 21  1  0  0  0  0
 10 11  1  0  0  0  0
 11 12  1  0  0  0  0
 12 13  2  0  0  0  0
M  END
>  <logS_expected>
-1.39

>  <CAS number>
58-55-9

>  <Kuehne_logS>
0.54

>  <Klopman_logS>
-1.07

>  <Huuskonen_logS>
-1.71

>  <Tetko_logS>
-0.69

>  <Gasteiger_logS>
-1.27

$$$$
antipyrine
  -ISIS-          3D

 26 27  0  0  0  0  0  0  0  0  1 V2000
```

```
  0.1029   1.2806   0.1321 C  0  0  0  0  0  0  0  0  0  0  0  0
  1.2894   1.9505   0.3575 C  0  0  0  0  0  0  0  0  0  0  0  0
  2.3756   1.2774   0.8860 C  0  0  0  0  0  0  0  0  0  0  0  0
  2.2780  -0.0681   1.1900 C  0  0  0  0  0  0  0  0  0  0  0  0
  1.0945  -0.7440   0.9666 C  0  0  0  0  0  0  0  0  0  0  0  0
  0.0014  -0.0706   0.4368 C  0  0  0  0  0  0  0  0  0  0  0  0
 -1.1988  -0.7518   0.2102 N  0  0  0  0  0  0  0  0  0  0  0  0
 -2.4364  -0.2170   0.2455 C  0  0  0  0  0  0  0  0  0  0  0  0
 -2.7106   0.9463   0.4797 O  0  0  0  0  0  0  0  0  0  0  0  0
 -3.3581  -1.2512  -0.0396 C  0  0  0  0  0  0  0  0  0  0  0  0
 -2.6621  -2.3884  -0.2412 C  0  0  0  0  0  0  0  0  0  0  0  0
 -3.2516  -3.7352  -0.5724 C  0  0  0  0  0  0  0  0  0  0  0  0
 -1.3317  -2.1117  -0.1002 N  0  0  0  0  0  0  0  0  0  0  0  0
 -0.2343  -3.0713  -0.2454 C  0  0  0  0  0  0  0  0  0  0  0  0
 -0.7465   1.8080  -0.2764 H  0  0  0  0  0  0  0  0  0  0  0  0
  1.3691   3.0012   0.1205 H  0  0  0  0  0  0  0  0  0  0  0  0
  3.3024   1.8035   1.0613 H  0  0  0  0  0  0  0  0  0  0  0  0
  3.1283  -0.5910   1.6023 H  0  0  0  0  0  0  0  0  0  0  0  0
  1.0190  -1.7949   1.2039 H  0  0  0  0  0  0  0  0  0  0  0  0
 -4.4321  -1.1481  -0.0875 H  0  0  0  0  0  0  0  0  0  0  0  0
 -3.3286  -3.8420  -1.6544 H  0  0  0  0  0  0  0  0  0  0  0  0
 -2.6092  -4.5208  -0.1745 H  0  0  0  0  0  0  0  0  0  0  0  0
 -4.2435  -3.8170  -0.1277 H  0  0  0  0  0  0  0  0  0  0  0  0
  0.0378  -3.4630   0.7347 H  0  0  0  0  0  0  0  0  0  0  0  0
 -0.5517  -3.8916  -0.8892 H  0  0  0  0  0  0  0  0  0  0  0  0
  0.6274  -2.5733  -0.6897 H  0  0  0  0  0  0  0  0  0  0  0  0
 1  6  2  0  0  0  0
 1  2  1  0  0  0  0
 1 15  1  0  0  0  0
 2  3  2  0  0  0  0
 2 16  1  0  0  0  0
 3  4  1  0  0  0  0
 3 17  1  0  0  0  0
 4  5  2  0  0  0  0
 4 18  1  0  0  0  0
 5  6  1  0  0  0  0
 5 19  1  0  0  0  0
 6  7  1  0  0  0  0
 7  8  1  0  0  0  0
 7 13  1  0  0  0  0
 8  9  2  0  0  0  0
 8 10  1  0  0  0  0
10 11  2  0  0  0  0
10 20  1  0  0  0  0
11 12  1  0  0  0  0
11 13  1  0  0  0  0
12 21  1  0  0  0  0
12 22  1  0  0  0  0
12 23  1  0  0  0  0
13 14  1  0  0  0  0
14 24  1  0  0  0  0
```

```
 14 25  1  0  0  0  0
 14 26  1  0  0  0  0
M  END
>  <logS_expected>
-0.56

>  <CAS number>
60-80-0

>  <Kuehne_logS>
-1.90

>  <Klopman_logS>
-2.76

>  <Huuskonen_logS>
-1.29

>  <Tetko_logS>
-0.89

>  <Gasteiger_logS>
-1.31

$$$$
atrazine
  -ISIS-            3D

 28 28  0  0  0  0  0  0  0  0  1 V2000
   -0.0160    1.3264    0.0093 N   0  0  0  0  0  0  0  0  0  0  0  0
    0.0021   -0.0041    0.0020 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.1625   -0.6513   -0.0125 N   0  0  0  0  0  0  0  0  0  0  0  0
    2.3014    0.0328   -0.0197 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.2767    1.3635   -0.0124 N   0  0  0  0  0  0  0  0  0  0  0  0
    3.5086   -0.6356   -0.0344 N   0  0  0  0  0  0  0  0  0  0  0  0
    4.7640    0.1195   -0.0423 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.8805   -0.7409    0.5526 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.1227    0.4974   -1.4809 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1831   -0.7110    0.0100 N   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4620    0.0034    0.0265 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.6106   -1.0073    0.0325 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.1199    2.0049    0.0021 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.0921    3.7407    0.0111 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    3.5260   -1.6055   -0.0395 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.6469    1.0252    0.5528 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.9975   -1.6466   -0.0426 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.8145   -0.1791    0.5467 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.6249   -1.0101    1.5774 H   0  0  0  0  0  0  0  0  0  0  0  0
    5.2398   -0.4083   -2.0760 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.3273    1.1104   -1.9047 H   0  0  0  0  0  0  0  0  0  0  0  0
    6.0568    1.0592   -1.4868 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
   -1.1693   -1.6809    0.0047 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5198    0.6244    0.9205 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5374    0.6339   -0.8594 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.5622   -0.4758    0.0448 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.5528   -1.6283   -0.8614 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.5352   -1.6379    0.9184 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  2  0  0  0  0
  1 13  1  0  0  0  0
  2  3  1  0  0  0  0
  2 10  1  0  0  0  0
  3  4  2  0  0  0  0
  4  5  1  0  0  0  0
  4  6  1  0  0  0  0
  5 13  2  0  0  0  0
  6  7  1  0  0  0  0
  6 15  1  0  0  0  0
  7  8  1  0  0  0  0
  7  9  1  0  0  0  0
  7 16  1  0  0  0  0
  8 17  1  0  0  0  0
  8 18  1  0  0  0  0
  8 19  1  0  0  0  0
  9 20  1  0  0  0  0
  9 21  1  0  0  0  0
  9 22  1  0  0  0  0
 10 11  1  0  0  0  0
 10 23  1  0  0  0  0
 11 12  1  0  0  0  0
 11 24  1  0  0  0  0
 11 25  1  0  0  0  0
 12 26  1  0  0  0  0
 12 27  1  0  0  0  0
 12 28  1  0  0  0  0
 13 14  1  0  0  0  0
M  END
>  <logS_expected>
-3.85

