NATIONAL INSTITUTE OF PUBLIC HEALTH AND ENVIRONMENTAL PROTECTION BILTHOVEN, THE NETHERLANDS

Report no.: 679101013

Soil-water partition coefficients for organic compounds.

G.J.M. Bockting, E.J. van de Plassche, J. Struijs, and J.H. Canton.

December 1993

This research was carried out on behalf of the Directorate General for Environmental Protection, Directorate of Chemicals, Safety, and Radiation Protection, in the frame of project no. 679101 'Setting integrated environmental quality objectives' (Quality objectives and risks).

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Acknowledgements

Hereby we express our gratitude to Mrs. R. Posthumus for carrying out the on-line literature search. Special gratitude goes to Dr. Z. Gerstl (The Volcani Center, Bet Dagan, Israel) for readily supplying an extensive data base with adsorption data. Mrs. Augustijn-Beckers (Gainesville University Florida) is thanked for her efforts to find data for compounds for which very little information was available. S. Karickhoff and L. Carreira (US-EPA, Athens) are thanked for their efforts with respect to the calculation of acid dissociation constants using SPARC. D. Ten Hulscher (RIZA, Lelystad) is thanked for her efforts to select K_{ow}s.

Preface

This report contains results of research carried out in the framework of the project 'Setting integrated environmental quality objectives'. The results have been discussed in the 'Setting integrated environmental quality objectives advisory group'. Members thereof are C.W.M. Bodar (Health Council), J.H.M. de Bruijn (Ministry of Housing, Physical Planning and the Environment), J.H. Canton (National Institute of Public Health and Environmental Protection), C.A.J. Denneman (Ministry of Housing, Physical Planning and the Environment), J.W. Everts (Ministry of Transport, Public Works and Water Management, Tidal Waters Division), M.P.M. Janssen (National Institute of Public Health and Environmental Protection), P. Leeuwangh (Winand Staring Centre for Integrated Land, Soil and Water Research), W. Ma (Institue for Forestry and Nature Research), E.J. van de Plassche (National Institute of Public Health and Environmental Protection), P.B.M. Stortelder (National Institute of Inland Water Management), J. Struijs (National Institute of Public Health and Environmental Protection), M. Vossen (National Institute of Inland Water Management), and J. van Wensem (Technical Committee on Soil Protection).

Contents

Summary

In the frame of the project 'Setting environmental quality objectives', organic carbon normalized partition coefficients (K_{oc}s) describing the partitioning of organic chemicals in soils and sediments were derived for, among others, halogenated biphenyls and benzyltoluenes, chlorinated anilines and nitrobenzenes, various pesticides, phthalate esters and organotin compounds. For that purpose a literature review with respect to adsorption experiments with soils and sediments was carried out.

According to the equilibrium partitioning method the K_{oc}s can be used to derive quality objectives for soils and sediments from ecotoxicologically based quality objectives for water when toxicity data for soil or sediment organisms are not available. Furthermore, the K_{oc}s can be used to harmonize quality objectives for different compartments (soil, sediment, interstitial water and surface water).

Samenvatting

In het kader van het project Integrale Normstelling (in Dutch INS) zijn op organisch koolstof genormeerde partitiecoëfficiënten voor de distributie van stoffen in bodems en sedimenten (K_{oc}s) afgeleid voor onder andere gehalogeneerde biphenylen and benzyltoluenen, gechloreerde anilines and nitrobenzenen, diverse pesticiden, phthalate esters en organotin verbindingen. Daartoe is een literatuurevaluatie uitgevoerd met betrekking tot adsorptie-experimenten met bodems en sedimenten. Volgens de evenwichtspartitie methode kunnen de K_{oc}s gebruikt worden voor de afleiding van Maximaal Toelaatbare Risiconivo's (MTR's) voor bodem en sediment uit ecotoxicologisch onderbouwde MTR's voor water als er geen toxicologische gegevens voor bodem- of sedimentorganismen beschikbaar zijn. Verder kunnen de partitiecoëfficiënten gebruikt worden voor het op elkaar afstemmen van de MTR's voor de verschillende compartimenten (bodem, sediment, poriewater, en oppervlaktewater).

1 INTRODUCTION

1.1 Objective and framework

In 1989 the Directorate-General for Environmental Protection started the project 'Setting environmental quality objectives' (INS). In this project action item A-35 of the National Environmental Policy Plan (1989) is worked out. Goal is to derive integrated quality objectives for air, ground- and surface water, sediment and soil for a great number of compounds, based on the risk philosophy of the Ministry of Housing, Physical Planning, and the Environment (Premises for risk mamagement, 1989). The project is carried out by the National Institute of Public Health and Environmental Protection.

The first sub-project (a) 'MILBOWA' resulted in the report 'Desire for levels' (Van de Meent et al., 1990). In this report a methodology was proposed for deriving these objectives for several compounds e.g., heavy metals, chlorophenols, pesticides and polycyclic aromatic hydrocarbons. Based on this report integrated environmental quality objectives for water, sediment and soil were proposed by the Minister of the Environment of The Netherlands for several compounds (Environmental quality standards for soil and water, 1991).
The second project (b) is devided into three sub-projects: 'Exotic Metals' (b-1), 'Volatile Compounds' (b-2) and 'Secondary Poisoning' (b-3). A third sub-project (c) includes a large number of organic compounds, such as chlorinated anilines and nitrobenzenes, various pesticides, phthalate esters and organotin compounds. The b-1 and b-2 subprojects were completed, whereas the b-3 and c sub-projects are still in progress (Van de Plassche and de Bruijn, 1992; Van de Plassche and Bockting, in press).

For deriving quality objectives almost the same methods are used as described in 'Desire for levels'. Maximum permissible concentrations (MPCs) are determined using extrapolation methods based on toxicity data. Because the compartments border on one another, chemicals may move from one compartment to another. Therefore, sets of independently derived MPCs may not be coherent in a sense that maintaining the concentration at MPC-level in one compartment may lead to exceedance in other compartments. To avoid this, MPCs have to be harmonized; MPCs leading to concentrations in other compartments that exceed the MPC, are adjusted downwards. For the harmonization procedure, models are used that relate for example concentrations in air to concentrations in soil or sediment and water (Van de Meent and De Bruijn, 1993). For water and soil (or sediment) it is assumed that concentrations can be related with simple partition coefficients (K_ps).

In order to derive integrated quality objectives the following had to be done:

1. derivation of MPCs for water, sediment, and soil based on ecotoxicological data.
2. derivation of partition coefficients in order to apply the equilibrium partitioning method and intercompartimental harmonization,
3. gathering information about actual concentrations in soil, sediment, groundwater, and surface water from the Netherlands,
4. proposing integrated quality objectives.

In this report based on literature data, soil-water partition coefficients are proposed for compounds included in the b3 and c sub-projects of INS. The compounds considered are shown in Table 1 together with their structural and empirical formula. The Chemical Abstracts (CAS) registration numbers of the compounds can be found in Appendix B. In addition to the values for the b3 and c compounds, experimental adsorption data for a large number of compounds that are not included in the INS project, are listed (appendix C and E). These data might be relevant, be it now for other projects, or in the future, when new compounds are considered in the INS-project.

1.2 Equilibrium partitioning

The soil-water partition coefficient (K_p) of a chemical is defined as the ratio of the concentration of a compound in the solid phase versus its concentration in the water phase:

$$K_p = \frac{C_{sorbed}}{C_{water}} \quad [l.kg^{-1}] \tag{1}$$

The calculate the total concentration of a chemical in soil a simple mass balance equation can be used:

$$\rho C_{soil} = \rho C_{ads} + \theta C_l \quad [mg/l] \tag{2}$$

where

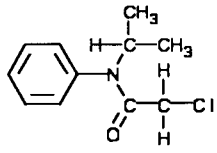
C_{soil} = the total concentration of the chemical in soil (mg/kg dry weight soil)
ρ = the soil dry bulk density (usually taken as 1.4-1.5 kg/l)
Θ = volumetric soil water content (often taken as 0.1)
C_l = the aqueous concentration of the contaminant in the porewater (mg/l)

Note that in the mass balance equation the contribution of the chemical that occurs in the gas-phase to the total concentration is assumed to be negligible.

Table 1. Formulas of the b3 and c compounds (CAS-registration numbers of the compounds are shown in Appendix B).

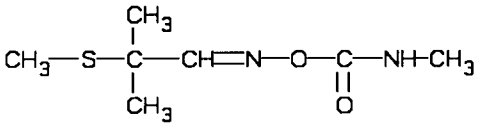
ACETANILIDES

propachlor $C_{11}H_{14}ClNO$

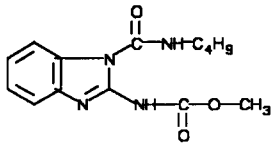


CARBAMATES

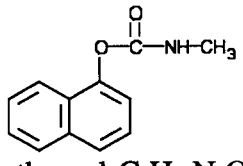
aldicarb $C_7H_{14}N_2O_2S$



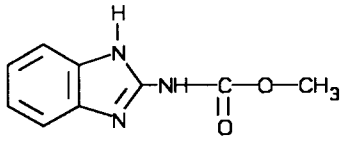
benomyl $C_{14}H_{18}N_4O_3$



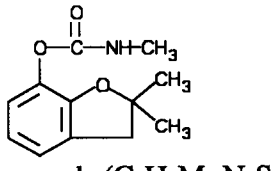
carbaryl $C_{12}H_{11}NO_2$



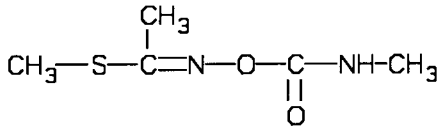
carbendazim $C_9H_9N_3O_3$ (acid)



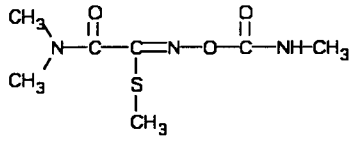
carbofuran $C_{12}H_{15}NO_3$



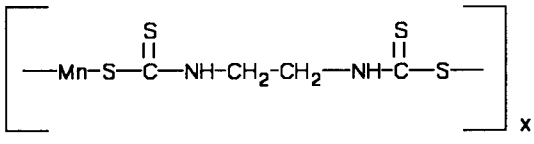
methomyl $C_5H_{10}N_2O_2S$



oxamyl $C_7H_{13}N_3O_3$

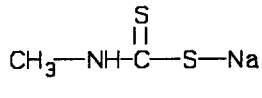


maneb $(C_4H_6MnN_2S_4)x$

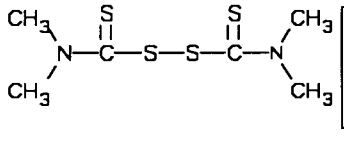


(polymeric)

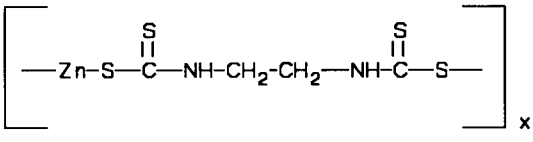
metham sodium $C_2H_4NNaS_2$



thiram $C_6H_{12}N_2S_4$



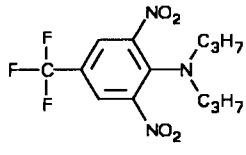
zineb $(C_4H_6N_2S_4Zn)x$



(polymeric)

DINITROANILINES

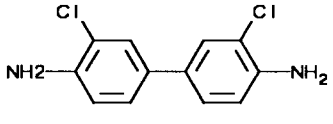
trifluralin $C_{13}H_{16}F_3N_3O_4$



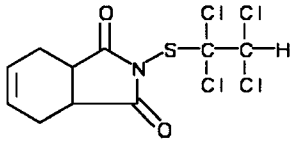
AROMATIC HALOGENATED HYDROCARBONS

Chlorinated pesticides

3,3-dichlorobenzidine $C_{12}H_{10}Cl_2N_2$



captafol $C_{10}H_9Cl_4NO_2S$



captan $C_9H_8Cl_3NO_2S$

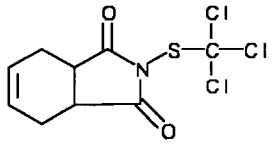
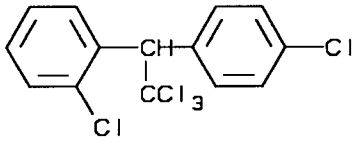
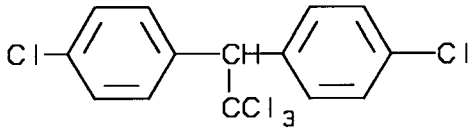


Table 1. (Continued) Formulas of the b3 and c compounds (CAS-registration numbers of the compounds are shown in Appendix B).

