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# Automatic log *P* estimation based on combined additive modeling methods

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## SUMMARY

A program for the automatic estimation of the logarithm of the partition coefficient between 1-octanol and water phases (log *P*) has been developed as a component of a system entitled CHEMICALC (Combined Handling of Estimation Methods Intended for Completely Automated Log *P* Calculation). Log *P* values are calculated based on additive group contributions to log *P*. Three sets of groups are defined, and their contributions have been derived from the experimental log *P* values of 1465 molecules. The system divides a structural formula of a compound of interest into the groups whose increments are provided and then calculates its log *P* value. All processing after structure input is fully automated. This system has been tested for predicting the log *P* values of 1686 compounds. The accuracy is sufficient for many practical purposes.

## INTRODUCTION

The logarithm of the partition coefficient between 1-octanol and water phases (usually expressed as log *P*) has been chosen as a parameter in QSAR studies by Hansch and Fujita, who have emphasized the importance of lipophilic properties in determining the transport properties of a drug and its interactions with receptor molecules [1]. Usually, before a new drug reaches the marketplace, a large number of candidate molecules is screened. Accurate log *P* values are necessary for reducing the actual number of molecules to be tested. Nevertheless, synthesis and experimental log *P* determinations may be costly and time consuming, especially if some compounds are as yet unknown or not readily available.

In recent years, log *P* has become a key parameter in studies of the environmental fate of organic chemicals. Log *P* also has legislative significance in many countries. For example, the Japanese government requires a manufacturer (or an importer) of a chemical substance to include a log *P*

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value in its specifications. Moreover, when selecting an optimal experimental condition to measure log $P$, one generally wants to know its rough estimate. Therefore, a reliable and convenient method for determination of log $P$ is desired.

Various methods for predicting log $P$ based on additive-constitutive characteristics have been attempted. The method of Rekker and de Kort [2] is easy and convenient for manual calculation, but provides a rough approximation for structurally complex compounds. While the method of Hansch and Leo [3] is more refined, the user is required to describe precisely a myriad of correction factors for some structural moieties. Chou and Jurs [4] computerized the approach of Hansch and Leo and elegantly developed the computer program CLOGP3 [5]. The methods of Rekker, and Hansch and Leo, however, are difficult to express systematically in computer programs and it appears that the physicochemical nature of correction factors used in such methods cannot be understood satisfactorily. Broto et al. [6] and Ghose and Crippen [7] tried to improve upon these methods by removing the correction factors; however, computerization of their approaches has yet to be completed to our knowledge. Klopman et al. [8], on the other hand, proposed a simple model for utilizing atomic charge densities and structural (atom and group) descriptors of a molecule to estimate log $P$ values. They showed that even neglect of charge densities can fit the partition coefficients of simple molecules.

From a practical viewpoint, we intended to develop an alternative method for simple and accurate calculation of log $P$ based on assumed additivity of group contribution. Full automatic calculation is performed easily and directly from a structural formula of a query compound. A program using this approach is to be incorporated in the system CHEMICALC (Combined Handling of Estimation Methods Intended for Completely Automatic Log $P$ Calculation). The present paper describes this new estimation method and the CHEMICALC system.

## METHOD

### *Estimation Method*

A log $P$ value is assumed to be calculated based on the following group-contribution model without any correction terms,

$$\log P = \sum_{i}^{N} n_i \cdot G_i \tag{1}$$

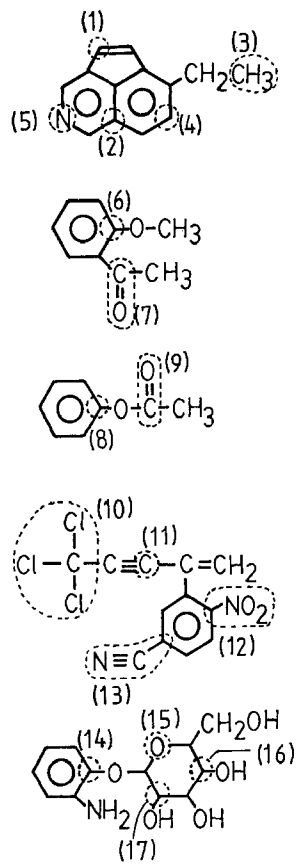
where $N$ is the total number of groups (i.e., partial structures) defined to be orthogonal, $n_i$ is the number of the $i$th group in the molecule, and $G_i$ is the group contribution to log $P$, so called increment, of the $i$th group. Clearly, the quality of this model (i.e., the precision of its predictions and their reliability) is critically dependent on the definition of a set of increments and on the values used. Any structure can be divided into groups, but their number can be considerable.

Orthogonality among groups is a factor which will lead to a single estimated value. The set of atoms is perfectly orthogonal, but it is usually not very accurate to estimate log $P$ for most molecules since few molecular properties are independent of structure. Generally, as the size of the fragments increases, more precise estimates would be available. But from a viewpoint of statistical reliability, the sheer volume of experimental data needed to determine their group values is a pro-

hibitive factor. The definition of what constitutes the best value of a group contribution is not very rigid. After considering statistical reliability of values, manageability of structural formulas, and implicit inclusion of the constitutive factors, we decided to make an essential set of a mixed level of groups to be stored in the Basic Group Table. Although the set of groups in this table constitutes a kind of closed system, there are special cases in which larger groups are arranged together according to their proper values of log *P*. Two supplementary tables are thus set up: (1) the Extended Group, which consists of larger groups with their values of contribution defined by the system, and (2) the User Defined Group, which consists of larger groups with their values of contribution defined by the user. Observed data also are very useful if available, so the system also contains an Observed Data Table.

*Definition and Notation of the Basic Group*

A Basic Group consists of a key group and its environment. A key group is taken to contain a central polyvalent atom (C, N, O, and S) and the attached atoms bonded to it. An attached atom is any atom bonded to only one other atom (e.g., H, halogens, O in CO group, N in CN group,




< Notation >

(1) CdH-(Cd)(Car)
(2) Carf-(Car)2(Carf)
(3) CH3-(C)
(4) CarH-(Car)2
(5) Nar-(Car)2
(6) Car-(Car)2(O)--(CO)
(7) CO-(Car)(C)
(8) Car-(O)(Car)2
(9) CO-(O)(C)
(10) CCl3-(Ct)
(11) Ct-(Ct)(Cd)
(12) CarNO2-(Car)2
(13) CarCN-(Car)2
(14) Car-(O)(Car)2--(N)
(15) O-(C)2--(O)
(16) CH-(O)(C)2--(O)2
(17) CH-(O)(C)2--(O)3

Fig. 1. Notation examples of the Basic Group.

etc.). Certain atomic groups, cyano, nitro, and such, are treated as univalent hetero atoms. The carbon and nitrogen atoms are categorized and the shorthand notation is used as follows:

C: single bonded ($sp^3$) carbon
Cd: double bonded (aliphatic $sp^2$) carbon
Ct: triple bonded (sp) carbon
Car: aromatic ($sp^2$) carbon
Carf: aromatic fused carbon
N: single bonded nitrogen
Nd: double bonded nitrogen
Nar: aromatic nitrogen

The group is defined by using the following notation as shown in Fig. 1. The key group is listed first, followed by the symbol, -, which indicates the group is bonded directly to the nearest neighbors. Parentheses are placed around the ligands not bonded to one another. A numerical subscript indicates how many of such ligands are attached. When hetero atoms are contained in the next-nearest neighbors (so-called $\beta$ atoms) to the key group, non-bonded interactions with other hetero atoms in that group (key group and all of its $\beta$ atoms) are taken into account. Such $\beta$ atoms are listed, followed by the symbol, --, in groups 6, 14, 15, 16, and 17 of Fig. 1.

*Outline of CHEMICALC System*

The basic system structure of CHEMICALC is shown in Fig. 2. This system requires the user to provide only a structural formula of a molecule of interest.

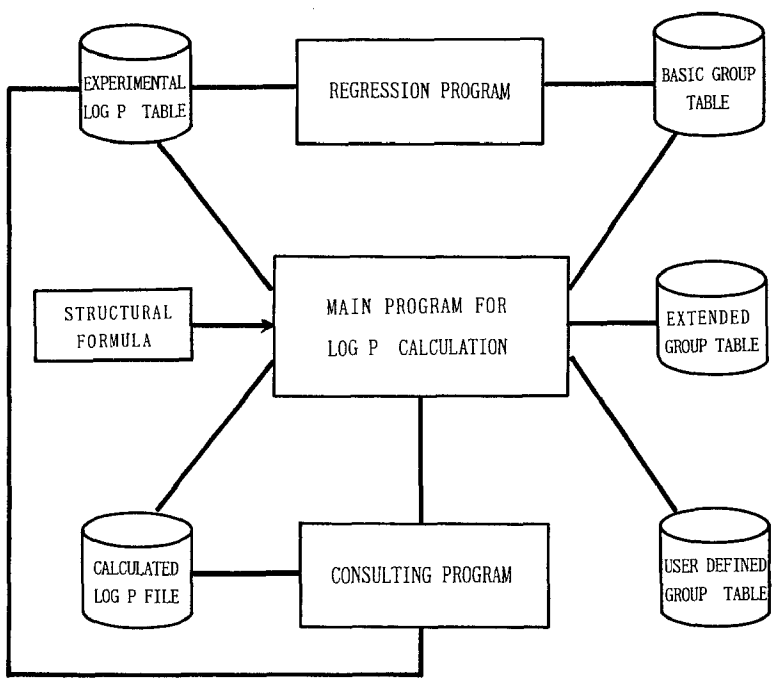



Fig. 2. Structure of CHEMICALC.

TABLE 1
COMMANDS FOR THE INTERACTIVE STRUCTURE INPUT

| Command | Function |
|---|---|
| A N1 L DX | Attachment of a chain or a ring L to atom N1. The direction parameter DX may be set for 8 main directions: U, upward; D, downward; R, rightward; L, leftward; as well as combinations RU, LU, RD and LD. |
| B N b M | Replace the bond type between atoms N and M with chemical bond b. |
| B N / M | Delete bonds between pairs of atoms N and M. |
| D N1....Nk | Delete atoms N1,...,Nk. |
| E X N1....Nk | Replace the atom type of atoms N1,...,Nk with chemical element X. |
| J N1....Nk | Formation of bonds connecting atoms N1,....,Nk. |
| H(HELP) | Display the list of commands. |
| CT | Show a connection table. |
| NEW | Abandon the structure. |
| ST | Display structural formula. |
| OK | Termination of the structure input. |

In the current personal computer version, input and output of structural formulas are based on the use of a character-type CRT. Entry of chemical structure is performed in the interactive mode using the set of commands listed in Table 1. One can initiate with a chain or a ring, add a chain or a ring, and alter atom and bond types. Figure 3 shows an aspect of input operation of a structural formula described with the limited set of characters printed by a line printer. During and/or after the generation of the structure, one can check the correctness of the structure on a display. For speedier operation or a routine procedure for simple structures, the user can use the direct mode to input a connection table.

After the structure has been entered, the structural information is stored in a connection table and is decomposed to partial structures according to the definition of the Basic Group. Then its log $P$ value is calculated by summing up $G_i$ values of constituent groups from Table 2. In this step, if a group in the query molecule contains $\beta$ hetero atoms and there is no corresponding group in the table, all $\beta$ atoms in the query molecule are omitted. Values of pure atomic fragments are used when the target group values are not available. The Extended Group and the User Defined Group that are present in the query molecule are identified automatically. In this step, the maximum substructure is preferably identified and the estimation results based on different pathways which use the Extended Group Table and/or the User Defined Group Table together with the Basic Group Table (it is applied to the remaining part of the structural formula) are available. This system also provides a consulting function to assist the user. The program has been written in Fortran 77 under the MS-DOS operating system on the NEC PC-9801 Personal Computer.

## RESULTS AND DISCUSSION

### *Increments of Basic Group Set*

The increments of the Basic Group Set were determined by using a least-squares method based on Eq. 1. Experimental log $P$ values of 1465 compounds containing carbon, hydrogen, oxygen, ni-

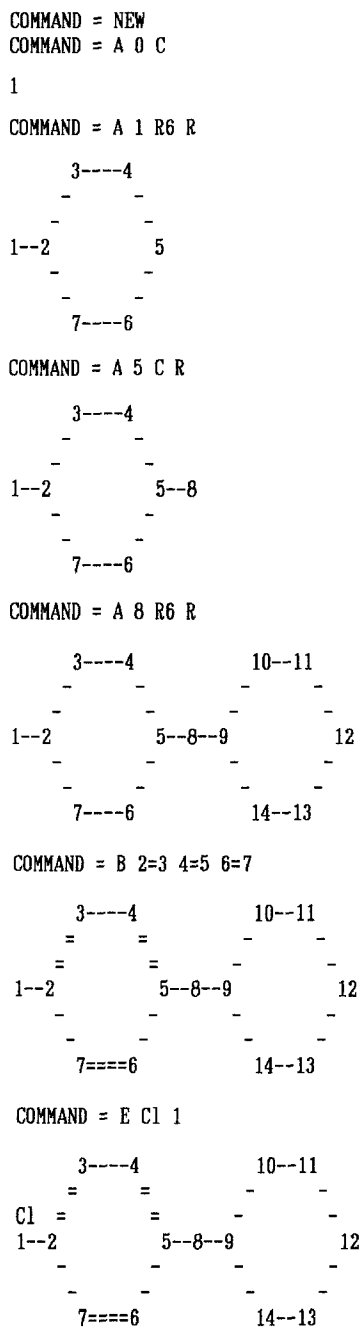



Fig. 3. An aspect in the structure input.

trogen, sulfur, and halogens were taken from the literature [3] and were used to determine 415 increments as shown in Table 2.

Some increments were assigned arbitrarily to circumvent a colinearity problem (i.e., this usually

TABLE 2
CONTRIBUTION VALUES TO LOG *P* OF THE BASIC GROUP SET*

| | Group* | Frequency of use | No. of compounds | $G_i$ | Remarks |
|---|---|---|---|---|---|
| 1 | $CH_3$-(Cal) | 536 | 341 | 0.764 | |
| 2 | $CH_3$-(Car) | 173 | 124 | 0.614 | |
| 3 | $CH_3$-(O) | 119 | 104 | 0.610 | |
| 4 | $CH_3$-(N) | 211 | 151 | 0.610 | ≡ $CH_3$-(O), assigned |
| 5 | $CH_3$-(S) | 19 | 18 | 0.610 | ≡ $CH_3$-(O), assigned |
| 6 | $CH_3$-(CO) | 119 | 115 | 0.773 | |
| 7 | $CH_3$-(CS) | 1 | 1 | 1.410 | |
| 8 | $CH_3$-(SO) | 3 | 2 | 0.773 | ≡ $CH_3$-(CO) |
| 9 | $CH_3$-($SO_2$) | 7 | 6 | 0.773 | ≡ $CH_3$-(CO) |
| 10 | $CH_2$-$(C)_2$--$(Cl)_2$ | 4 | 4 | 0.897 | |
| 11 | $CH_2$-$(C)_2$--(O)(Cl) | 1 | 1 | 0.897 | ≡ $CH_2$-$(C)_2$--$(Cl)_2$ |
| 12 | $CH_2$-$(C)_2$ | 467 | 198 | 0.536 | |
| 13 | $CH_2$-(Cd)(C) | 28 | 22 | 0.407 | |
| 14 | $CH_2$-(Ct)(C) | 2 | 2 | 0.232 | |
| 15 | $CH_2$-(Car)(C) | 78 | 73 | 0.369 | |
| 16 | $CH_2$-(C)(N′)--(N′) | 15 | 7 | 0.497 | |
| 17 | $CH_2$-(C)(N)--(S) | 2 | 1 | 0.556 | |
| 18 | $CH_2$-(C)(N)--(O) | 10 | 6 | 0.473 | |
| 19 | $CH_2$-(C)(N)--(O)(NO) | 5 | 3 | 0.820 | |
| 20 | $CH_2$-(C)(N)--(CO)(NO) | 2 | 1 | 0.979 | |
| 21 | $CH_2$-(Cal)(N′) | 117 | 81 | 0.291 | |
| 22 | $CH_2$-(C)(N′)--(N′)(NO) | 13 | 5 | 0.602 | |
| 23 | $CH_2$-(C)(O)--(N) | 10 | 6 | 0.473 | |
| 24 | $CH_2$-(C)(O)--(O) | 18 | 11 | 0.505 | |
| 25 | $CH_2$-(C)(O)--(F) | 1 | 1 | 0.370 | |
| 26 | $CH_2$-(C)(O)--(Cl) | 1 | 1 | 0.633 | |
| 27 | $CH_2$-(C)(O)--(Br) | 1 | 1 | 0.701 | |
| 28 | $CH_2$-(C)(O)--$(F)_3$ | 1 | 1 | 0.494 | |
| 29 | $CH_2$-(C)(O)--$(Cl)_3$ | 1 | 1 | 1.333 | |
| 30 | $CH_2$-(C)(O)--($NO_2$) | 1 | 1 | 1.250 | |
| 31 | $CH_2$-(C)(O) | 89 | 80 | 0.331 | |
| 32 | $CH_2$-(C)(S)--(CO) | 1 | 1 | 0.685 | |
| 33 | $CH_2$-(C)(S)--(N) | 2 | 1 | 0.657 | |
| 34 | $CH_2$-(C)(CO)--(O)(CO) | 2 | 1 | 0.797 | |
| 35 | $CH_2$-(C)(CO)--(N) | 2 | 1 | 0.493 | |
| 36 | $CH_2$-$(Cd)_2$ | 4 | 2 | 0.159 | |
| 37 | $CH_2$-(Cd)(Car) | 3 | 3 | 0.272 | |
| 38 | $CH_2$-$(Car)_2$ | 9 | 7 | 0.295 | |
| 39 | $CH_2$-(Cd)(O) | 7 | 6 | 0.414 | |
| 40 | $CH_2$-(Car)(N) | 4 | 4 | 0.257 | |
| 41 | $CH_2$-(Car)(O) | 19 | 19 | 0.213 | |
| 42 | $CH_2$-(C′)(S) | 10 | 9 | 0.392 | |
| 43 | $CH_2$-(C′)(CO) | 82 | 75 | 0.493 | |
| 44 | $CH_2$-(C′)(CS) | 2 | 2 | 0.493 | ≡ $CH_2$-(CO)(C′) |
| 45 | $CH_2$-(N′)(CO) | 6 | 6 | −0.731 | |
| 46 | $CH_2$-$(O)_2$ | 5 | 5 | 0.901 | |
| 47 | $CH_2$-(O)(CO) | 71 | 71 | 1.002 | |
| 48 | $CH_2$-(S)(CO) | 1 | 1 | 1.002 | ≡ $CH_2$-(O)(CO) |
| 49 | $CH_2$-$(CO)_2$ | 5 | 5 | 1.454 | |
| 50 | $CH_2F$-(C′) | 3 | 3 | −0.003 | |

TABLE 2 (continued)

| | Group* | Frequency of use | No. of compounds | $G_i$ | Remarks |
|---|---|---|---|---|---|
| 51 | $CH_2Cl$-(C)--(Cl) | 2 | 1 | 0.740 | |
| 52 | $CH_2Cl$-(C′) | 10 | 8 | 0.684 | |
| 53 | $CH_2Cl$-(CO) | 1 | 1 | 0.684 | ≡ $CH_2Cl$-(C′) |
| 54 | $CH_2Br$-(C′) | 7 | 7 | 0.816 | |
| 55 | $CH_2Br$-(CO) | 1 | 1 | 0.816 | ≡ $CH_2Br$-(C′) |
| 56 | $CH_2I$-(C′) | 2 | 2 | 1.112 | |
| 57 | $CH_2I$-(CO) | 1 | 1 | 1.112 | ≡ $CH_2I$-(C′) |
| 58 | $CH_2CN$-(C′) | 3 | 3 | −0.576 | |
| 59 | $CH_2NO_2$-(C′) | 7 | 7 | −0.383 | |
| 60 | $CH_2NCS$-(C′) | 3 | 3 | 0.874 | |
| 61 | CH-$(C)_3$--(O)$(Cl)_2$ | 1 | 1 | 1.528 | |
| 62 | CH-$(C')_3$ | 68 | 62 | 0.233 | |
| 63 | CH-$(C)_2$(N)--(O) | 1 | 1 | 0.070 | |
| 64 | CH-$(C)_2$(N)--(N)(NO) | 5 | 3 | 0.369 | |
| 65 | CH-$(C')_2$(N) | 20 | 18 | −0.179 | |
| 66 | CH-$(C)_2$(O)--(O) | 2 | 1 | 0.063 | |
| 67 | CH-$(C)_2$(O)--$(O)_2$ | 14 | 5 | 0.998 | |
| 68 | CH-$(C)_2$(O)--$(O)_3$ | 4 | 4 | 0.860 | |
| 69 | CH-$(C)_2$(O)--$(F)_3$ | 1 | 1 | 0.030 | |
| 70 | CH-$(C)_2$(O)--$(Cl)_2$ | 3 | 2 | 0.813 | |
| 71 | CH-$(C)_2$(O)--(Cl) | 1 | 1 | 0.462 | |
| 72 | CH-$(C)_2$(O)--$(Cl)_2$(CO) | 1 | 1 | 0.946 | |
| 73 | CH-$(C')_2$(O)--(N) | 5 | 4 | 0.267 | |
| 74 | CH-$(C')_2$(O) | 18 | 17 | −0.087 | |
| 75 | CH-$(C)_2$(S) | 1 | 1 | 0.401 | |
| 76 | CH-$(C')_2$(CO) | 7 | 7 | −0.259 | |
| 77 | CH-(C)$(O)_2$--(O) | 4 | 4 | 0.246 | |
| 78 | CH-(C)$(O)_2$--$(Cl)_3$ | 1 | 1 | 2.810 | |
| 79 | CH-(C)$(O)_2$ | 1 | 1 | 0.072 | |
| 80 | CH-(C)$(CO)_2$ | 1 | 1 | 1.623 | |
| 81 | CH-(Car)$(CO)_2$ | 1 | 1 | 1.485 | |
| 82 | CH-(C)(CO)(N) | 12 | 12 | −1.367 | |
| 83 | CH-(C′)(CO)(O) | 4 | 4 | 0.994 | |
| 84 | $CHF_2$-(C) | 1 | 1 | 0.014 | |
| 85 | $CHCl_2$-(C) | 1 | 1 | 1.026 | |
| 86 | CHCl-$(C)_2$--$(Cl)_2$ | 25 | 8 | 0.620 | |
| 87 | CHCl-$(C)_2$--(O)$(Cl)_2$ | 2 | 1 | 0.620 | ≡ CHCl-$(C)_2$--$(Cl)_2$ |
| 88 | CHCl-$(C)_2$--(O)(Cl) | 9 | 4 | 0.620 | ≡ CHCl-$(C)_2$--$(Cl)_2$ |
| 89 | CHCl-$(C)_2$--(S)$(Cl)_2$ | 2 | 1 | 0.620 | ≡ CHCl-$(C)_2$--$(Cl)_2$ |
| 90 | CHCl-$(C)_2$--(S)(Cl) | 2 | 1 | 0.620 | ≡ CHCl-$(C)_2$--$(Cl)_2$ |
| 91 | CHCl-$(C)_2$--(Cl) | 11 | 6 | 0.254 | |
| 92 | CHCl-$(C)_2$ | 1 | 1 | 0.372 | |
| 93 | CHCl-(C)(CO) | 1 | 1 | 0.372 | ≡ CHCl-$(C)_2$ |
| 94 | CHBr-(C)(CO) | 3 | 3 | 0.544 | |
| 95 | CHNCS-$(C')_2$ | 1 | 1 | 0.689 | |
| 96 | C-$(C)_3$(N) | 3 | 2 | −0.713 | |
| 97 | C-$(C)_3$(O)--$(Cl)_3$ | 1 | 1 | 0.415 | |
| 98 | C-$(C)_2$(Car)(O)--$(F)_6$ | 1 | 1 | 0.284 | |
| 99 | C-$(C')_3$(O) | 7 | 7 | −0.473 | |
| 00 | C-$(C')_2$$(CO)_2$ | 10 | 10 | 0.263 | |

TABLE 2 (continued)

| | Group* | Frequency of use | No. of compounds | $G_i$ | Remarks |
|---|---|---|---|---|---|
| 101 | C-$(C)_2$(CO)(O) | 1 | 1 | 0.491 | |
| 102 | C-(C)(Car)(CO)(N) | 1 | 1 | −0.067 | |
| 103 | C-$(C')_4$ | 18 | 13 | −0.064 | |
| 104 | C-$(C')_3$(CO) | 6 | 6 | −0.064 | ≡ C-$(C')_4$ |
| 105 | C-$(CO)_2(O)_2$ | 1 | 1 | 3.816 | |
| 106 | $CF_3$-(C)--(F)$(Cl)_2$ | 1 | 1 | 1.000 | |
| 107 | $CF_3$-(C′) | 33 | 31 | 1.203 | |
| 108 | $CF_3$-(O) | 2 | 2 | 1.770 | |
| 109 | $CF_3$-(S) | 2 | 2 | 1.438 | |
| 110 | $CF_3$-(CO) | 3 | 3 | 1.203 | |
| 111 | $CF_3$-$(SO_2)$ | 4 | 4 | 2.670 | |
| 112 | $CFCl_2$-(C)--$(F)_3$ | 1 | 1 | 1.820 | |
| 113 | $CCl_3$-(C′) | 9 | 8 | 1.374 | |
| 114 | $CCl_3$-(S) | 1 | 1 | 1.648 | |
| 115 | $CCl_3$-(CO) | 1 | 1 | 1.374 | |
| 116 | CCl-$(C)_2$(O)--$(Cl)_2$ | 1 | 1 | 1.348 | |
| 117 | CCl-$(C)_2$(S)--$(Cl)_2$ | 1 | 1 | 0.956 | |
| 118 | CBr-$(C)_2$(CO) | 1 | 1 | 0.197 | |
| 119 | $CNO_2$-$(C)_3$ | 1 | 1 | −1.282 | |
| 120 | $CdH_2$-(Cd) | 38 | 30 | 0.477 | |
| 121 | CdH-(Cd)(O) | 6 | 5 | 0.786 | |
| 122 | CdH-(Cd)(S) | 8 | 7 | 0.685 | |
| 123 | CdH-(Cd)(CO)--(CO) | 11 | 5 | 1.478 | |
| 124 | CdH-(Cd)(CO) | 33 | 28 | 0.718 | |
| 125 | CdH-(Cd)(Nd)--(Nd) | 1 | 1 | 2.634 | |
| 126 | CdH-(Cd)(Nd)--(Nd)(CO) | 1 | 1 | 2.634 | ≡ CdH-(Nd)(Cd)--(Nd) |
| 127 | CdH-(C′)(N′) | 55 | 53 | 0.641 | |
| 128 | CdH-(C′)(Cd) | 130 | 94 | 0.433 | |
| 129 | CdH-(Nd)(N′) | 12 | 11 | 2.552 | |
| 130 | CdH-(Nd)(S) | 2 | 2 | 2.111 | |
| 131 | CdH-(Nd)(CO) | 1 | 1 | 2.111 | ≡ CdH-(Nd)(S) |
| 132 | CdHBr-(Cd) | 1 | 1 | 1.093 | |
| 133 | CdHCN-(Cd) | 2 | 2 | −0.480 | |
| 134 | $CdHNO_2$-(Cd) | 16 | 16 | −0.214 | |
| 135 | Cd-(C)$(Cd)_2$ | 2 | 2 | 0.433 | |
| 136 | Cd-(C)(Cd)(Nd) | 1 | 1 | 2.286 | |
| 137 | Cd-(C)(Cd)(O) | 1 | 1 | −0.326 | |
| 138 | Cd-(C)(Cd)(CO)--(CO) | 1 | 1 | 1.210 | |
| 139 | Cd-(C)(Cd)(CO) | 3 | 3 | 0.608 | |
| 140 | Cd-(C)(N)(Nd)--$(F)_3$ | 10 | 10 | 2.443 | |
| 141 | Cd-(C)(N)(Nd) | 6 | 6 | 1.808 | |
| 142 | Cd-(C)(CO)(Nd) | 5 | 5 | 1.321 | |
| 143 | Cd-$(Cd)_2$ | 1 | 1 | 0.495 | |
| 144 | Cd-(Cd)$(C')_2$ | 23 | 17 | 0.246 | |
| 145 | Cd-$(Cd)_2$(Nd) | 3 | 3 | 2.083 | |
| 146 | Cd-(Cd)$(CO)_2$ | 1 | 1 | 1.256 | |
| 147 | Cd-(Cd)$(N)_2$ | 1 | 1 | 0.060 | |
| 148 | Cd-(Cd)(N)(Nd) | 4 | 4 | 2.504 | |
| 149 | Cd-(Cd)$(Nd)_2$ | 1 | 1 | 2.259 | |
| 150 | Cd-(Cd)(CO)(N) | 6 | 6 | 2.736 | |

TABLE 2 (continued)

| | Group* | Frequency of use | No. of compounds | $G_i$ | Remarks |
|---|---|---|---|---|---|
| 151 | Cd-(Cd)(CO)(O) | 5 | 5 | 2.367 | |
| 152 | Cd-(Cd)(CO)(S) | 1 | 1 | 1.464 | |
| 153 | Cd-(Cal)(Cd)(N) | 4 | 4 | 0.055 | |
| 154 | Cd-$(Car)_2$(Nd) | 5 | 5 | 1.497 | |
| 155 | Cd-(Car)(N)(Nd) | 1 | 1 | 2.504 | |
| 156 | Cd-$(N)_2$(Nd) | 2 | 2 | 3.295 | |
| 157 | Cd-(N)$(Nd)_2$ | 1 | 1 | 5.599 | |
| 158 | Cd-(N)(Nd)(O) | 2 | 2 | 4.204 | |
| 159 | Cd-(N)(Nd)(S) | 4 | 4 | 1.107 | |
| 160 | $CdF_2$-(Cd) | 1 | 1 | 0.763 | |
| 161 | CdF-(Cd)(CO) | 2 | 2 | 0.172 | |
| 162 | CdCl-(Cd)(CO) | 1 | 1 | 0.672 | |
| 163 | CdCl-$(Nd)_2$ | 1 | 1 | 2.942 | |
| 164 | CdBr-(Cd)(CO) | 1 | 1 | 0.812 | |
| 165 | CdI-(Cd)(CO) | 1 | 1 | 1.062 | |
| 166 | $CdNO_2$-(C)(Cd) | 2 | 2 | −0.718 | |
| 167 | CdI -$(Cd)_2$--(N)(Nd) | 1 | 1 | 1.978 | |
| 168 | $CdNO_2$-$(Cd)_2$--(N)(Nd) | 1 | 1 | 0.868 | |
| 169 | CdCN-$(Cd)_2$--(N)(Nd) | 1 | 1 | 0.518 | |
| 170 | CdCN-(Nd)(CO) | 11 | 11 | 3.548 | |
| 171 | CtH-(Ct) | 7 | 6 | 0.244 | |
| 172 | Ct-(Ct)(C′) | 9 | 7 | 0.201 | |
| 173 | CarH-$(Car')_2$ | 5012 | 1235 | 0.367 | |
| 174 | CarH-(Car)(Nar)--(Nar) | 21 | 9 | 0.560 | |
| 175 | CarH-(Car′)(Nar) | 160 | 117 | 0.367 | ≡ CarH-$(Car')_2$ |
| 176 | CarH-(Car)(NaO) | 22 | 20 | 0.367 | ≡ CarH-$(Car')_2$ |
| 177 | CarH-$(Nar)_2$ | 2 | 2 | 0.863 | |
| 178 | CarF-$(Car)_2$--(N) | 2 | 2 | 0.587 | |
| 179 | CarF-$(Car)_2$--(O) | 2 | 2 | 0.615 | ≡ CarF-$(Car)_2$--(CO) |
| 180 | CarF-$(Car)_2$--(O)(F) | 2 | 1 | 0.615 | ≡ CarF-$(Car)_2$--(CO) |
| 181 | CarF-$(Car)_2$--$(F)_2$ | 9 | 2 | 0.370 | |
| 182 | CarF-$(Car)_2$--(CO) | 4 | 3 | 0.615 | ≡ CarF-$(Car)_2$--(CO) |
| 183 | CarF-$(Car')_2$ | 28 | 25 | 0.615 | |
| 184 | CarF-(Car)(Nar) | 1 | 1 | 1.102 | |
| 185 | CarCl-$(Car)_2$--(N) | 5 | 5 | 1.420 | |
| 186 | CarCl-$(Car)_2$--(N)(Cl) | 1 | 1 | 1.650 | |
| 187 | CarCl-$(Car)_2$--(O) | 15 | 13 | 0.075 | |
| 188 | CarCl-$(Car)_2$--(O)(Cl) | 6 | 4 | 0.547 | |
| 189 | CarCl-$(Car)_2$--$(Cl)_2$ | 14 | 5 | 0.688 | |
| 190 | CarCl-$(Car)_2$--(Cl) | 24 | 13 | 0.956 | |
| 191 | CarCl-$(Car)_2$--(Br) | 1 | 1 | 0.956 | ≡ CarCl-$(Car)_2$--(Cl) |
| 192 | CarCl-$(Car)_2$--(I) | 1 | 1 | 0.939 | |
| 193 | CarCl-$(Car)_2$--$(NO_2)$ | 3 | 3 | 0.679 | |
| 194 | CarCl-$(Car)_2$--(CO) | 4 | 4 | 1.014 | ≡ CarCl-$(Car')_2$ |
| 195 | CarCl-$(Car)_2$--(CN) | 1 | 1 | 1.014 | ≡ CarCl-$(Car')_2$ |
| 196 | CarCl-$(Car)_2$--$(SO_2)$ | 1 | 1 | 1.014 | ≡ CarCl-$(Car')_2$ |
| 197 | CarCl-$(Car')_2$ | 88 | 76 | 1.014 | |
| 198 | CarCl-(Car)(Nar)--(Cl) | 3 | 2 | 1.280 | |
| 199 | CarCl-(Car)(Nar) | 6 | 6 | 1.233 | |
| 200 | CarBr-$(Car)_2$--(N) | 1 | 1 | 1.659 | |