>  <CAS number>
1912-24-9

>  <Kuehne_logS>
-3.95

>  <Klopman_logS>
-3.05

>  <Huuskonen_logS>
-3.51

>  <Tetko_logS>
```

-3.70

> <Gasteiger_logS>
-3.83

$$$$
phenobarbital
  -ISIS-   3D

 29 30 0 0 0 0 0 0 0 0 1 V2000
   -0.0187   1.5258   0.0104 C   0 0 0 0 0 0 0 0 0 0 0 0
    0.0021   -0.0041   0.0020 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.4333   -0.5336   0.0129 C   0 0 0 0 0 0 0 0 0 0 0 0
   -2.1137   -0.0275   1.2707 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.6686   -0.2776   2.3703 O   0 0 0 0 0 0 0 0 0 0 0 0
   -3.2329   0.7122   1.1202 N   0 0 0 0 0 0 0 0 0 0 0 0
   -3.7368   0.9970   -0.0861 C   0 0 0 0 0 0 0 0 0 0 0 0
   -4.7481   1.6687   -0.1295 O   0 0 0 0 0 0 0 0 0 0 0 0
   -3.2086   0.5957   -1.2479 N   0 0 0 0 0 0 0 0 0 0 0 0
   -2.0868   -0.1532   -1.3023 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.6191   -0.5089   -2.3627 O   0 0 0 0 0 0 0 0 0 0 0 0
   -1.3742   -2.0378   0.0846 C   0 0 0 0 0 0 0 0 0 0 0 0
   -2.5432   -2.7751   0.1079 C   0 0 0 0 0 0 0 0 0 0 0 0
   -2.4890   -4.1548   0.1738 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.2657   -4.7972   0.2159 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.0967   -4.0599   0.1916 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.1509   -2.6804   0.1214 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.0039   1.9031   0.0027 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.5459   1.8868   -0.8726 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.5289   1.8773   0.9072 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.5123   -0.3556   -0.8948 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.5293   -0.3651   0.8851 H   0 0 0 0 0 0 0 0 0 0 0 0
   -3.6854   1.0469   1.9101 H   0 0 0 0 0 0 0 0 0 0 0 0
   -3.6448   0.8505   -2.0760 H   0 0 0 0 0 0 0 0 0 0 0 0
   -3.4990   -2.2732   0.0751 H   0 0 0 0 0 0 0 0 0 0 0 0
   -3.4024   -4.7308   0.1927 H   0 0 0 0 0 0 0 0 0 0 0 0
   -1.2234   -5.8751   0.2680 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.8591   -4.5618   0.2249 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.7625   -2.1046   0.0987 H   0 0 0 0 0 0 0 0 0 0 0 0
  1 2 1 0 0 0 0
  1 18 1 0 0 0 0
  1 19 1 0 0 0 0
  1 20 1 0 0 0 0
  2 3 1 0 0 0 0
  2 21 1 0 0 0 0
  2 22 1 0 0 0 0
  3 4 1 0 0 0 0
  3 10 1 0 0 0 0
  3 12 1 0 0 0 0
  4 5 2 0 0 0 0
  4 6 1 0 0 0 0

```
 6  7  1  0  0  0  0
 6 23  1  0  0  0  0
 7  8  2  0  0  0  0
 7  9  1  0  0  0  0
 9 10  1  0  0  0  0
 9 24  1  0  0  0  0
10 11  2  0  0  0  0
12 13  2  0  0  0  0
12 17  1  0  0  0  0
13 14  1  0  0  0  0
13 25  1  0  0  0  0
14 15  2  0  0  0  0
14 26  1  0  0  0  0
15 16  1  0  0  0  0
15 27  1  0  0  0  0
16 17  2  0  0  0  0
16 28  1  0  0  0  0
17 29  1  0  0  0  0
M  END
>  <logS_expected>
-2.34

>  <CAS number>
50-06-6

>  <Kuehne_logS>
-2.41

>  <Klopman_logS>
-2.08

>  <Huuskonen_logS>
-2.97

>  <Tetko_logS>
-2.89

>  <Gasteiger_logS>
-2.80

$$$$
diuron
  -ISIS-            3D

 24 24  0  0  0  0  0  0  0  0  1 V2000
   -0.3698    0.3384    0.9882 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.2989    1.4581    0.5196 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.8517    2.1543    0.6085 N   0  0  0  0  0  0  0  0  0  0  0  0
    1.9720    1.6212    1.3875 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.9820    3.4441   -0.0738 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3693    2.0010   -0.0937 N   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  -2.6112    1.3575   -0.0341 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.7768    2.1044    0.0708 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.0014    1.4677    0.1296 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.0675    0.0867    0.0846 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.9063   -0.6613   -0.0200 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.9927   -2.3942   -0.0763 Cl  0  0  0  0  0  0  0  0  0  0  0  0
  -6.6079   -0.7102    0.1599 Cl  0  0  0  0  0  0  0  0  0  0  0  0
  -2.6794   -0.0285   -0.0854 C   0  0  0  0  0  0  0  0  0  0  0  0
   2.6043    1.0102    0.7433 H   0  0  0  0  0  0  0  0  0  0  0  0
   2.5570    2.4461    1.7940 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.5883    1.0105    2.2048 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.0207    3.7272   -0.5025 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.2984    4.2032    0.6416 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.7240    3.3617   -0.8680 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.2791    2.8374   -0.5765 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.7262    3.1826    0.1067 H   0  0  0  0  0  0  0  0  0  0  0  0
  -5.9082    2.0488    0.2112 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.7744   -0.6114   -0.1718 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  2  0  0  0  0
 2  3  1  0  0  0  0
 2  6  1  0  0  0  0
 3  4  1  0  0  0  0
 3  5  1  0  0  0  0
 4 15  1  0  0  0  0
 4 16  1  0  0  0  0
 4 17  1  0  0  0  0
 5 18  1  0  0  0  0
 5 19  1  0  0  0  0
 5 20  1  0  0  0  0
 6  7  1  0  0  0  0
 6 21  1  0  0  0  0
 7  8  2  0  0  0  0
 7 14  1  0  0  0  0
 8  9  1  0  0  0  0
 8 22  1  0  0  0  0
 9 10  2  0  0  0  0
 9 23  1  0  0  0  0
10 11  1  0  0  0  0
10 13  1  0  0  0  0
11 12  1  0  0  0  0
11 14  2  0  0  0  0
14 24  1  0  0  0  0
M  END
> <logS_expected>
-3.80

> <CAS number>
330-54-1

> <Kuehne_logS>
-3.38
```

> <Klopman_logS>
-2.85

> <Huuskonen_logS>
-2.86

> <Tetko_logS>
-3.01

> <Gasteiger_logS>
-3.70

$$$$
nitrofurantoin
  -ISIS-   3D

 23 24 0 0 0 0 0 0 0 0 2 V2000
    1.4322   4.2058   0.0154 O   0 0 0 0 0 0 0 0 0 0 0 0
    0.6796   3.2529   0.0164 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.0936   1.9730   0.0031 N   0 0 0 0 0 0 0 0 0 0 0 0
    2.3150   1.5581   -0.0121 N   0 0 0 0 0 0 0 0 0 0 0 0
    2.5783   0.2486   0.0795 C   0 0 0 0 0 0 0 0 0 0 0 0
    3.8847   -0.1881   0.1682 C   0 0 0 0 0 0 0 0 0 0 0 0
    4.9955   0.5851   0.1752 O   0 0 0 0 0 0 0 0 0 0 0 0
    6.0776   -0.1918   0.2744 C   0 0 0 0 0 0 0 0 0 0 0 0
    7.4799   0.3019   0.3127 N   0 3 0 0 0 0 0 0 0 0 0 0
    8.4765   -0.5532   0.4129 O   0 0 0 0 0 0 0 0 0 0 0 0
    7.7252   1.5941   0.2464 O   0 5 0 0 0 0 0 0 0 0 0 0
    5.7003   -1.5356   0.3373 C   0 0 0 0 0 0 0 0 0 0 0 0
    4.3393   -1.5884   0.2804 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.1197   1.1377   0.0096 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.2486   2.1491   0.0284 C   0 0 0 0 0 0 0 0 0 0 0 0
   -2.4386   1.9182   0.0396 O   0 0 0 0 0 0 0 0 0 0 0 0
   -0.6540   3.3585   0.0366 N   0 0 0 0 0 0 0 0 0 0 0 0
    1.7686   -0.4660   0.0839 H   0 0 0 0 0 0 0 0 0 0 0 0
    6.3672   -2.3809   0.4206 H   0 0 0 0 0 0 0 0 0 0 0 0
    3.7207   -2.4731   0.3089 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.1685   0.5252   -0.8907 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.1501   0.5125   0.9020 H   0 0 0 0 0 0 0 0 0 0 0 0
   -1.1337   4.2015   0.0527 H   0 0 0 0 0 0 0 0 0 0 0 0
  1 2 2 0 0 0 0
  2 3 1 0 0 0 0
  2 17 1 0 0 0 0
  3 4 1 0 0 0 0
  3 14 1 0 0 0 0
  4 5 2 0 0 0 0
  5 6 1 0 0 0 0
  5 18 1 0 0 0 0
  6 7 1 0 0 0 0
  6 13 2 0 0 0 0