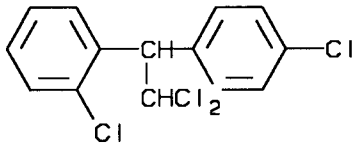
o,p'-DDT $C_{14}H_9Cl_5$



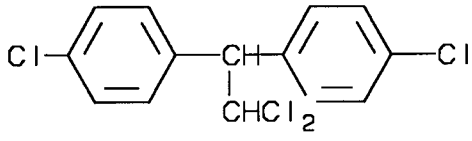
p,p'-DDT (= DDT) $C_{14}H_9Cl_5$



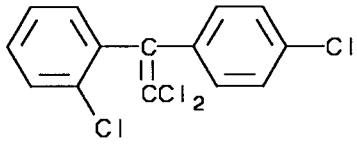
o,p'-DDD



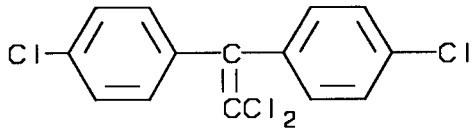
p,p'-DDD



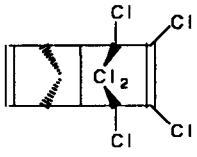
o,p'-DDE



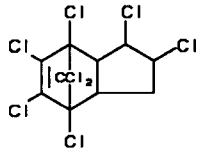
p,p'-DDE



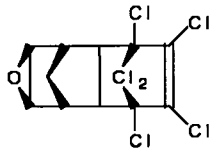
aldrin $C_{12}H_8Cl_6$



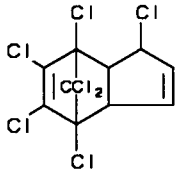
chlordane $C_{10}H_6Cl_8$



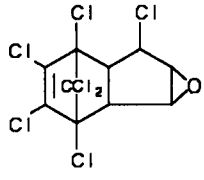
endrin $C_{12}H_8Cl_6O$



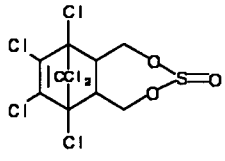
heptachlor $C_{10}H_5Cl_7$



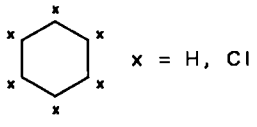
heptachlorepoxide $C_{10}H_5Cl_7O$



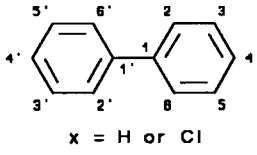
endosulfan $C_9H_8Cl_6O_3S$



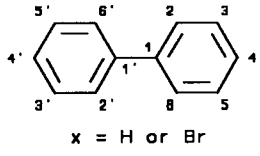
hexachlorocyclohexanes $C_6H_6Cl_6$



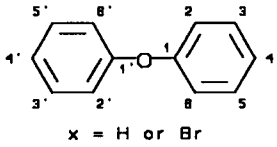
chlorinated biphenyls (PCBs)



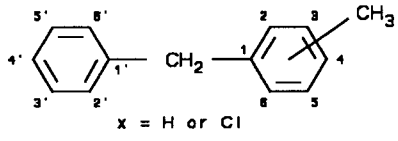
polybromine biphenyls (PBBs)



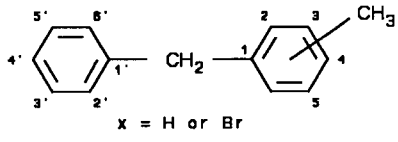
polybromine biphenyloxides



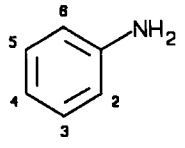
chlorinated benzyltoluenes (ugilecs)



dibromo benzyltoluenes (DBBTs)



chloroanilines



chloronitrobenzenes

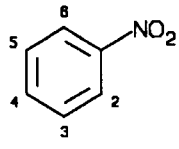
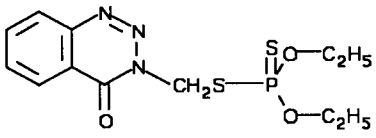


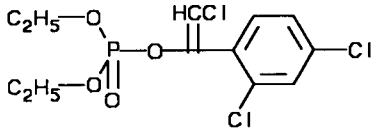
Table 1. (Continued) Formulas of the b3 and c compounds (CAS-registration numbers of the compounds are shown in Appendix B).

ORGANOPHOSPHATE PESTICIDES

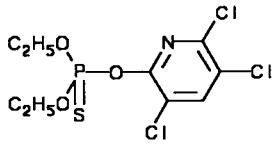
azinphos ethyl
$C_{12}H_{16}N_3O_3PS_2$



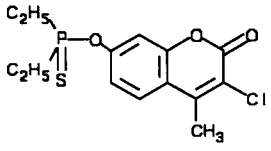
chlorfenvinphos
$C_{12}H_{14}Cl_3O_4P$



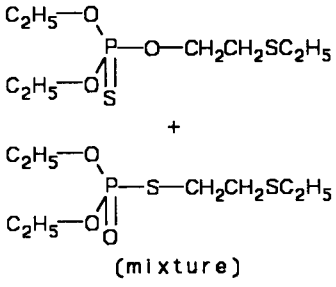
chlorpyrifos
$C_9H_{11}Cl_3NO_3PS_2$



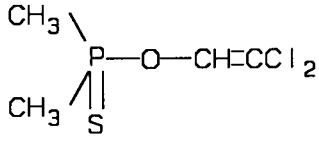
coumaphos $C_{14}H_{16}ClO_5PS$



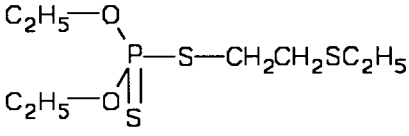
demeton $C_8H_{19}O_3PS_2$



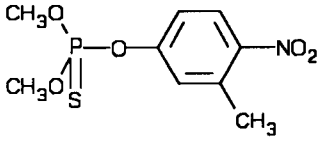
dichlorvos $C_4H_7Cl_2O_4P$



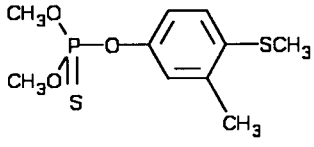
disulfoton $C_8H_{19}O_2PS_3$



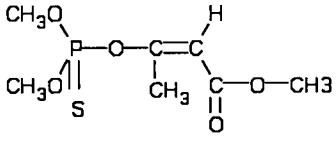
fenitrothion $C_9H_{12}NO_5PS$



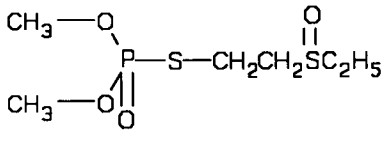
fenthion $C_{10}H_{15}O_3PS_2$



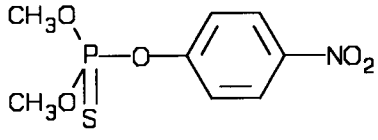
mevinphos $C_7H_{13}O_6P$



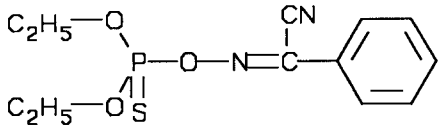
oxydemeton methyl
$C_6H_{15}O_4PS_2$



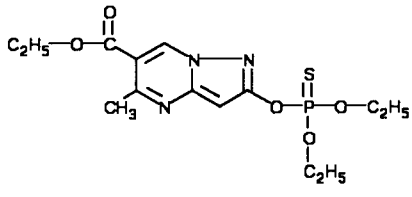
parathion-methyl $C_8H_{10}NO_5PS$



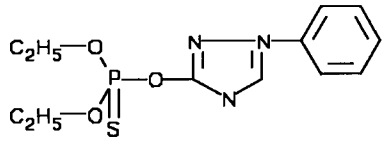
phoxim $C_{12}H_{15}N_2O_3PS$



pyrazophos $C_{14}H_{20}N_3O_5PS$



triazophos $C_{12}H_{16}N_3O_3PS$



trichlorfon $C_4H_8Cl_3O_4P$ (acid)

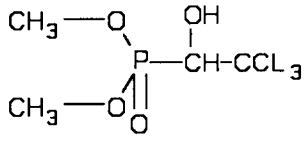
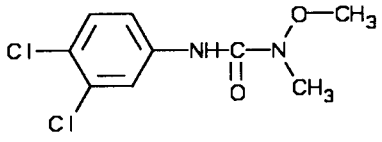


Table 1. (Continued) Formulas of the b3 and c compounds (CAS-registration numbers of the compounds are shown in Appendix B).

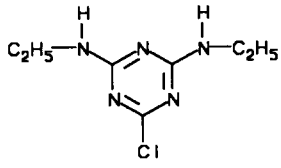
UREAS

linuron $C_9H_{10}Cl_2N_2O_2$



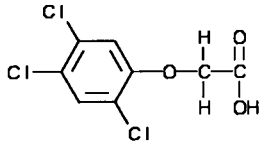
TRIAZINES

simazine $C_7H_{12}ClN_5$

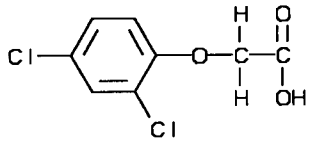


ACIDS

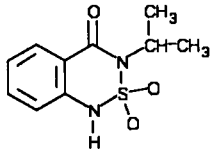
2,4,5-T $C_8H_5Cl_3O_3$



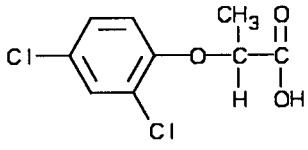
2,4-D $C_8H_6Cl_2O_3$



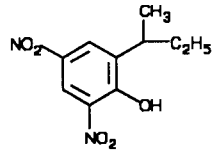
bentazone $C_{10}H_{12}N_2O_3S$



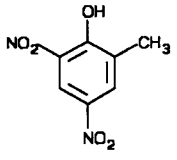
dichlorprop $C_9H_8Cl_2O_3$



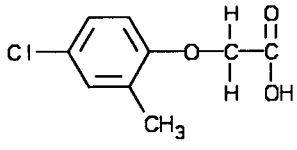
dinoseb $C_{10}H_{12}N_2O_5$



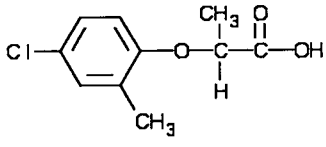
DNOC $C_7H_6N_2O_5$



MCPA $C_9H_9ClO_3$

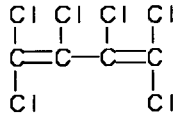


mecoprop $C_{10}H_{11}ClO_3$



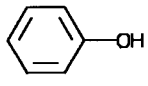
NON-AROMATIC HC HALOGENATED

hexachlorobutadiene C_4Cl_6

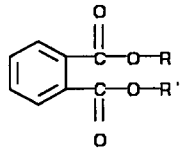


AROMATIC HC NON-HALOGENATED

phenol C_6H_6O

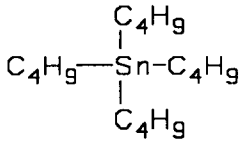


PHTHALATE ESTERS

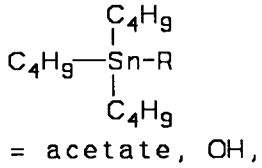


ORGANOTIN COMPOUNDS

tetrabutyltin



tributyltin compounds



triphenyltin compounds

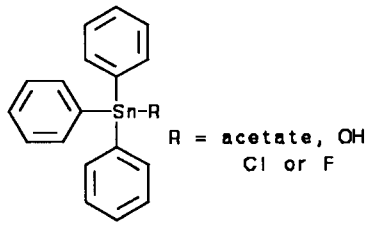
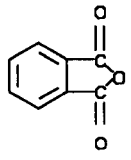


Table 1. (Continued) Formulas of the b3 and c compounds (CAS-registration numbers of the compounds are shown in Appendix B).

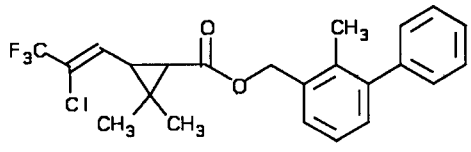
MISCELLANEOUS COMPOUNDS

phthalate anhydride $C_8H_4O_3$

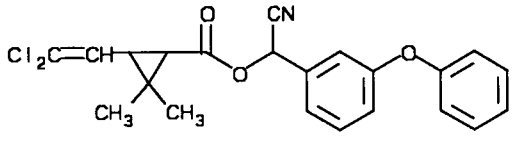


Pyrethroides

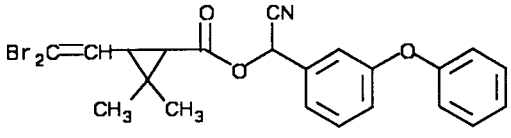
bifenthrin $C_{23}H_{22}ClF_3O_2$



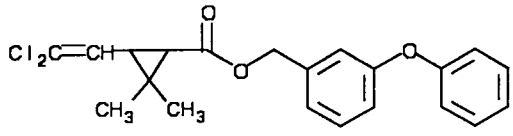
cypermethrin $C_{22}H_{19}Cl_2NO_3$



deltamethrin $C_{22}H_{19}Br_2NO_3$



permethrin $C_{21}H_{20}Cl_2O_3$



Assuming that adsorption processes determine the distribution of the contaminant over the solid phase and the porewater, total concentrations in soil can be related to the aqueous concentration after combining and equation 1 and 2:

$$C_{soil} = \frac{\rho K_p + \theta}{\rho} C_l \quad [mg.kg^{-1}] \tag{3}$$

For large K_ps (larger than approximately 1 l/kg) equation 3 can be approximated with:

$$C_{soil} = K_p C_l \quad [mg.kg^{-1}] \tag{4}$$

The equilibrium partitioning method (EP method) was originally proposed by Pavlou and Weston (1984) to develop sediment quality criteria. The concept has been described in detail by Shea (1988) and Di Toro et al. (1991). The method attempts to model the tendency of a chemical to move from one environmental compartment to another. The EP method is based on the premise that the distribution of contaminants in an environmental phase (e.g., sediment) is controlled by a continuous exchange with other environmental phases (water and biota) (Shea, 1988). These bio-geochemical exchange processes must be sufficiently rapid and reversible to have reached an equilibrium (or steady state) at the time of sample collection.