TABLE 2 (continued)

| | Group* | Frequency of use | No. of compounds | $G_i$ | Remarks |
|---|---|---|---|---|---|
| 201 | CarBr-$(Car)_2$--(O) | 13 | 9 | 0.075 | |
| 202 | CarBr-$(Car)_2$--$(O)_2$ | 2 | 2 | −0.021 | |
| 203 | CarBr-$(Car)_2$--(Cl) | 1 | 1 | 1.218 | |
| 204 | CarBr-$(Car)_2$--(Br) | 5 | 3 | 1.086 | |
| 205 | CarBr-$(Car)_2$--$(Br)_2$ | 1 | 1 | 0.429 | |
| 206 | CarBr-$(Car)_2$--(CO) | 2 | 2 | 1.276 | |
| 207 | CarBr-$(Car')_2$ | 38 | 37 | 1.276 | |
| 208 | CarBr-(Car)(Nar) | 1 | 1 | 1.094 | |
| 209 | CarI-$(Car)_2$--(N) | 2 | 2 | 2.101 | |
| 210 | CarI-$(Car)_2$--(O) | 5 | 5 | 1.626 | |
| 211 | CarI-$(Car)_2$--(Cl) | 1 | 1 | 1.586 | |
| 212 | CarI-$(Car)_2$--(CO) | 3 | 3 | 1.626 | ≡ CarI -$(Car)_2$--(O) |
| 213 | CarI-$(Car')_2$ | 18 | 18 | 1.661 | |
| 214 | $CarIO_2$-$(Car)_2$ | 1 | 1 | −3.165 | |
| 215 | CarIO-$(Car)_2$ | 1 | 1 | −3.445 | |
| 216 | CarCN-$(Car)_2$--(O) | 3 | 3 | −0.275 | ≡ CarCN-$(Car)_2$ |
| 217 | CarCN-$(Car)_2$--(Cl) | 1 | 1 | −0.030 | |
| 218 | CarCN-$(Car')_2$ | 21 | 21 | −0.275 | |
| 219 | CarCN-(Car)(Nar) | 2 | 2 | 0.140 | |
| 220 | $CarNO_2$-$(Car)_2$--(N) | 1 | 1 | 0.899 | |
| 221 | $CarNO_2$-$(Car)_2$--(O) | 9 | 7 | 0.093 | ≡ $CarNO_2$-$(Car')_2$ |
| 222 | $CarNO_2$-$(Car)_2$--$(O)_2$ | 1 | 1 | −0.343 | |
| 223 | $CarNO_2$-$(Car)_2$--(Cl) | 3 | 3 | 0.093 | ≡ $CarNO_2$-$(Car')_2$ |
| 224 | $CarNO_2$-$(Car)_2$--(CO) | 2 | 2 | 0.093 | ≡ $CarNO_2$-$(Car')_2$ |
| 225 | $CarNO_2$-$(Car)_2$--$(NO_2)$ | 4 | 2 | 0.056 | |
| 226 | $CarNO_2$-$(Car)_2$--$(SO_2)$ | 1 | 1 | 0.093 | ≡ $CarNO_2$-$(Car')_2$ |
| 227 | $CarNO_2$-$(Car')_2$ | 98 | 87 | 0.093 | |
| 228 | $CarNO_2$-(Car)(Nar) | 1 | 1 | 0.194 | |
| 229 | CarNO-$(Car')_2$ | 3 | 3 | 0.175 | |
| 230 | CarNCS-$(Car')_2$ | 21 | 19 | 1.430 | |
| 231 | Car-(Cal)$(Car')_2$ | 484 | 389 | 0.172 | |
| 232 | Car-(Cal)(Car)(Nar) | 16 | 15 | 0.242 | |
| 233 | Car-$(Car')_3$ | 51 | 25 | 0.233 | |
| 234 | Car-$(Car)_2$(N)--(N) | 8 | 4 | 0.652 | |
| 235 | Car-$(Car)_2$(N)--(O) | 6 | 6 | 0.395 | |
| 236 | Car-$(Car)_2$(N)--(Cl) | 4 | 4 | 0.250 | |
| 237 | Car-$(Car)_2$(N)--(CO)(O) | 2 | 2 | 0.749 | |
| 238 | Car-$(Car)_2$(N)--(S) | 3 | 2 | 0.451 | |
| 239 | Car-$(Car)_2$(N)--(CO) | 8 | 8 | 1.213 | |
| 240 | Car-$(Car)_2$(N)--$(CO)_2$ | 1 | 1 | 1.213 | ≡ Car-$(Car)_2$(N)--(CO) |
| 241 | Car-$(Car)_2$(N)--$(Nd)_2$ | 2 | 2 | 0.652 | ≡ Car-$(Car)_2$(N)--(N) |
| 242 | Car-$(Car)_2$(N)--(Nd) | 13 | 13 | 0.652 | ≡ Car-$(Car)_2$(N)--(N) |
| 243 | Car-$(Car)_2$(Nd)--(Nd)(N) | 2 | 2 | 0.652 | ≡ Car-$(Car)_2$(N)--(N) |
| 244 | Car-$(Car)_2$(Nd)--(N) | 12 | 12 | 0.652 | ≡ Car-$(Car)_2$(N)--(N) |
| 245 | Car-$(Car)_2$(Nd)--(O) | 1 | 1 | 0.652 | ≡ Car-$(Car)_2$(N)--(N) |
| 246 | Car-$(Car)_2$(Nd)--(S) | 1 | 1 | 0.652 | ≡ Car-$(Car)_2$(N)--(N) |
| 247 | Car-$(Car)_2$(Nd)--(CO) | 3 | 3 | 1.213 | |
| 248 | Car-$(Car)_2$(Nd)--$(SO_2)$ | 3 | 3 | 0.842 | |
| 249 | Car-$(Car')_2$(N') | 289 | 269 | 0.250 | |
| 250 | Car-$(Car)_2$(Nar) | 4 | 3 | 0.275 | |

TABLE 2 (continued)

| | Group* | Frequency of use | No. of compounds | $G_i$ | Remarks |
|---|---|---|---|---|---|
| 251 | Car-$(Car)_2$(O)--(N) | 9 | 9 | 0.652 | ≡ Car-$(Car)_2$(N)--(N) |
| 252 | Car-$(Car)_2$(O)--(Nd) | 1 | 1 | 0.652 | ≡ Car-$(Car)_2$(N)--(N) |
| 253 | Car-$(Car)_2$(O)--(O) | 39 | 22 | 0.771 | |
| 254 | Car-$(Car)_2$(O)--$(O)_2$ | 2 | 2 | 0.317 | |
| 255 | Car-$(Car)_2$(O)--(F) | 3 | 3 | 0.729 | |
| 256 | Car-$(Car)_2$(O)--$(F)_2$ | 1 | 1 | 1.992 | |
| 257 | Car-$(Car)_2$(O)--(F)(CO) | 1 | 1 | 0.323 | |
| 258 | Car-$(Car)_2$(O)--(Cl) | 8 | 8 | 2.013 | |
| 259 | Car-$(Car)_2$(O)--$(Cl)_2$ | 5 | 5 | 2.898 | |
| 260 | Car-$(Car)_2$(O)--(Cl)(CO) | 3 | 3 | 1.114 | |
| 261 | Car-$(Car)_2$(O)--(Br) | 6 | 5 | 1.890 | |
| 262 | Car-$(Car)_2$(O)--$(Br)_2$ | 5 | 4 | 3.039 | |
| 263 | Car-$(Car)_2$(O)--(Br)(CO) | 1 | 1 | 1.303 | |
| 264 | Car-$(Car)_2$(O)--(I) | 3 | 3 | 0.658 | ≡ Car-$(Car')_2$(O) |
| 265 | Car-$(Car)_2$(O)--(I)(CO) | 2 | 2 | 0.102 | |
| 266 | Car-$(Car)_2$(O)--(CO) | 45 | 44 | 1.689 | |
| 267 | Car-$(Car)_2$(O)--$(CO)_2$ | 2 | 2 | 0.466 | |
| 268 | Car-$(Car)_2$(O)--(CO)(CN) | 2 | 2 | 0.782 | |
| 269 | Car-$(Car)_2$(O)--(CO)(O) | 5 | 5 | 0.066 | |
| 270 | Car-$(Car)_2$(O)--(CO)(S) | 2 | 2 | 0.066 | ≡ Car-$(Car)_2$(O)--(CO)(O) |
| 271 | Car-$(Car)_2$(O)--(CN) | 1 | 1 | 1.519 | |
| 272 | Car-$(Car)_2$(O)--$(NO_2)$ | 7 | 6 | 1.403 | |
| 273 | Car-$(Car)_2$(O)--$(NO_2)_2$ | 2 | 2 | 1.064 | |
| 274 | Car-$(Car')_2$(O) | 354 | 306 | 0.658 | |
| 275 | Car-$(Car)_2$(S)--(N) | 3 | 2 | 0.451 | |
| 276 | Car-$(Car)_2$(S)--(Nd) | 1 | 1 | 1.033 | |
| 277 | Car-$(Car)_2$(S)--(O) | 2 | 2 | 0.636 | |
| 278 | Car-$(Car)_2$(S)--(CO) | 2 | 1 | 1.096 | |
| 279 | Car-$(Car)_2$(S) | 17 | 16 | 0.658 | ≡ Car-$(Car')_2$(O) |
| 280 | Car-$(Car)_2$(CO)--(N) | 1 | 1 | 1.198 | |
| 281 | Car-$(Car)_2$(CO)--(Nd) | 3 | 3 | 0.869 | |
| 282 | Car-$(Car)_2$(CO)--(O) | 4 | 4 | 1.044 | ≡ Car-$(Car')_2$(CO) |
| 283 | Car-$(Car)_2$(CO)--$(O)_2$ | 36 | 36 | 1.034 | |
| 284 | Car-$(Car)_2$(CO)--$(O)_3$ | 2 | 2 | −0.085 | |
| 285 | Car-$(Car)_2$(CO)--(S) | 2 | 1 | 0.993 | |
| 286 | Car-$(Car)_2$(CO)--$(F)_2$ | 1 | 1 | 0.706 | |
| 287 | Car-$(Car)_2$(CO)--(F)(O) | 2 | 2 | 0.748 | |
| 288 | Car-$(Car)_2$(CO)--(Cl)(O) | 3 | 3 | 0.522 | |
| 289 | Car-$(Car)_2$(CO)--(Br)(O) | 2 | 2 | 0.447 | |
| 290 | Car-$(Car)_2$(CO)--(I)(O) | 3 | 3 | 0.314 | |
| 291 | Car-$(Car)_2$(CO)--(O)$(NO_2)$ | 2 | 2 | 1.115 | |
| 292 | Car-$(Car)_2$(CO)--(O)(N) | 11 | 11 | 1.198 | |
| 293 | Car-$(Car)_2$(CO)--(CO) | 20 | 10 | 0.878 | |
| 294 | Car-$(Car')_2$(CO) | 173 | 164 | 1.044 | |
| 295 | Car-$(Car)_2$(CS) | 1 | 1 | 1.044 | ≡ Car-$(Car')_2$(CO) |
| 296 | Car-$(Car)_2$$(SO_2)$--(Nd)(N) | 4 | 3 | 0.936 | |
| 297 | Car-$(Car')_2$$(SO_2)$ | 46 | 44 | 1.044 | ≡ Car-$(Car')_2$(CO) |
| 298 | Car-$(Car)_2$(SO) | 6 | 4 | 1.044 | ≡ Car-$(Car')_2$(CO) |
| 299 | Car-(Car)(N')(Nar) | 12 | 12 | 1.368 | |
| 300 | Car-(Car)(Nar)(O) | 5 | 5 | 0.435 | |

TABLE 2 (continued)

| | Group* | Frequency of use | No. of compounds | $G_i$ | Remarks |
|---|---|---|---|---|---|
| 301 | Car-(Car)(Nar)(S) | 1 | 1 | 1.919 | |
| 302 | Car-(Car)(Nar)(CO) | 4 | 4 | 1.679 | |
| 303 | Car-(N)$(Nar)_2$ | 8 | 6 | 1.773 | |
| 304 | Carf-(Carf)$(Car)_2$--$(Nar)_2$ | 1 | 1 | 0.750 | |
| 305 | Carf-$(Car')_3$ | 201 | 119 | 0.230 | |
| 306 | Carf-$(C'ar)_2$(Nar)--(Nar) | 20 | 9 | 0.567 | |
| 307 | Carf-$(Car')_2$(Nar) | 66 | 56 | 0.479 | |
| 308 | Carf-$(Car')_2$(NarO) | 20 | 20 | 0.479 | ≡ Carf-$(Car')_2$(Nar) |
| 309 | CHO-(C) | 3 | 3 | −0.906 | |
| 310 | CHO-(Cd) | 2 | 2 | −1.264 | |
| 311 | CHO-(Car) | 11 | 11 | −1.223 | |
| 312 | CHO-(O) | 3 | 3 | −0.906 | |
| 313 | CHO-(N) | 11 | 11 | −0.906 | |
| 314 | CO-$(C)_2$ | 17 | 16 | −1.747 | |
| 315 | CO-(C)(Cd) | 8 | 8 | −1.908 | ≡ CO-(C)(Car) |
| 316 | CO-(C)(Car) | 34 | 31 | −1.908 | |
| 317 | CO-(C)(Nd) | 3 | 3 | −1.682 | |
| 318 | CO-$(Cd)_2$ | 8 | 7 | −2.856 | |
| 319 | CO-(Cd)(Car) | 19 | 11 | −2.238 | |
| 320 | CO-$(Car)_2$ | 7 | 7 | −2.587 | |
| 321 | CO-(C)(N)--(Br) | 1 | 1 | −1.212 | |
| 322 | CO-(C)(N)--(Cl) | 1 | 1 | −1.090 | |
| 323 | CO-(C)(N)--(I) | 1 | 1 | −1.178 | |
| 324 | CO-(C)(N)--$(Cl)_3$ | 1 | 1 | −0.210 | |
| 325 | CO-(C)(N)--$(F)_3$ | 3 | 3 | −0.959 | |
| 326 | CO-(Cal)(N) | 121 | 103 | −1.682 | |
| 327 | CO-(Car)(N) | 59 | 57 | −2.115 | |
| 328 | CO-(C)(O)--(Br) | 2 | 2 | −0.671 | |
| 329 | CO-(C')(O) | 318 | 312 | −1.357 | |
| 330 | CO-(C')(CO) | 5 | 3 | −1.316 | |
| 331 | CO-$(N)_2$ | 56 | 55 | −0.923 | |
| 332 | CO-(N)(Nd) | 8 | 8 | −0.923 | ≡ CO-$(N)_2$ |
| 333 | CO-(N)(O) | 80 | 73 | −1.471 | |
| 334 | CO-(N)(CO) | 3 | 2 | −1.138 | |
| 335 | CS-(C')(N) | 4 | 4 | −1.725 | |
| 336 | CS-$(N)_2$ | 7 | 7 | −1.600 | |
| 337 | $NH_2$-(C') | 179 | 171 | −1.177 | |
| 338 | $NH_2$-(N) | 10 | 10 | −0.274 | |
| 339 | $NH_2$-(CO) | 69 | 67 | −0.124 | |
| 340 | $NH_2$-(CS) | 3 | 3 | 0.070 | |
| 341 | $NH_2$-$(SO_2)$ | 25 | 25 | −0.124 | |
| 342 | NH-$(Cal)_2$ | 28 | 27 | −1.401 | |
| 343 | NH-$(Car)_2$ | 11 | 11 | −0.720 | |
| 344 | NH-(Cal)(Car) | 33 | 33 | −0.945 | |
| 345 | NH-(C')(CO) | 157 | 145 | −0.060 | |
| 346 | NH-(C')(CS) | 11 | 9 | −0.060 | ≡ NH-(C')(CO) |
| 347 | NH-(C')$(SO_2)$ | 13 | 13 | −0.060 | ≡ NH-(C')(CO) |
| 348 | NH-(C')(O) | 16 | 16 | −1.560 | |
| 349 | NH-(Car)(N) | 4 | 2 | −0.615 | |
| 350 | NH-(CO)(O) | 3 | 3 | −1.090 | |

TABLE 2 (continued)

| | Group* | Frequency of use | No. of compounds | $G_i$ | Remarks |
|---|---|---|---|---|---|
| 351 | NH-$(CO)_2$ | 52 | 37 | 1.002 | |
| 352 | NH-(CO)(N) | 6 | 6 | −0.060 | ≡ NH-(C′)(CO) |
| 353 | NH-(CO)(Nd) | 3 | 3 | 0.185 | |
| 354 | NH-(Cd)(Nd) | 5 | 5 | −0.577 | |
| 355 | NH-(Car)(Nd) | 14 | 14 | −0.329 | |
| 356 | NH-(CO)(CS) | 3 | 2 | 1.703 | |
| 357 | NH-(CO)$(SO_2)$ | 2 | 2 | −0.060 | ≡ NH-(C′)(CO) |
| 358 | N-$(Cal)_3$ | 16 | 15 | −1.654 | |
| 359 | N-$(Cal)_2$(Car) | 25 | 23 | −0.935 | |
| 360 | N-(C)$(Car)_2$ | 1 | 1 | −1.820 | |
| 361 | N-$(Car)_3$ | 1 | 1 | −0.510 | |
| 362 | N-(C)(Car)(Nd) | 6 | 6 | −0.385 | |
| 363 | N-(C)$(CO)_2$ | 2 | 2 | −0.220 | |
| 364 | N-(C)$(N)_2$ | 1 | 1 | −0.575 | |
| 365 | N-(Car)$(Nd)_2$ | 2 | 2 | −0.711 | |
| 366 | N-(C)(Cd)(N′) | 3 | 3 | −1.135 | |
| 367 | N-(Cd)(CO)(N) | 4 | 4 | −1.135 | ≡ N-(C)(Cd)(N′) |
| 368 | N-(Car)(CO)(N) | 2 | 2 | −1.135 | ≡ N-(C)(Cd)(N′) |
| 369 | N-(C)(Car)(CS) | 1 | 1 | −0.307 | |
| 370 | N-$(C')_2$(CO) | 39 | 39 | −1.014 | |
| 371 | N-$(C')_2(SO_2)$ | 2 | 2 | −0.353 | |
| 372 | NdH-(Cd) | 1 | 1 | −4.265 | |
| 373 | Nd-(C)(Cd) | 4 | 4 | −1.993 | |
| 374 | Nd-$(Cd)_2$ | 9 | 9 | −2.512 | |
| 375 | Nd-(Car)(Cd) | 26 | 25 | −2.893 | |
| 376 | Nd-(C)(Nd) | 1 | 1 | −0.175 | |
| 377 | Nd-(Cd)(N) | 20 | 20 | −0.983 | |
| 378 | Nd-(Cd)(Nd) | 11 | 7 | −0.928 | |
| 379 | Nd-(Car)(Nd) | 12 | 10 | −0.928 | ≡ Nd-(Cd)(Nd) |
| 380 | Nd-(Cd)(CO) | 10 | 10 | −2.352 | |
| 381 | Nd-(Cd)(O) | 6 | 6 | −0.983 | ≡ Nd-(Cd)(N) |
| 382 | Nd-$(N')_2$ | 11 | 11 | −0.928 | ≡ Nd-(Cd)(Nd) |
| 383 | NdNO-(Cd) | 1 | 1 | −2.452 | |
| 384 | NdBr-(Cd) | 1 | 1 | −0.678 | |
| 385 | NdCl-(Cd) | 1 | 1 | −0.538 | |
| 386 | Nar-$(Car')_2$ | 180 | 152 | −1.182 | |
| 387 | Nar-(Car)(Nar) | 2 | 1 | −1.094 | |
| 388 | NarO-$(Car')_2$ | 20 | 20 | −2.923 | |
| 389 | NNO-$(C)_2$ | 31 | 27 | −1.666 | |
| 390 | NNO-(C)(CO) | 3 | 3 | 0.397 | |
| 391 | OH-(Cal) | 91 | 76 | −1.287 | |
| 392 | OH-(Car)--(Nar) | 2 | 2 | −2.546 | |
| 393 | OH-(Car) | 194 | 180 | −1.102 | |
| 394 | OH-(CO) | 214 | 206 | 0.265 | |
| 395 | OH-(N′) | 7 | 7 | 0.265 | ≡ OH-(CO) |
| 396 | O-$(C')_2$ | 237 | 212 | −1.093 | |
| 397 | O-(C′)(CO) | 166 | 165 | −0.062 | |
| 398 | O-$(CO)_2$ | 1 | 1 | −1.130 | |
| 399 | O-(CO)(N) | 15 | 15 | 0.741 | |
| 400 | O-(C)$(SO_2)$ | 2 | 1 | 0.340 | |

TABLE 2 (continued)

| | Group* | Frequency of use | No. of compounds | $G_i$ | Remarks |
|---|---|---|---|---|---|
| 401 | O-(Cd)(Nd) | 2 | 2 | −0.797 | |
| 402 | O-(C)(N) | 2 | 1 | −0.797 | ≡ O-(Cd)(Nd) |
| 403 | O-(Car)(N) | 1 | 1 | 0.266 | |
| 404 | $ONO_2$-(C) | 1 | 1 | −0.017 | |
| 405 | SH-(C′) | 4 | 4 | 0.052 | |
| 406 | S-(C′)$_2$ | 34 | 34 | −0.361 | |
| 407 | S-(C)(S) | 2 | 1 | 0.275 | |
| 408 | $SO_2$-(Car)$_2$ | 2 | 2 | −3.358 | |
| 409 | $SO_2$-(C)(Car) | 6 | 6 | −2.849 | |
| 410 | $SO_2$-(C′)(N′) | 39 | 38 | −2.240 | |
| 411 | $SO_2$-(C)(O) | 2 | 2 | −2.240 | ≡ $SO_2$-(C′)(N′) |
| 412 | $SO_2$-(N)$_2$ | 1 | 1 | −1.501 | |
| 413 | $SO_2F$-(Car) | 2 | 2 | −0.559 | |
| 414 | SO-(C′)$_2$ | 5 | 5 | −3.003 | |
| 415 | SCN-(C′) | 3 | 3 | −0.198 | |
| *Pure atomic contributions* | | | | | |
| 416 | C-(X) | | | 0.288 | |
| 417 | H-(X) | | | 0.040 | |
| 418 | N-(X) | | | −0.523 | |
| 419 | O-(X) | | | −0.327 | |
| 420 | S-(X) | | | 0.079 | |
| 421 | F-(X) | | | 0.144 | |
| 422 | Cl-(X) | | | 0.471 | |
| 423 | Br-(X) | | | 0.796 | |
| 424 | I-(X) | | | 1.285 | |

*(C) = $sp^3$ C-atom; (Cd) = aliphatic $sp^2$ C-atom; (Ct) = sp C-atom; (Cal) = C, Cd, or Ct; (Car) = aromatic $sp^2$ C-atom; (Carf) = aromatic fused C-atom; (C′) = C, Cd, Ct, or Car; Car′ = Car or Carf; (N) = single bonded N-atom; (Nd) = double bonded N-atom; (N′) = N or Nd; (Nar) = aromatic N-atom; (X) = any atoms.

happens when more than two unique groups are found in a single molecule and cannot be separated reliably because of dependency on each other) and/or to increase the statistical significance of the increments for smaller segments. Most were assigned in the same way as previously done by Benson for the prediction of chemical thermodynamic data [9] (e.g., $CH_2$-(C)(N)--(O) was analogously assigned the same value as $CH_2$-(C)(O)--(N) and 3 potential groups, $CH_3$-(C), $CH_3$-(Cd), and $CH_3$-(Ct), were all fused into one, $CH_3$-(Cal), etc.).

Since the 415 groups are insufficient for the Basic Group Table to cover all of the structures which require their log $P$ values to be estimated, 9 pure atomic fragments (Nos. 416–424 in Table 1) were added as complements. Their increments were also obtained with Eq. 1 based on a data set of 250 typical compounds which were extracted from the entire set of 1465 compounds. The set includes compounds (shown in Appendix Table A1) with diversity of structure and has a wide range of observed log $P$ values from −1.73 to 6.11 [10] (i.e., the total number of entries of the Basic Group Table is 424).

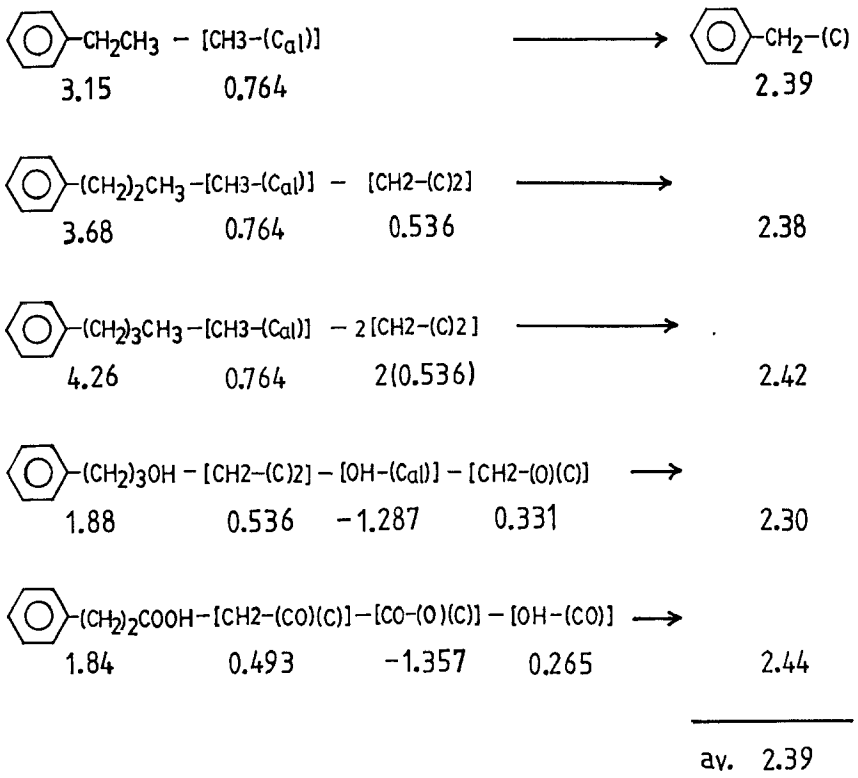



Fig. 4. Derivation of the group contribution to log $P$ for $C_6H_5CH_2$-(C).

*Increments of Extended Group Set*

The increments of the Extended Group Set are determined as follows. Initially, a molecule is divided into 2 parts, a target group (i.e., Extended Group) and the rest of the molecule. For the latter, a sum of increments is calculated by using the value of the Basic Group Set. Then the difference between the experimentally observed log $P$ and the estimated log $P$ value of the fragment is determined. To reduce the influence of potential errors as much as possible for any given molecule, the mean value based on several molecules was adopted. An example of this procedure is given in Fig. 4. Increments determined until now are shown in Table 3. 'C' in parentheses represents the neighboring carbon atom in the same manner as in Table 2. If one prefers to use a group connecting with different atoms, its increment is readily available from the value in Table 3 by using the increment in Table 2.

*Use of CHEMICALC*

This system has been tested for computing log $P$ values of 1686 molecular structures, of which 1465 were used for determining $G_i$ values. Although more than one value could be obtained for many compounds, the estimates using only the Basic Group Table are presented here.

The summary of estimation results is shown in Table 4 (the entire list of compounds used for

the calculation is shown in Appendix Tables A1 and A2). In this table, all compounds in the test set are classified into typical classes and their average absolute errors are shown. Excellent agreement of the calculated log $P$ values with experimental values was obtained for monofunctional compounds, but the average error for polyfunctional compounds was more than twice as large as that for monofunctional compounds. The error for polyfunctional compounds was most likely due to 2 factors: (i) eq. 1 and/or classification of the Basic Group was not complete; and (ii) the

TABLE 3
CONTRIBUTION VALUES TO LOG $P$ OF THE EXTENDED GROUP SET

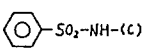
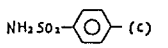
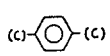
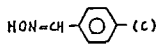
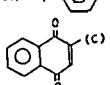
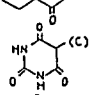
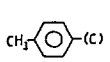
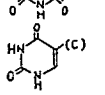
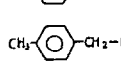
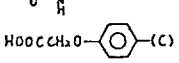
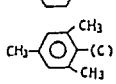
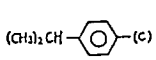
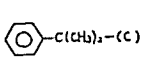
| Group | $G_i$ | Group | $G_i$ |
|---|---|---|---|
| $CH_2=CH-(C)$ | 1.03 |  | 0.16 |
| $CH_2=CHCH_2-(C)$ | 1.47 |  | 0.55 |
| $CH\equiv C-CH_2-(C)$ | 0.63 | | |
| $(CH_3)_2CH-(C)$ | 1.83 |  | 0.48 |
| $(CH_3)_3C-(C)$ | 2.40 |  | −0.60 |
| $CH_3CH_2\underset{CH_3}{CH}-(C)$ | 2.22 |  | −0.40 |
|  | 1.43 |  | 2.09 |
|  | 2.70 |  | −0.22 |
|  | 3.02 |  | −0.30 |
|  | 2.67 |  | 0.45 |
|  | 1.96 |  | 0.20 |
|  | 1.87 |  | 1.74 |
|  | 2.39 |  | 1.44 |
|  | 2.85 |  | 0.70 |
|  | 2.46 |  | −1.38 |
|  | 2.95 |  | 1.11 |
|  | 3.23 |  | 1.17 |
|  | 3.47 |  | 0.36 |
|  | 3.35 | | |

TABLE 3 (continued)

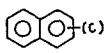
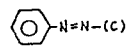
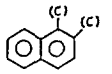
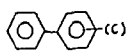
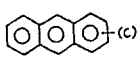
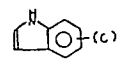
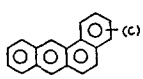
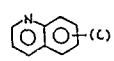
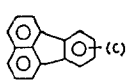
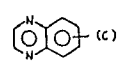
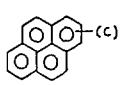
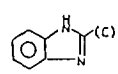
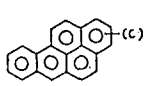
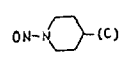
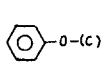
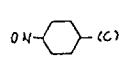
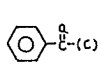
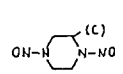
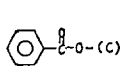
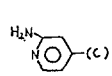
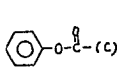
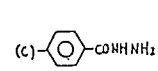
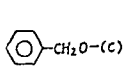
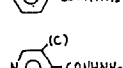
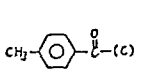
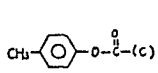
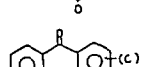
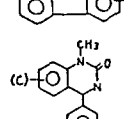
| Group | $G_i$ | Group | $G_i$ |
|---|---|---|---|
|  | 3.18 |  | 2.16 |
|  | 3.03 |  | 0.16 |
|  | 3.90 |  | −0.24 |
|  | 4.35 |  | 1.94 |
|  | 5.42 |  | 1.86 |
|  | 5.78 |  | 1.35 |
|  | 4.69 |  | 1.38 |
|  | 6.31 |  | 0.54 |
|  | 0.16 |  | 0.31 |
|  | 1.45 |  | 0.31 |
|  | 0.92 |  | −1.04 |
|  | 1.48 |  | 0.40 |
|  | 0.82 |  | −0.01 |
|  | 1.32 |  | −0.97 |
|  | 1.51 |  | 0.21 |
|  | 1.34 |  | 3.39 |
|  | 2.99 |  | 1.56 |

TABLE 4
ESTIMATION RESULTS FOR 1686 COMPOUNDS

| Compound class | No. of compounds[a] | Average absolute error[b] |
|---|---|---|
| Aliphatic hydrocarbons | 28 ( 28) | 0.20 |
| Aromatic hydrocarbons | 54 ( 53) | 0.17 |
| Nitriles (monofunctional) | 8 ( 7) | 0.31 |
| Alcohols and Phenols (monofunctional) | 52 ( 51) | 0.12 |
| Ethers (monofunctional) | 19 ( 19) | 0.18 |
| Aldehydes and ketones (monofunctional) | 25 ( 25) | 0.15 |
| Carboxylic acids and esters (monofunctional) | 42 ( 42) | 0.21 |
| Nitro compounds (monofunctional) | 20 ( 19) | 0.15 |
| Amides and Anilides (monofunctional) | 21 ( 21) | 0.19 |
| Amines and 1N-containing ring compounds | 99 ( 99) | 0.14 |
| 1S-containing compounds | 13 ( 13) | 0.06 |
| Halogenated hydrocarbons | 55 ( 40) | 0.11 |
| Other compounds | 1250 (1048) | 0.42 |
| Compounds not included in the data set | 221 ( 0) | 0.49[c] |
| All compounds | 1686 (1465) | 0.35 |

[a]: The numbers in parentheses denote number of compounds used for the determination of group values.
[b]: $\sum|\log P(\text{observed})-\log P(\text{estimated})|$/ Number of compounds.
[c]: Compounds whose observed log $P$ values are not available are excluded.

propagation of errors cannot be neglected for large or complex molecules when calculation is based on small-sized groups.

Although the set of compounds (see Table A2) not included in the basic set contained not only many structurally complex molecules, but also molecules containing more carbon atoms than the 1465 compounds used in the data set, the predicted values gave a correlation coefficient of 0.938 and an average absolute error of 0.49. The error distribution for the test set is also shown in Fig. 5. About 72% of the compounds in the test set could be calculated within a precision of 0.40 log $P$ units (equivalent to the precision of many experimental uncertainties); therefore, the usefulness of this system was confirmed.