```
  7  8  1  0  0  0  0
  8  9  1  0  0  0  0
  8 12  2  0  0  0  0
  9 10  2  0  0  0  0
  9 11  1  0  0  0  0
 12 13  1  0  0  0  0
 12 19  1  0  0  0  0
 13 20  1  0  0  0  0
 14 15  1  0  0  0  0
 14 21  1  0  0  0  0
 14 22  1  0  0  0  0
 15 16  2  0  0  0  0
 15 17  1  0  0  0  0
 17 23  1  0  0  0  0
M  CHG  2   9   1  11  -1
M  END
>  <logS_expected>
-3.47

>  <CAS number>
67-20-9

>  <Kuehne_logS>
-2.62

>  <Klopman_logS>
-2.19

>  <Huuskonen_logS>
-3.42

>  <Tetko_logS>
-3.09

>  <Gasteiger_logS>
-2.52

$$$$
phenytoin
  -ISIS-            3D

 31 33  0  0  0  0  0  0  0  0  1 V2000
    0.4555    0.1429   -0.2893 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.2714    1.3408   -0.1975 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2524    2.2495   -0.2416 N   0  0  0  0  0  0  0  0  0  0  0  0
    0.7745    3.5033   -0.1165 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.4129    4.5340   -0.1190 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7274    3.3570    0.0271 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9420    1.9015   -0.0459 N   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1884    3.9000    1.3551 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7936    5.1611    1.7609 C   0  0  0  0  0  0  0  0  0  0  0  0
```

-1.2165 5.6591 2.9791 C 0 0 0 0 0 0 0 0 0 0 0 0
-2.0345 4.8963 3.7913 C 0 0 0 0 0 0 0 0 0 0 0 0
-2.4300 3.6355 3.3851 C 0 0 0 0 0 0 0 0 0 0 0 0
-2.0107 3.1392 2.1650 C 0 0 0 0 0 0 0 0 0 0 0 0
-1.4384 4.0503 -1.1065 C 0 0 0 0 0 0 0 0 0 0 0 0
-1.1133 5.3539 -1.4320 C 0 0 0 0 0 0 0 0 0 0 0 0
-1.7656 5.9898 -2.4717 C 0 0 0 0 0 0 0 0 0 0 0 0
-2.7426 5.3221 -3.1862 C 0 0 0 0 0 0 0 0 0 0 0 0
-3.0670 4.0182 -2.8612 C 0 0 0 0 0 0 0 0 0 0 0 0
-2.4117 3.3808 -1.8243 C 0 0 0 0 0 0 0 0 0 0 0 0
2.1916 2.0326 -0.3498 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.7923 1.4376 0.0070 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.1545 5.7571 1.1263 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.9075 6.6441 3.2964 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.3643 5.2851 4.7434 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.0689 3.0393 4.0199 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.3228 2.1557 1.8460 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.3500 5.8756 -0.8738 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.5121 7.0085 -2.7256 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.2527 5.8192 -3.9981 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.8306 3.4967 -3.4192 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.6626 2.3609 -1.5728 H 0 0 0 0 0 0 0 0 0 0 0 0
1 2 2 0 0 0 0
2 3 1 0 0 0 0
2 7 1 0 0 0 0
3 4 1 0 0 0 0
3 20 1 0 0 0 0
4 5 2 0 0 0 0
4 6 1 0 0 0 0
6 7 1 0 0 0 0
6 8 1 0 0 0 0
6 14 1 0 0 0 0
7 21 1 0 0 0 0
8 9 2 0 0 0 0
8 13 1 0 0 0 0
9 10 1 0 0 0 0
9 22 1 0 0 0 0
10 11 2 0 0 0 0
10 23 1 0 0 0 0
11 12 1 0 0 0 0
11 24 1 0 0 0 0
12 13 2 0 0 0 0
12 25 1 0 0 0 0
13 26 1 0 0 0 0
14 15 2 0 0 0 0
14 19 1 0 0 0 0
15 16 1 0 0 0 0
15 27 1 0 0 0 0
16 17 2 0 0 0 0
16 28 1 0 0 0 0
17 18 1 0 0 0 0

```
 17 29  1  0  0  0  0
 18 19  2  0  0  0  0
 18 30  1  0  0  0  0
 19 31  1  0  0  0  0
M  END
>  <logS_expected>
-3.99

>  <CAS number>
57-41-0

>  <Kuehne_logS>
-5.25

>  <Klopman_logS>
-3.47

>  <Huuskonen_logS>
-3.40

>  <Tetko_logS>
-3.52

>  <Gasteiger_logS>
-3.18

$$$$
diazepam
  -ISIS-          3D

 33 35  0  0  0  0  0  0  0  0  1 V2000
   -0.0577   -0.0124    0.0075 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0486    1.2004    0.0099 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.1185    1.8400   -0.0136 N   0  0  0  0  0  0  0  0  0  0  0  0
    1.2748    3.2168    0.0407 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.4490    4.1081   -0.6410 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.6855    5.4870   -0.5294 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7204    5.9582    0.2461 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5391    5.0688    0.9245 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.0007    7.6666    0.3743 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -0.6772    3.6752   -1.4830 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4875    2.7196   -1.1936 N   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8943    4.3946   -2.7598 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.1625    5.0673   -3.3729 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0458    5.7355   -4.5620 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2999    5.7391   -5.1461 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3522    5.0737   -4.5428 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1549    4.3971   -3.3565 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.3193    3.7130    0.8237 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.3330    1.0257   -0.1034 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3568    1.9429    0.0331 C   0  0  0  0  0  0  0  0  0  0  0  0
```

```
   0.0506    6.1838   -1.0565 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.3505    5.4396    1.5332 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.1419    5.0654   -2.9176 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.7716    6.2571   -5.0375 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.4583    6.2639   -6.0767 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.3290    5.0804   -5.0034 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.9759    3.8739   -2.8889 H   0  0  0  0  0  0  0  0  0  0  0  0
   2.9610    3.0264    1.3559 H   0  0  0  0  0  0  0  0  0  0  0  0
   2.0613   -0.0293   -0.1380 H   0  0  0  0  0  0  0  0  0  0  0  0
   2.8812    1.2895   -1.0078 H   0  0  0  0  0  0  0  0  0  0  0  0
   2.9600    1.2111    0.7687 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.1794    1.2311    0.1017 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.3802    2.6144    0.8914 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  2  0  0  0  0
 2  3  1  0  0  0  0
 2 20  1  0  0  0  0
 3  4  1  0  0  0  0
 3 19  1  0  0  0  0
 4  5  2  0  0  0  0
 4 18  1  0  0  0  0
 5  6  1  0  0  0  0
 5 10  1  0  0  0  0
 6  7  2  0  0  0  0
 6 21  1  0  0  0  0
 7  8  1  0  0  0  0
 7  9  1  0  0  0  0
 8 18  2  0  0  0  0
 8 22  1  0  0  0  0
10 11  2  0  0  0  0
10 12  1  0  0  0  0
11 20  1  0  0  0  0
12 13  2  0  0  0  0
12 17  1  0  0  0  0
13 14  1  0  0  0  0
13 23  1  0  0  0  0
14 15  2  0  0  0  0
14 24  1  0  0  0  0
15 16  1  0  0  0  0
15 25  1  0  0  0  0
16 17  2  0  0  0  0
16 26  1  0  0  0  0
17 27  1  0  0  0  0
18 28  1  0  0  0  0
19 29  1  0  0  0  0
19 30  1  0  0  0  0
19 31  1  0  0  0  0
20 32  1  0  0  0  0
20 33  1  0  0  0  0
M  END
>  <logS_expected>
-3.76
```

> <CAS number>
439-14-5

> <Kuehne_logS>
-4.51

> <Klopman_logS>
-6.54

> <Huuskonen_logS>
-4.05

> <Tetko_logS>
-4.37

> <Gasteiger_logS>
-4.81

$$$$
testosterone
  -ISIS-   3D

 49 52 0 0 0 0 0 0 0 0 1 V2000
   -0.0186   1.5239   0.0104 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.4220   1.9967   -0.0008 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.8129   2.8355   -0.7854 O   0 0 0 0 0 0 0 0 0 0 0 0
    2.3182   1.3859   0.9868 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.0095   0.2081   1.5289 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.9652   -0.3675   2.5580 C   0 0 0 0 0 0 0 0 0 0 0 0
    3.2544   -1.8270   2.2010 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.9306   -2.5894   2.0914 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.2055   -4.0547   1.8062 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.9314   -4.8237   2.9158 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.5440   -6.2997   2.6271 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.2140   -6.2552   1.8343 C   0 0 0 0 0 0 0 0 0 0 0 0
    0.2034   -6.9969   2.5204 O   0 0 0 0 0 0 0 0 0 0 0 0
    0.8334   -4.7798   1.7679 C   0 0 0 0 0 0 0 0 0 0 0 0
    0.0114   -4.4002   3.0012 C   0 0 0 0 0 0 0 0 0 0 0 0
    0.1213   -4.3209   0.5098 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.1559   -2.8177   0.6693 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.1278   -2.0285   0.9085 C   0 0 0 0 0 0 0 0 0 0 0 0
    0.7720   -0.5625   1.1857 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.1610   -0.5248   2.3977 C   0 0 0 0 0 0 0 0 0 0 0 0
    0.0021   -0.0041   0.0020 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.5194   1.8827   0.9096 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.5364   1.8923   -0.8752 H   0 0 0 0 0 0 0 0 0 0 0 0
    3.2287   1.8905   1.2746 H   0 0 0 0 0 0 0 0 0 0 0 0
    3.8950   0.2014   2.5513 H   0 0 0 0 0 0 0 0 0 0 0 0
    2.5107   -0.3166   3.5474 H   0 0 0 0 0 0 0 0 0 0 0 0
    3.7804   -1.8714   1.2474 H   0 0 0 0 0 0 0 0 0 0 0 0