Potential biological effects of a certain contaminant concentration in the sediment can be estimated using appropriate water quality criteria and the partition coefficient for the contaminant between the aqueous phase and sediment phase. Rewriting equation 2 yields an equation that allows the derivation of sediment quality criteria from water quality criteria:

$$MPC_{sediment} = \frac{\rho K_p + \Theta}{\rho} MPC_{water} \quad (5)$$

where

MPC = the Maximum Permissible Concentration based on ecotoxicological data.

Again this equation can be simplified when K_ps are above approximately 10 l/kg.

$$MPC_{sediment} = K_p \, MPC_{water} \quad (6)$$

When the EP method is applied it is assumed that toxic effects are largely caused by exposure to pore water and hardly or not at all by uptake from particles (Van Leeuwen et al., 1992). Those opposing the EP method stress that this is not always valid (Landrum and Robbins, 1989).

Van de Meent et al. (1990) extended the EP method to soils to compensate for the lack of toxicity data for soil organisms. It is assumed that equation 1 that was originally proposed for the derivation of MPCs for sediments, can be applied also to derive MPCs for organisms living in terrestrial soils. In this report no distinction is made between K_ps for soils and sediments. For the sake of brevity the partition coefficients are usually termed soil-water partition coefficients.

A validation of the EP method for the derivation of MPCs for soils and sediments using literature data and field measurements is beyond the scope of this report, but will be undertaken by the National Institute of Public Health and Environmental Protection in the near future.

1.3 Approach

In order to collect the sometimes scarce data concerning the mobility of organic compounds in the environment, literature was selected from the Chemical Abstracts Data System (CAS) in April and July 1991. Relevant titles were selected using appropriate key words (shown in Appendix A) in combination with the CAS-registration number of the compound.

From the online search a recently published review on adsorption of organic substances by soils emerged (Gerstl, 1990). From the author a very extensive database containing experimentally determined K_{oc}s for 419 compounds was obtained. Approximately 4000 experimental K_{oc}s are listed together with a reference number that refers to easily accesible public literature. The reliability of Gerstl's data was tested with K_{oc}s that were already collected at that moment (K_{oc}s for chlorpyrifos, simazine and aldicarb). It was found that the K_{oc}s were derived in the same manner from the original sources. No errors were found.

In view of the limited time available it was decided to complement Gerstl's database with values from sources that were not covered by Gerstl: recently published data, data from grey literature and unpublished data. Naturally attention was directed to the b3 and c compounds.

Unpublished data or data published in grey literature were sought through consultation of experts in the field. Several authors of articles on the subject were approached with a request to supply unpublished data or private databases.

2 EXPERIMENTAL METHODS FOR THE DETERMINATION OF ORGANIC CARBON NORMALIZED SOIL-WATER PARTITION COEFFICIENTS

Adsorption can be caused by various intermolecular interactions of which 'hydrophobic bonding' caused by the repulsion of the molecule by water, is often considered most important for nonpolar, uncharged organic chemicals. Besides hydrophobic bonding, hydrogen bonding, charge tansfer, dipole interactions, chemisorption, ligand exchange and other interactions may play a role depending on characteristics of the chemical and the adsorbing surface considered. Hamaker and Thompson (1972) described in detail the intermolecular interactions involved in adsorption.

Lambert et al. (1965) observed a strong correlation between K_ps and the organic carbon content of soils. This led to the formulation of the organic carbon normalized soil-water partition coefficient (K_{oc}):

$$K_{oc} = \frac{K_p}{f_{oc}} \qquad [l.kg^{-1}] \tag{7}$$

The K_{oc} is normally considered to be independent of soil type. The correctness for nonpolar, hydrophobic compounds and especially the practical value of the concept was confirmed by later experiments (e.g., Karickhoff et al. 1979; Karickhoff 1984; Chiou et al. 1979).

2.1 Batch experiments

Batch experiments involve the shaking of soil, sediment or particulate matter with an aqueous solution containing the adsorbing chemical. After a certain equilibration period the suspension is either centrifugated or filtered and the aqueous concentration of the chemical is then determined. The adsorbed fraction is calculated from the decrease of the aqueous concentration. To derive an adsorption isotherm, the adsorbed fraction is measured for at least 4 to 5 initial concentrations. To determine the period required for equilibration of the adsorption process the progress of the adsorption should be determined. This is often done in a preliminary experiment.

To perform adsorption experiments at the very low aqueous concentrations that are usually found in the environment, it is often necessary to use a radioactive equivalent of the chemical to be tested. The chemical derives its radioactivity from a structural atom that is replaced by a radioactive isotope (usually ^{14}C, ^{2}H or ^{36}Cl). The adsorbed fraction of the chemical is determined from the decrease of radioactivity in the aqueous phase after equilibration. McCarty et al. (1988) stated that when radiolabled sorbants are used,

precautions should be taken to avoid artefacts resulting from radiochemical impurities. Often impurities are relatively polar oxidation products of the parent compound, particularly in the case of photosensitive substances such as polyaromatic hydrocarbons (Gollnick, 1968). The artefact might have lead in some experiments to underestimated partition coefficients, apparantly partially non-reversible adsorption in systems in which binding was fully reversible or apparantly decreasing partition coefficients as the sorbent concentration (or solid-solution ratio) is increased.

Experimental conditions for batch experiments should be chosen in such a way that reliable K_ps or adsorption isotherms are derived. For batch experiments this means that experimental conditions resulting in nearly complete or nearly no adsorption should be avoided. In these cases small analytical errors of the aqueous concentration will lead to a considerable error in the K_p (Bockting et al., 1992). Initial concentrations and particle concentrations should be chosen in such a way that adsorption will lie between 20 to 80 %.

A critical step in a batch batch experiment is always the separation of the solid and liquid phase (through centrifugation or filtration). Often a complete separation is not achieved due to the adsorption of the contaminant to a 'third-phase' (colloids and organic macromolecules) that can not be separated from the water phase using normal filtration and centrifugation techniques. The resulting overestimation of aqueous contaminant concentrations leads to an underestimation of K_ps. This holds especially for very hydrophobic compounds (e.g., PCBs and PAHs) that have a large affinity for the 'third-phase'.

A recent development in the study of contaminant adsorption is the application of the so called co-solvent method (Evers and Smedes, 1993, in press). Basically, the co-solvent method can be regarded as a modification of the batch method, where as an extra step a co-solvent (often methanol) is added to the soil(sediment)-water system. The co-solvent acts as an 'third-phase' to which the hydrophobic contaminant binds. This binding is relatively strong so that when co-solvent concentrations are high the macromolecule can not bind to colloids and organic macromolecules. Variation of the amount of co-solvent (e.g., 5 batches with 0 % to 30 % co-solvent) allows the quantification of the 'third-phase effect' caused by the binding to colloids and organic macromolecules and the calculation of a K_p corrected for this effect.

2.2 Column or leaching experiments

The potential of a chemical to leach to the groundwater from contaminated soils is usually tested in column experiments. Usually the chemicals are applied at the top of a soil filled column and subsequently the column is sprinkled for a certain period with water. At the bottom of the column the drain water is collected at given time intervals for analysis. From the progress of concentration in the drain water a so called retention factor (R_f) is calculated. Although the primary goal of column experiments is usually not the determination of a K_p or K_{oc}, but the determination of the leaching potential of a chemical in a particular soil, the R_f can be used to calculate a K_p according to Ross' (1989) equation:

$$K_p = \frac{\theta(R_f - 1)}{\rho} \quad [l/kg] \tag{8}$$

where

ρ = the soil dry bulk density (usually taken as 1.4-1.5 kg/l)
Θ = volumetric soil water content (often taken as 0.1)

2.3 In situ measurements

Measurements of the concentration of organic chemicals in porewater and solid phase of soils and sediments can give valuable information about the actual distribution of chemicals in the field.

Unfortunately, field data are very scarce, probably due to analytical problems associated with the usually low aqueous concentrations that are encountered in the field and difficulties associated with sampling porewater from soils and sediments. Futhermore, the data that are available are usually difficult to interpret because they are not necessarily related to an equilibrium situation and because degradation processes rather than adsorption might have determined the chemicals distribution. At the RIVM efforts are being made to measure the concentration of chemicals (PAHs and some organochlor pesticides) in the porewater and solid phase of field-contaminated sediments (Van den Hoop, 1993). The results will be reported soon.

Courto et al. (1992) derived K_{oc}s for 13 PAHs from measurements in filtered riverine water, sediments and suspended matter. For 10 compounds the in situ K_{oc}s were considerably higher (approximately two orders of magnitude) than values calculated from K_{ow}s using the regression equation proposed by Karickhoff et al. (1981). Similar

observations have been made by others (Kayal and Connell 1990; Readman et al. 1984). The authors attributed the deviations from laboratory studies to factors such as binding to particulate matter, dissolved organic carbon or deviations from equilibrium in the field situation. Although biological and chemical degradation is usually considered a relatively slow process for most PAHs, it cannot be excluded that degradation has lead to low aqueous concentrations and consequently to high K_{oc}s in the study of Courto et al.

3 ESTIMATION METHODS FOR ORGANIC CARBON NORMALIZED SOIL-WATER PARTITION COEFFICIENTS

Numerous reviews have been written on factors affecting the adsorption of organic compounds by soils and sediments and its prediction from K_{ow}, water solubility, and other parameters (e.g., Dragun, 1988; Karickhoff, 1981; Gerstl, 1990; Kenaga, 1980; Briggs, 1981; Calvet; 1989; Jaffé, 1991; Lyman et al, 1983). The relationships between the parameters are obtained from various data sets using regression analysis. Other articles concern the prediction of adsorption from molecular stucture using molecular connectivity indices (e.g., Sabljic, 1984 and 1987; Gerstl, 1990; Gerstl and Helling, 1987; Bahnick and Doucette, 1988; Evers et al., 1990), or adsorbability indices (Okouchi and Saegusa, 1989) and the parachor (e.g., Lambert, 1967; Hance, 1969). Banerjee and Howard (1998) presented the UNIFAC theory. The UNIFAC (UNIQUAC functional group Activity Coefficient) group contribution method is a semi-empirical method for the prediction of partition coefficients of liquid mixtures. The Flory-Huggins theory (Porter and Schmedding, 1983; Chin and Weber, 1989) utilizes molar volumes and solubility parameters. Attempts to quantify interactions between polymeric humic materials and hydrophobic compounds were quite promising. Kamlet et al. (1988) demonstrated that solvation properties, such as aqueous solubility and the partition behaviour of nonionic organic compounds between water and organic phases, can be modelled using LSERs (Linear Solvation Energy Relationships).

After statistical analysis of a large data set Gerstl (1990) concluded that the use of molecular connectivity indices alone are inadequate for predicting adsorption values with the exception of a few homologous groups.

The reader is referred to the literature mentioned above for a detailed description of the factors affecting adsorption and methods for the estimation of adsorption.

K_{oc}-K_{ow} relationships are frequently used because of their simplicity and because they appear to predict adsorption reasonably well. These relationships are regression equations obtained from various data sets and are usually expressed in log-log form:

$$\log K_{oc} = a \log K_{ow} + b \qquad [l.kg^{-1}] \tag{9}$$

where a and b are constants.

Reported values for a and b range from 0.4 to 1.0 and from -0.2 to 1.4, respectively. Each equation is derived from a different data set representing different chemicals (sometimes just one or two chemical classes). Many of the chemicals are pesticides. Aromatic and

polyaromatic hydrocarbons are also well represented. According to Lyman et al. (1990) the uncertainty associated with any value of K_{oc} estimated by one of these equations is generally less than one order of magnitude. This assumes that the estimated K_{oc} is to be used for an environmental system that does not differ significantly from one implied by the normal conditon of test (temperature, soil pH, chemical concentration, salinity, etc.). Attempts to extrapolate much beyond these conditons will invite additional errors.