## CONCLUSION

A computer-assisted system, CHEMICALC, for predicting log $P$ values from molecular structures has been implemented and tested. The method of calculation is based on the additive-constitutive character of log $P$, involves no correction factors (the constitutive factor is kept hidden in the group classification), and is thus convenient for computer use. Another predominant feature of this method is its combined handling of 3 sets of group contributions. Although this scheme affords more than one estimate to a query molecule, it is useful for reliably estimating log $P$ values. In fact, for structurally complex molecules, the most accurate prediction can be obtained by using larger sized groups, and, even in the calculation based on only the Basic Group Set, sufficiently ac-

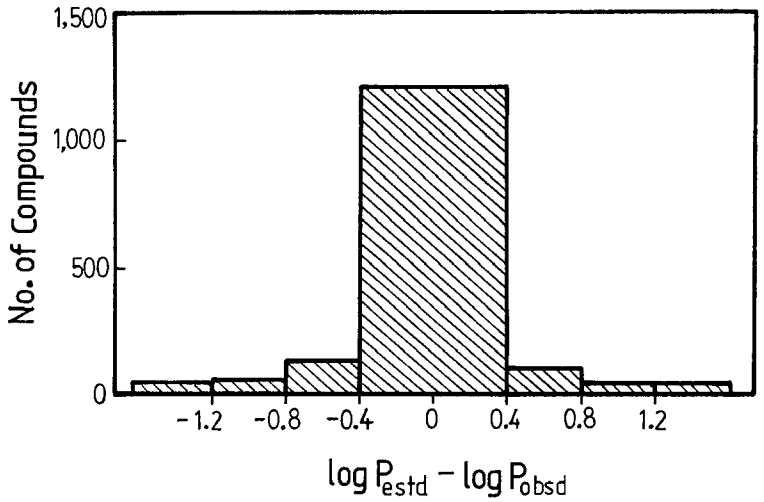



Fig. 5. Histograms of the error distribution in the prediction of log $P$ values for 1686 compounds.

curate predictions are possible. The increments of the Basic Group Set are also useful for the estimation of the distribution of lipophilicity on molecular structures.

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## APPENDIX

The list of the experimental and calculated (by using only the Basic Group Table) log $P$ values in the data set is shown in Table A1. The table is arranged in the order: aliphatic hydrocarbons, aromatic hydrocarbons, nitriles, alcohols, phenols, ethers and heterocycles with 1 O atom, aldehydes and ketones, carboxylic acids and esters, nitro compounds, amides and anilides, amines and 1 N-containing ring compounds, S-containing compounds, halogen containing compounds, and polyfunctional compounds. Compounds denoted by an asterisk are used for the determination of the contributions of the pure atomic fragments.

Table A2 shows the estimation results (based on only the Basic Group Table) for the compounds not included in the data set.