```
  3.8706   -2.2771    2.9793 H  0  0  0  0  0  0  0  0  0  0  0  0
  1.3655   -2.4898    3.0182 H  0  0  0  0  0  0  0  0  0  0  0  0
  2.7351   -4.1636    0.8597 H  0  0  0  0  0  0  0  0  0  0  0  0
  4.0099   -4.6859    2.8385 H  0  0  0  0  0  0  0  0  0  0  0  0
  2.5716   -4.5155    3.8975 H  0  0  0  0  0  0  0  0  0  0  0  0
  3.3194   -6.7802    2.0303 H  0  0  0  0  0  0  0  0  0  0  0  0
  2.4035   -6.8397    3.5635 H  0  0  0  0  0  0  0  0  0  0  0  0
  1.3590   -6.6549    0.8306 H  0  0  0  0  0  0  0  0  0  0  0  0
  0.5135   -7.9115    2.5706 H  0  0  0  0  0  0  0  0  0  0  0  0
 -0.1510   -3.3224    3.0120 H  0  0  0  0  0  0  0  0  0  0  0  0
 -0.9503   -4.9122    2.9685 H  0  0  0  0  0  0  0  0  0  0  0  0
  0.5498   -4.6955    3.9017 H  0  0  0  0  0  0  0  0  0  0  0  0
  0.7563   -4.4913   -0.3596 H  0  0  0  0  0  0  0  0  0  0  0  0
 -0.8182   -4.8619    0.3964 H  0  0  0  0  0  0  0  0  0  0  0  0
 -0.6374   -2.4472   -0.2357 H  0  0  0  0  0  0  0  0  0  0  0  0
 -0.8278   -2.6680    1.5144 H  0  0  0  0  0  0  0  0  0  0  0  0
  1.7433   -2.0712    0.0099 H  0  0  0  0  0  0  0  0  0  0  0  0
 -0.4143    0.5098    2.6293 H  0  0  0  0  0  0  0  0  0  0  0  0
 -1.0715   -1.0802    2.1727 H  0  0  0  0  0  0  0  0  0  0  0  0
  0.3381   -0.9772    3.2546 H  0  0  0  0  0  0  0  0  0  0  0  0
 -1.0227   -0.3736    0.0384 H  0  0  0  0  0  0  0  0  0  0  0  0
  0.4699   -0.3481   -0.9204 H  0  0  0  0  0  0  0  0  0  0  0  0
 1 21  1  0  0  0  0
 1  2  1  0  0  0  0
 1 22  1  0  0  0  0
 1 23  1  0  0  0  0
 2  3  2  0  0  0  0
 2  4  1  0  0  0  0
 4  5  2  0  0  0  0
 4 24  1  0  0  0  0
 5  6  1  0  0  0  0
 5 19  1  0  0  0  0
 6  7  1  0  0  0  0
 6 25  1  0  0  0  0
 6 26  1  0  0  0  0
 7  8  1  0  0  0  0
 7 27  1  0  0  0  0
 7 28  1  0  0  0  0
 8  9  1  0  0  0  0
 8 18  1  0  0  0  0
 8 29  1  0  0  0  0
 9 10  1  0  0  0  0
 9 14  1  0  0  0  0
 9 30  1  0  0  0  0
10 11  1  0  0  0  0
10 31  1  0  0  0  0
10 32  1  0  0  0  0
11 12  1  0  0  0  0
11 33  1  0  0  0  0
11 34  1  0  0  0  0
12 13  1  0  0  0  0
```

 12 14 1 0 0 0 0
 12 35 1 0 0 0 0
 13 36 1 0 0 0 0
 14 15 1 0 0 0 0
 14 16 1 0 0 0 0
 15 37 1 0 0 0 0
 15 38 1 0 0 0 0
 15 39 1 0 0 0 0
 16 17 1 0 0 0 0
 16 40 1 0 0 0 0
 16 41 1 0 0 0 0
 17 18 1 0 0 0 0
 17 42 1 0 0 0 0
 17 43 1 0 0 0 0
 18 19 1 0 0 0 0
 18 44 1 0 0 0 0
 19 20 1 0 0 0 0
 19 21 1 0 0 0 0
 20 45 1 0 0 0 0
 20 46 1 0 0 0 0
 20 47 1 0 0 0 0
 21 48 1 0 0 0 0
 21 49 1 0 0 0 0
M END
> <logS_expected>
-4.09

> <CAS number>
58-22-0

> <Kuehne_logS>
-4.62

> <Klopman_logS>
-5.17

> <Huuskonen_logS>
-3.98

> <Tetko_logS>
-4.13

> <Gasteiger_logS>
-4.52

$$$$
lindane
  -ISIS-   3D

 18 18 0 0 0 0 0 0 0 0 1 V2000
   -0.0187   1.5258   0.0104 C   0 0 0 0 0 0 0 0 0 0 0 0

```
    0.0021   -0.0041    0.0020 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.7421   -0.5109    1.2415 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.1775    0.0187    1.2307 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.1567    1.5485    1.2391 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8482    2.1726    1.2263 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    3.0495   -0.5786    2.6914 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -0.1019    0.0706    2.7250 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -1.6894   -0.6281    0.0148 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    1.4167    2.0553   -0.0004 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.2606    1.4739   -1.4838 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -0.8907    2.1230   -1.4503 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -0.5289    1.8773    0.9072 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5123   -0.3556   -0.8948 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.7568   -1.6008    1.2356 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.6876   -0.3328    0.3339 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.6465    1.9000    2.1359 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.4019    3.1452    0.0056 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1 10  1  0  0  0  0
  1 12  1  0  0  0  0
  1 13  1  0  0  0  0
  2  3  1  0  0  0  0
  2  9  1  0  0  0  0
  2 14  1  0  0  0  0
  3  4  1  0  0  0  0
  3  8  1  0  0  0  0
  3 15  1  0  0  0  0
  4  5  1  0  0  0  0
  4  7  1  0  0  0  0
  4 16  1  0  0  0  0
  5  6  1  0  0  0  0
  5 10  1  0  0  0  0
  5 17  1  0  0  0  0
 10 11  1  0  0  0  0
 10 18  1  0  0  0  0
M  END
> <logS_expected>
-4.60