In this chapter and chapter 5 experimental K_{oc}s are compared with predicted K_{ow}s using parameters for the regression equation proposed by Karickhoff (1981):

$$\log K_{oc} = 0.989 \log K_{ow} - 0.346 \tag{10}$$

and DiToro et al. (1991):

$$\log K_{oc} = \log K_{ow} \tag{11}$$

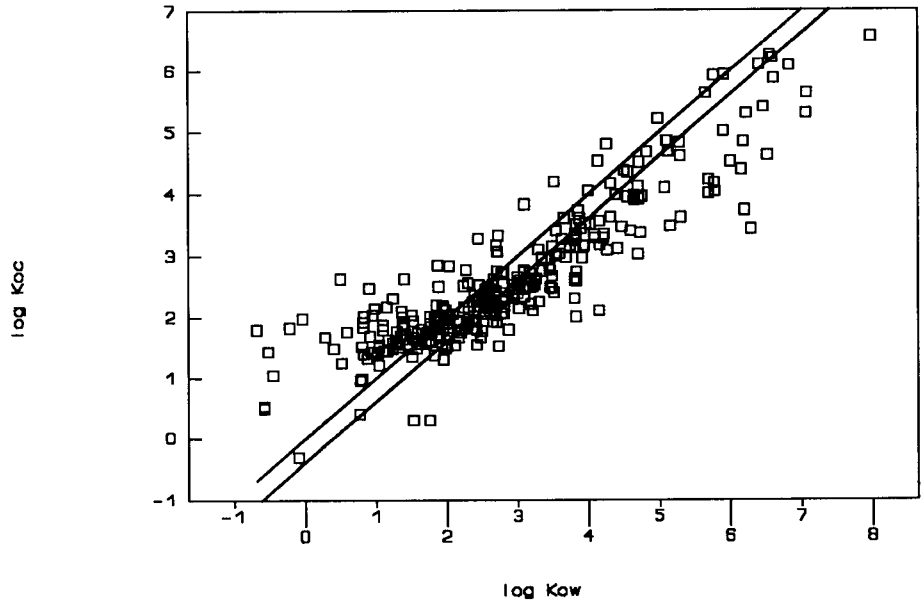


Figure 1 Relationship between experimental K_{oc}s and K_{ow}s (data from Gerstl, 1990). Regression lines (based on other datasets) proposed by Di Toro et al. (1991) (upper) and Karickhoff (1981) (lower) were added for comparison. Both relations are used frequently for the estimation of K_{oc}s for hydrophobic (non-ionic) compounds from K_{ow}s.

From Figure 1 it appears that considerable deviations from regression equations occur and that the large deviations are most frequent at low and high values of K_{ow} and K_{oc}. These observations are not surprising considering that, depending on the chemical and soil studied, a very different type of intermolecular interaction may dominate adsorption (see Chapter 2). Furthermore, the variability of physico-chemical characteristics of soil (and organic matter) and the variation associated with the different experimental methods employed for the determination of K_{ow}s and K_{oc}s, are reflected in Figure 1.
Naturally, when regression equations are being based on larger data sets the reliability of the estimated K_{oc}s is enhanced. However, Figure 1 suggests that accurate predictions can not be made with a single regression equation of the form of equation 5. An approach that potentially enhances the reliability of predictive equations for K_{oc} estimation was presented by Gerstl (1990). Based on a large database regression equations relating K_{ow} and K_{oc} were derived for compounds from 16 chemical groups, which are presented in Table 2.

Table 2. Regresssion equations of log K_{oc} with log K_{ow} for several chemical groups (after Gerstl, 1990).

		$\log K_{oc} = a \log K_{ow} + b$		
	Group	a	b	R^2
	All compounds	0.679	0.663	0.831
1	Acetanilides	-	-	-
2	Carbamates	0.433	0.919	0.863
3	Dinitroanilines	0.431	1.787	0.852
4	Aromatic hydrocarbons halogenated	0.722	0.417	0.855
5	Organophosorous pesticides	0.689	0.530	0.672
6	Ureas	0.545	0.943	0.713
7	Triazines	0.586	0.826	0.894
8	Triazoles	0.583	0.969	0.799
9	Acids	-	-	-
10	PAH	0.762	1.051	0.898
11	Non-aromatic hydrocarbons halogenated	0.827	-0.039	0.698
12	Aromatic hydrocarbons non-halogenated	0.529	0.916	0.664
13	Amides	0.253	1.776	0.808
14	Phthalate esters	-	-	-
15	Organotin compounds	-	-	-
16	Miscellaneous	0.556	0.863	0.745

This approach might enhance reliability because for chemicals with similar structural properties the same type of intermolecular interactions are likely to dominate adsorption.

In Chapter 4 K_{oc}s calculated with Gerstl's equations are compared with K_{oc}s calculated in a traditional manner (equation 5).

3.1 Taking into account acid dissociation

Some organic compounds contain acidic groups (e.g., hydroxyl or carboxyl groups) from which a proton can dissociate. Dissociation of a neutral acid yields negatively charged species. These species are, due to their low hydrophobicity probably much more mobile in soil than their parent acids. Therefore, a pH-dependent partition coefficient is sometimes calculated from K_{ow} and pK_a (Van de Meent et al. 1990). In such calculations it is normally assumed that adsorption of negative species can be neglected when compared to adsorption of the parent acid:

$$K_{oc} = K_{ow} * f_{nd} \qquad (12)$$

The non-dissociated fraction (f_{nd}) is calculated according to:

$$f_{nd} = \frac{1}{10^{pH-pKa} + 1} \qquad (13)$$

Here pK_a is the negative logarithmic value of the equilibrium constant for a acid dissociation reaction.

pK_as can be calculated from structural properties of the compounds. An overview of the available estimation methods is given by Lyman et al. (1990).

Karickhoff and co-workers developed a computer programme called SPARC (SPARC Performs Automated Reasoning in Chemistry) for the computation of a variety of reactivity parameters using computational algorithms based on fundamental chemical structure. The parameters that can be estimated include UV-visible absorption spectra and various equilibrium/rate constants including pK_as. An overview of the computational procedures was recently published by Karickhoff et al. (1991). Additional papers are in preparation describing in detail the chemical models and specific applications.

3.2 The marine environment

To allow the application of the K_{oc}s derived in this report for the marine environment, the literature was studied with respect to the influence of salinity on the adsorption of organic compounds.

Karickhoff et al. (1979) found that the logarithmic K_{oc} for pyrene increased with 0.06 units going from pure water to a sodium chloride solution concentration of 0.34 M. A similar, small increase was found by Schwartzenbach et al. (1992). Based on a thermodynamic approach, they concluded that an increase of the Cl^- concentration up to an ionic strength of 0.34 M would result in 0.09 units higher (logarithmic) K_{oc} for pyrene (the ionic strenght of seawater is around 0.7 M).

Although Karickhoff's and Schwartzenbach's results show a small discrepancy, it looks reasonable to conclude that K_{oc}s for hydrophobic compounds in the marine environment are not significantly different from K_{oc}s for fresh water systems.

Salinity might have a more pronounced effect on the adsorption of ionic or polar compounds. However, from a publication of Johnson and Westall (1990) it appeared that a general predictive equation for marine K_{oc}s for these compounds cannot be formulated yet. As a first approximation it is assumed here that the K_{oc}s for ionic and polar compounds are also valid for the marine environment.

4 DERIVING ORGANIC CARBON NORMALIZED SOIL-WATER PARTITION COEFFICIENTS FROM LITERATURE DATA

4.1 Batch experiments versus in situ measurements and column experiments

In view of the paucity of in situ measurements and the difficulties with the interpretation of the results, derivation of K_{oc}s from this type of experiments was not considered. When more in situ measurements become available in the future, attempts should be made to validate the extrapolation of laboratory data to the field.

Column experiments have advantages and disadvantages over batch experiments for the determination of contaminant mobility. In general terms it can be said that physico/chemical conditions of (terrestrial) soils in the field are reflected better in column experiments than in batch experiments. For example, particle concentrations in batch experiments are considerably lower than actual particle concentrations of soils. However, from results of column experiments it usually is not possible to decide whether the adsorption processes have reached an equilibrium situation. Most of the time this will probably not be the case.

Because of the problems associated with the other techniques described above it was decided to collect only K_{oc}s determined in batch experiments. Fortunately, most K_{oc}s found in the literature are determined in batch experiments.

4.2 Concentration dependency

In many experiments it is suggested that the K_p and K_{oc} for the adsorption of a chemical to a given soil is not constant, but dependent upon the equilibrium concentration of the aqueous phase. It is often suggested that K_{oc}s increase at low equilibrium concentrations. To describe the deviation from linearity of the adsorption process, several equations, relating aqueous concentrations with concentrations in the solid phase, called adsorption isotherms are used. Often experimental adsorption data are fitted using Freundlich's isotherm:

$$C_s = K_f C_e^N \qquad (14)$$

where

C_s = the amount of chemical adsorbed to the solid phase per kg solid phase [$mg.kg^{-1}$]
C_e = the aqueous equilibrium concentration of the chemical [$mg.l^{-1}$]
N = a dimensionless exponent
K_f = the Freundlich constant [$mg^{(1-N)}.l^N.kg^{-1}$]

N (sometimes indicated as 1/n in the literature) describes the deviation from linearity. Values for N found in the literature vary mostly between 0.7 and 1.2. Rao and Davidson (1980) found an average value of 0.87 for 26 chemicals.

The Freundlich isotherm is entirely empirical, in other words its validity is not supported by physico-chemical understanding of adsorption processes or experimental proof. Extrapolations of K_ps to concentrations outside the range where they were actually determined are therefore very questionable and resulting K_ps are therefore unreliable.

The unit of K_f depends on the units chosen for C_s and C_e and the value of N (equation 8). Because authors use different units for C_s and C_e (e.g. kg/kg, mg/kg, ug/kg, mole/kg) literature values for K_f cannot be compared directly. Care should be taken because in the literature the unit for K_f is often not given or is erroneously stated (e.g., $m^3.kg^{(-1)}$ or $l.kg^{-1}$).

Combining Freundlich's isotherm (equation 8) with the definition of the K_p (equation 5) leads to the formulation of a concentration dependent K_p:

$$K_p(C_e) = K_f C_e^{(1/n-1)} \quad [l.kg^{-1}] \qquad (15)$$

It is important to realize that K_f is in general not equal to K_p. From equation 6 it follows that this is only true if N = 1 (linear adsorption) or if the C_e = 1 (in the unit that was originally chosen for aqueous concentrations). It is often reported that experimental adsorption data are better described by a Freundlich equation than a linear regression equation. From the good fit of (non-linear) Freundlich isotherms it may seem that that adsorption of organic chemicals by soils is a concentration dependent, non-linear process. However, no conclusive evidence for non-linearity was found in the literature. Unfortunately, most authors do not indicate whether the enhancement of the goodness of fit after applying the Freundlich equation is statistically significant. Chiou et al. (1979) performed batch experiments over a very wide range of aqueous concentrations. No deviation from linearity was observed.

In this report it is assumed that the relation between the content associated with the solid phase and the aqueous concentration is approximately linear for the range of concentrations considered. To derive K_ps from adsorption data reported in the form of Freundlich isotherms the following approach was chosen. From the parameters of the Freundlich isotherm and the initial chemical concentration (C_i), C_e and the corresponding K_p (and K_{oc}) were calculated. K_ps for low aqeous concentrations are most relevant in the framework of this report, because environmental concentrations and MPCs for water are usually low. Therefore, K_{oc}s corresponding with the lowest experimental C_es were preferred over K_{oc}s corresponding with high C_es. In those cases where C_e could not be calculated, because the

experimental conditions were not described sufficiently, K_{oc}s were derived assuming that C_e was equal to 1 mg/l.

4.3 Reliability of experimental data

4.3.1 Organic carbon normalized soil-water partition coefficients

At the beginning of the literature research, after the decision was taken to derive K_{oc}s primarily from batch experiments, various methods for estimation of the reliablity of literature derived adsorption data were considered.

Most appealing was a method proposed by Kollig (1988) that attempts the quantification of the reliability of experimentally determined environmental parameters (e.g., K_{oc}s and solubility). The method involves the formulation of a set of evaluation criteria for each parameter considered. Each criterion is assigned a weight factor between 1 and 10, according to the importance of the criterion. Then for each experimental value, the so called Data Reliability Indicator (DRI) is calculated by adding the weight factors of criteria that are met and dividing by the maximum score. Kollig defines DRIs as the degree of confidence with which a literature value can be used. DRIs equal to 1 refer to values with maximum reliability and DRIs equal to zero or only slightly above zero refer to values with poor reliability.