TABLE A1
EXPERIMENTAL AND CALCULATED LOG $P$ VALUES IN THE DATA SET

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | *Aliphatic Hydrocarbons* | | | |
| | 1. Ethane | $C_2H_6$ | 1.81 | 1.53 |
| * | 2. Propane | $C_3H_8$ | 2.36 | 2.06 |
| * | 3. Butane | $C_4H_{10}$ | 2.89 | 2.60 |
| * | 4. Isobutane | $C_4H_{10}$ | 2.76 | 2.53 |
| * | 5. Neopentane | $C_5H_{12}$ | 3.11 | 2.99 |
| * | 6. Pentane | $C_5H_{12}$ | 3.39 | 3.14 |
| * | 7. 2,2-Dimethylbutane | $C_6H_{14}$ | 3.82 | 3.53 |
| * | 8. 2,3-Dimethylbutane | $C_6H_{14}$ | 3.85 | 3.52 |
| * | 9. Cyclopropane | $C_3H_6$ | 1.72 | 1.60 |
| * | 10. Cyclopentane | $C_5H_{10}$ | 3.00 | 2.68 |
| * | 11. Cyclohexane | $C_6H_{12}$ | 3.44 | 3.22 |
| * | 12. Ethylene | $C_2H_4$ | 1.13 | 0.95 |
| * | 13. Acetylene | $C_2H_2$ | 0.37 | 0.49 |
| | 14. Allen | $C_3H_4$ | 1.45 | 1.45 |
| * | 15. Propyne | $C_3H_4$ | 0.94 | 1.21 |
| * | 16. Propylene | $C_3H_6$ | 1.77 | 1.67 |
| * | 17. 1,3-Butadiene | $C_4H_6$ | 1.99 | 1.82 |
| | 18. 2-Butyne | $C_4H_6$ | 1.46 | 1.93 |
| | 19. Isobutene | $C_4H_8$ | 2.40 | 2.25 |
| * | 20. *cis*-2-Butene | $C_4H_8$ | 2.31 | 2.39 |
| | 21. *trans*-2-Butene | $C_4H_8$ | 2.33 | 2.39 |
| | 22. 1,4-Pentadiene | $C_5H_8$ | 1.48 | 1.98 |
| * | 23. 1-Pentyne | $C_5H_8$ | 1.98 | 1.98 |
| | 24. 1,3-Cyclohexadiene | $C_6H_8$ | 2.47 | 2.55 |
| * | 25. 1,4-Cyclohexadiene | $C_6H_8$ | 2.30 | 2.05 |
| * | 26. 1-Butene | $C_4H_8$ | 2.40 | 2.08 |
| * | 27. Cyclohexene | $C_6H_{10}$ | 2.86 | 2.75 |
| | 28. 1,5-Hexadiene | $C_6H_{10}$ | 2.45 | 2.63 |
| | *Aromatic Hydrocarbons* | | | |
| * | 29. Benzene | $C_6H_6$ | 2.15 | 2.20 |
| | 30. Toluene | $C_7H_8$ | 2.73 | 2.62 |
| * | 31. Phenylacetylene | $C_8H_6$ | 2.53 | 2.45 |
| | 32. Styrene | $C_8H_8$ | 2.95 | 2.92 |
| * | 33. Ethylbenzene | $C_8H_{10}$ | 3.15 | 3.14 |
| * | 34. *o*-Xylene | $C_8H_{10}$ | 3.12 | 3.04 |
| | 35. *m*-Xylene | $C_8H_{10}$ | 3.20 | 3.04 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | 36. *p*-Xylene | $C_8H_{10}$ | 3.15 | 3.04 |
| * | 37. Indene | $C_9H_8$ | 2.92 | 2.95 |
| | 38. Allylbenzene | $C_9H_{10}$ | 3.23 | 3.19 |
| * | 39. Cyclopropylbenzene | $C_9H_{10}$ | 3.27 | 3.31 |
| | 40. Indane | $C_9H_{10}$ | 3.33 | 3.09 |
| | 41. 1-Phenylpropene | $C_9H_{10}$ | 3.35 | 3.49 |
| | 42. Isopropylbenzene | $C_9H_{12}$ | 3.66 | 3.77 |
| * | 43. Propylbenzene | $C_9H_{12}$ | 3.68 | 3.67 |
| | 44. 1,3,5-Trimethylbenzene | $C_9H_{12}$ | 3.42 | 3.46 |
| | 45. 1,2,4-Trimethylbenzene | $C_9H_{12}$ | 3.65 | 3.46 |
| * | 46. Naphthalene | $C_{10}H_8$ | 3.37 | 3.40 |
| | 47. *t*-Butylbenzene | $C_{10}H_{14}$ | 4.11 | 4.23 |
| * | 48. Butylbenzene | $C_{10}H_{14}$ | 4.26 | 4.21 |
| | 49. 1,2,4,5-Tetramethylbenzene | $C_{10}H_{14}$ | 4.00 | 3.88 |
| * | 50. 1-Methylnaphthalene | $C_{11}H_{10}$ | 3.87 | 3.82 |
| | 51. 2-Methylnaphthalene | $C_{11}H_{10}$ | 3.86 | 3.82 |
| | 52. Acenaphthylene | $C_{12}H_8$ | 4.03 | 3.87 |
| * | 53. Biphenyl | $C_{12}H_{10}$ | 4.09 | 4.14 |
| | 54. Acenaphthene | $C_{12}H_{10}$ | 3.92 | 3.74 |
| | 55. 1,2-Dimethylnaphthalene | $C_{12}H_{12}$ | 4.31 | 4.23 |
| * | 56. 1,3-Dimethylnaphthalene | $C_{12}H_{12}$ | 4.42 | 4.23 |
| | 57. 1,4-Dimethylnaphthalene | $C_{12}H_{12}$ | 4.37 | 4.23 |
| | 58. 1,5-Dimethylnaphthalene | $C_{12}H_{12}$ | 4.38 | 4.23 |
| | 59. 1,7-Dimethylnaphthalene | $C_{12}H_{12}$ | 4.44 | 4.23 |
| | 60. 1,8-Dimethylnaphthalene | $C_{12}H_{12}$ | 4.26 | 4.23 |
| | 61. 2,3-Dimethylnaphthalene | $C_{12}H_{12}$ | 4.40 | 4.23 |
| | 62. 2,6-Dimethylnaphthalene | $C_{12}H_{12}$ | 4.31 | 4.23 |
| | 63. Hexamethylbenzene | $C_{12}H_{18}$ | 4.31 | 4.72 |
| | 64. Fluorene | $C_{13}H_{10}$ | 4.18 | 4.04 |
| * | 65. Diphenylmethane | $C_{13}H_{12}$ | 4.14 | 4.30 |
| | 66. 2,3,6-Trimethylnaphthalene | $C_{13}H_{14}$ | 4.73 | 4.65 |
| * | 67. Anthracene | $C_{14}H_{10}$ | 4.45 | 4.60 |
| | 68. Diphenylacetylene | $C_{14}H_{10}$ | 4.78 | 4.42 |
| | 69. Phenanthrene | $C_{14}H_{12}$ | 4.60 | 4.59 |
| | 70. 9,10-Dihydroanthracene | $C_{14}H_{12}$ | 4.25 | 4.21 |
| * | 71. Stilbene | $C_{14}H_{12}$ | 4.81 | 4.88 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | 72. Bibenzyl | $C_{14}H_{14}$ | 4.79 | 4.75 |
| * | 73. Pyrene | $C_{16}H_{10}$ | 4.88 | 5.05 |
| | 74. Fluoranthene | $C_{16}H_{10}$ | 5.22 | 5.06 |
| | 75. Benz[*a*]anthracene | $C_{18}H_{12}$ | 5.61 | 5.78 |
| | 76. Chrysene | $C_{18}H_{12}$ | 5.91 | 5.78 |
| | 77. Benzo[*b*]fluoranthene | $C_{20}H_{12}$ | 6.57 | 6.02 |
| | 78. Benzo[*k*]fluoranthene | $C_{20}H_{12}$ | 6.84 | 6.26 |
| | 79. Benzo[*g,h,i*]perylene | $C_{22}H_{12}$ | 7.10 | 6.70 |
| | 80. Indeno[1,2,3-*cd*]pyrene | $C_{22}H_{12}$ | 7.66 | 6.83 |
| | 81. Dibenz[*a,h*]anthracene | $C_{22}H_{14}$ | 5.97 | 7.00 |
| | *Nitriles* | | | |
| * | 82. Acrylonitrile | $C_3H_3N$ | −0.92 | 0.00 |
| * | 83. Propionitrile | $C_3H_5N$ | 0.16 | 0.19 |
| | 84. Benzonitrile | $C_7H_5N$ | 1.56 | 1.56 |
| * | 85. Benzylcyanide | $C_8H_7N$ | 1.56 | 1.43 |
| * | 86. Cinnamonitrile | $C_9H_7N$ | 1.96 | 1.96 |
| * | 87. Benzylacetonitrile | $C_9H_9N$ | 1.70 | 1.80 |
| * | 88. 3-Cyano-1-propylbenzene | $C_{10}H_{11}N$ | 2.21 | 3.03 |
| | *Alcohols* | | | |
| | 89. Methanol | $CH_4O$ | −0.77 | −0.68 |
| * | 90. Ethanol | $C_2H_6O$ | −0.31 | −0.19 |
| | 91. Allyl alcohol | $C_3H_6O$ | 0.17 | 0.04 |
| | 92. Propanol | $C_3H_8O$ | 0.25 | 0.34 |
| | 93. Isopropanol | $C_3H_8O$ | 0.05 | 0.15 |
| * | 94. Butanol | $C_4H_{10}O$ | 0.88 | 0.88 |
| | 95. Isobutanol | $C_4H_{10}O$ | 0.76 | 0.81 |
| * | 96. *s*-Butanol | $C_4H_{10}O$ | 0.61 | 0.69 |
| | 97. *t*-Butanol | $C_4H_{10}O$ | 0.35 | 0.53 |
| * | 98. 3-Methyl-2-butanol | $C_5H_{12}O$ | 1.28 | 1.15 |
| | 99. Pentanol | $C_5H_{12}O$ | 1.56 | 1.42 |
| | 100. Isopentanol | $C_5H_{12}O$ | 1.42 | 1.34 |
| | 101. 3-Pentanol | $C_5H_{12}O$ | 1.21 | 1.23 |
| | 102. 2,2-Dimethyl-1-Propanol | $C_5H_{12}O$ | 1.36 | 1.27 |
| | 103. *t*-Amyl alcohol | $C_5H_{12}O$ | 0.89 | 1.07 |
| * | 104. Cyclohexanol | $C_6H_{12}O$ | 1.23 | 1.31 |
| | 105. 3,3-Dimethyl-2-butanol | $C_6H_{14}O$ | 1.48 | 1.61 |
| * | 106. Hexanol | $C_6H_{14}O$ | 2.03 | 1.95 |
| * | 107. Benzyl alcohol | $C_7H_8O$ | 1.10 | 0.93 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| * | 108. 2-Phenylethanol | $C_8H_{10}O$ | 1.36 | 1.42 |
| * | 109. *m*-Methylbenzyl alcohol | $C_8H_{10}O$ | 1.60 | 1.35 |
| | 110. *p*-Methylbenzyl alcohol | $C_8H_{10}O$ | 1.59 | 1.35 |
| | 111. 1-Ethylcyclohexanol | $C_8H_{12}O$ | 1.73 | 1.37 |
| * | 112. Octanol | $C_8H_{18}O$ | 3.15 | 3.02 |
| | 113. Cinnamylalcohol | $C_9H_{10}O$ | 1.95 | 2.00 |
| | 114. 3-Phenylpropanol | $C_9H_{12}O$ | 1.88 | 1.96 |
| | 115. Phenylcyclopropylcarbinol | $C_{10}H_{12}O$ | 1.95 | 1.94 |
| * | 116. 1-Dodecanol | $C_{12}H_{26}O$ | 5.13 | 5.17 |
| | 117. Diphenylcarbinol | $C_{13}H_{12}O$ | 2.67 | 2.64 |
| * | 118. Phenyl-*o*-tolylcarbinol | $C_{14}H_{14}O$ | 3.06 | 3.29 |
| | 119. Phenyl-*p*-tolylcarbinol | $C_{14}H_{14}O$ | 3.13 | 3.29 |
| | *Phenols* | | | |
| * | 120. Phenol | $C_6H_6O$ | 1.46 | 1.39 |
| | 121. Cresol | $C_7H_8O$ | 1.96 | 1.81 |
| * | 122. *o*-Methylphenol | $C_7H_8O$ | 1.95 | 1.81 |
| | 123. *p*-Methylphenol | $C_7H_8O$ | 1.94 | 1.81 |
| * | 124. 2,4-Dimethylphenol | $C_8H_{10}O$ | 2.30 | 2.23 |
| | 125. 3,5-Dimethylphenol | $C_8H_{10}O$ | 2.31 | 2.23 |
| * | 126. *m*-Ethylphenol | $C_8H_{10}O$ | 2.40 | 2.33 |
| | 127. *o*-Ethylphenol | $C_8H_{10}O$ | 2.47 | 2.33 |
| | 128. *p*-Ethylphenol | $C_8H_{10}O$ | 2.26 | 2.33 |
| | 129. *o*-Propylphenol | $C_9H_{12}O$ | 2.93 | 2.87 |
| * | 130. *o*-Isopropylphenol | $C_9H_{12}O$ | 2.88 | 2.96 |
| * | 131. 1-Naphthalenol | $C_{10}H_8O$ | 2.98 | 2.59 |
| | 132. 2-Naphthalenol | $C_{10}H_8O$ | 2.84 | 2.59 |
| * | 133. *o*-*s*-Butylphenol | $C_{10}H_{14}O$ | 3.27 | 3.49 |
| | 134. *o*-*t*-Butylphenol | $C_{10}H_{14}O$ | 3.31 | 3.42 |
| | 135. *p*-*t*-Butylphenol | $C_{10}H_{14}O$ | 3.31 | 3.42 |
| | 136. Thymol | $C_{10}H_{14}O$ | 3.30 | 3.37 |
| | 137. 2-Phenylphenol | $C_{12}H_{10}O$ | 3.09 | 3.32 |
| | 138. 3-Phenylphenol | $C_{12}H_{10}O$ | 3.23 | 3.32 |
| * | 139. 4-Phenylphenol | $C_{12}H_{10}O$ | 3.20 | 3.32 |
| | *Ethers and Heterocycles with 1 O atom* | | | |
| * | 140. Ethylene oxide | $C_2H_4O$ | −0.30 | −0.08 |
| * | 141. Dimethyl ether | $C_2H_6O$ | 0.10 | 0.13 |
| * | 142. Furan | $C_4H_4O$ | 1.34 | 1.35 |
| | 143. 2,5-Dihydrofuran | $C_4H_6O$ | 0.46 | 0.60 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| * | 144. Ethyl vinyl ether | $C_4H_8O$ | 1.04 | 1.27 |
| * | 145. Tetrahydrofuran | $C_4H_8O$ | 0.46 | 0.64 |
| * | 146. Diethyl ether | $C_4H_{10}O$ | 0.89 | 1.09 |
| * | 147. Dipropyl ether | $C_6H_{14}O$ | 2.03 | 2.17 |
| * | 148. Butyl ethyl ether | $C_6H_{14}O$ | 2.03 | 2.17 |
| * | 149. Anisole | $C_7H_8O$ | 2.08 | 2.01 |
| * | 150. Benzofurane | $C_8H_6O$ | 2.67 | 2.42 |
| | 151. Benzyl methyl ether | $C_8H_{10}O$ | 1.35 | 1.74 |
| * | 152. Phenetole | $C_8H_{10}O$ | 2.51 | 2.50 |
| | 153. Allyl phenyl ether | $C_9H_{10}O$ | 2.94 | 2.72 |
| * | 154. Phenyl propyl ether | $C_9H_{12}O$ | 3.18 | 3.03 |
| | 155. 1-Methoxy-3-phenylpropane | $C_{10}H_{14}O$ | 2.70 | 2.76 |
| | 156. Dibenzofuran | $C_{12}H_8O$ | 4.12 | 3.63 |
| | 157. Diphenyl ether | $C_{12}H_{10}O$ | 4.21 | 3.89 |
| * | 158. Benzyl phenyl ether | $C_{13}H_{12}O$ | 3.79 | 3.62 |
| | *Aldehydes and Ketons* | | | |
| | 159. Acetone | $C_3H_6O$ | −0.24 | −0.20 |
| * | 160. 2-Butanone | $C_4H_8O$ | 0.26 | 0.28 |
| | 161. 2-Pentanone | $C_5H_{10}O$ | 0.91 | 0.82 |
| * | 162. 1-Hexyn-5-one | $C_6H_8O$ | 0.58 | 0.20 |
| | 163. Cyclohexanone | $C_6H_{10}O$ | 0.81 | 0.85 |
| * | 164. 1-Hexen-5-one | $C_6H_{10}O$ | 1.02 | 0.84 |
| | 165. Hexaldehyde | $C_6H_{12}O$ | 1.78 | 1.96 |
| * | 166. 2-Hexanone | $C_6H_{12}O$ | 1.38 | 1.36 |
| | 167. Benzaldehyde | $C_7H_6O$ | 1.48 | 1.65 |
| * | 168. 4-Cyclopropyl-2-Butanone | $C_7H_{12}O$ | 1.50 | 1.36 |
| | 169. *o*-Methylbenzaldehyde | $C_8H_8O$ | 2.26 | 2.08 |
| * | 170. Phenylacetaldehyde | $C_8H_8O$ | 1.78 | 1.59 |
| | 171. Acrylophenone | $C_9H_8O$ | 1.88 | 1.84 |
| * | 172. Cinnamaldehyde | $C_9H_8O$ | 1.90 | 1.89 |
| | 173. *p*-Methylacetophenone | $C_9H_{10}O$ | 2.28 | 2.16 |
| * | 174. Acetophenone | $C_8H_8O$ | 1.68 | 1.74 |
| | 175. 1-Phenyl-2-propanone | $C_9H_{10}O$ | 1.44 | 1.53 |
| * | 176. Propiophenone | $C_9H_{10}O$ | 2.19 | 2.23 |
| | 177. Metyl styryl ketone | $C_{10}H_{10}O$ | 2.07 | 2.02 |
| | 178. 9-Fluorenone | $C_{13}H_8O$ | 3.58 | 2.90 |
| | 179. Benzalacetophenone | $C_{15}H_{12}O$ | 3.08 | 3.78 |
| | 180. 5-Phenyl-2-pentanone | $C_{11}H_{14}O$ | 2.42 | 2.43 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | 181. 5-Isopropyltropalone | $C_{10}H_{12}O$ | 1.89 | 2.07 |
| | 182. 6-Isopropyltropalone | $C_{10}H_{12}O$ | 1.82 | 2.07 |
| | 183. Benzophenone | $C_{13}H_{10}O$ | 3.18 | 3.17 |
| | *Carboxylic acids and Esters* | | | |
| | 184. Formic acid | $CH_2O_2$ | −0.54 | −0.64 |
| * | 185. Acetic acid | $C_2H_4O_2$ | −0.17 | −0.32 |
| * | 186. Methyl acetate | $C_3H_6O_2$ | 0.18 | −0.04 |
| * | 187. Propionic acid | $C_3H_6O_2$ | 0.33 | 0.17 |
| | 188. Crotonic acid | $C_4H_6O_2$ | 0.72 | 0.82 |
| | 189. Ethyl acetate | $C_4H_8O_2$ | 0.73 | 0.45 |
| * | 190. Butyric acid | $C_4H_8O_2$ | 0.79 | 0.70 |
| | 191. Propyl formate | $C_4H_8O_2$ | 0.83 | 0.66 |
| * | 192. Propionic acid ethyl ester | $C_5H_{10}O_2$ | 1.21 | 0.93 |
| | 193. Hexanoic acid | $C_6H_{12}O_2$ | 1.88 | 1.77 |
| * | 194. Benzoic acid | $C_7H_6O_2$ | 1.87 | 1.79 |
| | 195. Phenyl formate | $C_7H_6O_2$ | 1.26 | 1.53 |
| | 196. Phenyl acetate | $C_8H_8O_2$ | 1.49 | 1.85 |
| * | 197. Benzoic acid methyl ester | $C_8H_8O_2$ | 2.12 | 2.07 |
| | 198. Phenylacetic acid | $C_8H_8O_2$ | 1.41 | 1.41 |
| | 199. *m*-Toluic acid | $C_8H_8O_2$ | 2.37 | 2.21 |
| * | 200. *p*-Toluic acid | $C_8H_8O_2$ | 2.27 | 2.21 |
| | 201. Cinnamic acid | $C_9H_8O_2$ | 2.08 | 2.07 |
| | 202. Benzyl acetate | $C_9H_{10}O_2$ | 1.96 | 1.57 |
| | 203. Ethyl benzoate | $C_9H_{10}O_2$ | 2.64 | 2.56 |
| | 204. Phenylacetic acid methyl ester | $C_9H_{10}O_2$ | 1.83 | 1.69 |
| | 205. 3-Phenylpropionic acid | $C_9H_{10}O_2$ | 1.84 | 1.78 |
| * | 206. *m*-Tolyl acetate | $C_9H_{10}O_2$ | 2.09 | 2.27 |
| | 207. *o*-Tolyl acetate | $C_9H_{10}O_2$ | 2.11 | 2.27 |
| | 208. *p*-Tolyl acetate | $C_9H_{10}O_2$ | 2.11 | 2.27 |
| | 209. *p*-Methylphenylacetic acid | $C_9H_{10}O_2$ | 1.86 | 1.83 |
| * | 210. Cinnamic acid methyl ester | $C_{10}H_{10}O_2$ | 2.62 | 2.34 |
| | 211. 1-Phenylethyl acetate | $C_{10}H_{12}O_2$ | 2.30 | 2.03 |
| | 212. 2-Phenylethyl acetate | $C_{10}H_{12}O_2$ | 2.42 | 2.06 |
| | 213. 4-Phenylbutyric acid | $C_{10}H_{12}O_2$ | 2.42 | 2.31 |
| * | 214. $\beta$-Phenylpropionic acid methyl ester | $C_{10}H_{12}O_2$ | 2.32 | 2.06 |
| * | 215. Decanoic acid | $C_{10}H_{20}O_2$ | 4.09 | 3.92 |
| | 216. 1-Naphthonic acid | $C_{11}H_8O_2$ | 3.10 | 3.02 |
| | 217. Cinnamic acid ethyl ester | $C_{11}H_{12}O_2$ | 2.99 | 2.83 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| * | 218. 4-Phenylbutyric acid methyl ester | $C_{11}H_{14}O_2$ | 2.77 | 2.60 |
| | 219. 2-Isopropylphenyl acetate | $C_{11}H_{14}O_2$ | 2.78 | 3.41 |
| | 220. Naphthalene-1-acetoxy | $C_{12}H_{10}O_2$ | 2.78 | 3.04 |
| * | 221. Dodecanoic acid | $C_{12}H_{24}O_2$ | 4.20 | 4.99 |
| | 222. Phenyl benzoate | $C_{13}H_{10}O_2$ | 3.59 | 3.95 |
| | 223. Ibuprofen | $C_{13}H_{18}O_2$ | 3.51 | 3.41 |
| * | 224. Benzyl benzoate | $C_{14}H_{12}O_2$ | 3.97 | 3.68 |
| | 225. $\alpha,\alpha$-Diphenyl propionic acid | $C_{15}H_{14}O_2$ | 2.58 | 3.62 |
| | *Nitro compounds* | | | |
| * | 226. Nitroethane | $C_2H_5NO_2$ | 0.18 | 0.38 |
| * | 227. Nitropropane | $C_3H_7NO_2$ | 0.87 | 0.91 |
| * | 228. 1-Nitrobutane | $C_4H_9NO_2$ | 1.47 | 1.45 |
| * | 229. 2-Methyl-2-nitropropane | $C_4H_9NO_2$ | 1.01 | 1.01 |
| * | 230. 1-Nitropentane | $C_5H_{11}NO_2$ | 2.01 | 1.99 |
| * | 231. Nitrobenzene | $C_6H_5NO_2$ | 1.85 | 1.93 |
| * | 232. *m*-Nitrotoluene | $C_7H_7NO_2$ | 2.45 | 2.35 |
| | 233. *o*-Nitrotoluene | $C_7H_7NO_2$ | 2.30 | 2.35 |
| * | 234. *p*-Nitrotoluene | $C_7H_7NO_2$ | 2.37 | 2.35 |
| | 235. $\alpha$-Nitrotoluene | $C_7H_7NO_2$ | 1.75 | 1.62 |
| * | 236. $\beta$-Nitrostyrene | $C_8H_7NO_2$ | 2.24 | 2.23 |
| * | 237. $\beta$-Nitroethylbenzene | $C_8H_9NO_2$ | 2.08 | 1.99 |
| | 238. 1,3-Dimethyl-2-nitrobenzene | $C_8H_9NO_2$ | 2.95 | 2.77 |
| | 239. 2-Methyl-$\beta$-nitrostyrene | $C_9H_9NO_2$ | 2.63 | 2.65 |
| | 240. $\beta$-Methyl-$\beta$-nitrostyrene | $C_9H_9NO_2$ | 2.52 | 2.49 |
| | 241. 4-Methyl-$\beta$-nitrostyrene | $C_9H_9NO_2$ | 2.66 | 2.65 |
| | 242. 1-Nitronaphthalene | $C_{10}H_7NO_2$ | 3.19 | 3.12 |
| | 243. $\beta$-Ethyl-$\beta$-nitro styrene | $C_{10}H_{11}NO_2$ | 2.86 | 2.89 |
| | 244. 2-Nitro-1-butenylbenzene | $C_{10}H_{11}NO_2$ | 2.86 | 3.64 |
| | *Amides and Anilides* | | | |
| * | 245. *N,N*-Dimethylformamide | $C_3H_7NO$ | −1.01 | −0.70 |
| * | 246. *N*-Methylacetamide | $C_3H_7NO$ | −1.05 | −0.36 |
| * | 247. Butylamide | $C_4H_9NO$ | −0.21 | −0.01 |
| * | 248. Benzamide | $C_7H_7NO$ | 0.64 | 0.64 |
| * | 249. Formanilide | $C_7H_7NO$ | 1.12 | 1.12 |
| * | 250. Oxindole | $C_8H_7NO$ | 1.16 | 0.64 |
| | 251. *p*-Methylformanilide | $C_8H_9NO$ | 1.61 | 1.54 |
| | 252. Phenylacetamide | $C_8H_9NO$ | 0.45 | 0.69 |
| * | 253. Acetoanilide | $C_8H_9NO$ | 1.16 | 1.12 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| * | 254. *m*-Methylbenzamide | $C_8H_9NO$ | 1.18 | 1.06 |
| * | 255. *N*-methylformanilide | $C_8H_9NO$ | 1.09 | 0.78 |
| * | 256. Allyl-isopropylacetamide | $C_8H_{15}NO$ | 1.14 | 1.05 |
| * | 257. Propyl-isopropylacetamide | $C_8H_{17}NO$ | 1.48 | 1.57 |
| * | 258. Cinnamamide | $C_9H_9NO$ | 1.41 | 1.35 |
| | 259. *y*-Phenylpropionamide | $C_9H_{11}NO$ | 1.15 | 1.06 |
| | 260. Propionanilide | $C_9H_{11}NO$ | 1.61 | 1.60 |
| | 261. *N-N*-Dimethylbenzamide | $C_9H_{11}NO$ | 0.62 | 0.97 |
| | 262. *N*-Methylacetanilide | $C_9H_{11}NO$ | 1.07 | 0.77 |
| | 263. *p*-Isopropylbenzamide | $C_{10}H_{13}NO$ | 2.14 | 2.21 |
| | 264. 4-Phenylbutyramide | $C_{10}H_{13}NO$ | 1.41 | 1.60 |
| * | 265. Cinnamanilide | $C_{15}H_{13}NO$ | 3.61 | 3.50 |
| | *Amines and 1 N-containing ring compounds* | | | |
| | 266. Methylamine | $CH_5N$ | −0.57 | −0.57 |
| | 267. Ethylamine | $C_2H_7N$ | −0.13 | −0.12 |
| | 268. Allylamine | $C_3H_7N$ | 0.03 | 0.02 |
| | 269. Isopropylamine | $C_3H_9N$ | −0.03 | 0.17 |
| * | 270. Methylethylamine | $C_3H_9N$ | 0.15 | 0.26 |
| | 271. Propylamine | $C_3H_9N$ | 0.48 | 0.41 |
| | 272. Trimethylamine | $C_3H_9N$ | 0.16 | 0.17 |
| * | 273. Pyrrole | $C_4H_5N$ | 0.75 | 0.75 |
| * | 274. Pyrrolidine | $C_4H_9N$ | 0.46 | 0.25 |
| | 275. Butylamine | $C_4H_{11}N$ | 0.88 | 0.95 |
| | 276. Isobutylamine | $C_4H_{11}N$ | 0.88 | 0.88 |
| * | 277. *s*-Butylamine | $C_4H_{11}N$ | 0.74 | 0.71 |
| | 278. *t*-Butylamine | $C_4H_{11}N$ | 0.40 | 0.40 |
| | 279. Diethylamine | $C_4H_{11}N$ | 0.57 | 0.71 |
| | 280. Ethyl-dimethylamine | $C_4H_{11}N$ | 0.70 | 0.62 |
| * | 281. Pyridine | $C_5H_5N$ | 0.64 | 0.65 |
| * | 282. Piperidine | $C_5H_{11}N$ | 0.85 | 0.79 |
| | 283. Amylamine | $C_5H_{13}N$ | 1.45 | 1.49 |
| | 284. Methylbutylamine | $C_5H_{13}N$ | 1.33 | 1.34 |
| * | 285. Aniline | $C_6H_7N$ | 0.90 | 0.91 |
| | 286. 2-Methylpyridine | $C_6H_7N$ | 1.11 | 1.14 |
| * | 287. 3-Methylpyridine | $C_6H_7N$ | 1.20 | 1.07 |
| | 288. 4-Methylpyridine | $C_6H_7N$ | 1.22 | 1.07 |
| | 289. 2,5-Dimethylpyridine | $C_6H_8N$ | 0.63 | 1.56 |
| | 290. 4,6-Dimethylpyridine | $C_6H_8N$ | 0.62 | 1.56 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | 291. Diallylamine | $C_6H_{11}N$ | 1.11 | 1.00 |
| * | 292. Allylpropylamine | $C_6H_{13}N$ | 1.33 | 1.39 |
| | 293. Cyclohexylamine | $C_6H_{13}N$ | 1.49 | 1.32 |
| | 294. Dimethylbutylamine | $C_6H_{15}N$ | 1.70 | 1.69 |
| | 295. Dipropylamine | $C_6H_{15}N$ | 1.73 | 1.78 |
| * | 296. Hexylamine | $C_6H_{15}N$ | 2.06 | 2.02 |
| | 297. Triethylamine | $C_6H_{15}N$ | 1.44 | 1.51 |
| | 298. *N*-Methylaniline | $C_7H_9N$ | 1.82 | 1.75 |
| | 299. Benzylamine | $C_7H_9N$ | 1.09 | 1.09 |
| * | 300. 2-Ethylpyridine | $C_7H_9N$ | 1.69 | 1.66 |
| | 301. 2,6-Lutidine | $C_7H_9N$ | 1.68 | 1.63 |
| | 302. *m*-Toluidine | $C_7H_9N$ | 1.40 | 1.33 |
| | 303. *o*-Toluidine | $C_7H_9N$ | 1.29 | 1.33 |
| * | 304. *p*-Toluidine | $C_7H_9N$ | 1.39 | 1.33 |
| | 305. Quinuclidine | $C_7H_{13}N$ | 1.20 | 1.06 |
| | 306. Heptylamine | $C_7H_{17}N$ | 2.57 | 2.56 |
| | 307. Propyl-isobutylamine | $C_7H_{17}N$ | 2.07 | 2.24 |
| * | 308. Propyl-*s*-butylamine | $C_7H_{17}N$ | 1.91 | 2.08 |
| | 309. Propylbutylamine | $C_7H_{17}N$ | 2.12 | 2.32 |
| | 310. Indole | $C_8H_7N$ | 2.00 | 2.02 |
| * | 311. *N*-Ethylaniline | $C_8H_{11}N$ | 2.16 | 2.20 |
| | 312. *N,N*-Dimethylaniline | $C_8H_{11}N$ | 2.31 | 2.37 |
| | 313. 2-Phenylethylamine | $C_8H_{11}N$ | 1.41 | 1.49 |
| | 314. 2-Ethylaniline | $C_8H_{11}N$ | 1.74 | 1.85 |
| | 315. *N*-Methylbenzylamine | $C_8H_{11}N$ | 1.52 | 1.47 |
| * | 316. 4-Propylpyridine | $C_8H_{11}N$ | 2.10 | 2.13 |
| | 317. *N*-Methyl-*o*-toluidine | $C_8H_{11}N$ | 2.16 | 2.17 |
| | 318. *N*-Methyl-*p*-toluidine | $C_8H_{11}N$ | 2.15 | 2.17 |
| * | 319. Dibutylamine | $C_8H_{19}N$ | 2.68 | 2.85 |
| | 320. Ethyl-diisopropylamine | $C_8H_{19}N$ | 2.68 | 2.58 |
| | 321. 2-Ethylhexylamine | $C_8H_{19}N$ | 2.82 | 3.02 |
| | 322. Quinoline | $C_9H_7N$ | 2.03 | 2.10 |
| | 323. Isoquinoline | $C_9H_7N$ | 2.09 | 1.85 |
| | 324. 2-Methylindole | $C_9H_9N$ | 2.53 | 2.20 |
| | 325. 3-Methylindole | $C_9H_9N$ | 2.60 | 2.60 |
| | 326. 5-Methylindole | $C_9H_9N$ | 2.68 | 2.44 |
| * | 327. 1,2,3,4-Tetrahydroquinoline | $C_9H_{11}N$ | 2.29 | 2.14 |
| | 328. Amphetamine | $C_9H_{13}N$ | 1.76 | 1.78 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| * | 329. *p*-Butylpyridine | $C_9H_{13}N$ | 3.13 | 2.66 |
| * | 330. *N,N*-Dimethylbenzylamine | $C_9H_{13}N$ | 1.79 | 1.83 |
| | 331. 3-Phenyl-propylamine | $C_9H_{13}N$ | 1.83 | 2.03 |
| * | 332. *N*-Propylaniline | $C_9H_{13}N$ | 2.45 | 2.73 |
| | 333. *N,N*-Dimethyl-*m*-toluidine | $C_9H_{13}N$ | 2.80 | 2.79 |
| | 334. *N,N*-Dimethyl-*o*-toluidine | $C_9H_{13}N$ | 2.85 | 2.79 |
| | 335. *N,N*-Dimethyl-*p*-toluidine | $C_9H_{13}N$ | 2.61 | 2.79 |
| * | 336. Tripropylamine | $C_9H_{21}N$ | 2.79 | 3.12 |
| | 337. 2-Methylquinoline | $C_{10}H_9N$ | 2.59 | 2.59 |
| | 338. 6-Methylquinoline | $C_{10}H_9N$ | 2.57 | 2.52 |
| | 339. 7-Methylquinoline | $C_{10}H_9N$ | 2.47 | 2.52 |
| | 340. 8-Methylquinoline | $C_{10}H_9N$ | 2.60 | 2.52 |
| | 341. 1-Naphtylamine | $C_{10}H_9N$ | 2.25 | 2.10 |
| | 342. 2-Naphtylamine | $C_{10}H_9N$ | 2.28 | 2.10 |
| | 343. *N*-Phenylpyrrole | $C_{10}H_9N$ | 3.08 | 3.30 |
| | 344. 1,2-Dimethylindole | $C_{10}H_{11}N$ | 2.82 | 2.82 |
| * | 345. *N*-Butylaniline | $C_{10}H_{15}N$ | 3.58 | 3.27 |
| | 346. *N,N*-Diethylaniline | $C_{10}H_{15}N$ | 3.31 | 3.26 |
| * | 347. 2-Phenylpyridine | $C_{11}H_9N$ | 2.63 | 2.63 |
| | 348. 4-Phenylpyridine | $C_{11}H_9N$ | 2.62 | 2.59 |
| | 349. *N*-Phenylpiperidine | $C_{11}H_{15}N$ | 2.78 | 3.34 |
| | 350. *p*-Hexylpyridine | $C_{11}H_{17}N$ | 4.35 | 3.74 |
| | 351. γ-Phenylpropyldimethylamine | $C_{11}H_{17}N$ | 2.73 | 2.86 |
| | 352. Carbazole | $C_{12}H_9N$ | 3.29 | 3.18 |
| | 353. *p*-Heptylpyridine | $C_{12}H_{19}N$ | 5.00 | 4.27 |
| | 354. 2-Aminobiphenyl | $C_{12}H_{11}N$ | 2.84 | 2.84 |
| | 355. Diphenylamine | $C_{12}H_{11}N$ | 3.34 | 3.45 |
| | 356. Acridine | $C_{13}H_9N$ | 3.40 | 3.54 |
| * | 357. *N*-Benzylaniline | $C_{13}H_{13}N$ | 3.13 | 3.40 |
| | 358. Diphenylmethylamine | $C_{13}H_{13}N$ | 3.16 | 2.96 |
| * | 359. *p*-Octylpyridine | $C_{13}H_{21}N$ | 5.42 | 4.81 |
| * | 360. *N*-Methyl-*N*-Benzylaniline | $C_{14}H_{15}N$ | 4.22 | 4.02 |
| * | 361. *p*-Nonylpyridine | $C_{14}H_{23}N$ | 6.11 | 5.34 |
| | 362. 2-Phenylquinoline | $C_{15}H_{11}N$ | 3.90 | 4.07 |
| * | 363. 2,6-Diphenylpyridine | $C_{17}H_{13}N$ | 4.82 | 4.61 |
| | 364. Triphenylamine | $C_{18}H_{15}N$ | 5.74 | 5.75 |
| | *S-containing compounds* | | | |
| * | 365. Thiophene | $C_4H_4S$ | 1.81 | 1.88 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| * | 366. Diethyl sulfide | $C_4H_{10}S$ | 1.95 | 1.95 |
| * | 367. 1-Butanethiol | $C_4H_{10}S$ | 2.28 | 2.28 |
| * | 368. Thiophenol | $C_6H_6S$ | 2.52 | 2.55 |
| * | 369. Methylthiobenzene | $C_7H_8S$ | 2.74 | 2.74 |
| * | 370. Benzothiophene | $C_8H_6S$ | 3.12 | 3.06 |
| * | 371. Phenylethyl sulfide | $C_8H_{10}S$ | 3.20 | 3.28 |
| * | 372. 2-Phenylthiophene | $C_{10}H_8S$ | 3.74 | 3.49 |
| * | 373. Diphenyl sulfide | $C_{12}H_{10}S$ | 4.45 | 4.45 |
| | 374. Dimethyl sulfoxide | $C_2H_6OS$ | −1.35 | −1.35 |
| | 375. Methylphenyl sulfoxide | $C_7H_8OS$ | 0.55 | 0.55 |
| | 376. Methylphenyl sulfone | $C_7H_8O_2S$ | 0.47 | 0.47 |
| | 377. Diphenyl sulfone | $C_{12}H_{10}O_2S$ | 2.40 | 2.40 |
| | *Halogen containing compounds* | | | |
| | 378. 1,2-Dichlorotetrafluoroethane | $C_2Cl_2F_4$ | 2.82 | 2.82 |
| * | 379. 1,1-Difluoroethylene | $C_2H_2F_2$ | 1.24 | 1.24 |
| | 380. 1,1,1-Trichloroethane | $C_2H_3Cl_3$ | 2.49 | 2.14 |
| * | 381. Vinylbromide | $C_2H_3Br$ | 1.57 | 1.57 |
| | 382. 1,1-Dichloroethane | $C_2H_4Cl_2$ | 1.79 | 1.79 |
| * | 383. 1,2-Dichloroethane | $C_2H_4Cl_2$ | 1.48 | 1.48 |
| * | 384. 1,1-Difluoroethane | $C_2H_4F_2$ | 0.75 | 0.84 |
| * | 385. Ethylbromide | $C_2H_5Br$ | 1.61 | 1.58 |
| * | 386. Ethylchloride | $C_2H_5Cl$ | 1.43 | 1.45 |
| * | 387. Ethyliodide | $C_2H_5I$ | 2.00 | 1.88 |
| * | 388. Chloropropane | $C_3H_7Cl$ | 2.04 | 1.98 |
| * | 389. 2-Chloropropane | $C_3H_7Cl$ | 1.90 | 1.90 |
| * | 390. 1-Bromopropane | $C_3H_7Br$ | 2.10 | 2.12 |
| * | 391. 1-Chlorobutane | $C_4H_9Cl$ | 2.64 | 2.52 |
| * | 392. 1-Fluoropentane | $C_5H_{11}F$ | 2.33 | 2.37 |
| * | 393. Hexachlorobenzene | $C_6Cl_6$ | 4.13 | 4.13 |
| | 394. *m*-Dibromobenzene | $C_6H_4Br_2$ | 3.75 | 4.02 |
| * | 395. *o*-Dibromobenzene | $C_6H_4Br_2$ | 3.64 | 3.64 |
| | 396. *o*-Dichlorobenzene | $C_6H_4Cl_2$ | 3.38 | 3.38 |
| | 397. *m*-Dichlorobenzene | $C_6H_4Cl_2$ | 3.38 | 3.50 |
| * | 398. *p*-Dichlorobenzene | $C_6H_4Cl_2$ | 3.38 | 3.50 |
| * | 399. Bromobenzene | $C_6H_5Br$ | 2.99 | 3.11 |
| * | 400. Chlorobenzene | $C_6H_5Cl$ | 2.84 | 2.85 |
| * | 401. Fluorobenzene | $C_6H_5F$ | 2.27 | 2.45 |
| * | 402. Iodobenzene | $C_6H_5I$ | 3.25 | 3.50 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | 403. Hexafluorobenzene | $C_6F_6$ | 2.22 | 2.22 |
| * | 404. Hexachlorocyclohexane | $C_6H_6Cl_6$ | 3.72 | 3.72 |
| * | 405. Tetrachlorocyclohexane | $C_6H_8Cl_4$ | 2.82 | 2.82 |
| * | 406. $\alpha,\alpha,\alpha$-Trichlorotoluene | $C_7H_5Cl_3$ | 2.92 | 3.38 |
| * | 407. $\alpha$-Bromotoluene | $C_7H_7Br$ | 2.92 | 2.82 |
| * | 408. *m*-Chlorotoluene | $C_7H_7Cl$ | 3.28 | 3.27 |
| * | 409. *p*-Chlorotoluene | $C_7H_7Cl$ | 3.33 | 3.27 |
| * | 410. 1-Methylpentachlorocyclohexane | $C_7H_9Cl_5$ | 4.04 | 4.05 |
| * | 411. $\beta$-Phenylethylbromide | $C_8H_9Br$ | 3.09 | 3.19 |
| * | 412. $\beta$-Phenylethylchloride | $C_8H_9Cl$ | 2.95 | 3.06 |
| | 413. $\gamma$-Phenylpropylbromide | $C_9H_{11}Br$ | 3.72 | 3.73 |
| | 414. $\gamma$-Phenylpropylchloride | $C_9H_{11}Cl$ | 3.55 | 3.60 |
| * | 415. $\gamma$-Phenylpropylfluoride | $C_9H_{11}F$ | 2.95 | 2.91 |
| * | 416. $\gamma$-Phenylpropyliodide | $C_9H_{11}I$ | 3.90 | 4.02 |
| | 417. $\alpha$-(2,2,2-Trichloroethyl)styrene | $C_{10}H_9Cl_3$ | 4.56 | 4.51 |
| | *Polyfunctional compounds* | | | |
| | 418. Trichloroacetamide | $C_2H_2Cl_3NO$ | 1.04 | 1.04 |
| | 419. Trifluoroacetamide | $C_2H_2F_3NO$ | 0.12 | 0.12 |
| | 420. Bromoacetic acid | $C_2H_3BrO_2$ | 0.41 | 0.41 |
| | 421. 2,2,2-Trichloroethanol | $C_2H_3Cl_3O$ | 1.42 | 1.42 |
| | 422. 2,2,2-Trichloroethandiol | $C_2H_3Cl_3O_2$ | 1.61 | 1.61 |
| | 423. 2,2,2-Trifluoroethanol | $C_2H_3F_3O$ | 0.41 | 0.41 |
| | 424. Bromoacetamide | $C_2H_4BrNO$ | −0.52 | −0.52 |
| * | 425. Chloroacetamide | $C_2H_4ClNO$ | −0.53 | −0.53 |
| | 426. Iodoacetamide | $C_2H_4INO$ | −0.19 | −0.19 |
| | 427. Mercaptoacetic acid | $C_2H_4O_2S$ | 0.09 | −0.04 |
| | 428. Hydroxyacetic acid | $C_2H_4O_3$ | −1.11 | −1.38 |
| | 429. 2-Bromoethanol | $C_2H_5BrO$ | 0.23 | 0.23 |
| * | 430. 2-Chloroethanol | $C_2H_5ClO$ | 0.03 | 0.03 |
| | 431. 2-Fluoroethanol | $C_2H_5FO$ | −0.92 | −0.92 |
| | 432. Acetaldoxime | $C_2H_5NO$ | −0.12 | 0.69 |
| | 433. Aminoacetic acid | $C_2H_5NO_2$ | −3.00 | −3.00 |
| | 434. 2-Nitroethanol | $C_2H_5NO_3$ | −0.42 | −0.42 |
| | 435. Dimethyldisulfide | $C_2H_6S_2$ | 1.77 | 1.77 |
| | 436. *N*-Nitrosodimethylamine | $C_2H_6N_2O$ | −0.57 | −0.45 |
| * | 437. Ethanolamine | $C_2H_7NO$ | −1.30 | −1.52 |
| | 438. $\alpha$-Bromopropionic acid | $C_3H_5BrO_2$ | 0.92 | 0.90 |
| | 439. 4-Iodopyrazole | $C_3H_3IN_2$ | 1.70 | 1.70 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| * | 440. Isoxazole | $C_3H_3NO$ | 0.08 | 0.08 |
| * | 441. Thiazole | $C_3H_3NS$ | 0.44 | 0.56 |
| | 442. 6-Azauracil | $C_3H_3N_3O_2$ | −0.29 | −0.29 |
| | 443. 4-Nitropyrazole | $C_3H_3N_3O_2$ | 0.59 | 0.59 |
| | 444. Imidazole | $C_3H_4N_2$ | −0.08 | −0.08 |
| * | 445. Pyrazole | $C_3H_4N_2$ | 0.13 | 0.16 |
| | 446. Hydantoin | $C_3H_4N_2O_2$ | −1.69 | −2.39 |
| | 447. 1,1,1-Trifluoro-2-propanol | $C_3H_5F_3O$ | 0.71 | 0.71 |
| * | 448. Ethylisothiocyanate | $C_3H_5NS$ | 1.47 | 1.64 |
| | 449. 1,3-Dichloropropane | $C_3H_6Cl_2$ | 2.00 | 2.27 |
| | 450. 2-Thioimidazolidone | $C_3H_6N_2S$ | −0.66 | −0.73 |
| * | 451. 3-Mercatpropionic acid | $C_3H_6O_2S$ | 0.43 | 0.43 |
| | 452. Lactic acid | $C_3H_6O_3$ | −0.62 | −0.62 |
| | 453. $\alpha$-Aminopropionic acid | $C_3H_7NO_2$ | −2.72 | −2.87 |
| | 454. Methyl-*N*-methyl carbamate | $C_3H_7NO_2$ | −0.06 | −0.37 |
| * | 455. Ethyl carbamate | $C_3H_7NO_2$ | −0.15 | −0.56 |
| | 456. *N*-Ethylurea | $C_3H_8N_2O$ | −0.74 | −0.05 |
| * | 457. Dimethoxymethane | $C_3H_8O_2$ | 0.00 | −0.07 |
| | 458. 2-Methoxyethanol | $C_3H_8O_2$ | −0.77 | −0.76 |
| * | 459. 1-Amino-2-propanol | $C_3H_9NO$ | −0.96 | −0.96 |
| | 460. 5-Bromouracil | $C_4H_3BrN_2O_2$ | −0.21 | −0.21 |
| | 461. 5-Chlorouracil | $C_4H_3ClN_2O_2$ | −0.35 | −0.35 |
| | 462. 5-Fluorouracil | $C_4H_3FN_2O_2$ | −0.95 | −0.85 |
| | 463. 2-Methyl-2-imidazoline | $C_4H_8N_2$ | 0.52 | 0.17 |
| | 464. *N*-Nitrosopyrrolidine | $C_4H_8N_2O$ | −0.19 | −0.01 |
| | 465. *N*-Nitrosothiomorpholine | $C_4H_8N_2OS$ | 0.40 | 0.40 |
| | 466. Butylnitrate | $C_4H_9NO_3$ | 2.15 | 2.15 |
| | 467. 1-Nitroso-trimethylurea | $C_4H_9N_3O_2$ | 0.36 | 0.29 |
| | 468. 5-Fluorouracil | $C_4H_3FN_2O_2$ | −0.85 | −0.85 |
| | 469. 5-Iodouracil | $C_4H_3IN_2O_2$ | 0.04 | 0.04 |
| * | 470. 4-Cyanopyrazole | $C_4H_3N_3$ | 0.24 | 0.24 |
| | 471. Pyrazine | $C_4H_4N_2$ | −0.22 | −0.12 |
| | 472. Pyridazine | $C_4H_4N_2$ | −0.72 | −0.72 |
| * | 473. Pyrimidine | $C_4H_4N_2$ | −0.40 | −0.40 |
| | 474. Pyrazine-2-one | $C_4H_4N_2O$ | −1.49 | −1.49 |
| | 475. 2-Pyrimidone | $C_4H_4N_2O$ | −1.62 | −1.62 |
| * | 476. 4-Pyrimidone | $C_4H_4N_2O$ | −1.38 | −2.86 |
| | 477. 2-Thiouracil | $C_4H_4N_2OS$ | −0.28 | −0.28 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | 478. Uracil | $C_4H_4N_2O_2$ | −1.07 | −0.30 |
| | 479. Barbituric acid | $C_4H_4N_2O_3$ | −1.41 | −0.83 |
| | 480. 2-Aminopyrazine | $C_4H_5N_3$ | −0.07 | −0.69 |
| | 481. 2-Aminopyrimidine | $C_4H_5N_3$ | −0.22 | −0.67 |
| | 482. 2-Amino-4-pyrimidone | $C_4H_5N_3O$ | −0.99 | −0.99 |
| * | 483. Cytosine | $C_4H_5N_3O$ | −1.73 | −1.73 |
| | 484. 2,3-Butanedione | $C_4H_6O_2$ | −1.34 | −1.09 |
| | 485. $\gamma$-Butyrolactone | $C_4H_6O_2$ | −0.64 | −0.06 |
| * | 486. Succinic acid | $C_4H_6O_4$ | −0.59 | −0.59 |
| * | 487. Malic acid | $C_4H_6O_5$ | −1.26 | −1.98 |
| | 488. $\alpha$-Bromobutyric acid | $C_4H_7BrO_2$ | 1.42 | 1.44 |
| | 489. 2,2,2-Trichloro-*t*-butanol | $C_4H_7Cl_3O$ | 2.03 | 2.03 |
| * | 490. *N*-Nitrosomorpholine | $C_4H_8N_2O_2$ | −0.44 | −0.17 |
| * | 491. *N,N'*-Dinitrosopiperazine | $C_4H_8N_4O_2$ | −0.85 | −0.92 |
| | 492. $\alpha$-Hydroxy-isobutyric acid | $C_4H_8O_3$ | −0.36 | −0.36 |
| | 493. 1-Nitroso-trimethylurea | $C_4H_9N_3O_2$ | 0.36 | 0.29 |
| | 494. *N,N*-Dimethylacetamide | $C_4H_9NO$ | −0.70 | −0.70 |
| * | 495. Morpholine | $C_4H_9NO$ | −1.08 | −0.60 |
| * | 496. *N*-Nitrosopiperazine | $C_4H_9N_3O$ | 0.18 | −0.87 |
| | 497. Piperazine | $C_4H_{10}N_2$ | −1.17 | −0.81 |
| | 498. *N*-Nitrosodiethylamine | $C_4H_{10}N_2O$ | 0.48 | 0.44 |
| * | 499. 2,3-Butanediol | $C_4H_{10}O_2$ | −0.92 | −0.92 |
| | 500. 2-Ethoxyethanol | $C_4H_{10}O_2$ | −0.54 | −0.28 |
| * | 501. Diethanolamine | $C_4H_{11}NO_2$ | −1.43 | −2.08 |
| | 502. 2,3,4,5,6-Pentachloropyridine | $C_5Cl_5N$ | 3.53 | 4.09 |
| * | 503. 2,3-Dichloropyridine | $C_5H_3Cl_2N$ | 2.11 | 2.21 |
| | 504. 2,5-Dichloropyridine | $C_5H_3Cl_2N$ | 2.40 | 2.17 |
| | 505. 2,6-Dichloropyridine | $C_5H_3Cl_2N$ | 2.15 | 2.39 |
| | 506. 3,5-Dichloropyridine | $C_5H_3Cl_2N$ | 2.56 | 1.95 |
| | 507. 2-Bromopyridine | $C_5H_4BrN$ | 1.38 | 1.38 |
| * | 508. 3-Bromopyridine | $C_5H_4BrN$ | 1.58 | 1.56 |
| | 509. 4-Bromopyridine | $C_5H_4BrN$ | 1.54 | 1.56 |
| | 510. 2-Chloropyridine | $C_5H_4ClN$ | 1.28 | 1.52 |
| | 511. 3-Chloropyridine | $C_5H_4ClN$ | 1.33 | 1.30 |
| | 512. 2-Nitropyridine | $C_5H_4N_2O_2$ | 0.48 | 0.48 |
| * | 513. 3-Nitropyridine | $C_5H_4N_2O_2$ | 0.60 | 0.38 |
| | 514. 5-Formyluracil | $C_5H_4N_2O_3$ | −1.03 | −1.03 |
| | 515. Hypoxanthine | $C_5H_4N_4O$ | −1.11 | 1.93 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | 516. Uric acid | $C_5H_4N_4O_3$ | −2.92 | 0.09 |
| | 517. 2-Hydroxypyridine | $C_5H_5NO$ | −0.58 | −0.38 |
| | 518. Pyridine 1-oxide | $C_5H_5NO$ | −1.30 | −1.09 |
| | 519. Adenine | $C_5H_5N_5$ | −0.16 | −0.98 |
| | 520. 2-Aminopyridine | $C_5H_6N_2$ | 0.58 | 0.48 |
| | 521. 3-Aminopyridine | $C_5H_6N_2$ | 0.20 | −0.64 |
| | 522. 4-Aminopyridine | $C_5H_6N_2$ | 0.26 | −0.64 |
| * | 523. 2-Methylpyrazine | $C_5H_6N_2$ | 0.23 | 0.17 |
| | 524. Thymine | $C_5H_6N_2O_2$ | −0.62 | 0.35 |
| | 525. 5-Ethyl-6-azauracil | $C_5H_7N_3O_2$ | 0.22 | 0.09 |
| * | 526. Acetylacetone | $C_5H_8O_2$ | 0.34 | −0.49 |
| | 527. 8-Valerolactone | $C_5H_8O_2$ | −0.35 | 0.48 |
| | 528. *N*-Nitroso-4-piperidone | $C_5H_8N_2O_2$ | −0.47 | −0.47 |
| | 529. 1,3-Diacetylurea | $C_5H_8N_2O_3$ | −0.68 | −0.74 |
| | 530. Butyl thiocyanate | $C_5H_9NS$ | 2.03 | 2.03 |
| | 531. *D*-Ribose | $C_5H_{10}O_5$ | −2.32 | −2.63 |
| | 532. *L*-Arabinose | $C_5H_{10}O_5$ | −3.02 | −2.63 |
| * | 533. *N*-Nitrosopiperidine | $C_5H_{10}N_2O$ | 0.63 | 0.52 |
| | 534. 3-Hydroxy-*N*-nitrosopiperidine | $C_5H_{10}N_2O_2$ | −0.47 | −0.50 |
| | 535. 4-Hydroxy-*N*-nitrosopiperidine | $C_5H_{10}N_2O_2$ | −0.89 | −1.39 |
| | 536. 2-Methylpropanoylurea | $C_5H_{10}N_2O_2$ | 0.04 | −0.42 |
| * | 537. 2-Methyl-*N*,*N*′-dinitrosopiperazine | $C_5H_{10}N_4O_2$ | −0.28 | −1.26 |
| | 538. 4-Methylmorpholine | $C_5H_{11}NO$ | −0.33 | −0.25 |
| | 539. Methionine | $C_5H_{11}NO_2S$ | −1.87 | −2.46 |
| | 540. *N*-Butylurea | $C_5H_{12}N_2O$ | 0.41 | 1.02 |
| * | 541. Diethoxymethane | $C_5H_{12}O_2$ | 0.84 | 0.90 |
| | 542. Isopropoxyethanol | $C_5H_{12}O_2$ | 0.05 | 0.07 |
| | 543. Propyl-*N*-methyl carbamate | $C_5H_{11}NO_2$ | 0.95 | 0.65 |
| | 544. 4-Methyl-*N*-nitrosopiperazine | $C_5H_{11}N_3O$ | 0.20 | −0.72 |
| | 545. *N*-Bromobenzoquinone monoimine | $C_6H_4BrNO$ | 1.12 | 1.12 |
| | 546. *N*-Chlorobenzoquinone monoimine | $C_6H_4ClNO$ | 1.26 | 1.26 |
| | 547. 2,5-Dichlorophenol | $C_6H_4Cl_2O$ | 3.20 | 3.10 |
| | 548. *N*-Hydroxybenzoquinone monoimine | $C_6H_5NO_2$ | 1.08 | 1.08 |
| | 549. *N*-Formylcyclobutane carboxyamide | $C_6H_9NO_2$ | −0.70 | −0.20 |
| | 550. 1,2-5,6-Dianhydrogalactitol | $C_6H_{10}O_4$ | −1.29 | 0.24 |
| | 551. 3-Methylbutanoylurea | $C_6H_{12}N_2O_2$ | 0.45 | 0.53 |
| | 552. Isoleucine | $C_6H_{13}NO_2$ | −1.69 | −1.34 |
| | 553. Pentyl carbamate | $C_6H_{13}NO_2$ | 1.35 | 1.05 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | 554. *t*-Pentyl carbamate | $C_6H_{13}NO_2$ | 0.94 | 0.70 |
| | 555. 1-Nitroso-3,3-diethyl-1-methylurea | $C_6H_{13}N_3O_2$ | 1.11 | 1.18 |
| | 556. 1-Nitrosodiisopropylamine | $C_6H_{14}N_2O$ | 1.63 | 1.03 |
| | 557. Pentachlorophenol | $C_6HCl_5O$ | 5.12 | 4.95 |
| | 558. Pentafluorophenol | $C_6HF_5O$ | 3.23 | 3.23 |
| * | 559. 2,3,4,6-Tetrachlorophenol | $C_6H_2Cl_4O$ | 4.10 | 4.42 |
| | 560. 2,6-Dibromo-4-nitrophenol | $C_6H_3Br_2NO_3$ | 3.05 | 2.91 |
| | 561. 2,4,6-Tribromophenol | $C_6H_3Br_3O$ | 3.96 | 4.10 |
| | 562. 2,4,6-Tribromoresorcinol | $C_6H_3Br_3O_2$ | 4.37 | 4.37 |
| * | 563. 2,6-Dichloro-4-nitrophenol | $C_6H_3Cl_2NO_3$ | 2.94 | 2.77 |
| | 564. 2,4,5-Trichlorophenol | $C_6H_3Cl_3O$ | 3.72 | 3.63 |
| | 565. 2,4,6-Trichlorophenol | $C_6H_3Cl_3O$ | 3.62 | 3.69 |
| * | 566. 1,3,5-Trinitrobenzene | $C_6H_3N_3O_6$ | 1.18 | 1.38 |
| | 567. 2,4,6-Trinitrophenol | $C_6H_3N_3O_7$ | 2.03 | 0.98 |
| | 568. 3-Bromo-1-nitrobenzene | $C_6H_4BrNO_2$ | 2.64 | 2.84 |
| | 569. 4-Bromo-1-nitrobenzene | $C_6H_4BrNO_2$ | 2.55 | 2.84 |
| | 570. 2,4-Dibromophenol | $C_6H_4Br_2O$ | 3.22 | 3.24 |
| | 571. 4-Chloro-1-nitrobenzene | $C_6H_4ClNO_2$ | 2.39 | 2.58 |
| | 572. 3-Chloro-1-nitrobenzene | $C_6H_4ClNO_2$ | 2.46 | 2.58 |
| | 573. 2-Chloro-1-nitrobenzene | $C_6H_4ClNO_2$ | 2.24 | 2.24 |
| | 574. 2,4-Dichlorophenol | $C_6H_4Cl_2O$ | 3.30 | 3.10 |
| | 575. 3-Iodonitrobenzene | $C_6H_4INO_2$ | 2.94 | 3.22 |
| | 576. 2-Cyanopyridine | $C_6H_4N_2$ | 0.50 | 0.43 |
| | 577. 3-Cyanopyridine | $C_6H_4N_2$ | 0.36 | 0.01 |
| * | 578. 4-Cyanopyridine | $C_6H_4N_2$ | 0.46 | 0.01 |
| | 579. *m*-Dinitrobenzene | $C_6H_4N_2O_4$ | 1.49 | 1.65 |
| | 580. *o*-Dinitrobenzene | $C_6H_4N_2O_4$ | 1.58 | 1.58 |
| | 581. *p*-Dinitrobenzene | $C_6H_4N_2O_4$ | 1.46 | 1.65 |
| * | 582. 2,4-Dinitrophenol | $C_6H_4N_2O_5$ | 1.50 | 1.59 |
| | 583. 2,5-Dinitrophenol | $C_6H_4N_2O_5$ | 1.75 | 1.59 |
| | 584. 2,6-Dinitrophenol | $C_6H_4N_2O_5$ | 1.25 | 1.25 |
| | 585. 3,5-Dinitrophenol | $C_6H_4N_2O_5$ | 2.32 | 0.84 |
| | 586. Quinone | $C_6H_4O_2$ | 0.20 | 0.20 |
| | 587. *m*-Bromophenol | $C_6H_5BrO$ | 2.63 | 2.30 |
| | 588. *o*-Bromophenol | $C_6H_5BrO$ | 2.35 | 2.33 |
| * | 589. *p*-Bromophenol | $C_6H_5BrO$ | 2.43 | 2.30 |
| | 590. *m*-Chlorophenol | $C_6H_5ClO$ | 2.50 | 2.04 |
| | 591. *o*-Chlorophenol | $C_6H_5ClO$ | 2.17 | 2.45 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | 592. *p*-Chlorophenol | $C_6H_5ClO$ | 2.35 | 2.04 |
| | 593. 2,3-Dichloroaniline | $C_6H_5Cl_2N$ | 2.78 | 2.78 |
| | 594. 3,4-Dichloroaniline | $C_6H_5Cl_2N$ | 2.69 | 2.09 |
| * | 595. 3,4-Dichlorobenzenesulfonamide | $C_6H_4Cl_2NO_2S$ | 1.44 | 1.69 |
| | 596. *m*-Fluorophenol | $C_6H_5FO$ | 1.93 | 1.64 |
| | 597. *o*-Fluorophenol | $C_6H_5FO$ | 1.71 | 1.71 |
| | 598. *p*-Fluorophenol | $C_6H_5FO$ | 1.81 | 1.64 |
| | 599. *m*-Iodophenol | $C_6H_5IO$ | 3.00 | 2.69 |
| | 600. *o*-Iodophenol | $C_6H_5IO$ | 2.65 | 2.65 |
| * | 601. *p*-Iodophenol | $C_6H_5IO$ | 2.91 | 2.69 |
| | 602. Iodosobenzene | $C_6H_5IO$ | −1.61 | −1.61 |
| | 603. Iodoxybenzene | $C_6H_5IO_2$ | −1.33 | −1.33 |
| | 604. Picolinic acid | $C_6H_5NO_2$ | −1.98 | −0.94 |
| | 605. 3-Hydroxypicolinic acid | $C_6H_5NO_3$ | −1.27 | −1.27 |
| | 606. *m*-Nitrophenol | $C_6H_5NO_3$ | 2.01 | 1.12 |
| | 607. *o*-Nitrophenol | $C_6H_5NO_3$ | 1.79 | 1.86 |
| | 608. *p*-Nitrophenol | $C_6H_5NO_3$ | 1.91 | 1.12 |
| | 609. 2-Nitroresorcinol | $C_6H_5NO_4$ | 1.36 | 1.36 |
| | 610. Benzotriazole | $C_6H_5N_3$ | 1.34 | 0.59 |
| | 611. *m*-Bromoaniline | $C_6H_6BrN$ | 2.10 | 1.82 |
| * | 612. *o*-Bromoaniline | $C_6H_6BrN$ | 2.29 | 2.20 |
| | 613. *p*-Bromoaniline | $C_6H_6BrN$ | 2.05 | 1.82 |
| | 614. *p*-Bromobenzenesulfonamide | $C_6H_6BrNO_2S$ | 1.36 | 1.42 |
| | 615. *m*-Chloroaniline | $C_6H_6ClN$ | 1.88 | 1.56 |
| | 616. *o*-Chloroaniline | $C_6H_6ClN$ | 1.90 | 1.96 |
| | 617. *p*-Chloroaniline | $C_6H_6ClN$ | 1.83 | 1.56 |
| | 618. *m*-Chlorobenzenesulfonamide | $C_6H_6ClNO_2S$ | 1.29 | 1.16 |
| | 619. *o*-Chlorobenzenesulfonamide | $C_6H_6ClNO_2S$ | 0.74 | 1.16 |
| * | 620. *p*-Chlorobenzenesulfonamide | $C_6H_6ClNO_2S$ | 0.84 | 1.16 |
| | 621. 2-Chloroisoniazid | $C_6H_6ClN_3O$ | 0.11 | −0.25 |
| | 622. *m*-Fluoroaniline | $C_6H_6FN$ | 1.30 | 1.16 |
| * | 623. *o*-Fluoroaniline | $C_6H_6FN$ | 1.26 | 1.13 |
| | 624. *p*-Fluoroaniline | $C_6H_6FN$ | 1.15 | 1.16 |
| | 625. 2-Fluoroisoniazid | $C_6H_6FN_3O$ | −0.11 | −0.38 |
| | 626. *m*-Iodoaniline | $C_6H_6IN$ | 2.98 | 2.20 |
| | 627. *o*-Iodoaniline | $C_6H_6IN$ | 3.34 | 2.64 |
| * | 628. *p*-Iodoaniline | $C_6H_6IN$ | 3.34 | 2.20 |
| | 629. Nicotinamide | $C_6H_6N_2O$ | −0.37 | −0.91 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | 630. 3-Hydroxypicolinamide | $C_6H_6N_2O_2$ | 0.65 | −1.09 |
| | 631. *m*-Nitroaniline | $C_6H_6N_2O_2$ | 1.37 | 0.63 |
| | 632. *o*-Nitroaniline | $C_6H_6N_2O_2$ | 1.44 | 1.44 |
| | 633. *p*-Nitroaniline | $C_6H_6N_2O_2$ | 1.39 | 0.63 |
| | 634. *o*-Nitrobenzenesulfonamide | $C_6H_6N_2O_4S$ | 0.34 | 0.24 |
| * | 635. *p*-Nitrobenzenesulfonamide | $C_6H_6N_2O_4S$ | 0.64 | 0.24 |
| | 636. *m*-Nitrobenzenesulfonamide | $C_6H_6N_2O_4S$ | 0.55 | 0.24 |
| * | 637. Resorcinol | $C_6H_6O_2$ | 0.80 | 0.58 |
| | 638. Catechol | $C_6H_6O_2$ | 0.88 | 0.81 |
| | 639. Hydroquinone | $C_6H_6O_2$ | 0.59 | 0.58 |
| * | 640. 1,3,5-Trihydroxybenzene | $C_6H_6O_3$ | 0.16 | −0.23 |
| | 641. 1-Hydroxypentachlorocyclohexane | $C_6H_7Cl_5O$ | 2.54 | 2.62 |
| | 642. *m*-Aminophenol | $C_6H_7NO$ | 0.17 | 0.10 |
| | 643. *o*-Aminophenol | $C_6H_7NO$ | 0.62 | −0.02 |
| | 644. *p*-Aminophenol | $C_6H_7NO$ | 0.04 | 0.10 |
| | 645. 2-Methoxypyridine | $C_6H_7NO$ | 1.39 | 1.68 |
| | 646. 4-Methoxypyridine | $C_6H_7NO$ | 1.00 | 0.46 |
| | 647. *N*-Phenylhydroxyamine | $C_6H_7NO$ | 0.79 | 0.79 |
| * | 648. Benzenesulfonamide | $C_6H_7NO_2S$ | 0.31 | 0.51 |
| | 649. *p*-Phenolsulfonamide | $C_6H_7NO_3S$ | 0.06 | −0.29 |
| | 650. 2-Aminonicotinamide | $C_6H_7N_3O$ | 0.88 | −1.09 |
| | 651. 6-Aminonicotinamide | $C_6H_7N_3O$ | 0.70 | −1.09 |
| | 652. Isoniazid | $C_6H_7N_3O$ | −1.14 | −1.12 |
| | 653. 2-Amino-4-picoline | $C_6H_8N_2$ | 0.56 | 0.90 |
| | 654. 2-Amino-5-methylpyridine | $C_6H_8N_2$ | 1.02 | 0.90 |
| | 655. *o*-Phenylenediamine | $C_6H_8N_2$ | 0.15 | 0.42 |
| | 656. *m*-Aminobenzenesulfonamide | $C_6H_8N_2O_2S$ | −1.20 | −0.78 |
| | 657. *N*-Phenylsulfamide | $C_6H_8N_2O_2S$ | 0.40 | 0.40 |
| * | 658. Sulfanilamide | $C_6H_8N_2O_2S$ | −0.72 | −0.78 |
| | 659. Pentylenetetrazole | $C_6H_{10}N_4$ | 0.14 | 0.20 |
| | 660. 4-Ketovaleric acid methyl ester | $C_6H_{10}O_3$ | −0.13 | −0.19 |
| * | 661. Adipic acid | $C_6H_{10}O_4$ | 0.08 | −0.13 |
| | 662. Bromisovalum | $C_6H_{11}BrN_2O_2$ | 1.14 | 0.58 |
| | 663. α-Chloro-isovalerylurea | $C_6H_{11}ClN_2O_2$ | 1.00 | 0.41 |
| | 664. 2-Azacycloheptanone | $C_6H_{11}NO$ | −0.19 | 0.65 |
| | 665. 2-Azacycloheptanthion | $C_6H_{11}NS$ | 0.75 | 0.61 |
| | 666. 2-Methyl-*N*-nitrosopiperidine | $C_6H_{12}N_2O$ | 0.71 | 0.82 |
| | 667. 3-Methyl-*N*-nitrosopiperidine | $C_6H_{12}N_2O$ | 0.99 | 0.99 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| * | 668. 4-Methyl-*N*-nitrosopiperidine | $C_6H_{12}N_2O$ | 1.05 | 0.99 |
| | 669. 2,6-Dimethyl-*N*-nitrosomorpholine | $C_6H_{12}N_2O_2$ | 0.32 | 0.94 |
| | 670. 2,6-Dimethyl-*N,N'*-dinitrosopiperazine | $C_6H_{12}N_4O_2$ | 0.08 | 0.14 |
| | 671. Leucine | $C_6H_{13}NO_2$ | −1.52 | −1.34 |
| * | 672. *N*-Nitrosodipropylamine | $C_6H_{14}N_2O$ | 1.63 | 1.52 |
| | 673. 2-Butoxyethanol | $C_6H_{14}O_2$ | 0.83 | 0.80 |
| | 674. Diethylacetal | $C_6H_{14}O_2$ | 0.84 | 0.84 |
| | 675. Busulfan | $C_6H_{14}O_6S_2$ | −0.52 | −0.52 |
| | 676. Di-isopropanolamine | $C_6H_{15}NO_2$ | −0.82 | −0.82 |
| * | 677. *N,N,N',N'*-Tetramethylethylenediamine | $C_6H_{16}N_2$ | 0.30 | 0.13 |
| | 678. *p*-Bromophenyl isothiocyanate | $C_7H_4BrNS$ | 4.03 | 4.17 |
| | 679. 3,5-Diiodosalicylic acid | $C_7H_4I_2O_3$ | 4.56 | 2.96 |
| | 680. 3-Cyano-1-nitrobenzene | $C_7H_4N_2O_2$ | 1.17 | 1.29 |
| | 681. 4-Cyano-1-nitrobenzene | $C_7H_4N_2O_2$ | 1.19 | 1.29 |
| | 682. 4-Nitrophenyl isothiocyanate | $C_7H_4N_2O_2S$ | 3.62 | 2.99 |
| | 683. *m*-Bromobenzoic acid | $C_7H_5BrO_2$ | 2.87 | 2.70 |
| | 684. *p*-Bromobenzoic acid | $C_7H_5BrO_2$ | 2.86 | 2.70 |
| | 685. 5-Bromosalicylic acid | $C_7H_5BrO_3$ | 2.87 | 2.91 |
| | 686. Zoxazolamine | $C_7H_5ClN_2O$ | 2.46 | 2.46 |
| | 687. 1-Phenyl-4-chlorotetrazole | $C_7H_5ClN_4$ | 1.48 | 0.73 |
| | 688. *m*-Chlorobenzoic acid | $C_7H_5ClO_2$ | 2.68 | 2.43 |
| | 689. *o*-Chlorobenzoic acid | $C_7H_5ClO_2$ | 1.98 | 1.91 |
| | 690. *p*-Chlorobenzoic acid | $C_7H_5ClO_2$ | 2.65 | 2.43 |
| | 691. *m*-Fluorobenzoic acid | $C_7H_5FO_2$ | 2.15 | 2.04 |
| * | 692. *p*-Fluorobenzoic acid | $C_7H_5FO_2$ | 2.07 | 2.04 |
| | 693. Trifluoromethoxybenzene | $C_7H_5F_3O$ | 3.17 | 3.17 |
| | 694. *m*-Trifluoromethylphenol | $C_7H_5F_3O$ | 2.95 | 2.40 |
| | 695. *o*-Trifluoromethylphenol | $C_7H_5F_3O$ | 2.80 | 2.40 |
| | 696. Phenyl-trifluoromethyl sulfone | $C_7H_5F_3O_2S$ | 2.68 | 2.70 |
| | 697. *m*-Iodobenzoic acid | $C_7H_5IO_2$ | 3.13 | 3.08 |
| | 698. *o*-Iodobenzoic acid | $C_7H_5IO_2$ | 2.40 | 2.32 |
| | 699. *p*-Iodobenzoic acid | $C_7H_5IO_2$ | 3.02 | 3.08 |
| | 700. *m*-Cyanophenol | $C_7H_5NO$ | 1.70 | 0.75 |
| | 701. *o*-Cyanophenol | $C_7H_5NO$ | 1.61 | 1.61 |
| * | 702. *p*-Cyanophenol | $C_7H_5NO$ | 1.60 | 0.75 |
| | 703. *m*-Nitrobenzoic acid | $C_7H_5NO_4$ | 1.83 | 1.51 |
| | 704. *p*-Nitrobenzoic acid | $C_7H_5NO_4$ | 1.89 | 1.51 |
| | 705. 5-Nitrosalicylic acid | $C_7H_5NO_5$ | 2.34 | 1.73 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | 706. Benzothiazole | $C_7H_5NS$ | 2.01 | 2.01 |
| | 707. Phenylisothiocyanate | $C_7H_5NS$ | 3.28 | 3.27 |
| | 708. Phenylthiocyanate | $C_7H_5NS$ | 2.54 | 2.30 |
| | 709. Trifluoromethyl thiobenzene | $C_7H_5F_3S$ | 3.57 | 3.57 |
| | 710. 3,5-Dinitrobenzamide | $C_7H_5N_3O_5$ | 0.83 | 0.09 |
| | 711. Trichloromethyl thiobenzene | $C_7H_5Cl_3S$ | 3.78 | 3.78 |
| | 712. *m*-Bromobenzamide | $C_7H_6BrNO$ | 1.65 | 1.55 |
| | 713. *p*-Bromobenzamide | $C_7H_6BrNO$ | 1.76 | 1.55 |
| | 714. 2-Bromo-4-aminobenzoic acid | $C_7H_6BrNO_2$ | 0.66 | 0.81 |
| | 715. 3-Bromo-4-aminobenzoic acid | $C_7H_6BrNO_2$ | 1.40 | 1.79 |
| | 716. *m*-Chlorobenzamide | $C_7H_6ClNO$ | 1.51 | 1.29 |
| * | 717. *p*-Chlorobenzamide | $C_7H_6ClNO$ | 1.51 | 1.29 |
| | 718. 2-Chloro-4-aminobenzoic acid | $C_7H_6ClNO_2$ | 0.50 | 0.62 |
| | 719. 3-Chloro-4-aminobenzoic acid | $C_7H_6ClNO_2$ | 1.52 | 1.55 |
| | 720. *m*-Fluorobenzamide | $C_7H_6FNO$ | 0.91 | 0.89 |
| | 721. *p*-Fluorobenzamide | $C_7H_6FNO$ | 0.91 | 0.89 |
| | 722. 2-Fluoro-4-aminobenzoic acid | $C_7H_6FNO_2$ | 0.46 | 0.45 |
| | 723. 3-Fluoro-4-aminobenzoic acid | $C_7H_6FNO_2$ | 0.58 | 0.71 |
| | 724. *p*-Trifluoromethylaniline | $C_7H_6F_3N$ | 1.95 | 1.92 |
| | 725. *p*-Iodobenzamide | $C_7H_6INO$ | 1.99 | 1.93 |
| | 726. 2-Iodo-4-aminobenzoic acid | $C_7H_6INO_2$ | 0.82 | 1.02 |
| | 727. 3-Iodo-4-aminobenzoic acid | $C_7H_6INO_2$ | 1.53 | 2.23 |
| | 728. 7-Azaindole | $C_7H_6N_2$ | 1.82 | 1.59 |
| | 729. Benzimidazole | $C_7H_6N_2$ | 1.46 | 1.49 |
| | 730. 4-Cyano-2-methylpyridine | $C_7H_6N_2$ | 0.81 | 0.50 |
| | 731. 2-Cyano-6-methylpyridine | $C_7H_6N_2$ | 0.84 | 0.92 |
| | 732. Indazole | $C_7H_6N_2$ | 1.82 | 1.22 |
| | 733. *p*-Cyanobenzenesulfonamide | $C_7H_6N_2O_2S$ | 0.23 | −0.13 |
| | 734. *m*-Nitrobenzamide | $C_7H_6N_2O_3$ | 0.77 | 0.37 |
| | 735. *p*-Nitrobenzamide | $C_7H_6N_2O_3$ | 0.82 | 0.37 |
| | 736. *p*-Nitroformanilide | $C_7H_6N_2O_3$ | 1.43 | 0.85 |
| | 737. 2,4-Dinitrotoluene | $C_7H_6N_2O_4$ | 1.98 | 2.07 |
| | 738. 2-Nitro-4-aminobenzoic acid | $C_7H_6N_2O_4$ | 0.38 | 0.29 |
| | 739. *o*-Phenylenethiourea | $C_7H_6N_2S$ | 1.66 | 1.05 |
| | 740. *m*-Hydroxybenzaldehyde | $C_7H_6O_2$ | 1.38 | 0.85 |
| | 741. *o*-Hydroxybenzaldehyde | $C_7H_6O_2$ | 1.70 | 1.88 |
| * | 742. *p*-Hydroxybenzaldehyde | $C_7H_6O_2$ | 1.35 | 0.85 |
| | 743. 1,2-Methylenedioxybenzene | $C_7H_6O_2$ | 2.08 | 1.73 |