> <CAS number>
58-89-9

> <Kuehne_logS>
-5.08

> <Klopman_logS>
-4.88

> <Huuskonen_logS>
-4.71
```

> <Tetko_logS>
-4.91

> <Gasteiger_logS>
-5.04

$$$$
parathion
  -ISIS-   3D

 32 32 0 0 0 0 0 0 0 0 2 V2000
   -0.5892   1.9173   -0.3202 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.4112   0.4059   -0.1632 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.6935   -0.2240   -0.1317 O   0 0 0 0 0 0 0 0 0 0 0 0
   -1.4319   -1.8039   0.0343 P   0 0 0 0 0 0 0 0 0 0 0 0
   -0.0746   -2.3343   -1.1272 S   0 0 0 0 0 0 0 0 0 0 0 0
   -0.9937   -2.1189   1.5512 O   0 0 0 0 0 0 0 0 0 0 0 0
   -0.4682   -3.4477   1.5619 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.1673   -3.8655   3.0026 C   0 0 0 0 0 0 0 0 0 0 0 0
   -2.7812   -2.6108   -0.3130 O   0 0 0 0 0 0 0 0 0 0 0 0
   -2.9514   -2.5305   -1.6589 C   0 0 0 0 0 0 0 0 0 0 0 0
   -2.5188   -3.5642   -2.4768 C   0 0 0 0 0 0 0 0 0 0 0 0
   -2.6934   -3.4805   -3.8446 C   0 0 0 0 0 0 0 0 0 0 0 0
   -3.2988   -2.3676   -4.3986 C   0 0 0 0 0 0 0 0 0 0 0 0
   -3.7307   -1.3361   -3.5856 C   0 0 0 0 0 0 0 0 0 0 0 0
   -3.5632   -1.4174   -2.2167 C   0 0 0 0 0 0 0 0 0 0 0 0
   -3.4842   -2.2803   -5.8644 N   0 3 0 0 0 0 0 0 0 0 0 0
   -3.1036   -3.1882   -6.5815 O   0 0 0 0 0 0 0 0 0 0 0 0
   -4.0173   -1.3004   -6.3535 O   0 5 0 0 0 0 0 0 0 0 0 0
    0.3889   2.3978   -0.3442 H   0 0 0 0 0 0 0 0 0 0 0 0
   -1.1195   2.1262   -1.2494 H   0 0 0 0 0 0 0 0 0 0 0 0
   -1.1638   2.3049   0.5211 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.1634   0.0184   -1.0045 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.1191   0.1971   0.7659 H   0 0 0 0 0 0 0 0 0 0 0 0
   -1.1997   -4.1311   1.1307 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.4496   -3.4802   0.9749 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.2335   -4.8792   3.0108 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.5642   -3.1821   3.4339 H   0 0 0 0 0 0 0 0 0 0 0 0
   -1.0851   -3.8330   3.5897 H   0 0 0 0 0 0 0 0 0 0 0 0
   -2.0456   -4.4335   -2.0446 H   0 0 0 0 0 0 0 0 0 0 0 0
   -2.3565   -4.2848   -4.4818 H   0 0 0 0 0 0 0 0 0 0 0 0
   -4.2030   -0.4677   -4.0207 H   0 0 0 0 0 0 0 0 0 0 0 0
   -3.9045   -0.6132   -1.5818 H   0 0 0 0 0 0 0 0 0 0 0 0
  1 2 1 0 0 0 0
  1 19 1 0 0 0 0
  1 20 1 0 0 0 0
  1 21 1 0 0 0 0
  2 3 1 0 0 0 0
  2 22 1 0 0 0 0
  2 23 1 0 0 0 0
  3 4 1 0 0 0 0

 4 5 2 0 0 0 0
 4 6 1 0 0 0 0
 4 9 1 0 0 0 0
 6 7 1 0 0 0 0
 7 8 1 0 0 0 0
 7 24 1 0 0 0 0
 7 25 1 0 0 0 0
 8 26 1 0 0 0 0
 8 27 1 0 0 0 0
 8 28 1 0 0 0 0
 9 10 1 0 0 0 0
10 11 2 0 0 0 0
10 15 1 0 0 0 0
11 12 1 0 0 0 0
11 29 1 0 0 0 0
12 13 2 0 0 0 0
12 30 1 0 0 0 0
13 14 1 0 0 0 0
13 16 1 0 0 0 0
14 15 2 0 0 0 0
14 31 1 0 0 0 0
15 32 1 0 0 0 0
16 17 2 0 0 0 0
16 18 1 0 0 0 0
M CHG 2 16   1 18 -1
M END
> <logS_expected>
-4.66

> <CAS number>
56-38-2

> <Kuehne_logS>
-4.59

> <Klopman_logS>
-3.94

> <Huuskonen_logS>
-4.13

> <Tetko_logS>
-4.31

> <Gasteiger_logS>
-3.66

$$$$
diazinon
  -ISIS-   3D

```
40 40  0  0  0  0  0  0  0  0  1 V2000
  -0.5080    1.4790    0.1119 O   0  0  0  0  0  0  0  0  0  0  0  0
  -0.2404   -0.1079    0.1588 P   0  0  0  0  0  0  0  0  0  0  0  0
   0.5466   -0.4796    1.5133 O   0  0  0  0  0  0  0  0  0  0  0  0
   1.0089   -1.8238    1.3668 C   0  0  0  0  0  0  0  0  0  0  0  0
   1.6367   -2.2933    2.6807 C   0  0  0  0  0  0  0  0  0  0  0  0
  -1.6468   -0.8907    0.1232 O   0  0  0  0  0  0  0  0  0  0  0  0
  -2.1041   -0.8167   -1.1503 C   0  0  0  0  0  0  0  0  0  0  0  0
  -1.7842   -1.7521   -2.0369 N   0  0  0  0  0  0  0  0  0  0  0  0
  -2.2266   -1.6842   -3.2765 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.9969   -0.6968   -3.6860 N   0  0  0  0  0  0  0  0  0  0  0  0
  -3.3587    0.2737   -2.8592 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.2406    1.3968   -3.3407 C   0  0  0  0  0  0  0  0  0  0  0  0
  -1.8405   -2.7655   -4.2527 C   0  0  0  0  0  0  0  0  0  0  0  0
  -0.3174   -2.8065   -4.3921 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.3424   -4.1173   -3.7412 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.9224    0.2395   -1.5484 C   0  0  0  0  0  0  0  0  0  0  0  0
   0.7865   -0.6085   -1.3135 S   0  0  0  0  0  0  0  0  0  0  0  0
   0.7482    2.1017   -0.1641 C   0  0  0  0  0  0  0  0  0  0  0  0
   0.6008    3.6203   -0.0493 C   0  0  0  0  0  0  0  0  0  0  0  0
   0.1694   -2.4712    1.1134 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.7539   -1.8672    0.5722 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.9894   -3.3186    2.5689 H   0  0  0  0  0  0  0  0  0  0  0  0
   2.4762   -1.6459    2.9340 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.8917   -2.2499    3.4752 H   0  0  0  0  0  0  0  0  0  0  0  0
  -5.2860    1.1287   -3.1886 H   0  0  0  0  0  0  0  0  0  0  0  0
  -4.0128    2.3035   -2.7801 H   0  0  0  0  0  0  0  0  0  0  0  0
  -4.0607    1.5708   -4.4015 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.2887   -2.5553   -5.2237 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.1308   -3.0167   -3.4210 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.0381   -3.5886   -5.0981 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.0402   -1.8434   -4.7565 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.8942   -4.3275   -2.7701 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.4275   -4.0880   -3.6418 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.0631   -4.8993   -4.4472 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.2048    1.0141   -0.8508 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.4916    1.7536    0.5530 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.0680    1.8430   -1.1735 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.5590    4.0953   -0.2598 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.1426    3.9684   -0.7664 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.2810    3.8790    0.9601 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1 18  1  0  0  0  0
 2  3  1  0  0  0  0
 2  6  1  0  0  0  0
 2 17  2  0  0  0  0
 3  4  1  0  0  0  0
 4  5  1  0  0  0  0
 4 20  1  0  0  0  0
 4 21  1  0  0  0  0
 5 22  1  0  0  0  0
```

```
 5 23  1  0  0  0  0
 5 24  1  0  0  0  0
 6  7  1  0  0  0  0
 7  8  2  0  0  0  0
 7 16  1  0  0  0  0
 8  9  1  0  0  0  0
 9 10  2  0  0  0  0
 9 13  1  0  0  0  0
10 11  1  0  0  0  0
11 12  1  0  0  0  0
11 16  2  0  0  0  0
12 25  1  0  0  0  0
12 26  1  0  0  0  0
12 27  1  0  0  0  0
13 14  1  0  0  0  0
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19 39  1  0  0  0  0
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>  <CAS number>
333-41-5