10 evaluation criteria were formulated:

1. Are the soils or sediments tested representative for Dutch soils and sediments?
2. Was the pH, f_{oc} and CEC (cation exchange capacity) and texture of the soil or sediment stated?
3. Were the Kps measured at more than one pH value? (only for ionic compounds)
4. Was adsorption tested for a minimum of 3 test concentrations, below the water solubility of the chemical?
5. Was the aqueous concentration lowered no more than 80% and not less than 20%?
6. Was the equilibration period shorter than the period in which more than 3% of the chemical is expected to decompose?
7. Were the reaction vessels capped? (only for volatile chemicals)
8. Was equilibration shown?
9. Was the stability of the chemical in water, soil or sediment shown?
10. Was the concentration of the chemical after equilibration determined in both the water and the sediment or soil, to allow calculation of a mass balance?

It soon emerged that this method of reliability estimation was impractical. Information essential for answering the 10 questions was often not found. Probably, because the space

available for the description of experimental methods is usually very limited in the public literature. The lack of information does not automatically mean that precautions, for example against volatilisation, were not taken by the experimentator. Furthermore, to answer question 3, 4, 6 and 7, information on the chemical's pK_a, solubility, degradation rate, and volatility is required. This information was generally not readily available and the estimation of reliable values for these parameters, would require time consuming additional literature studies. Particularly, the estimation of a reliable degradation rate proved to be a problem.

During the collection of experimental values it was gradually realized that the criterion of most importance for batch experiments is the mass balance requirement (amount of chemical in the soil = initially added amount of chemical - amount of chemical in water). This is the only way to prove that Kps determined in batch experiments are not in error due to analytical errors, incomplete separation of the solid and liquid phase, volatilisation, degradation or adsorption to the walls of the reaction vessel.

Unfortunately, until now few experimentators take the trouble to measure equilibrium concentrations in both the water and the soil or sediment. This is not surprising because the extraction of organic chemicals from soils or sediments for analysis is an elaborative procedure. It is often difficult to extract the chemical completely, whereas complete or at least nearly complete extraction is required for a proper calculation of the mass balance. Nevertheless, the importance of the mass balance requirement is gradually recognized and in recently published experiments sometimes the mass balance requirement is met (e.g., Opperhuizen et al., 1991; Von Oepen, 1991; Dao et al., 1986; Adams, et al., 1993).

The 10 evaluation criteria (except the mass balance requirement) and calculation of the DRI were now omitted. Only when the mass balance requirement was met, an experimental value is considered relatively reliable. However, exclusion of all values for which this criterion was not met, would have reduced the number of values dramatically, and was therefore not considered. At this moment the only practical way of estimating K_{oc}s for a large number of compounds with maximum reliablity, seems to be to collect a large number of values obtained with various soils by, preferably more than one experimentator. When for a chemical very few values are available, comparison of the experimental values with calculated values (e.g., from K_{ow}) may reveal data that are in error, or when deviations proof to be small, add to one's confidence in the experimental value.

4.3.2 Octanol-water partition coefficients

K_{ow}s are often selected form the MEDCHEM database (1992). Besides a large number of K_{ow}s from the literature the database contains a routine for estimation of K_{ow}s based on

structural properties of the compound (ClogP method). A description of the database and estimation method is given by Leo et al. (1971). Generally, the MEDCHEM database is considered the most extensive and reliable source for K_{ow}s available. The authors of the database indicate the value that is most reliable in their opinion with a star. K_{ow}s calculated with the ClogP method are less reliable than experimental values, but in an evaluation of the system (Verhaar and Hermens, 1990) it was concluded that the estimation method normally leads to reasonable values. Estimation is poor (and sometimes not possible at all) for compounds with structural phosphorus, sulfur, and metal atoms (organotin compounds, organophosphate pesticides and some carbamates).

4.4 Statistical analysis

To find out the nature of the distribution of K_{oc} data Gerstl (1990) performed statistical analysis of his adsorption data. The test included 13 compounds from different chemical groups for which adequate numbers of K_{oc}s were available. In all cases but one (pyrene) K_{oc}s were approximately log-normally distributed. It was concluded that, for most cases the use of an average log K_{oc} value (geometric mean) instead of an untransformed K_{oc} value is required.

5 RESULTS

5.1 Octanol-water partition coefficients

The K_{ow}s shown in Appendix B were selected mainly by Ten Hulsher (1992). Most values were found in the MEDCHEM database. Unfortunately, the values recommended in the MEDCHEM database (the star values) were sometimes based on old literature (1960-1970) or derived from non-evaluated sources (unpublished results, private communication) whereas recently published data based on more accurate analytical methods were available. In those cases Ten Hulscher proposed the use of a different value than the star value. Often this was a K_{ow} determined with the 'slow stirring' method (De Bruijn et al, 1989). This technique prevents the formation of octanol emulsions that, in the traditional 'shake-flask' technique, lead to an underestimation of the K_{ow} for relatively hydrophobic chemicals (log Kow > 4.5).

The MEDCHEM database does not contain K_{ow}s for ugilecs, the values shown were obtained from Van Haelst (1992).

The K_{ow}s for the o,p'-DDD and p,p'-DDD isomers (Appendix B) show a surprisingly large difference (one logarithmic unit). The value for the p,p'-isomer was determined experimentally, whereas the value for the o,p-DDD was calculated according to the ClogP method. Theoretically, one would expect a lower K_{ow} for o,p'-DDD than for p,p'-DDD because the chlorine atoms of this isomer show more overlap with the electron orbitals of the central methyl group of the molecule than for p,p'-DDD (Table 1). However, this effect cannot explain the large difference of one order of magnitude. It is believed that this difference is caused by an inaccuracy of the ClogP method. In Table 3 the experimental K_{ow} for p,p'-DDD is used for estimating the K_{oc} of both isomers.

The K_{ow}s for the chloronitrobenzenes (Appendix B) showed large variations (upto one order of magnitude) for the individual isomers depending on the author. Here the values taken from Opperhuizen et al. (1991) are recommended because they were determined with the 'slow stirring' method. The finally recommended K_{ow}s for the b3 and c compounds are presented in Table 3. Average values are presented for the isomers, however work is still in progress and more detailed information may become available in the near future (Opperhuizen, 1993, personal communication). Unfortunately, for some compounds (several dithiocarbamates, demeton and tetrabutyltin) no experimental K_{ow} was available and also calculation according to the ClogP method was not possible.

K_{ow}s for phthalates found in the literature often vary considerably. When for example K_{ow}s measured by Leyder and Boulanger (1983) are compared with data of Howard et al.

(1985), a variation upto one order of magnitude is observed. Sometimes variation is even larger. Howard et al. (1985) determined a log K_{ow} of 7.94 for di-2-ethylhexylphthalate, whereas Kenaga and Goring (1980) presented a value of 3.98. The large variation is probably a result of analystical problems and different experimental methods employed. because of the large uncertainity K_{ow}s for only 4 phthalates are recommended here. All these values originate from the MEDCHEM database and comparison with literature sources showed that deviations were within reasonable limits.

5.2 Acid dissociation constants

The pK_as shown in Table 3 were calculated by Karickhoff and Carreira (1992) using SPARC (Karickhoff et al., 1991). For most compounds no pK_a is given because these chemicals contain no groups from which a proton could dissociate in the presence of water.

5.3 Organic carbon normalized soil-water partition coefficients

Appendix C contains all the available experimental K_{oc}s (logarithmic) together with a number referring to the literature source. Appendix D contains the references corresponding to these numbers. Reference numbers below 1000 refer to data collected by Gerstl. Reference numbers above 1000 refer to data added in 1992 and 1993 at the RIVM. Appendix E contains average log K_{oc}s calculated from the data in Appendix C. In the second column standard deviations are shown. N refers to the number of K_{oc}s used for calculation of averages and standard deviation. The average standard deviation for 270 compounds is 0.28 (approximately a factor 2).

Average experimental K_{oc}s for the b3 and c compounds are shown in Table 3. In addition to the experimental values Table 3 contains K_{oc}s estimated from K_{ow}s according to the equations of Di Toro et al. (1991) and Gerstl (1990) (Table 2), and eventually pK_as (equation 6 and 7) when acids are concerned. The last column of Table 3 shows K_{oc}s recommended for the derivation of MPCs for soil and sediment according to the EP-method and harmonization of MPCs for soil, sediment and water. Experimental K_{oc}s were preferred over calculated values.

The relation between the recommended K_{oc} and K_{ow}s for the b3 and c compounds is shown in Figure 2.

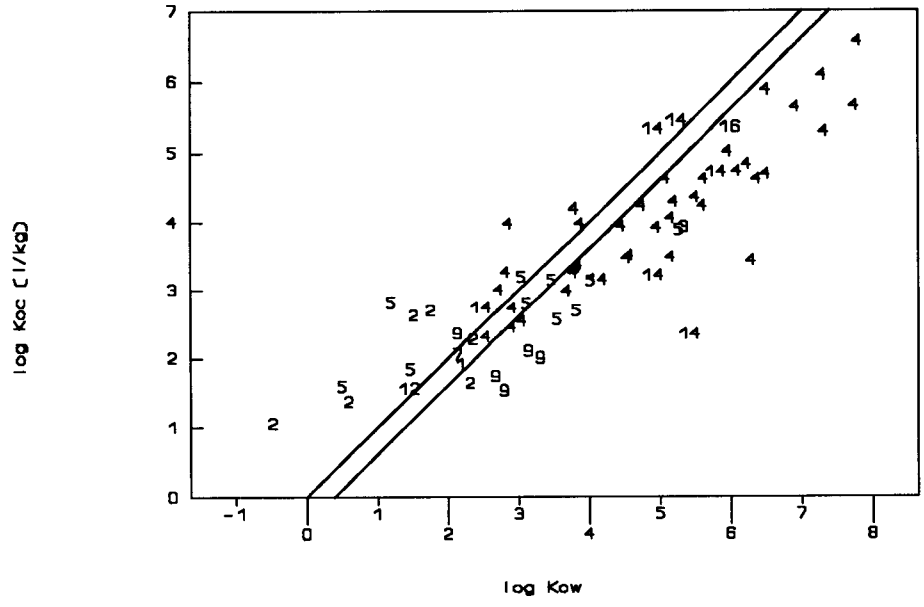


Figure 2 K_{oc} versus K_{ow} for the b3 and c compounds. The numbers refer to the chemical groups (Table 2). Regression lines proposed by Di Toro et al. (1991) (upper) and Karickhoff (1981) (lower) were added for comparison. Both relations are used frequently for the estimation of K_{oc}s for hydrophobic (non-ionic) compounds from K_{ow}s.

5.3.1 Acetanilides

For propachlor 11 experimental K_{oc}s were available. Considering the relatively large standard deviation (0.41, logarithmic) the average K_{oc} value is in good agreement with the value predicted from the K_{ow} using Di Toro's equation.

5.3.2 Carbamates

For all carbamates, except benomyl, maneb, metham sodium and thiram, experimental K_{oc}s were found. For aldicarb, carbofuran and oxamyl the standard deviations (0.33 - 0.38) are larger than the average standard deviation (0.28). For aldicarb the large deviation might be

a result from experimental difficulties associated with the rapid transformations that occurs when this compound is introduced in the soil. The structural sulfur atom of aldicarb (Table 1) undergoes rapid oxidation in soil to form aldicarb sulfone and sulfoxide (RIVM, 1993). Literature in which the adsorption of these metabolites was studied in detail showed that these compounds are more mobile than the parent compound aldicarb (Appendix C). Because of the rapid oxidation of aldicarb it is likely that the K_{oc}s shown in Table 3 do not reflect the adsorption of the parent compound only, but also reflect the influence of the weaker adsorption of metabolites.

Prediction of K_{oc}s according to the equation of Di Toro et al. (1991) leads in three cases to K_{oc}s that are significantly different (one overestimation and 2 underestimations) from the average experimental K_{oc}s.

For the dithiocarbamates, K_{oc} and K_{ow} data were scarce. Only for metham sodium and thiram data were available. Here the K_{oc} estimated from the K_{ow} value seems to underestimate considerably. Prediction of the adsorption of maneb and zineb is very troublesome because for these compounds no K_{oc} and K_{ow} (neither measured nor calculated) is available. Even when values for these parameters would have been available the prediction would remain troublesome because the compounds may form polymeric colloids in water. The mobility of colloids is difficult to predict and can certainly not be predicted properly using only a K_{ow}. Therefore, no K_{oc}s are recommended for maneb and thiram.

Table 3. Partitioning data and recommended K_{oc} values for INS-b3 and c compounds.