TABLE A1 (continued)

| | Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|---|
| | 744. Tropolone | $C_7H_6O_2$ | 0.53 | 0.67 |
| | 745. *m*-Hydroxybenzoic acid | $C_7H_6O_3$ | 1.50 | 0.98 |
| | 746. Salicylic acid | $C_7H_6O_3$ | 2.26 | 2.01 |
| | 747. *p*-Hydroxybenzoic acid | $C_7H_6O_3$ | 1.58 | 0.98 |
| | 748. 2,4-Dihydroxybenzoic acid | $C_7H_6O_4$ | 1.44 | 1.20 |
| | 749. 2,6-Dihydroxybenzoic acid | $C_7H_6O_4$ | 2.20 | 2.20 |
| | 750. *m*-Chlorobenzyl alcohol | $C_7H_7ClO$ | 1.94 | 1.58 |
| * | 751. *p*-Chlorobenzyl alcohol | $C_7H_7ClO$ | 1.96 | 1.58 |
| | 752. 2-Methyl-4-chlorophenol | $C_7H_7ClO$ | 2.78 | 2.46 |
| | 753. 3-Methyl-4-chlorophenol | $C_7H_7ClO$ | 3.10 | 2.46 |
| | 754. *p*-Fluorosulfonyltoluene | $C_7H_7FO_2S$ | 2.74 | 2.74 |
| | 755. 2-Acetylpyridine | $C_7H_7NO$ | 0.83 | 0.83 |
| | 756. 4-Acetylpyridine | $C_7H_7NO$ | 0.54 | 0.20 |
| | 757. 3-Acetylpyridine | $C_7H_7NO$ | 0.43 | 0.20 |
| | 758. Benzaldoxime | $C_7H_7NO$ | 1.75 | 1.93 |
| | 759. *o*-Aminobenzoic acid | $C_7H_7NO_2$ | 1.21 | 1.61 |
| | 760. *p*-Aminobenzoic acid | $C_7H_7NO_2$ | 0.83 | 0.49 |
| | 761. *m*-Hydroxybenzamide | $C_7H_7NO_2$ | 0.39 | −0.17 |
| | 762. *o*-Hydroxybenzamide | $C_7H_7NO_2$ | 1.28 | 0.86 |
| | 763. *p*-Hydroxybenzamide | $C_7H_7NO_2$ | 0.25 | −0.17 |
| | 764. 3-Hydroxy-4-aminobenzoic acid | $C_7H_7NO_3$ | −0.32 | −0.18 |
| | 765. *m*-Nitroanisole | $C_7H_7NO_3$ | 2.16 | 1.74 |
| | 766. *p*-Nitroanisole | $C_7H_7NO_3$ | 2.03 | 1.74 |
| | 767. *m*-Nitrobenzyl alcohol | $C_7H_7NO_3$ | 1.21 | 0.66 |
| | 768. *p*-Nitrobenzyl alcohol | $C_7H_7NO_3$ | 1.26 | 0.66 |
| | 769. Thiobenzamide | $C_7H_7NS$ | 1.49 | 1.46 |
| | 770. 1-Methylbenzotriazole | $C_7H_7N_3$ | 1.13 | 1.14 |
| | 771. *m*-Aminobenzamide | $C_7H_8N_2O$ | 0.33 | −0.65 |
| | 772. *p*-Aminobenzamide | $C_7H_8N_2O$ | 0.02 | −0.65 |
| | 773. Benzoylhydrazine | $C_7H_8N_2O$ | 0.19 | 0.43 |
| | 774. *N*-Phenylurea | $C_7H_8N_2O$ | 0.83 | 0.98 |
| | 775. 2,4-Diaminobenzoic acid | $C_7H_8N_2O_2$ | −1.14 | 0.32 |
| | 776. 3,4-Diaminobenzoic acid | $C_7H_8N_2O_2$ | −0.70 | 0.00 |
| | 777. *p*-Nitro-*N*-methylaniline | $C_7H_8N_2O_2$ | 2.04 | 1.48 |
| | 778. Phenylthiourea | $C_7H_8N_2S$ | 0.73 | 0.73 |
| | 779. Theobromine | $C_7H_8N_4O_2$ | −0.78 | 2.23 |
| * | 780. *p*-Methiophenol | $C_7H_8OS$ | 1.78 | 1.93 |
| | 781. *m*-Hydroxybenzyl alcohol | $C_7H_8O_2$ | 0.49 | 0.12 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 782. *p*-Hydroxybenzyl alcohol | $C_7H_8O_2$ | 0.25 | 0.12 |
| 783. *o*-Hydroxybenzyl alcohol | $C_7H_8O_2$ | 0.73 | 0.12 |
| 784. *m*-Methoxyphenol | $C_7H_8O_2$ | 1.58 | 1.20 |
| 785. *o*-Methoxyphenol | $C_7H_8O_2$ | 1.32 | 1.43 |
| 786. *p*-Methoxyphenol | $C_7H_8O_2$ | 1.37 | 1.20 |
| 787. 3-Methoxypentachlorocyclohexane | $C_7H_9Cl_5O$ | 3.51 | 3.43 |
| 788. *m*-Aminobenzyl alcohol | $C_7H_9NO$ | −0.05 | −0.36 |
| 789. *m*-Methoxyaniline | $C_7H_9NO$ | 0.93 | 0.72 |
| 790. *o*-Methoxyaniline | $C_7H_9NO$ | 0.95 | 0.86 |
| 791. *p*-Methoxyaniline | $C_7H_9NO$ | 0.95 | 0.72 |
| 792. *m*-Methylbenzenesulfonamide | $C_7H_9NO_2S$ | 0.85 | 0.93 |
| 793. *o*-Methylbenzenesulfonamide | $C_7H_9NO_2S$ | 0.84 | 0.93 |
| 794. *p*-Methylbenzenesulfonamide | $C_7H_9NO_2S$ | 0.82 | 0.93 |
| 795. *m*-Methioaniline | $C_7H_9NS$ | 1.45 | 1.45 |
| 796. *o*-Methioaniline | $C_7H_9NS$ | 1.20 | 1.44 |
| 797. *o*-Phenyleneurea | $C_7H_6N_2O$ | 1.12 | 1.73 |
| 798. 1-Phenyltetrazole | $C_7H_6N_4$ | 1.09 | 1.09 |
| 799. 2,5-Dihydroxybenzoic acid | $C_7H_6O_4$ | 1.74 | 1.20 |
| 800. Benzohydroxamic acid | $C_7H_7NO_2$ | 0.26 | −0.06 |
| 801. Isonicotinic acid methylester | $C_7H_7NO_2$ | 0.87 | 0.52 |
| 802. Nicotinic acid methylester | $C_7H_7NO_2$ | 0.81 | 0.52 |
| 803. *o*-Phenylcarbamate | $C_7H_7NO_2$ | 1.08 | 0.84 |
| 804. Salicylamide | $C_7H_7NO_2$ | 0.89 | 0.86 |
| 805. *p*-Aminosalicylic acid | $C_7H_7NO_3$ | 0.87 | 0.71 |
| 806. 2-Acetaminopyridine | $C_7H_8N_2O$ | 0.61 | 0.69 |
| 807. 3-Acetaminopyridine | $C_7H_8N_2O$ | 0.41 | −0.43 |
| 808. 4-Acetaminopyridine | $C_7H_8N_2O$ | 0.59 | −0.43 |
| 809. Thiophene,2-carboxylic acid ethylester | $C_7H_8O_2S$ | 2.33 | 2.33 |
| 810. 2-Furoic acid ethyl ester | $C_7H_8O_3$ | 1.52 | 2.60 |
| 811. 1-Hydroxymethylpentachlorocyclohexane | $C_7H_9Cl_5O$ | 2.94 | 2.94 |
| 812. 3-Methoxypentachlorocyclohexane | $C_7H_9Cl_5O$ | 3.51 | 3.51 |
| 813. 1-Methiopentachlorocyclohexane | $C_7H_9Cl_5S$ | 3.75 | 3.75 |
| 814. 3-Methiopentachlorocyclohexane | $C_7H_9Cl_5S$ | 3.85 | 3.85 |
| 815. Methanesulfonanilide | $C_7H_9NO_2S$ | 0.95 | 0.56 |
| 816. 2-Methylisoniazid | $C_7H_9N_3O$ | −0.37 | −0.63 |
| 817. 2-Methoxyisoniazid | $C_7H_9N_3O_2$ | −0.10 | −0.09 |
| 818. 1-*H*-2-Methoxytetrachlorocycloxane | $C_7H_{10}Cl_4O$ | 2.99 | 2.99 |
| 819. 3-Methio-4-amino-6-*N*-Pr-1,2,4-triazine-5-one | $C_7H_{12}N_4OS$ | 1.01 | −0.51 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 820. 3-Methoxy-4-amino-6-isoPr-1,2,4-triazine-5-one | $C_7H_{12}N_4O_2$ | −0.06 | 1.86 |
| 821. 1,3-Diallylurea | $C_7H_{12}N_2O$ | 0.64 | 1.36 |
| 822. Carbromal | $C_7H_{13}BrN_2O_2$ | 1.54 | 1.07 |
| 823. 2-Azacyclooctanone | $C_7H_{13}NO$ | 0.24 | 1.19 |
| 824. 2-Azacyclooctanthione | $C_7H_{13}NS$ | 1.00 | 1.14 |
| 825. 6-Isopropyl-4-amino-3-meamino-1,2,4-triazine-5-one | $C_7H_{13}N_5O$ | 0.30 | 0.64 |
| 826. 2,6-Dimethyl-*N*-nitrosopiperidine | $C_7H_{14}N_2O$ | 1.36 | 1.11 |
| 827. 3,5-Dimethyl-*N*-nitrosopiperidine | $C_7H_{14}N_2O$ | 1.53 | 1.45 |
| 828. *o*-Hexylcarbamate | $C_7H_{15}NO_2$ | 1.85 | 1.58 |
| 829. *o*-*t*-Hexylcarbamate | $C_7H_{15}NO_2$ | 1.45 | 1.23 |
| 830. *o*-Pentyl-*N*-methylcarbamate | $C_7H_{15}NO_2$ | 1.96 | 1.72 |
| 831. 1-Nitrosotriethyl urea | $C_7H_{15}N_3O_2$ | 1.54 | 1.63 |
| 832. Phthalic anhydride | $C_8H_4O_3$ | −0.62 | −0.29 |
| 833. *p*-Trifluoroacetamide bromobenzene | $C_8H_5BrF_3NO$ | 3.34 | 3.18 |
| 834. 2-Chloroquinoxaline | $C_8H_5ClN_2$ | 2.23 | 1.84 |
| 835. 5-Chloroquinoxaline | $C_8H_5ClN_2$ | 1.75 | 1.92 |
| 836. 6-Chloroquinoxaline | $C_8H_5ClN_2$ | 2.10 | 2.01 |
| 837. 2-Chloro-5-nitro-$\beta$-nitrostyrene | $C_8H_5ClN_2O_4$ | 2.23 | 2.60 |
| 838. 2,4-Dichloro-$\beta$-nitrostyrene | $C_8H_5Cl_2NO_2$ | 3.26 | 3.52 |
| 839. 2-Trifluoromethyl benzimidazole | $C_8H_5F_3N_2$ | 2.58 | 2.58 |
| 840. Trifluoroacetophenone | $C_8H_5F_3O$ | 2.15 | 2.15 |
| 841. *m*-Trifluoromethyl benzoic acid | $C_8H_5F_3O_2$ | 2.95 | 2.80 |
| 842. *m*-Cyanobenzoic acid | $C_8H_5NO_2$ | 1.48 | 1.15 |
| 843. *p*-Cyanobenzoic acid | $C_8H_5NO_2$ | 1.56 | 1.15 |
| 844. 4-Carboxyphenylisothiocyanate | $C_8H_5NO_2S$ | 3.52 | 2.85 |
| 845. 3-Bromo-4-chlorophenoxyacetic acid | $C_8H_6BrClO_3$ | 2.75 | 2.49 |
| 846. 5-Bromo-indole | $C_8H_6BrN$ | 3.00 | 2.93 |
| 847. 3-Chloro-5-fluorophenoxyacetic acid | $C_8H_6ClFO_3$ | 2.20 | 2.21 |
| 848. 4-Chloro-3-iodophenoxyacetic acid | $C_8H_6ClIO_3$ | 3.10 | 3.10 |
| 849. 4-Chloro-$\beta$-nitrostyrene | $C_8H_6ClNO_2$ | 2.44 | 2.87 |
| 850. 3-Chloro-$\beta$-nitrostyrene | $C_8H_6ClNO_2$ | 2.57 | 2.87 |
| 851. 2-Chloro-$\beta$-nitrostyrene | $C_8H_6ClNO_2$ | 2.85 | 2.87 |
| 852. 4-Chloro-3-nitrophenoxyacetic acid | $C_8H_6ClNO_5$ | 1.85 | 1.35 |
| 853. 2,4-Dichlorophenoxyacetic acid | $C_8H_6Cl_2O_3$ | 2.81 | 3.02 |
| 854. 3,4-Dichlorophenoxyacetic acid | $C_8H_6Cl_2O_3$ | 2.81 | 2.49 |
| 855. 5-Fluoro-3-iodophenoxyacetic acid | $C_8H_6FIO_3$ | 2.42 | 2.85 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 856. *p*-Trifluoromethylbenzamide | $C_8H_6F_3NO$ | 1.71 | 1.65 |
| 857. Quinoxaline | $C_8H_6N_2$ | 1.32 | 1.18 |
| 858. Cinnoline-4-one | $C_8H_6N_2O$ | 0.82 | −0.19 |
| 859. *m*-Cyanobenzamide | $C_8H_6N_2O$ | 0.52 | 0.00 |
| 860. *p*-Cyanobenzamide | $C_8H_6N_2O$ | 0.48 | 0.00 |
| 861. *p*-Cyanoformanilide | $C_8H_6N_2O$ | 1.08 | 0.48 |
| 862. Quinazoline-4-one | $C_8H_6N_2O$ | 0.77 | 1.03 |
| 863. Quinazoline-2-one | $C_8H_6N_2O$ | 0.80 | −0.80 |
| 864. Quinazoline-2,4-dione | $C_8H_6N_2O_2$ | 0.55 | 1.78 |
| 865. Quinazoline-2,3-dione | $C_8H_6N_2O_2$ | 0.20 | 0.38 |
| 866. 2-Nitro-$\beta$-nitrostyrene | $C_8H_6N_2O_4$ | 1.80 | 1.95 |
| 867. 3-Nitro-$\beta$-nitrostyrene | $C_8H_6N_2O_4$ | 1.82 | 1.95 |
| 868. 4-Nitro-$\beta$-nitrostyrene | $C_8H_6N_2O_4$ | 1.89 | 1.95 |
| 869. Piperonal | $C_8H_6O_3$ | 1.05 | 1.18 |
| 870. Isophthalic acid | $C_8H_6O_4$ | 1.66 | 1.37 |
| 871. *p*-Bromoacetophenone | $C_8H_7BrO$ | 2.43 | 2.65 |
| 872. 2-Bromophenylacetate | $C_8H_7BrO_2$ | 2.20 | 2.79 |
| 873. *m*-Bromophenylacetic acid | $C_8H_7BrO_2$ | 2.37 | 2.32 |
| 874. *p*-Bromophenylacetic acid | $C_8H_7BrO_2$ | 2.31 | 2.32 |
| 875. 2-Bromophenoxyacetic acid | $C_8H_7BrO_3$ | 2.10 | 2.25 |
| 876. 3-Bromophenoxyacetic acid | $C_8H_7BrO_3$ | 2.22 | 2.22 |
| 877. 4-Bromophenoxyacetic acid | $C_8H_7BrO_3$ | 2.45 | 2.22 |
| 878. 2-(2,4,6-Tribromophenoxy)ethanol | $C_8H_7Br_3O_2$ | 3.42 | 3.83 |
| 879. *p*-Chloroacetophenone | $C_8H_7ClO$ | 2.35 | 2.39 |
| 880. 2-Chlorophenylacetate | $C_8H_7ClO_2$ | 2.18 | 2.91 |
| 881. 3-Chlorophenylacetate | $C_8H_7ClO_2$ | 2.32 | 2.49 |
| 882. *m*-Chlorophenylacetic acid | $C_8H_7ClO_2$ | 2.09 | 2.06 |
| 883. *p*-Chlorophenylacetic acid | $C_8H_7ClO_2$ | 2.12 | 2.06 |
| 884. *m*-Chlorophenoxyacetic acid | $C_8H_7ClO_3$ | 2.03 | 1.96 |
| 885. *o*-Chlorophenoxyacetic acid | $C_8H_7ClO_3$ | 2.02 | 2.37 |
| 886. *p*-Chlorophenoxyacetic acid | $C_8H_7ClO_3$ | 1.99 | 1.96 |
| 887. 2-Fluorophenylacetate | $C_8H_7FO_2$ | 1.76 | 2.17 |
| 888. 3-Fluorophenylacetate | $C_8H_7FO_2$ | 1.74 | 2.10 |
| 889. *m*-Fluorophenyl acetic acid | $C_8H_7FO_2$ | 1.65 | 1.66 |
| 890. *o*-Fluorophenyl acetic acid | $C_8H_7FO_2$ | 1.50 | 1.66 |
| 891. *p*-Fluorophenyl acetic acid | $C_8H_7FO_2$ | 1.55 | 1.66 |
| 892. *m*-Fluorophenoxyacetic acid | $C_8H_7FO_3$ | 1.48 | 1.56 |
| 893. *o*-Fluorophenoxyacetic acid | $C_8H_7FO_3$ | 1.26 | 1.63 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 894. *p*-Fluorophenoxyacetic acid | $C_8H_7FO_3$ | 1.41 | 1.56 |
| 895. 2-Iodophenylacetate | $C_8H_7IO_2$ | 2.55 | 3.11 |
| 896. *m*-Iodophenylacetic acid | $C_8H_7IO_2$ | 2.62 | 2.70 |
| 897. *p*-Iodophenylacetic acid | $C_8H_7IO_2$ | 2.64 | 2.70 |
| 898. 2-Iodophenoxyacetic acid | $C_8H_7IO_3$ | 2.19 | 2.57 |
| 899. 3-Iodophenoxyacetic acid | $C_8H_7IO_3$ | 2.44 | 2.60 |
| 900. 4-Iodophenoxyacetic acid | $C_8H_7IO_3$ | 2.69 | 2.60 |
| 901. *m*-Acetylnitrobenzene | $C_8H_7NO_3$ | 1.42 | 1.47 |
| 902. *p*-Acetylnitrobenzene | $C_8H_7NO_3$ | 1.49 | 1.47 |
| 903. 3-Hydroxy-$\beta$-nitrostyrene | $C_8H_7NO_3$ | 2.07 | 1.42 |
| 904. 4-Hydroxy-$\beta$-nitrostyrene | $C_8H_7NO_3$ | 2.12 | 1.42 |
| 905. 2-Nitrophenylacetate | $C_8H_7NO_4$ | 1.55 | 2.32 |
| 906. 3-Nitrophenylacetate | $C_8H_7NO_4$ | 1.82 | 1.57 |
| 907. 4-Nitrophenylacetate | $C_8H_7NO_4$ | 1.49 | 1.57 |
| 908. *m*-Nitrophenylacetic acid | $C_8H_7NO_4$ | 1.45 | 1.13 |
| 909. *p*-Nitrophenylacetic acid | $C_8H_7NO_4$ | 1.39 | 1.13 |
| 910. *m*-Nitrophenoxyacetic acid | $C_8H_7NO_5$ | 1.37 | 1.04 |
| 911. *o*-Nitrophenoxyacetic acid | $C_8H_7NO_6$ | 1.22 | 1.78 |
| 912. *p*-Nitrophenoxyacetic acid | $C_8H_7NO_5$ | 1.48 | 1.04 |
| 913. Benzylisothiocyanate | $C_8H_7NS$ | 2.83 | 2.88 |
| 914. Benzylthiocyanate | $C_8H_7NS$ | 1.99 | 2.20 |
| 915. 2-Aminoquinazoline-4-one | $C_8H_7N_3O$ | 0.60 | 0.60 |
| 916. 1-Carboxymethylbenzotriazole | $C_8H_7N_3O_2$ | −1.88 | −1.29 |
| 917. 3,5-Dinitro-4-methylbenzamide | $C_8H_7N_3O_5$ | 0.68 | 0.51 |
| 918. *N*-Methyl-3-bromophenylcarbamate | $C_8H_8BrNO_2$ | 2.25 | 2.22 |
| 919. *N*-Methyl-4-bromophenylcarbamate | $C_8H_8BrNO_2$ | 2.17 | 2.22 |
| 920. *p*-Chloroacetanilide | $C_8H_8ClNO$ | 1.87 | 1.76 |
| 921. *N*-Methyl-4-chlorophenylcarbamate | $C_8H_8ClNO_2$ | 2.01 | 1.96 |
| 922. *N*-Methyl-2-chlorophenylcarbamate | $C_8H_8ClNO_2$ | 1.64 | 1.44 |
| 923. *N*-Methyl-3-chlorophenylcarbamate | $C_8H_8ClNO_2$ | 2.03 | 1.96 |
| 924. *N*-Methyl-2-bromophenylcarbamate | $C_8H_8BrNO_2$ | 1.77 | 1.63 |
| 925. *N*-Methyl-2-fluorophenylcarbamate | $C_8H_8FNO_2$ | 1.25 | 1.27 |
| 926. *N*-Methyl-3-fluorophenylcarbamate | $C_8H_8FNO_2$ | 1.48 | 1.56 |
| 927. *N*-Methyl-4-fluorophenylcarbamate | $C_8H_8FNO_2$ | 1.28 | 1.56 |
| 928. *N*-Methyl-2-iodophenylcarbamate | $C_8H_8INO_2$ | 1.96 | 1.84 |
| 929. *N*-Methyl-3-iodophenylcarbamate | $C_8H_8INO_2$ | 2.52 | 2.61 |
| 930. *N*-Methyl-4-iodophenylcarbamate | $C_8H_8INO_2$ | 2.46 | 2.61 |
| 931. Isophthalamide | $C_8H_8N_2O_2$ | −0.21 | −0.92 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 932. *p*-Nitroacetanilide | $C_8H_8N_2O_3$ | 1.66 | 0.84 |
| 933. *N*-Methyl-2-nitrophenylcarbamate | $C_8H_8N_2O_4$ | 1.02 | 1.11 |
| 934. *N*-Methyl-3-nitrophenylcarbamate | $C_8H_8N_2O_4$ | 1.39 | 1.04 |
| 935. *N*-Methyl-4-nitrophenylcarbamate | $C_8H_8N_2O_4$ | 1.47 | 1.04 |
| 936. Phenylthioacetic acid | $C_8H_8O_2S$ | 1.91 | 2.04 |
| 937. *m*-Acetylphenol | $C_8H_8O_2$ | 1.39 | 0.93 |
| 938. *p*-Acetylphenol | $C_8H_8O_2$ | 1.35 | 0.93 |
| 939. *o*-Hydroxyacetophenone | $C_8H_8O_2$ | 1.92 | 1.96 |
| 940. *p*-Methiobenzoic acid | $C_8H_8O_2S$ | 2.74 | 2.33 |
| 941. Vanillin | $C_8H_8O_3$ | 1.31 | 0.88 |
| 942. *m*-Carbomethoxyphenol | $C_8H_8O_3$ | 1.89 | 1.26 |
| 943. *p*-Carbomethoxyphenol | $C_8H_8O_3$ | 1.96 | 1.26 |
| 944. *m*-Hydroxyphenylacetate | $C_8H_8O_3$ | 1.23 | 1.04 |
| 945. *m*-Hydroxyphenylacetic acid | $C_8H_8O_3$ | 0.85 | 0.60 |
| 946. *o*-Hydroxyphenylacetic acid | $C_8H_8O_3$ | 0.85 | 0.60 |
| 947. Isovanillin | $C_8H_8O_3$ | 0.97 | 0.88 |
| 948. *m*-Methoxybenzoic acid | $C_8H_8O_3$ | 2.02 | 1.60 |
| 949. *o*-Methoxybenzoic acid | $C_8H_8O_3$ | 1.59 | 2.63 |
| 950. *p*-Methoxybenzoic acid | $C_8H_8O_3$ | 1.96 | 1.60 |
| 951. Methyl salicyate | $C_8H_8O_3$ | 2.46 | 2.29 |
| 952. Phenoxyacetic acid | $C_8H_8O_3$ | 1.26 | 1.31 |
| 953. *o*-Vanillin | $C_8H_8O_3$ | 1.37 | 0.17 |
| 954. *m*-Hydroxyphenoxyacetic acid | $C_8H_8O_4$ | 0.76 | 0.50 |
| 955. *o*-Hydroxyphenoxyacetic acid | $C_8H_8O_4$ | 0.85 | 0.50 |
| 956. *p*-Hydroxyphenoxyacetic acid | $C_8H_8O_4$ | 0.65 | 0.50 |
| 957. 4,5,6-Tribromo-2-trifluoromethylbenzimidazole | $C_8H_2Br_3F_3N_2$ | 4.08 | 3.86 |
| 958. 5,6-Dibromo-2-trifluoromethylbenzimidazole | $C_8H_3Br_2F_3N_2$ | 4.15 | 4.02 |
| 959. 5-Chloro-6-nitro-2-trifluoromethylbenzimidazole | $C_8H_3ClF_3N_3O_2$ | 3.21 | 2.62 |
| 960. 2-Trifluoromethyl-5,6-dichlorobenzimidazole | $C_8H_3Cl_2F_3N_2$ | 3.99 | 3.76 |
| 961. 2-Trifluoromethyl-5,6-dinitrobenzimidazole | $C_8H_3F_3N_4O_4$ | 3.89 | 1.96 |
| 962. 2-Trifluoromethyl-5-bromobenzimidazole | $C_8H_4BrF_3N_2$ | 3.57 | 3.49 |
| 963. 2-Trifluoromethyl-5-chlorobenzimidazole | $C_8H_4BrF_3N_2$ | 3.39 | 3.23 |
| 964. 2-Trifluoromethyl-5-nitrobenzimidazole | $C_8H_4F_3N_3O_2$ | 2.68 | 2.31 |
| 965. *m*-$CF_3$-Trifluoromethane sulfonanilide | $C_8H_5F_6NO_2S$ | 4.50 | 3.46 |
| 966. *p*-$CF_3$-Trifluoromethane sulfonanilide | $C_8H_5F_6NO_2S$ | 4.47 | 3.46 |
| 967. Trifluoroacetanilide | $C_8H_6F_3NO$ | 2.21 | 2.27 |
| 968. 7-Chloro-3-methyl-2*H*-1,2,4-benzothiodiazine 1,1-dioxide | $C_8H_7ClN_2O_2S$ | 1.20 | 1.27 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 969. 6-Chloro-3-methyl-2*H*-1,2,4-benzothiodiazine 1,1-dioxide | $C_8H_7ClN_2O_2S$ | 1.21 | 1.27 |
| 970. 8-Chloro-3-methyl-2*H*-1,2,4-benzothiodiazine 1,1-dioxide | $C_8H_7ClN_2O_2S$ | 0.62 | 0.62 |
| 971. 5-Chloro-2(methylthio)benzimidazole | $C_8H_7ClN_2S$ | 3.22 | 0.94 |
| 972. 2,3-Dichloro-*N*-methylphenylcarbamate | $C_8H_7Cl_2NO_2$ | 2.48 | 2.74 |
| 973. 2,5-Dichloro-*N*-methylphenylcarbamate | $C_8H_7Cl_2NO_2$ | 2.44 | 2.32 |
| 974. *N*-Methyl-3,4-dichlorophenylcarbamate | $C_8H_7Cl_2NO_2$ | 2.80 | 2.69 |
| 975. *N*-Methyl-3,5-dichlorophenylcarbamate | $C_8H_7Cl_2NO_2$ | 3.03 | 2.80 |
| 976. 3-Amino-4-chlorophenoxyacetic acid | $C_8H_8ClNO_3$ | 1.16 | 1.07 |
| 977. 4-Methylphenylisothiocyanate | $C_8H_7NS$ | 3.92 | 3.68 |
| 978. *p*-Fluoroacetanilide | $C_8H_8FNO$ | 1.47 | 1.36 |
| 979. *p*-Acetamide-benzenesulfonylfluoride | $C_8H_8FNO_3S$ | 2.17 | 1.23 |
| 980. *p*-Iodoacetanilide | $C_8H_8INO$ | 2.46 | 2.41 |
| 981. *N*-Methyl-2-iodophenylcarbamate | $C_8H_8INO_2$ | 1.94 | 2.21 |
| 982. 3-Methyl-1,2,4-benzothiodiazine-1,1-dioxide | $C_8H_8N_2O_2S$ | 0.29 | 0.63 |
| 983. *p*-Methoxybenzaldehyde | $C_8H_8O_2$ | 1.59 | 1.46 |
| 984. 3,4-Methylenedioxy benzyl alcohol | $C_8H_8O_3$ | 1.05 | 0.46 |
| 985. *p*-Hydroxybenzoic acid methyl ester | $C_8H_8O_3$ | 1.92 | 1.26 |
| 986. Mandelic acid | $C_8H_8O_3$ | 0.62 | 0.62 |
| 987. *p*-Methylsulfonylbenzoic acid | $C_8H_8O_4S$ | 0.67 | 0.39 |
| 988. 1-Acetoxypentachlorocyclohexane | $C_8H_9Cl_5O_2$ | 3.40 | 3.40 |
| 989. *p*-Aminoacetophenone | $C_8H_9NO$ | 0.41 | 0.45 |
| 990. Ethyl-4-pyridyl ketone | $C_8H_9NO$ | 0.77 | 0.68 |
| 991. *o*-Methylbenzaldoxime | $C_8H_9NO$ | 2.53 | 2.35 |
| 992. *p*-Aminophenylacetate | $C_8H_9NO_2$ | −0.16 | 0.55 |
| 993. *o*-Benzylcarbamate | $C_8H_9NO_2$ | 1.20 | 0.56 |
| 994. *N*-Phenylglycine | $C_8H_9NO_2$ | 0.62 | −0.68 |
| 995. *m*-Hydroxyacetoanilide | $C_8H_9NO_2$ | 0.73 | 0.31 |
| 996. *o*-Hydroxyacetoanilide | $C_8H_9NO_2$ | 0.72 | 0.80 |
| 997. *p*-Hydroxyacetoanilide | $C_8H_9NO_2$ | 0.36 | 0.31 |
| 998. *m*-Methoxybenzamide | $C_8H_9NO_2$ | 0.85 | 0.45 |
| 999. *o*-Methoxybenzamide | $C_8H_9NO_2$ | 0.87 | 1.63 |
| 1000. *p*-Methoxybenzamide | $C_8H_9NO_2$ | 0.86 | 0.45 |
| 1001. *m*-Methoxyformanilide | $C_8H_9NO_2$ | 1.25 | 0.93 |
| 1002. *p*-Methoxyformanilide | $C_8H_9NO_2$ | 1.03 | 0.93 |
| 1003. 2-Methyl-4-aminobenzoic acid | $C_8H_9NO_2$ | 0.31 | 0.91 |
| 1004. 3-Methyl-4-aminobenzoic acid | $C_8H_9NO_2$ | 0.54 | 0.91 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1005. *N*-Methylphenylcarbamate | $C_8H_9NO_2$ | 1.24 | 1.51 |
| 1006. Nicotinic acid ethyl ester | $C_8H_9NO_2$ | 1.32 | 1.01 |
| 1007. Isonicotinic acid ethyl ester | $C_8H_9NO_2$ | 1.43 | 1.01 |
| 1008. Phenoxyacetamide | $C_8H_9NO_2$ | 0.76 | 0.76 |
| 1009. Picolinic acid ethyl ester | $C_8H_9NO_2$ | 0.87 | −0.17 |
| 1010. 2-Methoxy-4-aminobenzoic acid | $C_8H_9NO_3$ | −0.38 | 1.32 |
| 1011. *p*-Nitrophenetole | $C_8H_9NO_3$ | 2.53 | 2.22 |
| 1012. Thioacetanilide | $C_8H_9NS$ | 1.71 | 1.71 |
| 1013. Sulfanilacetamide | $C_8H_{10}N_2O_3S$ | −0.96 | −1.62 |
| 1014. 1-Methyl-1-phenyl-2-thiourea | $C_8H_{10}N_2S$ | 0.85 | 0.85 |
| 1015. Caffeine | $C_8H_{10}N_4O_2$ | −0.07 | −1.39 |
| 1016. 1,3-Dimethoxybenzene | $C_8H_{10}O_2$ | 2.21 | 1.82 |
| 1017. *o*-Dimethoxybenzene | $C_8H_{10}O_2$ | 2.21 | 1.82 |
| 1018. *m*-Ethoxyphenol | $C_8H_{10}O_2$ | 1.98 | 1.68 |
| 1019. *o*-Ethoxyphenol | $C_8H_{10}O_2$ | 1.68 | 1.91 |
| 1020. *p*-Ethoxyphenol | $C_8H_{10}O_2$ | 1.81 | 1.68 |
| 1021. *o*-Methoxybenzyl alcohol | $C_8H_{10}O_2$ | 1.13 | 0.74 |
| 1022. *p*-Methoxybenzyl alcohol | $C_8H_{10}O_2$ | 1.10 | 0.74 |
| 1023. *m*-Dimethylaminophenol | $C_8H_{11}NO$ | 1.57 | 1.56 |
| 1024. *N,N*-Dimethylbenzenesulfonamide | $C_8H_{11}NO_2S$ | 1.35 | 1.51 |
| 1025. *p*-Ethylbenzenesulfonamide | $C_8H_{11}NO_2S$ | 1.31 | 1.45 |
| 1026. 3,6-Dimethoxy-1,2,4,5-tetrachlorocyclohexane | $C_8H_{12}Cl_4O_2$ | 3.15 | 3.14 |
| 1027. Barbital | $C_8H_{12}N_2O_3$ | 0.65 | 0.58 |
| 1028. 4-Pentylpyrazole | $C_8H_{14}N_2$ | 2.96 | 2.93 |
| 1029. Heptanoic acid | $C_8H_{14}O_3$ | 0.55 | 0.22 |
| 1030. *N*-Nitroso-octamethyleneimine | $C_8H_{16}N_2O$ | 2.04 | 2.04 |
| 1031. *N*-Nitroso-dibutylamine | $C_8H_{18}N_2O$ | 1.92 | 2.59 |
| 1032. Quinoline-1-oxide | $C_9H_7NO$ | 0.36 | 0.36 |
| 1033. 6-Chloro-4-nitroquinoline-1-oxide | $C_9H_5ClN_2O_3$ | 1.41 | 0.73 |
| 1034. 8-Fluoro-4-nitroquinoline-1-oxide | $C_9H_5FN_2O_3$ | 1.00 | 0.33 |
| 1035. 6-Cyanoquinoxaline | $C_9H_5N_3$ | 1.01 | 0.72 |
| 1036. 4,5-Dinitroquinoline-1-oxide | $C_9H_5N_3O_5$ | 0.95 | −0.19 |
| 1037. 4,6-Dinitroquinoline-1-oxide | $C_9H_5N_3O_5$ | 0.90 | −0.19 |
| 1038. 4,8-Dinitroquinoline-1-oxide | $C_9H_5N_3O_5$ | 0.76 | −0.19 |
| 1039. 3-Bromoquinoline | $C_9H_6BrN$ | 3.03 | 3.01 |
| 1040. 6-Bromoquinoline | $C_9H_6BrN$ | 2.83 | 3.01 |
| 1041. 7-Bromoquinoline | $C_9H_6BrN$ | 2.92 | 3.01 |
| 1042. 2-Chloroquinoline | $C_9H_6ClN$ | 2.71 | 2.96 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1043. 6-Chloroquinoline | $C_9H_6ClN$ | 2.73 | 2.74 |
| 1044. 8-Chloroquinoline | $C_9H_6ClN$ | 2.33 | 2.74 |
| 1045. 4-Chloro-8-quinolinol | $C_9H_6ClNO$ | 2.67 | 1.93 |
| 1046. 4-Chloroquinoline-1-oxide | $C_9H_6ClNO$ | 1.08 | 1.00 |
| 1047. 3-Cyano-4-chlorophenoxyacetic acid | $C_9H_6ClNO_3$ | 1.56 | 1.56 |
| 1048. 1,1,1,3,3,3-Hexafluoro-2-phenyl-2-propanol | $C_9H_6F_6O$ | 3.41 | 3.41 |
| 1049. 3-Nitroquinoline | $C_9H_6N_2O_2$ | 1.97 | 1.82 |
| 1050. 4-Nitroquinoline | $C_9H_6N_2O_2$ | 2.06 | 1.82 |
| 1051. 5-Nitroquinoline | $C_9H_6N_2O_2$ | 1.86 | 1.82 |
| 1052. 6-Nitroquinoline | $C_9H_6N_2O_2$ | 1.84 | 1.82 |
| 1053. 7-Nitroquinoline | $C_9H_6N_2O_2$ | 1.82 | 1.82 |
| 1054. 8-Nitroquinoline | $C_9H_6N_2O_2$ | 1.40 | 1.82 |
| 1055. 3-Nitroquinoline-1-oxide | $C_9H_6N_2O_3$ | 0.56 | 0.08 |
| 1056. 4-Nitroquinoline-1-oxide | $C_9H_6N_2O_3$ | 1.02 | 0.08 |
| 1057. 5-Nitroquinoline-1-oxide | $C_9H_6N_2O_3$ | 0.49 | 0.08 |
| 1058. 6-Nitroquinoline-1-oxide | $C_9H_6N_2O_3$ | 0.39 | 0.08 |
| 1059. 7-Nitroquinoline-1-oxide | $C_9H_6N_2O_3$ | 0.36 | 0.08 |
| 1060. 8-Nitroquinoline-1-oxide | $C_9H_6N_2O_3$ | 0.04 | 0.08 |
| 1061. Coumarin | $C_9H_6O_2$ | 1.39 | 2.03 |
| 1062. 1,3-Indandione | $C_9H_6O_2$ | 0.61 | 0.86 |
| 1063. Ninhydrin | $C_9H_6O_4$ | 0.65 | 0.65 |
| 1064. 3-Carboxy-4-chlorophenoxyacetic acid | $C_9H_7ClO_5$ | 1.07 | 1.02 |
| 1065. 3-Trifluoromethylphenylacetic acid | $C_9H_7F_3O_2$ | 2.62 | 2.42 |
| 1066. *m*-Trifluoromethylphenylacetic acid | $C_9H_7F_3O_2$ | 2.62 | 2.42 |
| 1067. *p*-Trifluoromethylphenylacetic acid | $C_9H_7F_3O_2$ | 2.45 | 2.42 |
| 1068. *m*-Trifluoromethylphenoxyacetic acid | $C_9H_7F_3O_3$ | 2.36 | 2.32 |
| 1069. *m*-Trifluoromethylthiophenoxyacetic acid | $C_9H_7F_3O_3S$ | 2.86 | 2.68 |
| 1070. *m*-Trifluoromethoxyphenoxyacetic acid | $C_9H_7F_3O_4$ | 2.48 | 2.28 |
| 1071. *m*-Trifluoromethylsulfonylphenoxyacetic acid | $C_9H_7F_3O_5S$ | 2.19 | 1.81 |
| 1072. 4-Hydroxyquinoline | $C_9H_7NO$ | 0.58 | 1.29 |
| 1073. 2-Quinolinol | $C_9H_7NO$ | 1.26 | 1.06 |
| 1074. 8-Quinolinol | $C_9H_7NO$ | 1.96 | 1.29 |
| 1075. $\alpha$-Quinolone | $C_9H_7NO$ | 1.26 | 1.30 |
| 1076. 2-Cyanophenylacetate | $C_9H_7NO_2$ | 1.33 | 1.33 |
| 1077. *m*-Cyanophenylacetic acid | $C_9H_7NO_2$ | 1.18 | 0.77 |
| 1078. *N*-Methylindol-2,3-dione | $C_9H_7NO_2$ | 0.58 | 0.74 |
| 1079. 4-Cyano-phenoxyacetic acid | $C_9H_7NO_3$ | 0.93 | 0.67 |
| 1080. 3-Cyano-phenoxyacetic acid | $C_9H_7NO_3$ | 0.95 | 0.67 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1081. 8-Aminoquinoline | $C_9H_8N_2$ | 1.79 | 0.80 |
| 1082. 2-Aminoquinoline | $C_9H_8N_2$ | 1.87 | 1.92 |
| 1083. 3-Aminoquinoline | $C_9H_8N_2$ | 1.63 | 0.80 |
| 1084. 4-Aminoquinoline | $C_9H_8N_2$ | 1.63 | 0.80 |
| 1085. 5-Aminoquinoline | $C_9H_8N_2$ | 1.16 | 0.80 |
| 1086. 6-Aminoquinoline | $C_9H_8N_2$ | 1.28 | 0.80 |
| 1087. 2-Methylquinoxaline | $C_9H_8N_2$ | 1.61 | 1.65 |
| 1088. 5-Methylquinoxaline | $C_9H_8N_2$ | 2.04 | 1.78 |
| 1089. 2-Phenylimidazole | $C_9H_8N_2$ | 1.88 | 1.88 |
| 1090. 5-Amino-8-hydroxyquinoline | $C_9H_8N_2O$ | −0.11 | −0.01 |
| 1091. 4-Aminoquinoline-1-oxide | $C_9H_8N_2O$ | 0.05 | −0.94 |
| 1092. 2-Methoxyquinoxaline | $C_9H_8N_2O$ | 2.31 | 2.00 |
| 1093. 3-Methyl-quinazoline-4-one | $C_9H_8N_2O$ | 0.69 | 0.87 |
| 1094. *N*-Methyl-4-cyanophenylcarbamate | $C_9H_8N_2O_2$ | 0.95 | 0.87 |
| 1095. *N*-Methyl-3-cyanophenylcarbamate | $C_9H_8N_2O_2$ | 0.97 | 0.87 |
| 1096. *N*-Methyl-2-cyanophenylcarbamate | $C_9H_8N_2O_2$ | 0.86 | 0.87 |
| 1097. 8-Sulfonamidoquinoline | $C_9H_8N_2O_2S$ | 0.36 | 0.41 |
| 1098. 2-Methioquinoxaline | $C_9H_8N_2S$ | 2.79 | 2.77 |
| 1099. Aspirin | $C_9H_8O_4$ | 1.23 | 1.23 |
| 1100. *m*-Carboxyphenylacetic acid | $C_9H_8O_4$ | 1.14 | 0.99 |
| 1101. *p*-Formylphenoxyacetic acid | $C_9H_8O_4$ | 0.79 | 0.76 |
| 1102. *m*-Carboxyphenoxyacetic acid | $C_9H_8O_5$ | 1.11 | 0.90 |
| 1103. 5-Methoxyindole | $C_9H_9NO$ | 2.06 | 1.83 |
| 1104. *p*-Acetylformanilide | $C_9H_9NO_2$ | 0.94 | 0.66 |
| 1105. *N*-Acetyl-*o*-aminobenzoic acid | $C_9H_9NO_3$ | 1.88 | 1.82 |
| 1106. *N*-Acetyl-*p*-aminobenzoic acid | $C_9H_9NO_3$ | 1.31 | 0.70 |
| 1107. 4-Methoxy-$\beta$-nitrostyrene | $C_9H_9NO_3$ | 2.20 | 2.03 |
| 1108. 3-Methoxy-$\beta$-nitrostyrene | $C_9H_9NO_3$ | 2.37 | 2.03 |
| 1109. 2-Phenethylisothiocyanate | $C_9H_9NS$ | 3.47 | 3.25 |
| 1110. 1-Phenethylisothiocyanate | $C_9H_9NS$ | 3.46 | 3.46 |
| 1111. Sulfathiazole | $C_9H_9N_3O_2S_2$ | 0.05 | −1.16 |