>  <Kuehne_logS>
-4.98

>  <Klopman_logS>
-5.29

>  <Huuskonen_logS>
-4.01

>  <Tetko_logS>
-3.43

>  <Gasteiger_logS>
-2.66
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$$$$
phenolphthalein
  -ISIS-   3D

 38 41 0 0 0 0 0 0 0 0 1 V2000
    0.0021   -0.0041   0.0020 O   0 0 0 0 0 0 0 0 0 0 0 0
   -0.0144   1.2105   0.0087 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.0769   1.9940   0.0025 O   0 0 0 0 0 0 0 0 0 0 0 0
    0.6603   3.3869   0.0140 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.8476   3.3805   0.0283 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.7960   4.3760   0.0427 C   0 0 0 0 0 0 0 0 0 0 0 0
   -3.1421   4.0486   0.0538 C   0 0 0 0 0 0 0 0 0 0 0 0
   -3.5362   2.7225   0.0504 C   0 0 0 0 0 0 0 0 0 0 0 0
   -2.5930   1.7154   0.0365 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.1862   4.0738   1.2479 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.3890   3.6741   1.8006 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.8731   4.3019   2.9319 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.1516   5.3345   3.5132 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.6259   5.9539   4.6260 O   0 0 0 0 0 0 0 0 0 0 0 0
    0.9453   5.7339   2.9565 C   0 0 0 0 0 0 0 0 0 0 0 0
    0.4680   5.1064   1.8221 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.1626   4.0871   -1.2223 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.3545   3.6935   -1.8022 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.8175   4.3341   -2.9352 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.0851   5.3728   -3.4915 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.5381   6.0042   -4.6064 O   0 0 0 0 0 0 0 0 0 0 0 0
    0.8892   5.7654   -2.9081 C   0 0 0 0 0 0 0 0 0 0 0 0
    0.4281   5.1182   -1.7781 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.2349   2.0374   0.0184 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.4918   5.4122   0.0457 H   0 0 0 0 0 0 0 0 0 0 0 0
   -3.8862   4.8313   0.0655 H   0 0 0 0 0 0 0 0 0 0 0 0
   -4.5872   2.4742   0.0591 H   0 0 0 0 0 0 0 0 0 0 0 0
   -2.9046   0.6813   0.0343 H   0 0 0 0 0 0 0 0 0 0 0 0
    2.9503   2.8703   1.3476 H   0 0 0 0 0 0 0 0 0 0 0 0
    3.8122   3.9889   3.3637 H   0 0 0 0 0 0 0 0 0 0 0 0
    3.1709   6.6932   4.3234 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.3816   6.5372   3.4074 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.4688   5.4199   1.3857 H   0 0 0 0 0 0 0 0 0 0 0 0
    2.9243   2.8849   -1.3687 H   0 0 0 0 0 0 0 0 0 0 0 0
    3.7489   4.0268   -3.3874 H   0 0 0 0 0 0 0 0 0 0 0 0
    2.1737   5.5279   -5.3649 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.3175   6.5740   -3.3390 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.5050   5.4206   -1.3260 H   0 0 0 0 0 0 0 0 0 0 0 0
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  3 4 1 0 0 0 0
  4 5 1 0 0 0 0
  4 10 1 0 0 0 0
  4 17 1 0 0 0 0

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 5 24 1 0 0 0 0
 6 7 1 0 0 0 0
 6 25 1 0 0 0 0
 7 8 2 0 0 0 0
 7 26 1 0 0 0 0
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 8 27 1 0 0 0 0
 9 24 2 0 0 0 0
 9 28 1 0 0 0 0
10 11 2 0 0 0 0
10 16 1 0 0 0 0
11 12 1 0 0 0 0
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13 14 1 0 0 0 0
13 15 1 0 0 0 0
14 31 1 0 0 0 0
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16 33 1 0 0 0 0
17 18 2 0 0 0 0
17 23 1 0 0 0 0
18 19 1 0 0 0 0
18 34 1 0 0 0 0
19 20 2 0 0 0 0
19 35 1 0 0 0 0
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22 23 2 0 0 0 0
22 37 1 0 0 0 0
23 38 1 0 0 0 0
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> <CAS number>
77-09-8

> <Kuehne_logS>
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> <Klopman_logS>
-4.48

> <Huuskonen_logS>
-3.99

> <Tetko_logS>

-4.31

> <Gasteiger_logS>
-4.62

$$$$
malathion
 -ISIS-   3D

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   -0.8966   2.1199   0.2878 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.7238   0.6053   0.4184 C   0 0 0 0 0 0 0 0 0 0 0 0
   -2.0199   -0.0406   0.3126 O   0 0 0 0 0 0 0 0 0 0 0 0
   -2.1128   -1.3769   0.3988 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.1180   -2.0422   0.5646 O   0 0 0 0 0 0 0 0 0 0 0 0
   -3.4580   -2.0473   0.2890 C   0 0 0 0 0 0 0 0 0 0 0 0
   -3.2852   -3.5619   0.4196 C   0 0 0 0 0 0 0 0 0 0 0 0
   -2.6848   -3.9607   2.0843 S   0 0 0 0 0 0 0 0 0 0 0 0
   -2.3475   -6.0422   1.8652 P   0 0 0 0 0 0 0 0 0 0 0 0
   -1.6344   -6.7256   3.4454 S   0 0 0 0 0 0 0 0 0 0 0 0
   -3.7412   -6.7806   1.5418 O   0 0 0 0 0 0 0 0 0 0 0 0
   -4.4767   -6.8289   2.7660 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.3138   -6.2940   0.6568 O   0 0 0 0 0 0 0 0 0 0 0 0
   -0.2398   -5.3679   0.8323 C   0 0 0 0 0 0 0 0 0 0 0 0
   -4.6106   -4.2406   0.1877 C   0 0 0 0 0 0 0 0 0 0 0 0
   -4.7149   -5.0853   -0.6699 O   0 0 0 0 0 0 0 0 0 0 0 0
   -5.6753   -3.9066   0.9337 O   0 0 0 0 0 0 0 0 0 0 0 0
   -6.9523   -4.5605   0.7103 C   0 0 0 0 0 0 0 0 0 0 0 0
   -7.9896   -4.0007   1.6858 C   0 0 0 0 0 0 0 0 0 0 0 0
    0.0763   2.6048   0.3673 H   0 0 0 0 0 0 0 0 0 0 0 0
   -1.3407   2.3528   -0.6800 H   0 0 0 0 0 0 0 0 0 0 0 0
   -1.5486   2.4811   1.0831 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.0718   0.2441   -0.3769 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.2797   0.3724   1.3862 H   0 0 0 0 0 0 0 0 0 0 0 0
   -4.1100   -1.6861   1.0843 H   0 0 0 0 0 0 0 0 0 0 0 0
   -3.9021   -1.8144   -0.6788 H   0 0 0 0 0 0 0 0 0 0 0 0
   -2.5642   -3.9104   -0.3199 H   0 0 0 0 0 0 0 0 0 0 0 0
   -5.4333   -7.3230   2.5959 H   0 0 0 0 0 0 0 0 0 0 0 0
   -3.9074   -7.3857   3.5103 H   0 0 0 0 0 0 0 0 0 0 0 0
   -4.6506   -5.8147   3.1257 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.5370   -5.5682   0.0943 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.6114   -4.3516   0.7018 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.1744   -5.4774   1.8346 H   0 0 0 0 0 0 0 0 0 0 0 0
   -7.2800   -4.3775   -0.3131 H   0 0 0 0 0 0 0 0 0 0 0 0
   -6.8443   -5.6332   0.8709 H   0 0 0 0 0 0 0 0 0 0 0 0
   -8.9482   -4.4916   1.5180 H   0 0 0 0 0 0 0 0 0 0 0 0
   -7.6618   -4.1836   2.7091 H   0 0 0 0 0 0 0 0 0 0 0 0
   -8.0976   -2.9280   1.5251 H   0 0 0 0 0 0 0 0 0 0 0 0
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  1 21 1 0 0 0 0