COMPOUND	Log Kow	pK_a/pK_b[a] [1]	log K_{oc} experimental average	STD	N	log K_{oc} estimated [2]	[3][b]	log K_{oc} recommended
ACETANILIDES								
propachlor	2.18		1.91	0.41	11		2.18	1.91 m
CARBAMATES								
aldicarb	1.13		1.22	0.33	27	1.41	1.13	1.22 m
benomyl	2.12					1.84	2.12	1.84 c
carbaryl	2.36		2.26	0.26	25	1.94	2.36	2.26 m
carbendazim	1.52	2.30	2.61	0.22	12	1.58	-2.18 (-4.18)	2.61 m
carbofuran	2.32		1.63	0.34	54	1.92	2.32	1.63 m
methomyl	0.60		1.36	0.05	3	1.18	0.60	1.36 m
oxamyl	-0.47		1.05	0.38	26	0.72	-0.47	1.05 m
Dithiocarbamates								
maneb								
metham-sodium			2.43	0.23	2			2.43 m
thiram	1.76		2.69		8	1.68	1.76	2.69 m
zineb								
DINITROANILINES								
trifluralin	5.34		3.93	0.25	27	4.09	5.34	3.93 m
AROMATIC HALOGENATED HYDROCARBONS								
Chlorinated pesticides								
3,3-dichlorobenzidine	3.51	2.30				2.95	3.51	2.95 c
captafol	3.83		3.32		1	3.18	3.83	3.32 m
captan	2.54		2.30		1	2.25	2.54	2.30 m
p,p'-DDT	6.91		5.63	0.61	31	5.41	6.91	5.63 m
o,p'-DDT	6.61					5.19	6.61	5.63 m
o,p'-DDD	5.19					4.91	6.22	4.91 c
p,p'-DDD	6.22					4.91	6.22	4.91 c
o,p'-DDE						1.79		4.82 m
p,p'-DDE	6.96		4.82		2	5.44	6.96	4.82 m
aldrin	6.50					5.11	6.50	5.11 c
chlordane	5.80					4.60	5.80	4.60 c
endrin	5.20		4.29		1	4.17	5.20	4.29 m
heptachlor	5.58					4.45	5.58	4.45 c
heptachlorepoxide	3.49					2.94	3.49	2.94 c
endosulfan			4.13		1			3.11 c
a-endosulfan	3.83					3.18	3.83	3.11 c
b-endosulfan	3.62					3.03	3.62	3.11 c
a-HCH	3.78		3.25	0.12	14	3.14	3.78	3.25 m
b-HCH	3.84		3.36	0.15	17	3.19	3.84	3.36 m
y-HCH	3.69		2.98	0.28	94	3.08	3.69	2.98 m
Polychlorinated biphenyls (IUPAC-number)								
2-CB (1)	4.53		3.47		1	3.69	4.53	see
2,2'-DI-CB (4)	4.96		3.92		1	4.00	4.96	text
2,4-DI-CB (7)	5.30					4.24	5.30	
2,4'-DI-CB (8)	5.15		3.48	0.77	5	4.14	5.15	
2,5-DI-CB (9)	5.16					4.14	5.16	
2,6-DI-CB (10)	4.98					4.01	4.98	
4,4'-DI-CB (15)	5.46					4.36	5.46	

Table 3. (continued) Partitioning data and recommended K_{oc} values for INS-b3 and c compounds.

COMPOUND	Log Kow	pK_a/pK_b[a] [1]	log K_{oc} experimental average	STD	N	log K_{oc} estimated [2]	[3][b]	log K_{oc} recommended
2,2',5-TRI-CB (18)	5.60		4.23	0.37	7		5.60	
2,4,4'-TRI-CB (28)	5.62		4.62	0.88	3	4.47	5.62	
2,4,5-TRI-CB (29)	5.90					4.68	5.90	
2,4,6-TRI-CB (30)	5.71					4.54	5.71	
2',3,4-TRI-CB (33)	5.87					4.66	5.87	
3,4,4'-TRI-CB (37)	5.90					4.68	5.90	
2,2',3,3'-TETRA-CB (40)	6.18					4.88	6.18	
2,2',3,5'-TETRA-CB (44)	6.67					5.23	6.67	
2,2',4,4'-TETRA-CB (47)	6.29		3.43		1		6.29	
2,2',4,5-TETRA-CB (48)	5.73					4.55	5.73	
2,2',5,5'-TETRA-CB (52)	6.09		4.73	1.20	5	4.81	6.09	
2,2',6,6'-TETRA-CB (54)	5.96		5.01	0.33	6	4.72	5.96	
2,3,4,5-TETRA-CB (61)	6.41					5.04	6.41	
2,3',4,4'-TETRA-CB (66)	6.67					5.23	6.67	
2,3',4',5-TETRA-CB (70)	6.23		4.84	0.12	5		6.23	
3,3',4,4'-TETRA-CB (77)	6.63					5.20	6.63	
2,2',3,4,5'-PENTA-CB (87)	6.37		4.62	0.17	2		6.37	
2,2',3,4,6-PENTA-CB (88)	7.51					5.84	7.51	
2,2',4,5,5'-PENTA-CB (101)	6.50		5.87	0.50	9	5.11	6.50	
2,3,4,5,6-PENTA-CB (116)	6.75					5.29	6.75	
2,3',4,4',5-PENTA-CB (118)	7.12					5.56	7.12	
2,2',3,3',4,4'-HEXA-CB (128)	7.32		5.29		1	5.70	7.32	
2,2',3,3',4,5-HEXA-CB (129)	8.26					6.38	8.26	
2,2',3,3',6,6'-HEXA-CB (136)	7.12					5.56	7.12	
2,2',3,4,4',5'-HEXA-CB (138)	7.90					6.12	7.90	
2,2',4,4',5,5'-HEXA-CB (153)	7.75		5.65	0.71	40	6.01	7.75	
2,2',4,4',6,6'-HEXA-CB (155)	7.29		6.08		1	5.68	7.29	
2,2',3,3',5,6-HEXA-CB (134)	8.18					6.32	8.18	
2,2',3,3',4,4',6-HEPTA-CB (171)	6.68					5.24	6.68	
2,2',3,4,4',5,5'-HEPTA-CB (180)	8.04						8.04	
2,2',3,4,5,5'6-HEPTA-CB (185)	7.79		6.56	0.52	3		7.79	
2,2',3,3',4,4',5,5'-OCTA-CB (194)	9.64					7.38	9.64	
2,2',3,3',5,5',6,6'-OCTA-CB (202)	7.73					6.00	7.73	
2,2',3,3',4,4',5,5,'6-NONA-CB (206)	10.40					7.93	10.40	
2,2,3,3',4,5,5',6,6'-NONA-CB (208)	8.16					6.31	8.16	
DECA-CB (209)	8.72					6.72	8.72	
Polybromine biphenyls (PBBs)								
4-bromo-biphenyl	4.89							see text
Polybromine biphenyls oxides (PBBOs)								
4-bromo-biphenyloxide	4.28							see text
Chlorinated benzyltoluenes (ugilecs)								
chloro-methyl-diphenylmethanes								see
2,2',4,4'-chloro-3-methyl-	7.20					5.62	7.20	text
2,2',4,4'-chloro-5-methyl-	7.76					6.02	7.76	
2,2',4,5'-chloro-5-methyl-	7.54					5.86	7.54	
2,2',4,6'-chloro-3-methyl-	7.33					5.71	7.33	
2,2',4,6'-chloro-5-methyl-	7.03					5.49	7.03	
2,2',5,5'-chloro-4-methyl-	7.49					5.82	7.49	
2,3',4,4'-chloro-5-methyl-	7.39					5.75	7.39	
2,3',4,4'-chloro-6-methyl-	7.48					5.82	7.48	
2,3',4,6'-chloro-6-methyl-	7.08					5.53	7.08	

Table 3. (continued) Partitioning data and recommended K_{oc} values for INS-b3 and c compounds.

COMPOUND	Log Kow	pK_a/pK_b[a] [1]	log K_{oc} experimental average	STD	N	log K_{oc} estimated [2]	[3][b]	log K_{oc} recommended
Bromine ugilecs (DBBTs)								see text
Chloroanilines								
chloroaniline			2.55	0.35	16			
2-chloroaniline	1.93	2.62 base				1.81	1.93	2.55 m
3-chloroaniline	1.91	3.67 base				1.80	1.91	2.55 m
4-chloroaniline	1.88	4.07 base				1.77	1.88	2.55 m
2,3-dichloroaniline	2.86	1.44 base				2.48	2.86	2.85 m
2,4-dichloroaniline	2.91	1.83 ba:	2.72	0.18	4	2.52	2.91	2.85 m
2,5-dichloroaniline	2.92	1.43 base				2.53	2.92	2.85 m
2,6-dichloroaniline	2.82	0.39 ba:	3.25		1	2.45	2.82	2.85 m
3,4-dichloroaniline	2.72	2.89 ba:	2.99	0.70	5	2.38	2.72	2.85 m
3,5-dichloroaniline	2.90	2.49 ba:	2.44	0.08	2	2.51	2.90	2.85 m
2,3,4-trichloroaniline	3.68	0.66 ba:	2.97	0.60	3	3.07	3.68	2.97 m
2,3,5-trichloroaniline		0.26 base						2.97 m
2,4,5-trichloroaniline	3.69	0.65 base				3.08	3.69	2.97 m
2,4,6-trichloroaniline	3.69	-0.39 base				3.08	3.69	2.97 m
3,4,5-trichloroaniline	3.32	1.71 base				2.81	3.32	2.97 m
2,3,4,5-tetrachloroaniline	4.57	-0.52 ba:	3.51	0.66	2	3.71	4.57	3.67 m
2,3,5,6-tetrachloroaniline	4.46	-1.95 ba:	3.94		1	3.63	4.46	3.67 m
pentachloroaniline	5.08	-2.73 ba:	4.62		1	4.08	5.08	4.62 m
Chloronitrobenzenes								
2-chloronitrobenzene	3.31					2.81	3.31	2.84 c
3-chloronitrobenzene	3.39					2.86	3.39	2.84 c
4-chloronitrobenzene								2.84 c
2,3-dichloronitrobenzene	3.87		3.97		1	3.21	3.87	3.16 c
3,4-dichloronitrobenzene								3.16 c
2,6-dichloronitrobenzene								3.16 c
2,4-dichloronitrobenzene								3.16 c
3,5-dichloronitrobenzene	3.79		4.19		1	3.15	3.79	3.16 c
2,5-dichloronitrobenzene	3.74					3.12	3.74	3.16 c
2,3,4-trichloronitrobenzene								3.38 c
3,4,5-trichloronitrobenzene								3.38 c
2,3,6-trichloronitrobenzene								3.38 c
2,4,5-trichloronitrobenzene								3.38 c
2,3,5-trichloronitrobenzene	4.11					3.38	4.11	3.38 c
2,4,6-trichloronitrobenzene								3.38 c
2,3,4,5-tetrachloronitrobenzene	4.74		4.23		1	3.84	4.74	4.14 m
2,3,5,6-tetrachloronitrobenzene	5.15		4.05		1	4.14	5.15	4.14 m
2,3,4,6-tetrachloronitrobenzene								4.14 m
pentachloronitrobenzene	5.50		4.36	0.18	4	4.39	5.50	4.36 m
ORGANOPHOSPHATE PESTICIDES								
azinphos-ethyl	3.40					2.87	3.40	2.87 c
chlorfenvinphos	3.82		2.68	0.18	3	3.16	3.82	2.68 m
chlorpyrifos	5.27		3.88	0.33	34	4.16	5.27	3.88 m
coumaphos	3.98					3.27	3.98	3.27 c

Table 3. (continued) Partitioning data and recommended K_{oc} values for INS-b3 and c compounds.

COMPOUND	Log Kow	pK_a/pK_b [1]	log K_{oc} experimental average	STD	N	log K_{oc} estimated [2]	[3][b]	log K_{oc} recommended
demeton								
dichlorvos	1.47		1.83	0.34	5	1.54	1.47	1.83 m
disulfoton	4.02		3.12	0.39	28	3.30	4.02	3.12 m
fenitrothion	3.47		3.13	0.33	10	2.92	3.47	3.13 m
fenthion	4.09					3.35	4.09	3.35 c
mevinphos	1.20		2.80	0.73	21	1.36	1.20	2.80 m
oxydemeton-methyl	-0.12					0.45	-0.12	0.45 c
parathion-methyl	3.04		3.17	0.46	16	2.62	3.04	3.17 m
phoxim	4.39							
pyrazophos	3.62	2.09 base				3.02	3.62	3.02 c
triazophos	3.55	0.89 ba:	2.55	0.06	3	2.98	3.55	2.55 m
trichlorfon	0.51		1.58	0.19	6	0.88	0.51	1.58 m
UREAS								
linuron	3.11	3.50 ba:	2.78	0.29	137	2.64	3.11	2.78 m
TRIAZINES								
simazine	2.14		2.04	0.36	265	2.08	2.14	2.04 m
ACIDS								
2,4,5-T	3.31	3.00	1.99	0.38	33		0.31 (-1.69)	1.99 m
2,4-D	2.81	3.10 aci	1.66	0.56	58		-0.09 (-2.09)	1.66 m
bentazone	2.80	5.00 est	1.52	0.37	6		1.76 (-0.20)	1.52 m
dichlorprop	3.13	3.50					0.63 (-1.37)	3.13 c
dinoseb	3.14	4.40	2.09		1		1.53 (-0.46)	2.09 m
DNOC	2.14	4.20	2.34	0.26	12		0.33 (-1.66)	2.34 m
MCPA	2.68	3.10	1.73	0.03	5		-0.22 (-2.22)	1.73 m
mecoprop	2.99	3.49					0.48 (-1.52)	2.99 c
NON AROMATIC HC HALOGENATED								
hexachlorobutadiene	4.78					3.91	4.78	3.91 c
AROMATIC HC NON-HALOGENATED								
phenol	1.46		1.55	0.52	10	1.69	1.46	1.55 m
PHTHALATE ESTERS								
benzylbutyl PA (BBP)	4.91		3.21	1.44	2		4.91	3.21 m
dibutyl PA								
diethyl PA (DEP)	2.47		2.73	0.62	4		2.47	2.73 m
diisobutyl PA (DBP)	4.11		3.14		1		4.11	3.14 m
diisooctyl PA								
dimethyl PA	1.53		2.33	0.27	5		5.42	2.33 m
dioctyl PA								
di(2-ethyl-hexyl) PA (DEHP)			5.44	0.41	4		5.24	5.44 m
dihexyl phthalate (DHP)			4.72	0.04	3		5.80	5.44 m
diisodecyl phthalate (DIDP)			5.33	0.39	3		4.91	5.33 m
ditridecyl phthalate (DTDP)			5.53	1.13	3		5.36	5.53 m
ORGANOTIN COMPOUNDS								
tetrabutyltin								
tributyltin	3.64		4.10		30		3.64	4.10 m

Table 3. (continued) Partitioning data and recommended K_{oc} values for INS-b3 and c compounds.