| 1112. *DL*-*p*-Chlorophenylalanine | $C_9H_{10}ClNO_2$ | −0.48 | −0.61 |
| 1113. Phenylalanine | $C_9H_{11}NO_2$ | −1.35 | −1.26 |
| 1114. *DL*-*p*-Fluorophenylalanine | $C_9H_{10}FNO_2$ | −1.89 | −1.01 |
| 1115. 5,6-Dimethylbenzimidazole | $C_9H_{10}N_2$ | 2.35 | 2.32 |
| 1116. *p*-*N*-Acetylaminobenzamide | $C_9H_{10}N_2O_2$ | 0.01 | −0.45 |
| 1117. *p*-Nitrophenylalanine | $C_9H_{10}N_2O_4$ | −1.25 | −1.53 |
| 1118. 3-Ureido-phenoxyacetic acid | $C_9H_{10}N_2O_4$ | 0.26 | 0.09 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1119. *o*-Hydroxypropiophenone | $C_9H_{10}O_2$ | 2.54 | 2.45 |
| 1120. *p*-Hydroxypropiophenone | $C_9H_{10}O_2$ | 2.03 | 1.42 |
| 1121. *p*-Methoxyacetophenone | $C_9H_{10}O_2$ | 1.82 | 1.55 |
| 1122. *p*-Hydroxybenzoic acid ethyl ester | $C_9H_{10}O_3$ | 2.47 | 1.74 |
| 1123. 2-Methoxyphenylacetate | $C_9H_{10}O_3$ | 1.38 | 1.18 |
| 1124. 4-Methoxyphenylacetate | $C_9H_{10}O_3$ | 1.54 | 1.66 |
| 1125. *m*-Methoxyphenylacetic acid | $C_9H_{10}O_3$ | 1.50 | 1.22 |
| 1126. *p*-Methoxyphenylacetic acid | $C_9H_{10}O_3$ | 1.42 | 1.22 |
| 1127. *m*-Methylphenoxyacetic acid | $C_9H_{10}O_3$ | 1.78 | 1.73 |
| 1128. *o*-Methylphenoxyacetic acid | $C_9H_{10}O_3$ | 1.98 | 1.73 |
| 1129. *p*-Methylphenoxyacetic acid | $C_9H_{10}O_3$ | 1.86 | 1.73 |
| 1130. 2-Methoxyphenoxyacetic acid | $C_9H_{10}O_4$ | 0.98 | 1.34 |
| 1131. 4-Methoxyphenoxyacetic acid | $C_9H_{10}O_4$ | 1.23 | 1.12 |
| 1132. 3-Methoxyphenoxyacetic acid | $C_9H_{10}O_4$ | 1.38 | 1.12 |
| 1133. *m*-Methylsulfonylphenylacetic acid | $C_9H_{10}O_4S$ | 0.06 | 0.01 |
| 1134. *m*-Methylsulfonylphenoxyacetic acid | $C_9H_{10}O_5S$ | 0.01 | −0.09 |
| 1135. 1,1-Dimethyl-3-*p*-chlorophenylurea | $C_9H_{11}ClN_2O$ | 1.94 | 1.96 |
| 1136. 1,1-Dimethyl-3-*m*-chlorophenylurea | $C_9H_{11}ClN_2O$ | 2.00 | 1.96 |
| 1137. 3-Methylthiophenoxyacetic acid | $C_9H_{10}O_3S$ | 1.90 | 1.85 |
| 1138. *o*-Aminobenzoic acid ethyl ester | $C_9H_{11}NO_2$ | 2.57 | 2.38 |
| 1139. *N*-Dimethylphenylcarbamate | $C_9H_{11}NO_2$ | 1.69 | 1.17 |
| 1140. *p*-Ethoxybenzamide | $C_9H_{11}NO_2$ | 1.30 | 0.93 |
| 1141. *N*-Phenylethylcarbamate | $C_9H_{11}NO_2$ | 2.30 | 1.58 |
| 1142. *o*-Methoxyacetanilide | $C_9H_{11}NO_2$ | 0.98 | 1.42 |
| 1143. *p*-Methoxyacetanilide | $C_9H_{11}NO_2$ | 1.03 | 0.92 |
| 1144. Tsumacide | $C_9H_{11}NO_2$ | 1.70 | 1.93 |
| 1145. *N*-methyl-o-tolylcarbamate | $C_9H_{11}NO_2$ | 1.46 | 1.93 |
| 1146. *N*-methyl-*p*-tolylcarbamate | $C_9H_{11}NO_2$ | 1.66 | 1.93 |
| 1147. *N*-Methyl-4-methylthiophenylcarbamate | $C_9H_{11}NO_2S$ | 1.92 | 2.05 |
| 1148. *N*-Methyl-2-methylthiophenylcarbamate | $C_9H_{11}NO_2S$ | 1.51 | 1.44 |
| 1149. 2-Ethoxy-4-aminobenzoic acid | $C_9H_{11}NO_3$ | 0.16 | 1.81 |
| 1150. *N*-Methyl-2-methoxyphenylcarbamate | $C_9H_{11}NO_3$ | 0.81 | 0.84 |
| 1151. *N*-Methyl-3-methoxyphenylcarbamate | $C_9H_{11}NO_3$ | 1.30 | 1.32 |
| 1152. *N*-Methyl-4-methoxyphenylcarbamate | $C_9H_{11}NO_3$ | 1.20 | 1.32 |
| 1153. 2-Tyrosine | $C_9H_{11}NO_3$ | −2.26 | −2.07 |
| 1154. 1-Propylbenzotriazole | $C_9H_{11}N_3$ | 2.13 | 2.12 |
| 1155. 1-Isopropylbenzotriazole | $C_9H_{11}N_3$ | 1.98 | 1.88 |
| 1156. 1,1-Dimethyl-3-*p*-nitrophenylurea | $C_9H_{11}N_3O_3$ | 1.51 | 1.03 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1157. Nornicotine | $C_9H_{12}N_2$ | 0.17 | 0.24 |
| 1158. *m*-Dimethylaminobenzamide | $C_9H_{12}N_2O$ | 0.95 | 0.81 |
| 1159. *p*-Dimethylaminobenzamide | $C_9H_{12}N_2O$ | 1.14 | 0.81 |
| 1160. *p*-Aminophenylalanine | $C_9H_{12}N_2O_2$ | −2.20 | −2.55 |
| 1161. 1-Phenyl-3-ethylthiourea | $C_9H_{12}N_2S$ | 1.42 | 1.42 |
| 1162. *o*-Isopropoxyphenol | $C_9H_{12}O_2$ | 2.09 | 2.26 |
| 1163. 1,2,3-Trimethoxybenzene | $C_9H_{12}O_3$ | 1.53 | 1.51 |
| 1164. *N,N*-Dimethyl-*o*-anisidine | $C_9H_{13}NO$ | 1.63 | 2.32 |
| 1165. *N,N*-Dimethyl-*p*-anisidine | $C_9H_{13}NO$ | 1.42 | 2.18 |
| 1166. *p*-Propylbenzenesulfonamide | $C_9H_{13}NO_2S$ | 1.64 | 1.99 |
| 1167. Probarbital | $C_9H_{14}N_2O_3$ | 0.97 | 1.04 |
| 1168. *N*-Methyl-5-butylbarbituric acid | $C_9H_{14}N_2O_3$ | 1.10 | 1.10 |
| 1169. 1,3-Dibutyryl urea | $C_9H_{16}N_2O_3$ | 1.40 | 1.30 |
| 1170. Azelaic acid | $C_9H_{16}O_4$ | 1.57 | 1.48 |
| 1171. 4-Tertbutyl-*N*-nitrosopiperidine | $C_9H_{18}N_2O$ | 1.96 | 2.45 |
| 1172. 2,2,6,6-Tetramethyl-*N*-nitrosopiperidine | $C_9H_{18}N_2O$ | 2.49 | 1.57 |
| 1173. Meprobamate | $C_9H_{18}N_2O_4$ | 0.70 | −0.12 |
| 1174. Hexamethylmelamine | $C_9H_{18}N_6$ | 2.52 | 2.63 |
| 1175. 2-Chloro-1,4-naphthoquinone | $C_{10}H_5ClO_2$ | 2.15 | 0.14 |
| 1176. 7-Trifluoromethylquinoline | $C_{10}H_6F_3N$ | 3.02 | 3.10 |
| 1177. 8-Trifluoromethylquinoline | $C_{10}H_6F_3N$ | 2.50 | 3.10 |
| 1178. 4-Hydroxy-7-trifluoromethylquinoline | $C_{10}H_6F_3NO$ | 2.05 | 2.29 |
| 1179. 1,4-Naphthoquinone | $C_{10}H_6O_2$ | 1.78 | 1.70 |
| 1180. 2-Hydroxy-1,4-naphthoquinone | $C_{10}H_6O_3$ | 1.38 | 0.55 |
| 1181. 2-Trifluoromethyl-4,7-dichloro-5,6-dimethyl-benzimidazole | $C_{10}H_7Cl_2F_3N_2$ | 3.19 | 4.31 |
| 1182. 3,4,5-Tri-Cl-$C_6H_2NHN{=}C(CN)COOCH_3$ | $C_{10}H_6Cl_3N_3O_2$ | 5.22 | 5.01 |
| 1183. 2,4,5-Tri-Cl-$C_6H_2NHN{=}C(CN)COOCH_3$ | $C_{10}H_6Cl_3N_3O_2$ | 5.15 | 5.74 |
| 1184. 3,4-Dichloro-$C_6H_3NHN{=}C(CN)CO\text{-}CH_3$ | $C_{10}H_7Cl_2N_3O$ | 4.56 | 4.36 |
| 1185. 3,5-Dichloro-$C_6H_3NHN{=}C(CN)CO\text{-}CH_3$ | $C_{10}H_7Cl_2N_3O$ | 4.68 | 4.48 |
| 1186. 3,5-Dichloro-$C_6H_3NHN{=}C(CN)COOCH_3$ | $C_{10}H_7Cl_2N_3O_2$ | 4.50 | 4.81 |
| 1187. 2-Nitroso-1-naphthol | $C_{10}H_7NO_2$ | 2.57 | 2.39 |
| 1188. 1-Nitroso-2-naphthol | $C_{10}H_7NO_2$ | 2.28 | 2.39 |
| 1189. 2-Cl-$C_6H_4NHN{=}C(CN)CO\text{-}CH_3$ | $C_{10}H_8ClN_3O$ | 4.01 | 4.24 |
| 1190. 3-Cl-$C_6H_4NHN{=}C(CN)CO\text{-}CH_3$ | $C_{10}H_8ClN_3O$ | 3.91 | 3.83 |
| 1191. 4-Cl-$C_6H_4NHN{=}C(CN)CO\text{-}CH_3$ | $C_{10}H_8ClN_3O$ | 4.13 | 3.83 |
| 1192. 3-Cl-$C_6H_4NHN{=}C(CN)COOCH_3$ | $C_{10}H_8ClN_3O_2$ | 3.56 | 4.16 |
| 1193. *N*-Formyl-*p*-cyanostrylamine | $C_{10}H_8N_2O$ | 1.58 | 1.47 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1194. 2-Methyl-4-nitroquinoline-1-oxide | $C_{10}H_8N_2O_3$ | 1.25 | 0.57 |
| 1195. 3-Methyl-4-nitroquinoline-1-oxide | $C_{10}H_8N_2O_3$ | 1.06 | 0.50 |
| 1196. 5-Methyl-4-nitroquinoline-1-oxide | $C_{10}H_8N_2O_3$ | 1.36 | 0.50 |
| 1197. 6-Methyl-4-nitroquinoline-1-oxide | $C_{10}H_8N_2O_3$ | 1.43 | 0.50 |
| 1198. 7-Methyl-4-nitroquinoline-1-oxide | $C_{10}H_8N_2O_3$ | 1.42 | 0.50 |
| 1199. 8-Methyl-4-nitroquinoline-1-oxide | $C_{10}H_8N_2O_3$ | 1.59 | 0.50 |
| 1200. Hymecromone | $C_{10}H_8O_3$ | 1.58 | 1.80 |
| 1201. 6-Methoxyquinoline | $C_{10}H_9NO$ | 2.20 | 1.90 |
| 1202. 7-Methoxyquinoline | $C_{10}H_9NO$ | 2.37 | 1.90 |
| 1203. 8-Methoxyquinoline | $C_{10}H_9NO$ | 1.84 | 1.90 |
| 1204. *N*-Methyl-*α*-quinolone | $C_{10}H_9NO$ | 1.45 | 0.96 |
| 1205. *N*-Methyl-4-quinolone | $C_{10}H_9NO$ | 0.44 | 2.68 |
| 1206. 2-Methyl-8-quinolinol | $C_{10}H_9NO$ | 2.33 | 1.77 |
| 1207. 4-Methyl-8-quinolinol | $C_{10}H_9NO$ | 2.41 | 1.73 |
| 1208. Indole-3-acetic acid | $C_{10}H_9NO_2$ | 1.41 | 1.23 |
| 1209. 5-Methoxy-8-quinolinol | $C_{10}H_9NO_2$ | 2.06 | 1.09 |
| 1210. 4-Methyl-5,8-dihydroxyquinoline | $C_{10}H_9NO_2$ | 1.59 | 0.89 |
| 1211. 3-Acetamido-4-chlorophenoxyacetic acid | $C_{10}H_{10}ClNO_4$ | 0.75 | 1.28 |
| 1212. 6,7-Dimethylquinoxaline | $C_{10}H_{10}N_2$ | 2.29 | 2.20 |
| 1213. Sulfadiazine | $C_{10}H_{10}N_4O_2S$ | −0.13 | −0.21 |
| 1214. Benzoylacetone | $C_{10}H_{10}O_2$ | 2.52 | 1.45 |
| 1215. 4-Acetyl-phenoxyacetic acid | $C_{10}H_{10}O_4$ | 0.87 | 0.85 |
| 1216. 3-Acetyl-phenoxyacetic acid | $C_{10}H_{10}O_4$ | 0.98 | 0.85 |
| 1217. 2-Acetyl-phenoxyacetic acid | $C_{10}H_{10}O_4$ | 1.25 | 1.88 |
| 1218. 1,1-Dimethyl-3-*m*-$CF_3$-phenylurea | $C_{10}H_{11}F_3N_2O$ | 2.36 | 2.32 |
| 1219. 3-Allyloxy-4-aminobenzoic acid | $C_{10}H_{11}NO_3$ | 0.42 | 1.15 |
| 1220. *N*-Methyl-3-acetylphenylcarbamate | $C_{10}H_{11}NO_3$ | 0.90 | 1.05 |
| 1221. *N*-Methyl-4-acetylphenylcarbamate | $C_{10}H_{11}NO_3$ | 1.01 | 1.05 |
| 1222. *m*-Acetamide-phenoxyacetic acid | $C_{10}H_{11}NO_4$ | 0.48 | 0.22 |
| 1223. Sulfamethoxazole | $C_{10}H_{11}N_3O_3S$ | 0.88 | 0.88 |
| 1224. 2,5-Dimethyl-4-chloro-*N*-methylphenylcarbamate | $C_{10}H_{12}ClNO_2$ | 2.95 | 3.00 |
| 1225. Serotonin | $C_{10}H_{12}N_2O$ | 0.21 | 0.54 |
| 1226. *m*-Diacetamidobenzene | $C_{10}H_{12}N_2O_2$ | 0.50 | 0.03 |
| 1227. 4-Dimethylamino-*β*-nitrostyrene | $C_{10}H_{12}N_2O_2$ | 2.67 | 2.39 |
| 1228. Allobarbital | $C_{10}H_{12}N_2O_3$ | 0.94 | 0.61 |
| 1229. 4-Ethoxyphenylacetate | $C_{10}H_{12}O_3$ | 1.95 | 2.14 |
| 1230. Ethylmandelate | $C_{10}H_{12}O_3$ | 0.91 | 1.39 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1231. *p*-Hydroxybenzoic acid propyl ester | $C_{10}H_{12}O_3$ | 3.04 | 2.28 |
| 1232. *o*-Methylphenoxyacetic acid methyl ester | $C_{10}H_{12}O_3$ | 2.08 | 2.01 |
| 1233. 3-Ethylphenoxyacetic acid | $C_{10}H_{12}O_3$ | 2.25 | 2.25 |
| 1234. 2-Ethylphenoxyacetic acid | $C_{10}H_{12}O_3$ | 2.53 | 2.25 |
| 1235. *N*-Phenylmorpholine | $C_{10}H_{13}NO$ | 1.36 | 1.95 |
| 1236. 4-Ethoxyacetanilide | $C_{10}H_{13}NO_2$ | 1.58 | 1.41 |
| 1237. 2,3-Dimethyl-4-hydroxyacetanilide | $C_{10}H_{13}NO_2$ | 1.06 | 1.14 |
| 1238. 2,5-Dimethyl-4-hydroxyacetanilide | $C_{10}H_{13}NO_2$ | 1.09 | 1.14 |
| 1239. 2,6-Dimethyl-4-hydroxyacetanilide | $C_{10}H_{13}NO_2$ | 0.80 | 1.14 |
| 1240. *N,N*-Dimethylphenoxyacetamide | $C_{10}H_{13}NO_2$ | 0.77 | 0.93 |
| 1241. 3,5-Dimethyl-4-hydroxyacetanilide | $C_{10}H_{13}NO_2$ | 1.60 | 1.14 |
| 1242. 3-Ethyl-4-hydroxyacetanilide | $C_{10}H_{13}NO_2$ | 1.79 | 1.24 |
| 1243. Fusaric acid | $C_{10}H_{13}NO_2$ | −1.29 | 1.07 |
| 1244. *m*-Methoxy-*N,N*-dimethylbenzamide | $C_{10}H_{13}NO_2$ | 1.00 | 0.78 |
| 1245. *o*-Methoxy-*N,N*-dimethylbenzamide | $C_{10}H_{13}NO_2$ | 0.71 | 1.96 |
| 1246. *p*-Methoxy-*N,N*-dimethylbenzamide | $C_{10}H_{13}NO_2$ | 0.96 | 0.78 |
| 1247. *N*-Methyl-2-ethylphenylcarbamate | $C_{10}H_{13}NO_2$ | 1.93 | 2.45 |
| 1248. *N*-Methyl-3-ethylphenylcarbamate | $C_{10}H_{13}NO_2$ | 2.20 | 2.45 |
| 1249. *N*-Methyl-4-ethylphenylcarbamate | $C_{10}H_{13}NO_2$ | 2.23 | 2.45 |
| 1250. *N*-Methyl-2,3-dimethylphenylcarbamate | $C_{10}H_{13}NO_2$ | 1.95 | 2.35 |
| 1251. *N*-Methyl-2,5-dimethylphenylcarbamate | $C_{10}H_{13}NO_2$ | 2.03 | 2.35 |
| 1252. *N*-Methyl-3,4-dimethylphenylcarbamate | $C_{10}H_{13}NO_2$ | 2.09 | 2.35 |
| 1253. *N*-Methyl-3,5-dimethylphenylcarbamate | $C_{10}H_{13}NO_2$ | 2.23 | 2.35 |
| 1254. *m*-Tolyl-*N,N*-dimethylcarbamate | $C_{10}H_{13}NO_2$ | 2.05 | 1.59 |
| 1255. *o*-Tolyl-*N,N*-dimethylcarbamate | $C_{10}H_{13}NO_2$ | 1.86 | 1.59 |
| 1256. *p*-Tolyl-*N,N*-dimethylcarbamate | $C_{10}H_{13}NO_2$ | 2.03 | 1.59 |
| 1257. *N*-Methyl-3-methyl-4-methylthiophenylcarbamate | $C_{10}H_{13}NO_2S$ | 2.47 | 2.47 |
| 1258. 3-Methoxyphenyl-*N,N*-dimethylcarbamate | $C_{10}H_{13}NO_3$ | 1.60 | 0.97 |
| 1259. 4-Methoxyphenyl-*N,N*-dimethylcarbamate | $C_{10}H_{13}NO_3$ | 1.53 | 0.97 |
| 1260. *N*-Methyl-2-ethoxyphenylcarbamate | $C_{10}H_{13}NO_3$ | 1.24 | 1.32 |
| 1261. *N*-Methyl-3-ethoxyphenylcarbamate | $C_{10}H_{13}NO_3$ | 1.75 | 1.80 |
| 1262. *N*-Methyl-4-ethoxyphenylcarbamate | $C_{10}H_{13}NO_3$ | 1.63 | 1.80 |
| 1263. 2-Propoxy-4-aminobenzoic acid | $C_{10}H_{13}NO_3$ | 0.70 | 2.34 |
| 1264. 4-Sulfamoylbenzoic acid propyl ester | $C_{10}H_{13}NO_4S$ | 1.75 | 1.40 |
| 1265. 1-*s*-Butylbenzotriazole | $C_{10}H_{13}N_3$ | 2.31 | 2.42 |
| 1266. 3,5-Dimethoxy-4-bromophenethylamine | $C_{10}H_{14}BrNO_2$ | 2.03 | 3.18 |
| 1267. Anabasine | $C_{10}H_{14}N_2$ | 0.97 | 0.78 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1268. Nicotine | $C_{10}H_{14}N_2$ | 1.17 | 0.60 |
| 1269. Nikethamide | $C_{10}H_{14}N_2O$ | 0.33 | 0.31 |
| 1270. *N*-Methyl-3-dimethylaminophenylcarbamate | $C_{10}H_{14}N_2O_2$ | 1.43 | 1.68 |
| 1271. Ephedrine | $C_1OH_{15}NO$ | 1.12 | 1.03 |
| 1272. *p*-Butylbenzenesulfonamide | $C_{10}H_{15}NO_2S$ | 2.45 | 2.53 |
| 1273. 5-Butyl-5-ethylbarbituric acid | $C_{10}H_{16}N_2O_3$ | 1.89 | 1.65 |
| 1274. 2,6-Di-Cl-4-$CF_3$-$C_6H_2NHN=C(CN)COOCH_3$ | $C_{11}H_6Cl_2F_3N_3O_2$ | 4.36 | 6.63 |
| 1275. 2-$CF_3$-4-Cl-$C_6H_3NHN=C(CN)COOCH_3$ | $C_{11}H_7ClF_3N_3O_2$ | 4.66 | 5.17 |
| 1276. 2-$NO_2$-4-$CF_3$-$C_6H_3NHN=C(CN)COOCH_3$ | $C_{11}H_7F_3N_4O_4$ | 3.44 | 5.05 |
| 1277. 2,4,5-Tri-Cl-$C_6H_2NHN=C(CN)COOC_2H_5$ | $C_{11}H_8Cl_3N_3O_2$ | 5.21 | 6.23 |
| 1278. 3,4,5-Tri-Cl-$C_6H_2NHN=C(CN)COOC2H_5$ | $C_{11}H_8Cl_3N_3O_2$ | 5.03 | 5.50 |
| 1279. 3-$CF_3$-$C_6H_4NHN=C(CN)COOCH_3$ | $C_{11}H_8F_3N_3O_2$ | 3.78 | 4.52 |
| 1280. 4-$SO_2CF_3$-$C_6H_4NHN=C(CN)COOCH_3$ | $C_{11}H_8F_3N_3O_4S$ | 4.22 | 4.01 |
| 1281. 4-$SCF_3$-$C_6H_4NHN=C(CN)COOCH_3$ | $C_{11}H_8F_3N_3O_2S$ | 4.27 | 4.88 |
| 1282. 1-Isothiocyanonaphthalene | $C_{11}H_7NS$ | 4.34 | 4.46 |
| 1283. 2-Isothiocyanonaphthalene | $C_{11}H_7NS$ | 4.34 | 4.46 |
| 1284. 4-Acetyl-7-chloroquinoline | $C_{11}H_8ClNO$ | 2.62 | 2.29 |
| 1285. 6-Methyl-1,4-naphthoquinone | $C_{11}H_8O_2$ | 2.10 | 2.12 |
| 1286. 2-Methyl-1,4-naphthoquinone | $C_{11}H_8O_2$ | 2.20 | 2.20 |
| 1287. 2-Methoxy-1,4-naphthoquinone | $C_{11}H_8O_3$ | 1.35 | 1.35 |
| 1288. 2-Methyl-3-hydroxy-1,4-naphthoquinone | $C_{11}H_8O_3$ | 1.20 | 1.20 |
| 1289. Alclofenac | $C_{11}H_{11}ClO_3$ | 1.06 | 2.99 |
| 1290. 4,5-Dimethyl-8-quinolinol | $C_{11}H_{11}NO$ | 2.71 | 2.12 |
| 1291. 4-Methyl-5-methoxy-8-quinolinol | $C_{11}H_{11}NO_2$ | 2.75 | 1.51 |
| 1292. 7-Dimethylaminoquinoline | $C_1H_{12}N_2$ | 2.71 | 2.26 |
| 1293. Antipyrine | $C_1H_{12}N_2O$ | 0.23 | 0.28 |
| 1294. 5-Ethyl-5-phenylhydantoin | $C_{11}H_{12}N_2O_2$ | 1.53 | 1.58 |
| 1295. *DL*-Tryptophan | $C_{11}H_{12}N_2O_2$ | −1.04 | −1.40 |
| 1296. Sulfamerazine | $C_{11}H_{12}N_4O_2S$ | 0.17 | 0.28 |
| 1297. Sulfaperine | $C_{11}H_{12}N_4O_2S$ | 0.34 | 0.21 |
| 1298. 2-Acetylphenyldimethylcarbamate | $C_{11}H_{13}NO_3$ | 0.93 | 0.52 |
| 1299. 3-Acetylphenyldimethylcarbamate | $C_{11}H_{13}NO_3$ | 1.18 | 0.71 |
| 1300. *N*-Methyl-4-propionylphenylcarbamate | $C_{11}H_{13}NO_3$ | 1.55 | 2.34 |
| 1301. *N*-Methyl-3-propionylphenylcarbamate | $C_{11}H_{13}NO_3$ | 1.49 | 2.34 |
| 1302. 4-Phenyl-*N*-nitrosopiperidine | $C_{11}H_{14}N_2O$ | 2.59 | 2.23 |
| 1303. 3-Isopropylphenoxyacetic acid | $C_{11}H_{14}O_3$ | 2.59 | 2.88 |
| 1304. 4-Isopropylphenoxyacetic acid | $C_{11}H_{14}O_3$ | 2.69 | 2.88 |
| 1305. 3-Propylphenoxyacetic acid | $C_{11}H_{14}O_3$ | 2.71 | 2.78 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1306. *o*-Isopropylphenoxyacetic acid | $C_{11}H_{14}O_3$ | 2.84 | 2.88 |
| 1307. *p*-Hydroxybenzoic acid butyl ester | $C_{11}H_{14}O_3$ | 3.57 | 2.82 |
| 1308. 4-Butoxybenzamide | $C_{11}H_{15}NO_2$ | 2.48 | 2.01 |
| 1309. 3-Isopropyl-4-hydroxyacetanilide | $C_{11}H_{15}NO_2$ | 2.20 | 1.87 |
| 1310. 2,4,5-Trimethyl-*N*-methylphenylcarbamate | $C_{11}H_{15}NO_2$ | 2.52 | 2.77 |
| 1311. 2,3,5-Trimethyl-4-hydroxyacetanilide | $C_{11}H_{15}NO_2$ | 1.30 | 1.56 |
| 1312. 2,3,6-Trimethyl-4-hydroxyacetanilide | $C_{11}H_{15}NO_2$ | 1.24 | 1.56 |
| 1313. 2-Amino-5-phenylvaleric acid | $C_{11}H_{15}NO_2$ | −0.36 | −0.19 |
| 1314. 2-Butoxy-4-aminobenzoic acid | $C_{11}H_{15}NO_3$ | 1.24 | 2.88 |
| 1315. Baygon | $C_{11}H_{15}NO_3$ | 1.58 | 1.67 |
| 1316. *N*-Methyl-3-isopropoxyphenylcarbamate | $C_{11}H_{15}NO_3$ | 1.96 | 2.15 |
| 1317. 1-Pentylbenzotriazole | $C_{11}H_{15}N_3$ | 3.22 | 3.19 |
| 1318. 2-Pentylbenzotriazole | $C_{11}H_{15}N_3$ | 3.63 | 2.83 |
| 1319. 5-Allyl-5-butylbarbituric acid | $C_{11}H_{16}N_2O_3$ | 1.35 | 1.67 |
| 1320. Inpea | $C_{11}H_{10}N_2O_3$ | 1.28 | 1.13 |
| 1321. *p*-Diethylaminobenzyl alcohol | $C_{11}H_{17}NO$ | 2.29 | 1.99 |
| 1322. 2,3-Dimethoxyamphetamine | $C_{11}H_{17}NO_2$ | 1.49 | 1.63 |
| 1323. 2,4-Dimethoxyamphetamine | $C_{11}H_{17}NO_2$ | 1.75 | 1.40 |
| 1324. 2,5-Dimethoxyamphetamine | $C_{11}H_{17}NO_2$ | 1.88 | 1.40 |
| 1325. 3,4-Dimethoxyamphetamine | $C_{11}H_{17}NO_2$ | 1.00 | 1.63 |
| 1326. Mescaline | $C_{11}H_{17}NO_3$ | 0.78 | 0.80 |
| 1327. 5-Ethyl-5-isoamyl-2-thiobarbituric acid | $C_{11}H_{18}N_2O_2S$ | 2.98 | 2.84 |
| 1328. 5-Amyl-5-ethylbarbituric acid | $C_{11}H_{18}N_2O_3$ | 2.24 | 2.19 |
| 1329. Amobarbital | $C_{11}H_{18}N_2O_3$ | 2.07 | 2.11 |
| 1330. Pentobarbital | $C_{11}H_{18}N_2O_3$ | 2.03 | 2.11 |
| 1331. 1,10-Phenanthroline | $C_{12}H_8N_2$ | 1.78 | 2.17 |
| 1332. 1,7-Phenanthroline | $C_{12}H_8N_2$ | 2.51 | 2.51 |
| 1333. 4,7-Phenanthroline | $C_{12}H_8N_2$ | 2.05 | 1.99 |
| 1334. Phenazine | $C_{12}H_8N_2$ | 2.84 | 2.84 |
| 1335. 4-Benzoylpyridine | $C_{12}H_9NO$ | 1.98 | 1.62 |
| 1336. 2-Acetamido-1,4-naphthoquinone | $C_{12}H_9NO_3$ | 1.29 | 1.23 |
| 1337. Phenothiazine | $C_{12}H_9NS$ | 3.78 | 3.48 |
| 1338. Azobenzene | $C_{12}H_{10}N_2$ | 3.82 | 2.31 |
| 1339. Harmalol | $C_{12}H_{12}N_2O$ | 2.19 | 2.19 |
| 1340. Phenylsulfoxide | $C_{12}H_{10}OS$ | 2.06 | 2.70 |
| 1341. 6,7-Dimethyl-1,4-naphthoquinone | $C_{12}H_{10}O_2$ | 2.49 | 2.54 |
| 1342. 2-Naphthoxyacetic acid | $C_{12}H_{10}O_3$ | 2.53 | 2.50 |
| 1343. *o*-Phenoxyaniline | $C_{12}H_{11}NO$ | 2.46 | 2.74 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1344. *p*-Phenoxyaniline | $C_{12}H_{11}NO$ | 2.36 | 2.60 |
| 1345. Carbaryl | $C_{12}H_{11}NO_2$ | 2.34 | 2.70 |
| 1346. Benzidine | $C_{12}H_{12}N_2$ | 1.34 | 1.55 |
| 1347. Hydrazobenzene | $C_{12}H_{12}N_2$ | 2.94 | 2.94 |
| 1348. Dapsone | $C_{12}H_{12}N_2O_2S$ | 0.97 | −0.19 |
| 1349. Sulfamethazine | $C_{12}H_{14}N_4O_2S$ | 0.32 | 0.77 |
| 1350. *o*-*t*-Butylphenoxyacetic acid | $C_{12}H_{16}O_3$ | 3.33 | 3.34 |
| 1351. 3-Butylphenoxyacetic acid | $C_{12}H_{16}O_3$ | 3.18 | 3.32 |
| 1352. 4-*s*-Butylphenoxyacetic acid | $C_{12}H_{16}O_3$ | 3.12 | 3.41 |
| 1353. 3-*t*-Butylphenoxyacetic acid | $C_{12}H_{16}O_3$ | 2.96 | 3.34 |
| 1354. *o*-*s*-Butylphenoxyacetic acid | $C_{12}H_{16}O_3$ | 3.32 | 3.41 |
| 1355. $\beta$-Phenylglucopyraroside | $C_{12}H_{16}O_6$ | −0.71 | −0.24 |
| 1356. Arbutin | $C_{12}H_{16}O_7$ | −1.35 | −1.05 |
| 1357. 3-*t*-Butyl-4-hydroxyacetanilide | $C_{12}H_{17}NO_2$ | 2.85 | 2.34 |
| 1358. 3,5-Diethyl-4-hydroxyacetanilide | $C_{12}H_{17}NO_2$ | 2.36 | 2.18 |
| 1359. *N*-Methyl-2-*s*-butylphenylcarbamate | $C_{12}H_{17}NO_2$ | 2.78 | 3.61 |
| 1360. *N*-Methyl-2-*t*-butylphenylcarbamate | $C_{12}H_{17}NO_2$ | 2.65 | 3.54 |
| 1361. *N*-Methyl-3-methyl-4-isopropylphenylcarbamate | $C_{12}H_{17}NO_2$ | 3.11 | 3.50 |
| 1362. *N*-Methyl-3-methyl-5-isopropylphenylcarbamate | $C_{12}H_{17}NO_2$ | 3.10 | 3.50 |
| 1363. *N*-Methyl-3-methyl-6-isopropylphenylcarbamate | $C_{12}H_{17}NO_2$ | 2.84 | 3.50 |
| 1364. *N*-Methyl-3-*t*-butylphenylcarbamate | $C_{12}H_{17}NO_2$ | 2.93 | 3.54 |
| 1365. *N*-Methyl-4-*s*-butylphenylcarbamate | $C_{12}H_{17}NO_2$ | 3.20 | 3.61 |
| 1366. *N*-Methyl-4-*t*-butylphenylcarbamate | $C_{12}H_{17}NO_2$ | 3.06 | 3.54 |
| 1367. 2-Isopropylphenyldimethylcarbamate | $C_{12}H_{17}NO_2$ | 2.65 | 2.73 |
| 1368. 2,3,5,6-Tetramethyl-4-hydroxyacetanilide | $C_{12}H_{17}NO_2$ | 1.44 | 1.98 |
| 1369. *N*-Methyl-2-butylthiophenylcarbamate | $C_{12}H_{17}NO_2S$ | 2.98 | 3.05 |
| 1370. Bufexamic | $C_{12}H_{17}NO_3$ | 1.47 | 1.36 |
| 1371. *N*-Methyl-3-butoxyphenylcarbamate | $C_{12}H_{17}NO_3$ | 2.96 | 2.88 |
| 1372. *N*-Methyl-4-butoxyphenylcarbamate | $C_{12}H_{17}NO_3$ | 2.86 | 2.88 |
| 1373. 2-Pentoxy-4-aminobenzoic acid | $C_{12}H_{17}NO_3$ | 1.55 | 3.42 |
| 1374. 2-Isopentoxy-4-aminobenzoic acid | $C_{12}H_{17}NO_3$ | 1.47 | 3.34 |
| 1375. Tolbutamide | $C_{12}H_{18}N_2O_3S$ | 2.34 | 2.14 |
| 1376. Thioxanthon | $C_{13}H_8OS$ | 3.99 | 3.99 |
| 1377. 3,4,4′-Trichlorocarbanilide | $C_{13}H_9Cl_3N_2O$ | 2.91 | 4.95 |
| 1378. Niflumic acid | $C_{13}H_9F_3N_2O_2$ | 1.59 | 3.61 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1379. 4-Biphenylisothiocyanate | $C_{13}H_9NS$ | 4.66 | 5.19 |
| 1380. 4-Isothiocyanodiphenyl ether | $C_{13}H_9NOS$ | 4.75 | 4.96 |
| 1381. 4-Isothiocyanodiphenylsulfoxide | $C_{13}H_9NOS_2$ | 4.40 | 3.76 |
| 1382. 4-Isothiocyanoazobenzene | $C_{13}H_9N_3S$ | 5.55 | 3.38 |
| 1383. 4-Aminosalicylic acid,4-bromophenylester | $C_{13}H_{10}BrNO_3$ | 3.46 | 3.78 |
| 1384. 4-Aminosalicylic acid,2-bromophenylester | $C_{13}H_{10}BrNO_3$ | 3.74 | 3.01 |
| 1385. 4-Aminosalicylic acid,3-bromophenylester | $C_{13}H_{10}BrNO_3$ | 3.84 | 3.78 |
| 1386. 3′-Chloro-*N*-phenylanthoanilic acid | $C_{13}H_{10}ClNO_2$ | 2.43 | 4.78 |
| 1387. 4-Aminosalicylic acid,4-chlorophenylester | $C_{13}H_{10}ClNO_3$ | 3.60 | 3.52 |
| 1388. 4-Aminosalicylic acid,2-chlorophenylester | $C_{13}H_{10}ClNO_3$ | 3.72 | 3.03 |
| 1389. 4-Aminosalicylic acid,3-chlorophenylester | $C_{13}H_{10}ClNO_3$ | 3.90 | 3.52 |
| 1390. 1-(3,4-Dichlorophenyl)-3-phenylurea | $C_{13}H_{10}Cl_2N_2O$ | 4.70 | 4.31 |
| 1391. 4-Aminosalicylic acid,4-fluorophenylester | $C_{13}H_{10}FNO_3$ | 3.27 | 3.12 |
| 1392. 4-Aminosalicylic acid,2-fluorophenylester | $C_{13}H_{10}FNO_3$ | 3.29 | 2.78 |
| 1393. 4-Aminosalicylic acid,3-fluorophenylester | $C_{13}H_{10}FNO_3$ | 3.42 | 3.12 |
| 1394. 1-Aminoacridine | $C_{13}H_{10}N_2$ | 2.47 | 2.25 |
| 1395. 2-Aminoacridine | $C_{13}H_{10}N_2$ | 2.62 | 2.25 |
| 1396. 3-Aminoacridine | $C_{13}H_{10}N_2$ | 2.19 | 2.25 |
| 1397. 4-Aminoacridine | $C_{13}H_{10}N_2$ | 3.26 | 2.25 |
| 1398. 9-Aminoacridine | $C_{13}H_{10}N_2$ | 2.74 | 2.25 |
| 1399. 4-Isothiocyanodiphenylamine | $C_{13}H_{10}N_2S$ | 4.94 | 4.51 |
| 1400. *o*-Hydroxybenzophenone | $C_{13}H_{10}O_2$ | 3.52 | 3.39 |
| 1401. *p*-Hydroxybenzophenone | $C_{13}H_{10}O_2$ | 3.07 | 2.36 |
| 1402. *o*-Phenoxybenzoic acid | $C_{13}H_{10}O_3$ | 2.84 | 4.50 |
| 1403. *p*-Phenoxybenzoic acid | $C_{13}H_{10}O_3$ | 3.21 | 3.48 |
| 1404. *N*-Benziliden aniline | $C_{13}H_{11}N$ | 1.84 | 1.84 |
| 1405. Benzanilide | $C_{13}H_{11}NO$ | 2.70 | 2.79 |
| 1406. *N*-Phenylanthranilic acid | $C_{13}H_{11}NO_2$ | 4.36 | 4.15 |
| 1407. Salicylanilide | $C_{13}H_{11}NO_2$ | 3.27 | 3.16 |
| 1408. Phenyl-4-aminosalicylate | $C_{13}H_{11}NO_3$ | 3.15 | 2.87 |
| 1409. 3,6-Diaminoacridine | $C_{13}H_{11}N_3$ | 1.10 | 0.95 |
| 1410. 4,4′-Dihydroxydiphenylmethane | $C_{13}H_{12}O_2$ | 2.91 | 2.69 |
| 1411. *o*-Phenoxyanisole | $C_{13}H_{12}O_2$ | 2.92 | 3.93 |
| 1412. Di-(*p*-aminophenyl)methane | $C_{13}H_{14}N_2$ | 1.59 | 1.72 |
| 1413. $N^1$-(4-Methylphenyl)sulfanilamide | $C_{13}H_{14}N_2O_2S$ | 2.00 | 2.18 |
| 1414. $N^1$-(2-Methoxyphenyl)sulfanilamide | $C_{13}H_{14}N_2O_3S$ | 1.56 | 1.71 |
| 1415. $N^1$-(4-Methoxyphenyl)sulfanilamide | $C_{13}H_{14}N_2O_3S$ | 1.51 | 1.57 |
| 1416. Benzylacetoacetic acid ethyl ester | $C_{13}H_{16}O_3$ | 2.52 | 2.25 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1417. 4-Cyclopentylphenoxyacetic acid | $C_{13}H_{16}O_3$ | 3.41 | 3.49 |
| 1418. Aminopyrene | $C_{13}H_{17}N_3O$ | 1.00 | 1.86 |
| 1419. Heptabarbital | $C_{13}H_{18}N_2O_3$ | 2.17 | 2.41 |
| 1420. 2-*s*-Butylphenyldimethylcarbamate | $C_{13}H_{19}NO_2$ | 3.31 | 3.27 |
| 1421. *N*-Methyl-3-methyl-4-*t*-butylphenylcarbamate | $C_{13}H_{19}NO_2$ | 3.38 | 3.96 |
| 1422. *N*-Methyl-3-methyl-5-*t*-butylphenylcarbamate | $C_{13}H_{19}NO_2$ | 3.35 | 3.96 |
| 1423. *N*-methyl-3-methyl-6-*t*-butylphenylcarbamate | $C_{13}H_{19}NO_2$ | 3.14 | 3.96 |
| 1424. 2-Methyl-5-*t*-butyl-4-hydroxyacetanilide | $C_{13}H_{19}NO_2$ | 2.67 | 2.76 |
| 1425. Probenecid | $C_{13}H_{19}NO_4S$ | 3.21 | 3.05 |
| 1426. 4,4′-Diisothiocyanatebiphenyl | $C_{14}H_8N_2S_2$ | 5.50 | 6.26 |
| 1427. DFDT | $C_{14}H_9Cl_3F_2$ | 4.62 | 6.11 |
| 1428. 4-Isothiocyanobenzophenone | $C_{14}H_9NOS$ | 4.88 | 4.23 |
| 1429. 4-Isothiocyanophenylbenzoate | $C_{14}H_9NO_2S$ | 4.90 | 5.01 |
| 1430. 3′-$CF_3$-*N*-phenylanthranilic acid | $C_{14}H_{10}F_3NO_2$ | 5.62 | 5.16 |
| 1431. Benzil | $C_{14}H_{10}O_2$ | 3.38 | 3.04 |
| 1432. 4-Isothiocyanodiphenylmethane | $C_{14}H_{11}NS$ | 4.40 | 5.37 |
| 1433. *m*-Phenylphenoxyacetic acid | $C_{14}H_{12}O_3$ | 3.18 | 3.24 |
| 1434. *o*-Phenylphenoxyacetic acid | $C_{14}H_{12}O_3$ | 2.83 | 3.24 |
| 1435. 2-$CF_3$-4-Cl-$C_6H_3$NHN=C(CN)CO-*t*-Bu | $C_{14}H_{13}ClF_3N_3O$ | 5.67 | 6.30 |
| 1436. 2-Cl-5-$CF_3$-$C_6H_3$NHN=C(CN)CO-*t*-Bu | $C_{14}H_{13}ClF_3N_3O$ | 5.31 | 6.70 |
| 1437. 4-Aminosalicylic acid,2-tolyl ester | $C_{14}H_{13}NO_3$ | 3.14 | 3.29 |
| 1438. 4-Aminosalicylic acid,4-tolyl ester | $C_{14}H_{13}NO_3$ | 3.38 | 3.29 |
| 1439. 4-Aminosalicylic acid,3-tolyl ester | $C_{14}H_{13}NO_3$ | 3.64 | 3.29 |
| 1440. 4-Aminosalicylic acid,2-methoxyphenyl ester | $C_{14}H_{13}NO_4$ | 2.88 | 2.20 |
| 1441. 4-Aminosalicylic acid,4-methoxyphenyl ester | $C_{14}H_{13}NO_4$ | 3.07 | 2.68 |