 1 22 1 0 0 0 0
 2 3 1 0 0 0 0
 2 23 1 0 0 0 0
 2 24 1 0 0 0 0
 3 4 1 0 0 0 0
 4 5 2 0 0 0 0
 4 6 1 0 0 0 0
 6 7 1 0 0 0 0
 6 25 1 0 0 0 0
 6 26 1 0 0 0 0
 7 8 1 0 0 0 0
 7 15 1 0 0 0 0
 7 27 1 0 0 0 0
 8 9 1 0 0 0 0
 9 10 2 0 0 0 0
 9 11 1 0 0 0 0
 9 13 1 0 0 0 0
11 12 1 0 0 0 0
12 28 1 0 0 0 0
12 29 1 0 0 0 0
12 30 1 0 0 0 0
13 14 1 0 0 0 0
14 31 1 0 0 0 0
14 32 1 0 0 0 0
14 33 1 0 0 0 0
15 16 2 0 0 0 0
15 17 1 0 0 0 0
17 18 1 0 0 0 0
18 19 1 0 0 0 0
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19 37 1 0 0 0 0
19 38 1 0 0 0 0
M END
> <logS_expected>
-3.37

> <CAS number>
121-75-5

> <Kuehne_logS>
-3.48

> <Klopman_logS>
-2.94

> <Huuskonen_logS>
-3.24

> <Tetko_logS>

-3.73

> <Gasteiger_logS>
-2.79

$$$$
chlorpyriphos
  -ISIS-   3D

 29 29 0 0 0 0 0 0 0 0 1 V2000
    0.2396   1.4192   -0.4195 C   0 0 0 0 0 0 0 0 0 0 0 0
    0.1486   -0.0967   -0.2329 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.2246   -0.4899   -0.1908 O   0 0 0 0 0 0 0 0 0 0 0 0
   -1.2453   -2.0877   0.0062 P   0 0 0 0 0 0 0 0 0 0 0 0
   -0.0054   -2.8714   -1.1432 S   0 0 0 0 0 0 0 0 0 0 0 0
   -0.8661   -2.4455   1.5294 O   0 0 0 0 0 0 0 0 0 0 0 0
   -0.6017   -3.8493   1.5704 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.3695   -4.2825   3.0193 C   0 0 0 0 0 0 0 0 0 0 0 0
   -2.7165   -2.6504   -0.3270 O   0 0 0 0 0 0 0 0 0 0 0 0
   -2.8689   -2.5768   -1.6736 C   0 0 0 0 0 0 0 0 0 0 0 0
   -2.4280   -3.5623   -2.4371 N   0 0 0 0 0 0 0 0 0 0 0 0
   -2.5561   -3.5315   -3.7512 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.9576   -4.8548   -4.7022 Cl 0 0 0 0 0 0 0 0 0 0 0 0
   -3.1617   -2.4582   -4.3790 C   0 0 0 0 0 0 0 0 0 0 0 0
   -3.3251   -2.4301   -6.1071 Cl 0 0 0 0 0 0 0 0 0 0 0 0
   -3.6379   -1.4034   -3.6116 C   0 0 0 0 0 0 0 0 0 0 0 0
   -3.4921   -1.4690   -2.2359 C   0 0 0 0 0 0 0 0 0 0 0 0
   -4.0747   -0.1817   -1.2274 Cl 0 0 0 0 0 0 0 0 0 0 0 0
    1.2870   1.7191   -0.4516 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.2477   1.7002   -1.3532 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.2558   1.9181   0.4134 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.6440   -0.5957   -1.0658 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.6358   -0.3777   0.7007 H   0 0 0 0 0 0 0 0 0 0 0 0
   -1.4539   -4.3916   1.1611 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.2870   -4.0689   0.9786 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.1678   -5.3532   3.0505 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.4828   -3.7401   3.4286 H   0 0 0 0 0 0 0 0 0 0 0 0
   -1.2582   -4.0628   3.6110 H   0 0 0 0 0 0 0 0 0 0 0 0
   -4.1148   -0.5532   -4.0766 H   0 0 0 0 0 0 0 0 0 0 0 0
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  1 21 1 0 0 0 0
  2 3 1 0 0 0 0
  2 22 1 0 0 0 0
  2 23 1 0 0 0 0
  3 4 1 0 0 0 0
  4 5 2 0 0 0 0
  4 6 1 0 0 0 0
  4 9 1 0 0 0 0
  6 7 1 0 0 0 0

```
  7  8  1  0  0  0  0
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  7 25  1  0  0  0  0
  8 26  1  0  0  0  0
  8 27  1  0  0  0  0
  8 28  1  0  0  0  0
  9 10  1  0  0  0  0
 10 11  2  0  0  0  0
 10 17  1  0  0  0  0
 11 12  1  0  0  0  0
 12 13  1  0  0  0  0
 12 14  2  0  0  0  0
 14 15  1  0  0  0  0
 14 16  1  0  0  0  0
 16 17  2  0  0  0  0
 16 29  1  0  0  0  0
 17 18  1  0  0  0  0
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>  <logS_expected>
-5.49

>  <CAS number>
2921-88-2

>  <Kuehne_logS>
-3.75

>  <Klopman_logS>
-5.77

>  <Huuskonen_logS>
-5.61

>  <Tetko_logS>
-5.31

>  <Gasteiger_logS>
-4.79

$$$$
prostaglandin_E2
  -ISIS-            3D

 57 57  0  0  0  0  0  0  0  0  1 V2000
   -0.0187    1.5258    0.0104 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0021   -0.0041    0.0020 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4333   -0.5336    0.0129 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4126   -2.0635    0.0045 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8479   -2.5931    0.0153 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8272   -4.1229    0.0069 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2398   -4.5980    1.2199 O   0  0  0  0  0  0  0  0  0  0  0  0
```

-4.2368 -4.6438 -0.1063 C 0 0 0 0 0 0 0 0 0 0 0 0
-4.5774 -5.3960 -1.1232 C 0 0 0 0 0 0 0 0 0 0 0 0
-5.9870 -5.9169 -1.2364 C 0 0 0 0 0 0 0 0 0 0 0 0
-6.6367 -5.4461 -2.5624 C 0 0 0 0 0 0 0 0 0 0 0 0
-6.2204 -4.1187 -2.8891 O 0 0 0 0 0 0 0 0 0 0 0 0
-6.0775 -6.4662 -3.5852 C 0 0 0 0 0 0 0 0 0 0 0 0
-6.0513 -7.7834 -2.8303 C 0 0 0 0 0 0 0 0 0 0 0 0
-6.0756 -8.8881 -3.3176 O 0 0 0 0 0 0 0 0 0 0 0 0
-5.9887 -7.4553 -1.3531 C 0 0 0 0 0 0 0 0 0 0 0 0
-4.7068 -8.0273 -0.7443 C 0 0 0 0 0 0 0 0 0 0 0 0
-4.7748 -9.5327 -0.7531 C 0 0 0 0 0 0 0 0 0 0 0 0
-3.8218 -10.2281 -1.3225 C 0 0 0 0 0 0 0 0 0 0 0 0
-3.8899 -11.7336 -1.3313 C 0 0 0 0 0 0 0 0 0 0 0 0
-3.7846 -12.2405 -2.7710 C 0 0 0 0 0 0 0 0 0 0 0 0
-3.8537 -13.7689 -2.7799 C 0 0 0 0 0 0 0 0 0 0 0 0
-3.7500 -14.2682 -4.1980 C 0 0 0 0 0 0 0 0 0 0 0 0
-3.6328 -13.4822 -5.1082 O 0 0 0 0 0 0 0 0 0 0 0 0
-3.7877 -15.5861 -4.4499 O 0 0 0 0 0 0 0 0 0 0 0 0
1.0039 1.9031 0.0027 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.5459 1.8868 -0.8726 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.5289 1.8773 0.9072 H 0 0 0 0 0 0 0 0 0 0 0 0
0.5123 -0.3556 -0.8948 H 0 0 0 0 0 0 0 0 0 0 0 0
0.5293 -0.3651 0.8851 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.9435 -0.1821 0.9097 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.9605 -0.1726 -0.8702 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.9024 -2.4150 -0.8923 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.8854 -2.4246 0.8875 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.3581 -2.2415 0.9121 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.3751 -2.2320 -0.8677 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.2409 -4.4737 -0.8424 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.7875 -4.2661 1.9444 H 0 0 0 0 0 0 0 0 0 0 0 0
-4.9661 -4.3969 0.6510 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.8481 -5.6429 -1.8805 H 0 0 0 0 0 0 0 0 0 0 0 0
-6.5829 -5.5947 -0.3825 H 0 0 0 0 0 0 0 0 0 0 0 0
-7.7234 -5.5066 -2.5045 H 0 0 0 0 0 0 0 0 0 0 0 0
-6.6568 -3.8854 -3.7199 H 0 0 0 0 0 0 0 0 0 0 0 0
-6.7357 -6.5367 -4.4512 H 0 0 0 0 0 0 0 0 0 0 0 0
-5.0708 -6.1837 -3.8930 H 0 0 0 0 0 0 0 0 0 0 0 0
-6.8596 -7.8666 -0.8429 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.8484 -7.6989 -1.3303 H 0 0 0 0 0 0 0 0 0 0 0 0
-4.6029 -7.6742 0.2816 H 0 0 0 0 0 0 0 0 0 0 0 0
-5.6093 -10.0383 -0.2899 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.9874 -9.7226 -1.7857 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.0664 -12.1379 -0.7426 H 0 0 0 0 0 0 0 0 0 0 0 0
-4.8375 -12.0570 -0.9006 H 0 0 0 0 0 0 0 0 0 0 0 0
-4.6080 -11.8362 -3.3597 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.8370 -11.9171 -3.2017 H 0 0 0 0 0 0 0 0 0 0 0 0
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17 48 1 0 0 0 0
18 19 2 0 0 0 0
18 49 1 0 0 0 0
19 20 1 0 0 0 0
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21 53 1 0 0 0 0
21 54 1 0 0 0 0
22 23 1 0 0 0 0