COMPOUND	Log Kow	pK_a/pK_b[a] [1]	log K_{oc} experimental average	STD	N	log K_{oc} estimated [2]	[3][b]	log K_{oc} recommended
triphenyltin	3.28		4.34		1		3.28	4.34 c
MISCELANEOUS COMPOUNDS								
phthalateacid-anhydride	1.60						1.60	1.60 c
Pyrethoides								
bifenthrin	6.00		5.35	0.16	4		6.00	4.87 m
cypermethrin	6.05						6.05	4.87 m
deltamethrin	6.20						6.20	4.87 m
permethrin	6.50		4.39	0.34	9		6.50	4.87 m

[a]: pK_as above 9 lead to an insignificant disocciated fraction (< 1%) and are therefore not shown.
[b]: For acids K_{oc}s were calculated according to equations 12 and 13 assuming a pH of 6.
The calculated Koc at pH 8 is shown between brackets.
[c]: m=measured; c=calculated from K_{ow}

[1] Karickhoff, S. and Carreira (US EPA, Athens) (1992, personal communication). pKa's calculated with SPARC
[2] Gerstl (1990) The regression equations for the chemical groups shown in Table 2 were applied.
[3] Di Toro et al. (1991)

5.3.3 Dinitroanilines

For trifluralin 27 K_{oc}s were available. The average K_{oc} is approximately one unit (logarithmic) lower than the values predicted according to the equation of Di Toro et al.

5.3.4 Aromatic halogenated hydrocarbons

Chlorinated pesticides

For all organochlor pesticides (except for DDD, chlordane, heptachlor and heptachlor epoxide) experimental K_{oc}s were available. In view of the probably insignificant differences in the K_{ow}s for DDT and DDE isomers the same (experimental) K_{oc} value is recommended. For the DDD isomers an average K_{oc} value calculated from the experimental K_{ow} according to Gerstl's equation is recommended. For the endosulfan isomeres only one experimental K_{oc} was available. It was not clear which of the isomers was tested in the experiment. Surprisingly the experimental value is about one (logarithmic) unit higher than the values predicted from the K_{ow}s using Gerstl's equation. Because the experimental value relates to only one measurement it was ignored. The recommended K_{oc}s are based on the values predicted according to Gerstl's equation using an average K_{ow} for the isomers.

The K_{oc}s predicted according to the equation of Di Toro et al. tend to overestimate adsorption when experimental adsorption data are compared.

Polychorinated biphenyls

Because the PCBs form a homologous group it is expected that for these compounds adsorption is caused by the same intermolecular interactions. A regression equation relating K_{oc}s and K_{ow}s was calculated (Figure 3) to allow prediction of K_{oc}s for all PCBs:

$$\log K_{oc} = 0.83 * \log K_{ow} - 0.37 \qquad (16)$$

In 2.1 it was already stated that the so-called 'third-phase effect' may play an important role when K_{oc}s for highly hydrophobic compounds (such as PCBs) are determined in ordinary batch-experiments. Experiments of Evers and Smedes (1993, in press) with polyaromatic hydrocarbons and PCBs indicated that the underestimation of the K_{oc} due to the 'third-phase effect' is very significant (the underestimation amounts typically 1-2 logarithmic units for tri-, tetra, penta- and hexachlorobiphenyls). Although the results of Evers and Smedes (1993, in press) do not yet have an official status and are still unpublished, they are shown here in Figure 4. Based on the data from Evers and Smedes

(1993, in press), calculated K_{ow}s (Hawker and Connell., 1988) an alternative regression equation relating K_{oc}s and K_{ow}s for PCBs was calculated:

$$\log K_{oc} = 1.39 * \log K_{ow} - 1.52 \qquad (17)$$

At this moment a choice for one of the equations (16 or 17) would be more or less arbitrary; equation 15 may be preferred because it relies on a larger number of data of several authors, but equation 16 may be preferred because it eliminates the 'third-phase effects' which certainly plays an important role for the PCBs. Here the choice is not made. In the future (when all eco-toxicological literature for the PCBs is reviewed and the final values for the K_{oc}s are needed for the application of the EP method and intercomparimental harmonization) more evidence might be available that allows a well founded choice of one of the two predictive equations. Which equation will be used is crucial because the predicted K_{oc}s can differ enormously. K_{oc}s predicted from K_{ow}s above 5.5 (logarithmic) using the equation based on the co-solvent method (equation 16) are than two orders of magnitude larger than those predicted with the equation based on K_{oc}s determined in a tradititional manner (equation 15).

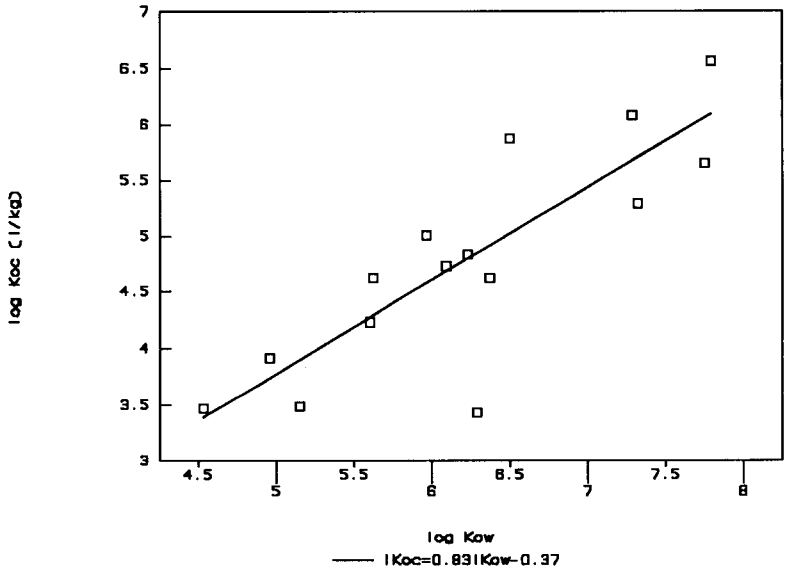


Figure 3 Linear regression analysis of logarithmic K_{oc} and K_{ow} data for polychorinated biphenyls (Table 3). (R^2 = 0.70).

Polybromine biphenyl, polybromine biphenyl oxides, ugilecs and bromine ugilecs.

No experimental K_{oc}s were available for these compounds. Because the molecular structures of these compounds resemble the structure of PCBs it is recommended to derive K_{oc}s from K_{ow}s using the same regression as for PCBs (either equation 10 or 11).

Choroanilines and chloronitrobenzenes

Chloroanilines contain an amine ($-NH_2$) group that behaves as a base (depending on the pH $-NH_3^+$ groups are formed). This renders the molecule a polar character. Due to this polar character interactions with soil particles may differ form the 'normal hydrophobic interactions' and binding may occur to specific surface groups of, for example, organic matter. The K_{oc}s recommended here were all based on experimental data. Because differences in the K_{ow}s and K_{oc}s for the isomers appeared insignificant average values were proposed. The K_{oc}s predicted with the equations of Gerstl or Di Toro et al. deviate considerably from the experimental values.

For the chloronitrobenzenes few adsorption data were available. Again the differences between the isomers appeared insignificant.

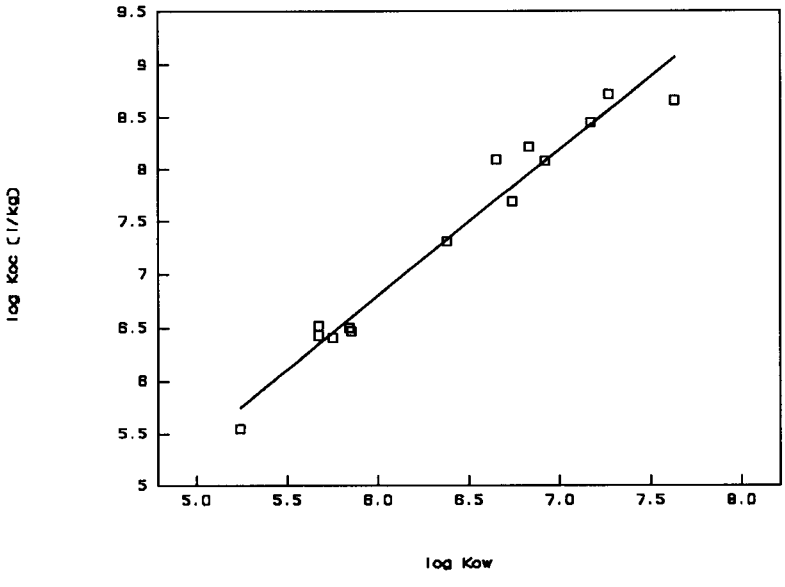


Figure 4 Linear regression analysis for polychorinated biphenyls using K_{oc}s from Evers and Smedes (1993, in press) and K_{ow}s from Hawker and Connell (1988). ($R^2 = 0.96$).

5.3.5 Organophosphate pesticides

Experimental K_{oc}s were available for most organophosphate pesticides. Comparison with the K_{oc}s predicted using the equation of Di Toro et al. showed that estimation often overestimates (but in 2 cases underestimates) adsorption considerably. For demeton and phoxim neither a K_{oc} nor a K_{ow} was available. Consequently, for these compounds no K_{oc} can be recommended here.

5.3.6 Ureas

For linuron a very large number (127) of K_{oc}s were available. The standard deviation is slightly higher than the average value (0.28).

5.3.7 Triazines

For simazine the largest number of K_{oc}s were found (265). The standard deviation is higher than the average value (0.28). Because the recommended K_{oc} is based on a very large number of data it is considered one of the most reliable values presented here.

5.3.8 Acids

Experimental K_{oc}s were found for 4 of the 8 acids considered in INS.

As stated in 3.1 dissociation of acids normally yields negatively charged species. These species are due, to their low hydrophobicity probably much more mobile in soil than their parent acids. In 3.1 an approach, that is sometimes applied to calculate a pH-dependent partition coefficient, was explained. Here the validity of this approach was tested with experimental K_{oc}s. Besides these experimental data, Table 3 contains K_{oc}s for acids that were estimated from K_{ow}s according to the equations of Di Toro et al. (1991) and pK_as (equation 6 and 7). Comparison of the experimental and calculated K_{oc}s for pH 6, shows that in all cases (except bentazon) the formulation of pH-dependent K_{oc}s leads to a severe underestimation (ususally 1-2 orders of magnitude) of adsorption. The calculation of pH-dependent K_{oc}s for pH 8, apparently leads to very low, and therefore unrealistic, K_{oc}s.

It is thought that the correction for acid dissociation is appropriate only when a minor fraction of the compound is dissociated. As soon as the dissociated fraction exceeds approximately 80 % the adsorption is dominated by characteristics of the dissociated molecule and the assumption of negligble adsorption does not longer hold.

Based on these observations, pH-depedent K_{oc}s are not recommended for these compounds. The recommended values are, when available, average experimental K_{oc}s. When no experimental data are available the recommended K_{oc}s were derived from K_{ow}s according to Di Toro's equation.

The standard deviation of the average K_{oc}s for the acids are all high compared to the average standard deviation (0.28). This is probably a result of the varying pHs of the adsorption experiments.

5.3.10 Non aromatic hydrocarbons, halogenated

No K_{oc}s were available for hexachlorobutadiene. The recommended value is based upon Gerstl's group equation for non aromatic hydrocarbons (halogenated) (Table 2).

5.3.11 Aromatic hydrocarbons, non-halogenated

For phenol 10 experimental K_{oc}s were available. The average K_{oc} is in good agreement with the value estimated according to Di Toro's and Gerstl's equations.