TABLE A1 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1442. 4-Aminosalicylic acid,3-methoxyphenyl ester | $C_{14}H_{13}NO_4$ | 3.25 | 2.68 |
| 1443. Naproxen | $C_{14}H_{14}O_3$ | 3.18 | 2.41 |
| 1444. 2-Me-4-Cl-$C_6H_3$NHN=C(CN)CO-*t*-Bu | $C_{14}H_{16}ClN_3O$ | 4.31 | 5.71 |
| 1445. Reposal | $C_{14}H_{18}N_2O_3$ | 2.53 | 2.44 |
| 1446. 4-Cyclohexylphenoxyacetic acid | $C_{14}H_{18}O_3$ | 3.79 | 4.03 |
| 1447. Chlorambucil | $C_{14}H_{19}Cl_2NO_2$ | 1.70 | 3.21 |
| 1448. *p*-Hydroxybenzoic acid heptyl ester | $C_{14}H_{20}O_3$ | 4.83 | 4.42 |
| 1449. 3,5-Dipropyl-4-hydroxyacetanilide | $C_{14}H_{21}NO_2$ | 3.16 | 3.25 |
| 1450. Lidocaine | $C_{14}H_{22}N_2O$ | 2.26 | 0.91 |
| 1451. 2-Isothiocyano anthracene | $C_{15}H_9NS$ | 5.70 | 5.65 |
| 1452. 2-Phenyl-1,3-indanedione | $C_{15}H_{10}O_2$ | 2.90 | 2.90 |
| 1453. 1-Me-4-phenyl-7-chloroquinazolin-2-one | $C_{15}H_{11}ClN_2O$ | 2.36 | 2.28 |
| 1454. 1-Me-4-phenyl-6-chloroquinazolin-2-one | $C_{15}H_{11}ClN_2O$ | 2.38 | 2.28 |
| 1455. 1-Me-4-phenyl-6-fluoroquinazolin-2-one | $C_{15}H_{11}FN_2O$ | 1.87 | 1.96 |
| 1456. 4-Isothiocyanostilbene | $C_{15}H_{11}NS$ | 5.85 | 5.94 |
| 1457. 1-Methyl-4-phenylquinazolin-2-one | $C_{15}H_{12}N_2O$ | 1.79 | 1.72 |
| 1458. 1-Methyl-4-phenyl-6-OH-quinazolin-2-one | $C_{15}H_{12}N_2O_2$ | 1.72 | 0.90 |
| 1459. 9-Carboxy-9,10-dihydroanthracene | $C_{15}H_{12}O_2$ | 2.67 | 2.55 |
| 1460. 3-Benzamido-phenoxyacetic acid | $C_{15}H_{13}NO_4$ | 1.99 | 1.90 |
| 1461. 4-Aminosalicylic acid-2,6-dimethylphenylester | $C_{15}H_{16}N_2O$ | 3.38 | 3.71 |
| 1462. 1,1-Diphenyl-3,3-dimethylurea | $C_{15}H_{16}N_2O$ | 2.80 | 2.44 |
| 1463. Parthenin | $C_{15}H_{18}O_4$ | 0.77 | 0.06 |
| 1464. *α,α′*-diethyl-4,4′-Stilbenedid | $C_{18}H_{20}O_2$ | 5.07 | 5.23 |
| 1465. Estrone | $C_{18}H_{22}O_2$ | 2.76 | 3.66 |