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 22 55  1  0  0  0  0
 22 56  1  0  0  0  0
 23 24  2  0  0  0  0
 23 25  1  0  0  0  0
 25 57  1  0  0  0  0
M  END
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-2.47

>  <CAS number>
363-24-6

>  <Kuehne_logS>
NaN

>  <Klopman_logS>
-4.21

>  <Huuskonen_logS>
-3.29

>  <Tetko_logS>
-3.52

>  <Gasteiger_logS>
-3.07

$$$$
p,p´-DDT
  -ISIS-          3D

 28 29  0  0  0  0  0  0  0  0  1 V2000
    0.1230    1.7750   -0.1785 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.4853    0.5173   -0.6234 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.8192    0.2080   -0.8109 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.7920    1.1574   -0.5534 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.4289    2.4160   -0.1082 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.4678    0.7695   -0.7882 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    1.0946    2.7241    0.0789 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3320    2.1136    0.0198 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5152    2.7765    1.3607 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8158    4.1241    1.4299 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9843    4.7326    2.6594 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8523    3.9927    3.8210 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5515    2.6441    3.7511 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0633    4.7564    5.3657 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -1.3884    2.0356    2.5209 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7895    3.0660   -1.0867 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7677    2.2029   -2.6696 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -3.4638    3.6352   -0.7356 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -0.6760    4.4822   -1.1591 Cl  0  0  0  0  0  0  0  0  0  0  0  0
```

```
   -0.2742   -0.2239   -0.8240 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.1022   -0.7748   -1.1581 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.1878    3.1575    0.0933 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.8109    3.7067    0.4261 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9260    1.2004   -0.0182 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9185    4.7016    0.5231 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2188    5.7854    2.7134 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4480    2.0661    4.6576 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1580    0.9819    2.4661 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  2  0  0  0  0
  1  7  1  0  0  0  0
  1  8  1  0  0  0  0
  2  3  1  0  0  0  0
  2 20  1  0  0  0  0
  3  4  2  0  0  0  0
  3 21  1  0  0  0  0
  4  5  1  0  0  0  0
  4  6  1  0  0  0  0
  5  7  2  0  0  0  0
  5 22  1  0  0  0  0
  7 23  1  0  0  0  0
  8  9  1  0  0  0  0
  8 16  1  0  0  0  0
  8 24  1  0  0  0  0
  9 10  2  0  0  0  0
  9 15  1  0  0  0  0
 10 11  1  0  0  0  0
 10 25  1  0  0  0  0
 11 12  2  0  0  0  0
 11 26  1  0  0  0  0
 12 13  1  0  0  0  0
 12 14  1  0  0  0  0
 13 15  2  0  0  0  0
 13 27  1  0  0  0  0
 15 28  1  0  0  0  0
 16 17  1  0  0  0  0
 16 18  1  0  0  0  0
 16 19  1  0  0  0  0
M  END
> <logS_expected>
-7.15

> <CAS number>
50-29-3

> <Kuehne_logS>
-7.75

> <Klopman_logS>
-8.00
```

> <Huuskonen_logS>
-7.67

> <Tetko_logS>
-7.59

> <Gasteiger_logS>
-7.86

$$$$
chlordane
  -ISIS-   3D

 24 26 0 0 0 0 0 0 0 0 1 V2000
    0.0021   -0.0041   0.0020 Cl 0 0 0 0 0 0 0 0 0 0 0 0
   -0.0224   1.7987   0.0119 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.4177   2.3672   0.0012 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.8550   2.2745   -1.4736 C   0 0 0 0 0 0 0 0 0 0 0 0
    0.5489   2.2614   -2.3156 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.6151   2.3468   -1.3092 C   0 0 0 0 0 0 0 0 0 0 0 0
   -1.9951   1.3220   -1.8535 Cl 0 0 0 0 0 0 0 0 0 0 0 0
    0.6057   3.6092   -3.1018 C   0 0 0 0 0 0 0 0 0 0 0 0
   -0.4886   3.7472   -4.5281 Cl 0 0 0 0 0 0 0 0 0 0 0 0
    0.4470   4.6819   -2.0175 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.5476   4.7019   -1.2873 C   0 0 0 0 0 0 0 0 0 0 0 0
    1.8505   5.7473   0.0652 Cl 0 0 0 0 0 0 0 0 0 0 0 0
    2.5284   3.6284   -1.8623 C   0 0 0 0 0 0 0 0 0 0 0 0
    4.2710   3.8043   -1.4340 Cl 0 0 0 0 0 0 0 0 0 0 0 0
    2.1489   3.7091   -3.3859 C   0 0 0 0 0 0 0 0 0 0 0 0
    2.7700   2.3026   -4.3277 Cl 0 0 0 0 0 0 0 0 0 0 0 0
    2.6132   5.2840   -4.1308 Cl 0 0 0 0 0 0 0 0 0 0 0 0
   -0.9422   5.6975   -1.7889 Cl 0 0 0 0 0 0 0 0 0 0 0 0
   -0.5785   2.1714   0.8722 H   0 0 0 0 0 0 0 0 0 0 0 0
    1.4200   3.4050   0.3346 H   0 0 0 0 0 0 0 0 0 0 0 0
    2.0705   1.7625   0.6308 H   0 0 0 0 0 0 0 0 0 0 0 0
    2.4892   1.4095   -1.6679 H   0 0 0 0 0 0 0 0 0 0 0 0
    0.4762   1.3893   -2.9655 H   0 0 0 0 0 0 0 0 0 0 0 0
   -0.9344   3.3814   -1.1831 H   0 0 0 0 0 0 0 0 0 0 0 0
  1 2 1 0 0 0 0
  2 3 1 0 0 0 0
  2 6 1 0 0 0 0
  2 19 1 0 0 0 0
  3 4 1 0 0 0 0
  3 20 1 0 0 0 0
  3 21 1 0 0 0 0
  4 5 1 0 0 0 0
  4 13 1 0 0 0 0
  4 22 1 0 0 0 0
  5 6 1 0 0 0 0
  5 8 1 0 0 0 0
  5 23 1 0 0 0 0

```
  6  7  1  0  0  0  0
  6 24  1  0  0  0  0
  8  9  1  0  0  0  0
  8 15  1  0  0  0  0
  8 10  1  0  0  0  0
 10 11  2  0  0  0  0
 10 18  1  0  0  0  0
 11 12  1  0  0  0  0
 11 13  1  0  0  0  0
 13 14  1  0  0  0  0
 13 15  1  0  0  0  0
 15 16  1  0  0  0  0
 15 17  1  0  0  0  0
M  END
>  <logS_expected>
-6.86

>  <CAS number>
57-74-9

>  <Kuehne_logS>
-6.51

>  <Klopman_logS>
-7.55

>  <Huuskonen_logS>
-7.29

>  <Tetko_logS>
-7.23

>  <Gasteiger_logS>
-7.66

$$$$
```