TABLE A2
ESTIMATION RESULTS FOR THE COMPOUNDS NOT INCLUDED IN THE DATA SET

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 1. Methyl bromide | $CH_3Br$ | 1.19 | 1.20 |
| 2. Methyl chloride | $CH_3Cl$ | 0.91 | 0.88 |
| 3. Methyl fluoride | $CH_3F$ | 0.51 | 0.55 |
| 4. Methyl iodide | $CH_3I$ | 1.51 | 1.69 |
| 5. Nitromethane | $CH_3NO_2$ | −0.33 | −0.77 |
| 6. Tetrachloroethylene | $C_2Cl_4$ | 2.60 | 2.60 |
| 7. Hexafluoroethane | $C_2F_6$ | 2.00 | 2.00 |
| 8. Acetonitrile | $C_2H_3N$ | −0.34 | 0.17 |
| 9. 2-Br,2-Cl,1,1,1-Trifluoroethane | $C_2HBrClF_3$ | 2.30 | 2.80 |
| 10. Trichloroethylene | $C_2HCl_3$ | 2.29 | 2.03 |
| 11. 2,2,3,3,3-Pentafluoropropanol | $C_3H_3F_5O$ | 1.23 | 0.82 |
| 12. Methoxyflurane | $C_3H_4Cl_2F_2O$ | 2.21 | 1.12 |
| 13. Pentafluoropropionic acid ethyl ester | $C_5H_5F_5O_2$ | 2.12 | 1.46 |
| 14. 3,4-Dichloro-*N*-nitrosopiperidine | $C_5H_8Cl_2N_2O$ | 1.04 | 0.08 |
| 15. 3,5,6-Trichloro-2-pyridinol | $C_5H_2Cl_3NO$ | 2.27 | 0.88 |
| 16. Nitrosobenzene | $C_6H_5NO$ | 2.01 | 2.01 |
| 17. 2,3,4,5,6-Pentachlorophenol | $C_6HCl_5O$ | 5.07 | 4.95 |
| 18. 1-*H*-Pentachlorocyclohexane | $C_6H_7Cl_5$ | 3.53 | 3.27 |
| 19. Allylglycidyl ether | $C_6H_{10}O_2$ | – | 1.15 |
| 20. Citric acid | $C_6H_8O_7$ | −1.72 | −2.48 |
| 21. Histidine | $C_6H_9N_3O_2$ | −2.52 | −1.66 |
| 22. Trifluoromethylbenzene | $C_7H_5F_3$ | 3.01 | 3.21 |
| 23. Saccharin | $C_7H_5NO_3S$ | 0.91 | 0.48 |
| 24. 5-Nitro-benzimidazole | $C_7H_5N_3O_2$ | 1.64 | 1.62 |
| 25. Bromothiazide | $C_7H_6BrN_3O_4S_2$ | 0.00 | −0.87 |
| 26. Chlorothiazide | $C_7H_6ClN_3O_4S_2$ | −0.27 | −1.14 |
| 27. Fluorothiazide | $C_7H_6FN_3O_4S_2$ | −0.29 | −1.53 |
| 28. Sulfaguanidine | $C_7H_{10}N_4O_2S$ | −1.22 | −1.22 |
| 29. α-Chlorotoluene | $C_7H_7Cl$ | 2.30 | 2.69 |
| 30. *o*- Chlorotoluene | $C_7H_7Cl$ | 3.42 | 3.27 |
| 31. Hydrobromothiazide | $C_7H_8BrN_3O_4S_2$ | 0.08 | −0.89 |
| 32. Hydrochlorothiazide | $C_7H_8ClN_3O_4S_2$ | −0.07 | −1.16 |
| 33. Glycerylmonobutyrate | $C_7H_{14}O_4$ | −0.17 | −0.19 |
| 34. 4-Vinylcyclohexene | $C_8H_{12}$ | – | 3.36 |
| 35. *p*-Di(trichloromethyl)benzene | $C_8H_4Cl_6$ | 4.62 | 4.56 |
| 36. 2-Chloro-1-ethylbenzene | $C_8H_9Cl$ | 2.95 | 3.78 |

TABLE A2 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 37. 1,4-Dimethyltetrachlorocyclohexane | $C_8H_{12}Cl_4$ | 4.40 | 4.38 |
| 38. 4,5,6,7-Tetrabromo-2-trifluoromethylbenzimidazole | $C_8HBr_4F_3N_2$ | 4.81 | 3.72 |
| 39. 4,5,6,7-Tetrachloro-2-trifluoromethylbenzimidazole | $C_8HCl_4F_3N_2$ | 3.97 | 4.34 |
| 40. 4,5,7-Trichloro-2-trifluoromethylbenzimidazole | $C_8H_2Cl_3F_3N_2$ | 3.78 | 4.07 |
| 41. 4,5,6-Trichloro-2-trifluoromethylbenzimidazole | $C_8H_2Cl_3F_3N_2$ | 3.87 | 3.74 |
| 42. 2-Trifluoromethyl-4,7-dichlorobenzimidazole | $C_8H_3Cl_2F_3N_2$ | 2.87 | 3.48 |
| 43. 2-Trifluoromethyl-4,5-dichlorobenzimidazole | $C_8H_3Cl_2F_3N_2$ | 3.49 | 3.47 |
| 44. 2-Trifluoromethyl-4,6-dichlorobenzimidazole | $C_8H_3Cl_2F_3N_2$ | 3.49 | 3.47 |
| 45. 4,5,6,7-Tetrachloro-2-methylbenzimidazole | $C_8H_4Cl_4N_2$ | 2.83 | 3.27 |
| 46. 3-$CF_3$-6-Cl-1,2,4-benzothiadiazine−1,1-dioxide | $C_8H_4ClF_3N_2O_2S$ | 1.65 | 2.35 |
| 47. 3-Methyl-5-I-7-Cl-1,2,4-benzothiadiazine−1,1-dioxide | $C_8H_6ClIN_2O_2S$ | 1.81 | 1.97 |
| 48. 3-Methyl-5-$NO_2$-7-Cl-1,2,4-benzothiadiazine−1,1-dioxide | $C_8H_6ClN_3O_4S$ | 0.85 | 0.41 |
| 49. 3-Methyl-6-$NO_2$-7-Cl-1,2,4-benzothiadiazine−1,1-dioxide | $C_8H_6ClN_3O_4S$ | 1.42 | 0.66 |
| 50. 3-Chloromethyl-6-Cl-1,2,4-benzothiadiazine−1,1-dioxide | $C_8H_6Cl_2N_2O_2S$ | 1.68 | 1.19 |
| 51. 3-Methyl-7-F-1,2,4-benzothiadiazine−1,1-dioxide | $C_8H_7FN_2O_2S$ | 0.62 | 0.87 |
| 52. 5-Chloro-3-methyl-2*H*-1,2,4-benzothiadiazine−1,1-dioxide | $C_8H_7ClN_2O_2S$ | 0.72 | 1.38 |
| 53. 3-Methyl-6-$NH_2$-7-Cl-1,2,4-benzothiadiazine−1,1-dioxide | $C_8H_8ClN_3O_2S$ | 0.63 | 0.38 |
| 54. 1-(3,3,3-Trifluoroethoxy)pentachlorocyclohexane | $C_8H_8Cl_5F_3O$ | 4.06 | 4.52 |
| 55. Methyl-*N*(2-F-phenyl)carbamate | $C_8H_8FNO_2$ | 1.66 | 1.32 |
| 56. Methyl-*N*(2-Cl-phenyl)carbamate | $C_8H_8ClNO_2$ | 2.13 | 2.16 |
| 57. Methyl-*N*(2-Br-phenyl)carbamate | $C_8H_8BrNO_2$ | 2.25 | 2.39 |
| 58. Methyl-*N*(2-$NO_2$-phenyl)carbamate | $C_8H_8N_2O_4$ | 2.07 | 1.63 |
| 59. Methyl-*N*(2-I-phenyl)carbamate | $C_8H_8INO_2$ | 2.44 | 2.84 |
| 60. 6-Azauridine | $C_8H_{11}N_3O_6$ | −2.14 | −3.21 |
| 61. Ethyltartrate | $C_8H_{14}O_6$ | −0.29 | −1.23 |
| 62. 3-Chloro-4-nitroquinoline-1-oxide | $C_9H_5ClN_2O_3$ | 1.33 | 0.73 |
| 63. 4,8-Dihydroxyquinoline | $C_9H_7NO_2$ | 0.62 | 0.47 |

TABLE A2 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 64. Methyl-*N*(2-$CF_3$-phenyl)carbamate | $C_9H_8F_3NO_2$ | 2.13 | 2.11 |
| 65. Sulfamethizole | $C_9H_{10}N_4O_2S_2$ | 0.26 | −0.77 |
| 66. Methyl-*N*(2-methyl-phenyl)carbamate | $C_9H_{11}NO_2$ | 1.69 | 1.52 |
| 67. Methyl-*N*(2-methoxy-phenyl)carbamate | $C_9H_{11}NO_3$ | 1.84 | 1.40 |
| 68. 2,4,6-Trimethylphenol | $C_9H_{12}O$ | 2.86 | 2.65 |
| 69. Ethylidenenorbornene | $C_9H_{12}$ | – | 3.92 |
| 70. Isophorone | $C_9H_{14}O$ | – | 2.18 |
| 71. 5-Propyl-5-ethylbarbituric acid | $C_9H_{14}N_2O_3$ | 0.66 | 1.12 |
| 72. 4-Cyanoquinoline | $C_{10}H_6N_2$ | 1.98 | 1.45 |
| 73. Benzal malononitrile | $C_{10}H_6N_2$ | 2.18 | 2.26 |
| 74. Methyl-*N*(2-ethoxy-phenyl)carbamate | $C_{10}H_{13}NO_3$ | 2.40 | 1.89 |
| 75. 2-Amino-1,4-naphtoquinone | $C_{10}H_7NO_2$ | 1.88 | 1.05 |
| 76. Safrole | $C_{10}H_{10}O_2$ | – | 2.71 |
| 77. Inosine | $C_{10}H_{12}N_4O_5$ | −2.08 | −4.04 |
| 78. Adenosine | $C_{10}H_{13}N_5O_4$ | −1.23 | −3.18 |
| 79. Cimetidine | $C_{10}H_{16}N_6S$ | – | 0.97 |
| 80. 1-Hydroxyadamantane | $C_{10}H_{16}O$ | 2.14 | 2.16 |
| 81. 2-Cl-5-$CF_3$-$C_6H_3NHN{=}C(CN)CO$-$CH_3$ | $C_{11}H_7ClF_3N_3O$ | 5.08 | 4.19 |
| 82. 2-Cl-5-$CF_3$-$C_6H_3NHN{=}C(CN)COOCH_3$ | $C_{11}H_7ClF_3N_3O_2$ | 4.42 | 5.57 |
| 83. 3-$CHF_2$-4-Cl-$C_6H_3NHN{=}C(CN)COOCH_3$ | $C_{11}H_8ClF_2N_3O_2$ | 3.83 | 4.58 |
| 84. Fenclozic acid | $C_{11}H_8ClNO_2S$ | 3.29 | 2.44 |
| 85. 4-$SCF_3$-$C_6H_4NHN{=}C(CN)COCH_3$ | $C_{11}H_8F_3N_3OS$ | 5.04 | 4.55 |
| 86. 2-$CF_3$-$C_6H_4NHN{=}C(CN)COOCH_3$ | $C_{11}H_8F_3N_3O_2$ | 3.72 | 4.52 |
| 87. 4-$CF_3$-$C_6H_4NHN{=}C(CN)COOCH_3$ | $C_{11}H_8F_3N_3O_2$ | 3.79 | 4.52 |
| 88. 3,4-DiCl-$C_6H_3NHN{=}C(CN)COOC_2H_5$ | $C_{11}H_9Cl_2N_3O_2$ | 4.66 | 5.18 |
| 89. 3,5-DiCl-$C_6H_3NHN{=}C(CN)COOC_2H_5$ | $C_{11}H_9Cl_2N_3O_2$ | 3.82 | 5.29 |
| 90. 2-$CH_3$-4-Cl-$C_6H_3NHN{=}C(CN)COCH_3$ | $C_{11}H_{10}ClN_3O$ | 4.28 | 4.25 |
| 91. 2-Cl-$C_6H_4NHN{=}C(CN)COOC_2H_5$ | $C_{11}H_{10}ClN_3O_2$ | 3.38 | 5.05 |
| 92. 3-Cl-$C_6H_4NHN{=}C(CN)COOC_2H_5$ | $C_{11}H_{10}ClN_3O_2$ | 3.94 | 4.64 |
| 93. 2,4-$(NH_2)_2$-5(3,4-DiCl-Ph)-6-Methyl-pyrimidine | $C_{11}H_{10}Cl_2N_4$ | 2.82 | 2.76 |
| 94. Sulfapyridine | $C_{11}H_{11}N_3O_2S$ | 0.02 | 0.94 |
| 95. 1-Phenyl-3,5-dimethyl-4-nitrosopyrazole | $C_{11}H_{11}N_3O$ | 2.28 | 3.89 |
| 96. 8-Dimethylaminoquinoline | $C_{11}H_{12}N_2$ | 2.73 | 2.26 |
| 97. Salfalene | $C_{11}H_{12}N_4O_3S$ | 0.70 | 0.81 |
| 98. Sulfamethoxypyridazine | $C_{11}H_{12}N_4O_3S$ | 0.40 | 0.60 |
| 99. Sulfamonomethoxine | $C_{11}H_{12}N_4O_3S$ | 0.85 | 0.92 |
| 100. Polythiazide | $C_{11}H_{13}ClF_3N_3O_4S_3$ | 1.13 | 0.03 |

TABLE A2 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 101. Sulfisoxazole | $C_{11}H_{13}N_3O_3S$ | 1.15 | 2.04 |
| 102. Tubercidin | $C_{11}H_{14}N_4O_4$ | −0.80 | −1.84 |
| 103. 1-Allyl-3,4-dimethoxybenzene | $C_{11}H_{14}O_2$ | – | 3.03 |
| 104. Metron S | $C_{11}H_{25}N$ | – | 3.90 |
| 105. 3,5-Di$CF_3$-$C_6H_3NHN{=}C(CN)COOCH_3$ | $C_{12}H_7F_6N_3O_2$ | 5.16 | 5.53 |
| 106. 2,4,5,2′,4′,5′-PCB | $C_{12}H_4Cl_6$ | 6.72 | 7.90 |
| 107. 2,4,5,2′,5′-PCB | $C_{12}H_5Cl_5$ | 6.11 | 7.26 |
| 108. 4-Nitrophenyl-2,4,6-trichlorophenyl ether | $C_{12}H_6Cl_3NO_3$ | – | 5.92 |
| 109. 2,5-CN-$C_6H_3NHN{=}C(CN)COOCH_3$ | $C_{12}H_7N_5O_2$ | 2.81 | 2.23 |
| 110. 4,4′-PCB | $C_{12}H_8Cl_2$ | 5.58 | 5.43 |
| 111. 3-$CF_3$-4-Cl-$C_6H_3NHN{=}C(CN)COOC_2H_5$ | $C_{12}H_9ClF_3N_3O_2$ | 4.86 | 5.65 |
| 112. Propyzamide | $C_{12}H_{11}Cl_2NO$ | – | 4.26 |
| 113. Phenobarbital | $C_{12}H_{12}N_2O_3$ | 1.42 | 1.31 |
| 114. Pyrimethamine | $C_{12}H_{13}ClN_4$ | 2.69 | 2.75 |
| 115. Vitavax | $C_{12}H_{13}NO_2S$ | 2.14 | 1.51 |
| 116. Cyclopentobarbital | $C_{12}H_{14}N_2O_3$ | 1.51 | 1.34 |
| 117. Sulfsomidine | $C_{12}H_{14}N_4O_2S$ | −0.30 | 0.41 |
| 118. Sulfadimethoxine | $C_{12}H_{14}N_4O_4S$ | 1.33 | −0.14 |
| 119. 4-Chloro-phenyl-*β*-*D*-glucopyranoside | $C_{12}H_{15}ClO_6$ | 0.26 | 0.41 |
| 120. 2-Iodo-phenyl-*β*-*D*-glucopyranoside | $C_{12}H_{15}O_6I$ | 0.27 | 1.02 |
| 121. 4-Iodo-phenyl-*β*-*D*-glucopyranoside | $C_{12}H_{15}O_6I$ | 0.75 | 1.05 |
| 122. 2-Nitro-phenyl-*β*-*D*-glucopyranoside | $C_{12}H_{15}NO_8$ | −0.78 | 0.24 |
| 123. 4-Nitro-phenyl-*β*-*D*-glucopyranoside | $C_{12}H_{15}NO_8$ | −0.44 | −0.51 |
| 124. Cyclobarbital | $C_{12}H_{16}N_2O_3$ | 1.77 | 1.87 |
| 125. Hexobarbital | $C_{12}H_{16}N_2O_3$ | 1.49 | 0.41 |
| 126. Methyl-*N*(4-n-butyl-phenyl)carbamate | $C_{12}H_{17}NO_2$ | 3.68 | 3.11 |
| 127. Methyl-*N*(3,4-diethoxyphenyl)carbamate | $C_{12}H_{17}NO_4$ | 2.09 | 1.91 |
| 128. 2-Amino-phenyl-*β*-*D*-glucopyranoside | $C_{12}H_{17}NO_6$ | −1.23 | −1.39 |
| 129. Aspergillic acid | $C_{12}H_{20}N_2O_2$ | 1.81 | 2.03 |
| 130. Sotalol | $C_{12}H_{20}N_2O_3S$ | −1.51 | −0.24 |
| 131. Hexachlorophene | $C_{13}H_6Cl_6O_2$ | 7.54 | 7.10 |
| 132. 2,4,5-TriCl-$C_6H_2NHN{=}C(CN)CO$-*t*-Bu | $C_{13}H_{12}Cl_3N_3O$ | 5.86 | 6.87 |
| 133. 2-$SO_2$Et-5-$CF_3$-$C_6H_5NHN{=}C(CN)COCH_3$ | $C_{13}H_{12}F_3N_3O_3S$ | 4.22 | 3.15 |
| 134. 3-Cl-$C_6H_4NHN{=}C(CN)CO$-*t*-Bu | $C_{13}H_{14}ClN_3O$ | 4.62 | 5.29 |
| 135. 3-$CF_3$-phenyl-*β*-*D*-glucopyranoside | $C_{13}H_{15}F_3O_6$ | 0.49 | 0.60 |
| 136. 2-$CH_2OH$-phenyl-*β*-*D*-glucopyranoside | $C_{13}H_{18}O_7$ | −1.22 | −1.39 |
| 137. 2-Methyl-phenyl-*β*-*D*-glucopyranoside | $C_{13}H_{18}O_6$ | −0.16 | 0.18 |
| 138. 3-Methyl-phenyl-*β*-*D*-glucopyranoside | $C_{13}H_{18}O_6$ | −0.20 | 0.18 |

TABLE A2 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 139. 4-Methoxy-phenyl-β-*D*-glucopyranoside | $C_{13}H_{18}O_7$ | −0.73 | −0.43 |
| 140. Ethyl-*N*(3,4-diethoxyphenyl)carbamate | $C_{13}H_{19}NO_4$ | 2.50 | 2.40 |
| 141. Rantidine | $C_{13}H_{22}N_4O_3S$ | – | −2.12 |
| 142. DDT | $C_{14}H_9Cl_5$ | 6.19 | 6.92 |
| 143. 2-Butylthio-1,4-naphthoquinone | $C_{14}H_{14}O_2S$ | 3.29 | 2.80 |
| 144. α-Aminoazotoluene | $C_{14}H_{15}N_3$ | – | 1.86 |
| 145. Trimethoprim | $C_{14}H_{18}N_4O_3$ | 0.91 | 0.44 |
| 146. Allyl-*N*(3,4-diethoxyphenyl)carbamate | $C_{14}H_{19}NO_4$ | 2.76 | 2.63 |
| 147. 3-Ethyl-phenyl-β-*D*-glucopyranoside | $C_{14}H_{20}O_6$ | 0.31 | 0.70 |
| 148. Alachlor | $C_{14}H_{20}ClNO_2$ | – | 2.43 |
| 149. *n*-Propyl-*N*(3,4-diethoxyphenyl)carbamate | $C_{14}H_{21}NO_4$ | 2.91 | 2.94 |
| 150. Isopropyl-*N*(3,4-diethoxyphenyl)carbamate | $C_{14}H_{21}NO_4$ | 2.82 | 2.75 |
| 151. Practolol | $C_{14}H_{22}N_2O_3$ | 0.79 | −0.13 |
| 152. Clonazepam | $C_{15}H_{10}ClN_3O_3$ | 2.41 | 1.30 |
| 153. Lorazepan | $C_{15}H_{10}Cl_2N_2O_2$ | 2.38 | 1.99 |
| 154. Apigenin | $C_{15}H_{10}O_5$ | 1.74 | 3.31 |
| 155. Oxazepam | $C_{15}H_{11}ClN_2O_2$ | 2.17 | 1.35 |
| 156. Nitrazepam | $C_{15}H_{11}N_3O_3$ | 2.12 | 0.65 |
| 157. 1,2-Diphenyl-3,5-pyrazolidinedione | $C_{15}H_{12}N_2O_2$ | 1.45 | −0.01 |
| 158. 5,5-Diphenyl-hydantoin | $C_{15}H_{12}N_2O_2$ | 2.47 | 2.64 |
| 159. 4,5-(-$OCF_2CF_2O$-)$C_6H_3NHN{=}C(CN)CO$-*t*-Bu | $C_{15}H_{13}F_4N_3O_3$ | 4.96 | 4.42 |
| 160. 3,5-$DiCF_3$-$C_6H_3NHN{=}C(CN)CO$-*t*-Bu | $C_{15}H_{13}F_6N_3O$ | 5.44 | 6.66 |
| 161. Sulfaphenazole | $C_{15}H_{14}N_4O_2S$ | 1.52 | 1.00 |
| 162. Vernolepin | $C_{15}H_{16}O_5$ | 0.31 | 0.05 |
| 163. Vernomenin | $C_{15}H_{16}O_5$ | −0.14 | 0.05 |
| 164. Bisphenol A | $C_{15}H_{16}O_2$ | 3.32 | 3.86 |
| 165. α-Cyclopropyl-α-(4-methoxyphenyl)-5-pyrimidine methanol | $C_{15}H_{18}N_2O_2$ | – | 0.77 |
| 166. *N*-Sulfanilyl-3,4-xylanide | $C_{15}H_{16}N_2O_3S$ | 2.19 | 0.89 |
| 167. Helenalin | $C_{15}H_{18}O_4$ | 0.87 | 0.15 |
| 168. Ambrosin | $C_{15}H_{18}O_3$ | 1.03 | 2.06 |
| 169. Meperidine | $C_{15}H_{21}NO_2$ | 1.68 | 2.23 |
| 170. Physostigmine | $C_{15}H_{21}N_3O_2$ | 1.58 | 1.68 |
| 171. Isobutyl-*N*(3,4-diethoxyphenyl)carbamate | $C_{15}H_{23}NO_4$ | 3.36 | 3.40 |
| 172. *n*-Butyl-*N*(3,4-diethoxyphenyl)carbamate | $C_{15}H_{23}NO_4$ | 3.46 | 3.47 |
| 173. Diazepam | $C_{16}H_{13}ClN_2O$ | 2.82 | 1.23 |
| 174. Cyclopentyl-*N*(3,4-diethoxyphenyl)carbamate | $C_{16}H_{23}NO_4$ | 3.33 | 3.36 |
| 175. Nialamide | $C_{16}H_{18}N_4O_2$ | 0.87 | −0.02 |

TABLE A2 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 176. 4-*t*-Butyl-phenyl-β-*D*-glucopyranoside | $C_{16}H_{24}O_6$ | 1.18 | 1.80 |
| 177. Carbinoxamine | $C_{16}H_{19}ClN_2O$ | – | 2.44 |
| 178. Prochlonol | $C_{16}H_{14}Cl_2O$ | – | 4.85 |
| 179. Benzo[*a*]acridine | $C_{17}H_{11}N$ | – | 4.73 |
| 180. Benzo[*c*]fluorene | $C_{17}H_{12}$ | – | 5.17 |
| 181. Ellipticine | $C_{17}H_{14}N_2$ | 4.80 | 3.67 |
| 182. Triflupromazine | $C_{18}H_{19}F_3N_2S$ | 5.19 | 4.25 |
| 183. Promethazine | $C_{17}H_{20}N_2S$ | 2.88 | 2.87 |
| 184. Diphenhydramine | $C_{17}H_{21}NO$ | 3.27 | 4.24 |
| 185. Cocaine | $C_{17}H_{21}NO_4$ | 2.09 | 0.51 |
| 186. Benzyl-*N*(3,4-diethoxyphenyl)carbamate | $C_{18}H_{21}NO_4$ | 3.29 | 3.52 |
| 187. Trimeprazine | $C_{18}H_{22}N_2S$ | 3.44 | 3.37 |
| 188. Metrizamide | $C_{18}H_{22}I_3N_3O_8$ | −1.89 | −1.86 |
| 189. Mebhydroline | $C_{19}H_{20}N_2$ | – | 3.47 |
| 190. Nalorphine | $C_{19}H_{21}NO_3$ | 1.51 | 1.07 |
| 191. Triprolidine | $C_{19}H_{22}N_2$ | 3.92 | 3.85 |
| 192. Diphenylpyraline | $C_{19}H_{23}NO$ | – | 3.36 |
| 193. Homochlorocyclizine | $C_{19}H_{23}ClN_2$ | – | 3.90 |
| 194. Ethopropazine | $C_{19}H_{24}N_2S$ | 4.77 | 4.17 |
| 195. Levomepromazine | $C_{19}H_{24}N_2OS$ | 3.39 | 3.51 |
| 196. Quinine | $C_{20}H_{24}N_2O_2$ | 1.73 | 2.14 |
| 197. 4-Androstene-3,17-dione | $C_{19}H_{26}O_2$ | 2.75 | 3.48 |
| 198. Testosterone | $C_{19}H_{28}O_2$ | 3.32 | 3.90 |
| 199. Benzo[*a*]pyrene | $C_{20}H_{12}$ | 6.50 | 6.24 |
| 200. Phenolphthalein | $C_{20}H_{14}O_4$ | 2.41 | 3.18 |
| 201. Phenolphthalol | $C_{20}H_{18}O_3$ | 3.27 | 3.36 |
| 202. Elephantin | $C_{20}H_{22}O_7$ | 1.05 | 2.60 |
| 203. Perochloperazine | $C_{20}H_{24}ClN_3S$ | 3.55 | 3.65 |
| 204. Perazine | $C_{20}H_{25}N_3S$ | 2.90 | 3.00 |
| 205. Buguinolate | $C_{20}H_{27}NO_5$ | 2.18 | 4.44 |
| 206. Dibucaine | $C_{20}H_{29}N_3O_2$ | 4.40 | 4.43 |
| 207. 17-Methyltestosterone | $C_{20}H_{30}O_2$ | 3.36 | 4.28 |
| 208. Prostaglandin E2 | $C_{20}H_{32}O_5$ | 1.35 | 1.40 |
| 209. Prostaglandin E1 | $C_{20}H_{34}O_5$ | 2.00 | 1.87 |
| 210. Haloperidol | $C_{21}H_{23}ClFNO_2$ | 4.30 | 3.43 |
| 211. Trifluoperazine | $C_{21}H_{24}F_3N_3S$ | 3.90 | 3.98 |
| 212. Thioridazine | $C_{21}H_{26}N_2S_2$ | 5.79 | 4.60 |
| 213. Clemastine | $C_{21}H_{26}ClNO$ | – | 4.86 |

TABLE A2 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 214. Progesterone | $C_{21}H_{30}O_2$ | 3.87 | 4.15 |
| 215. Pipamperone | $C_{21}H_{30}FN_3O_2$ | 2.40 | 1.56 |
| 216. Benzo[*b*]chrysene | $C_{22}H_{14}$ | – | 6.98 |
| 217. Thioproperazine | $C_{22}H_{30}N_4O_2S_2$ | 0.83 | 2.27 |

TABLE A2 (continued)

| Compound | Empirical formula | Log $P_{obsd}$ | Log $P_{estd}$ |
|---|---|---|---|
| 218. Flupentixol | $C_{23}H_{25}F_3N_2OS$ | 3.83 | 3.80 |
| 219. Coronene | $C_{24}H_{12}$ | – | 7.16 |
| 220. Etorphine | $C_{25}H_{33}NO_4$ | 1.86 | 1.79 |
| 221. Prostaglandin F2$\alpha$ | $C_{29}H_{34}O_5$ | 2.28 | 2.27 |