5.3.12 Phthalate esters

For the phthalates only few adsorption data were available. Estimation form the K_{ow} according to Di Toro's equation, was often poor when compared with the experimental K_{oc}s. Similar to the PCBs a regression analysis was attempted, but the correlation was poor ($R^2 = 0.24$). Therefore no reliable regression equation can be given here. The recommended K_{oc}s were derived from the K_{ow}s according to Di Toro's equation. The reliability of the K_{oc}s for the phthalates is considered very poor.

5.3.13 Organotin compounds

For tetrabutyltin neither a K_{oc} nor a K_{ow} is available and therefore no K_{oc} is recommended.

The structure of tributyltin and triphenyltin in water deserves comment. Dissolution of tributyltin and triphenyltin compounds (usually salts of acetate or chloride) in pure water is likely to produce hydrated $(C_4H_9)_3Sn^+$ or $(C_6H_5)_3Sn^+$ ions, that behave as monoprotic acids (Royal Soc. Chem., 1991). The dissociated form can be represented as $(C_4H_9)_3SnOH$ or $(C_6H_5)_3SnOH$. However, acid dissociation of these compounds, does not yield negative species as 'normal' acids do (see 3.1) but neutral species that are not expected to be much more mobile than their parent molecule. Therefore calculation of a pH dependent K_p from the K_{ow} (equation 6 and 7) was not considered for these compounds.

The ionic character of these compounds may however be responsable for the relatively large standard deviation of the average K_{oc} for tributyl- and triphenyltin and the large deviation from the value estimated according to Di Toro's equation. The recommened value for triphenyltin is derived from the K_{ow} according to Di Toro's equation.

5.3.14 Miscellaneous compounds

For phthalateacid-anhydride the recommended K_{oc} was based on the K_{ow} and calculated according to Di Toro's equation.

For 2 of the 4 pyrethroides no experimental K_{oc}s were avaible. Comparison with the values estimated according to Di Toro's equation showed that Di Toro's equation overestimates adsorption by more than 1 order of magnitude. Because of this large discrepancy, the structural similarity of the pyrethroides (Table 1) and the relatively small differences in the K_{ow}s, none of the recommended K_{oc}s was based on Di Toro's equation. The recommended K_{oc}s for the compounds for which no experimental K_{oc}s were available (cypermethrin and deltamethrin) is the average of all K_{oc}s available for pyrethroides.

6 DISCUSSION AND CONCLUSIONS

K_{oc}s are often estimated from K_{ow}s using equations of the ones proposed by Karickhoff (1981) and Di Toro et al. (1991) (equations 6 and 7). These equations are used not only for hydrophobic (non-ionic) compounds, for which they were originally derived, but also for compounds that can not be classified as hydrophobic. Analysis of K_{ow} data and nearly all K_{oc} data available at this moment, showed that this may lead to considerable deviations. Applying the equations that were derived for hydrophobic compounds, to compounds with low K_{ow}s, normally leads to considerable underestimation of adsorption (shown in Figure 1). Because most experimentators did not take the trouble of checking the mass balance, which is usually a laborious procedure, it is possible that experimental artefacts caused by particulary, volatilization or degradation of the test compound, produced too high experimental K_{oc}s. Among the compounds with low K_{ow}s many readily biodegradable and volatile componds are found. However, it is thought that not these experimental artefacts, but processes other than hydrophobic partitioning are the main cause of the relatively strong sorption that was observed.

For estimation of K_{oc}s for PCB and PBB congeners two regression equations relating K_{oc} and K_{ow} were derived. The K_{oc}s predicted with these equations can differ more than two orders of magnitude (logarithmic) for hydrophobic compounds. The difference is most likely a reflection of the 'third phase effect' which results from strong adsorption of hydrophobic compounds to colloids and dissolved organic matter. The equation that predicts high K_{oc}s is based on K_{oc}s that were determined with the relatively new co-solvent method that allows elimination of the third phase effect. At this moment none of these equations could be given preference because the validity of the co-solvent is not yet fully accepted. However, it is is expected that in the near future more experimental data become available that may support the results obtained with co-solvent method, so that an a scientifically sound choice can be made.

Care should be taken when an correction for acid dissociation is applied when estimating K_{oc}s from K_{ow} data, as is sometimes done (e.g., for chlorinated phenols). In this report analysis of K_{ow} and pK_a data and experimental K_{oc}s for acidic compounds showed that this may lead to a severe underestimation of the K_{oc} (usually 2 orders of magnitude or more depending on the compound and pH). Apparently, the assumption made for the correction (negligible adsorption of the dissociated fraction) is generally not valid.

The pitfalls associated with estimating K_{oc}s for acidic compounds shows again that estimating adsorption from K_{ow} data only is hazardous and that available experimental K_{oc} should not be neglected.

The average standard deviations for the experimental (logarithmic) K_{oc}s was 0.28 (approximately a factor 2). For K_{oc}s calculated from K_{ow}s it is concluded that a higher standard deviation (approximately a factor 10) is applicable.

Whenever possible, experimental determination of adsorption is recommended. If this is not possible use should be made of the proper group equations relating K_{ow} and K_{oc} as derived by Gerstl (1990).

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Appendix A Search profile used for selection of titles from the Chemical Abstracts Data System

s1 sorption or adsorption or desorption or partitioning or partition
s2 distribution or complexation or langmuir or freundlich or bioavailability
s3 complex(w)formation or fractionation or precipitation or coprecipitation
s4 remobili?ation or mobili?ation or interaction? or koc or kd or kp
s5 s1 or s2 or s3 or s4
s6 liquid(w)solid or suspended(w)matter or suspended(w)particles or sediment?
s7 sludge or soil? or particulate(w)matter or solid(w)phase or liquid(w)phase
s8 suspended(w)solid? or suspended(w)material? or interstitial(w)water
s9 porewater or groundwater or dissolved(w)matter or dissolved(w)phase
s10 third(w)phase or suspended(w)sediment
s11 s6 or s7 or s8 or s9 or s10
s12 s5 and s11

Appendix B K_{ow}'s (and CAS regsitration numbers) for the b and c compounds selected from the MEDCHEM database and the literature. A * indicates the value that is recommended in the database.

COMPOUND	CAS-Number	Log Kow	Reference
ACETANILIDES			
propachlor	1918-16-17	2.18 *	Gould and Hansch (unpublished)
CARBAMATES			
aldicarb	116-06-3	1.13 *	Bowman and Sans (1983)
benomyl	17804-35-2	2.12 *	Austin and Briggs (1976)
carbaryl	63-25-2	2.36 *	Fujita et al. (1974)
carbendazim	10605-21-7	1.52 *	Austin and Briggs (1976)
carbofuran	1563-66-2	2.32 *	Metcalf and Lu (in press)
methomyl	16752-77-5	0.60 *	Drabeck and Bachman (1983)
oxamyl	23135-22-0	-0.47 *	Briggs (1981)
Dithiocarbamates			
maneb	12427-38-2		
metham-sodium	137-42-8		
thiram	137-26-8	1.76	ClogP method
zineb	12122-67-7		
DINITROANILINES			
trifluralin	1582-09-8	5.34 *	Kenaga and Goring (1987)
AROMATIC HALOGENATED HYDROCARBONS			
Chlorinated pesticides			
3,3-dichlorobenzidine	91-94-1	3.51 *	Banerjee et al. (1980)
captafol	2425-06-1	3.83	Briggs (1981)
captan	133-06-2	2.54	Briggs (1981)
p,p'-DDT	50-29-3	6.91 *	De Bruijn et al. (1989)
o,p'-DDT	789-02-6	6.61	ClogP method
o,p'-DDD	53-19-0	5.19	ClogP method
p,p'-DDD	72-54-8	6.22 *	De Bruijn et al. (1989)
o,p'-DDE	3424-82-6		
p,p'-DDE	72-55-9	6.96 *	De Bruijn et al. (1989)
aldrin	309-00-2	6.50 *	De Bruijn et al. (1989)
chlordane	57-74-9	5.80	ClogP method
endrin	72-20-8	5.20 *	De Bruijn et al. (1989)
heptachlor	76-44-8	5.58	DeKock and Lord (1987)
heptachlorepoxide	1024-57-3	3.49	ClogP method
endosulfan			
a-endosulfan	57-74-9	3.83 *	Hermens and Leeuwangh (1982)
b-endosulfan	959-98-8	3.62	Callahan et al. (1979)
a-HCH	319-84-6	3.78	De Bruijn et al. (1989)
b-HCH	319-85-7	3.84	De Bruijn et al. (1989)
y-HCH	58-89-9	3.69	De Bruijn et al. (1989)

Appendix B K_{ow}'s (and CAS regsitration numbers) for the b and c compounds selected from the MEDCHEM database and the literature. A * indicates the value that is recommended in the database.

COMPOUND	CAS-Number	Log Kow	Reference
Polychlorinated biphenyls (IUPAC-number)			
2-CB (1)		4.53	De Bruijn et al. (1989)
2,2'-DI-CB (4)		4.96	De Bruijn et al. (1989)
2,4-DI-CB (7)		5.30	Gerstl (1991)
2,4'-DI-CB (8)		5.15	Gerstl (1991)
2,5-DI-CB (9)		5.16	Gerstl (1991)
2,6-DI-CB (10)		4.98	De Bruijn et al. (1989)
4,4'-DI-CB (15)		5.46	Gerstl (1991)
2,2',5-TRI-CB (18)		5.60	*
2,4,4'-TRI-CB (28)		5.62	* Chiou et al. (1983)
2,4,5-TRI-CB (29)		5.90	De Bruijn et al. (1989)
2,4,6-TRI-CB (30)		5.71	De Bruijn et al. (1989)
2',3,4-TRI-CB (33)		5.87	De Bruijn et al. (1989)
3,4,4'-TRI-CB (37)		5.90	Gerstl (1991)
2,2',3,3'-TETRA-CB (40)		6.18	De Bruijn et al. (1989)
2,2',3,5'-TETRA-CB (44)		6.67	Gerstl (1991)
2,2',4,4'-TETRA-CB (47)		6.29	*
2,2',4,5-TETRA-CB (48)		5.73	Gerstl (1991)
2,2',5,5'-TETRA-CB (52)		6.09	* Rapaport and Eisenreich (1984)
2,2',6,6'-TETRA-CB (54)		5.96	De Bruijn et al. (1989)
2,3,4,5-TETRA-CB (61)		6.41	De Bruijn et al. (1989)
2,3',4,4'-TETRA-CB (66)		6.67	Gerstl (1991)
2,3',4',5-TETRA-CB (70)		6.23	*
3,3',4,4'-TETRA-CB (77)		6.63	De Bruijn et al. (1989)
2,2',3,4,5'-PENTA-CB (87)		6.37	*
2,2',3,4,6-PENTA-CB (88)		7.51	Gerstl (1991)
2,2',4,5,5'-PENTA-CB (101)		6.50	* Doucette and Andren (1988)
2,3,4,5,6-PENTA-CB (116)		6.75	De Bruijn et al. (1989)
2,3',4,4',5-PENTA-CB (118)		7.12	* Rapaport and Eisenreich (1984)
2,2',3,3',4,4'-HEXA-CB (128)		7.32	De Bruijn et al. (1989)
2,2',3,3',4,5-HEXA-CB (129)		8.26	Gerstl (1991)
2,2',3,3',6,6'-HEXA-CB (136)		7.12	De Bruijn et al. (1989)
2,2',3,4,4',5'-HEXA-CB (138)		7.90	* Shaw and Connel (1982)
2,2',4,4',5,5'-HEXA-CB (153)		7.75	* Rapaport and Eisenreich (1984)
2,2',4,4',6,6'-HEXA-CB (155)		7.29	De Bruijn et al. (1989)
2,2',3,3',5,6-HEXA-CB		8.18	Gerstl (1991)
2,2',3,3',4,4',6-HEPTA-CB (171)		6.68	Gerstl (1991)
2,2',3,4,4',5,5'-HEPTA-CB (180)		8.04	ClogP, unreliable
2,2',3,4,5,5'6-HEPTA-CB (185)		7.79	ClogP, unreliable
2,2',3,3',4,4',5,5'-OCTA-CB (194)		9.64	Gerstl (1991)
2,2',3,3',5,5',6,6'-OCTA-CB (202)		7.73	De Bruijn et al. (1989)
2,2',3,3',4,4',5,5'6-NONA-CB (206)		10.40	Gerstl (1991)
2,2,3,3',4,5,5',6,6'-NONA-CB (208)		8.16	Gerstl (1991)
DECA-CB (209)		8.72	De Bruijn et al. (1989)
Polybromine biphenyls (PBBs)			
4-bromo-biphenyl		4.89	ClogP
Polybromine biphenyls oxides (PBBOs)			
4-bromo-biphenyloxide		4.28	ClogP

Appendix B K_{ow}'s (and CAS regsitration numbers) for the b and c compounds selected from the MEDCHEM database and the literature. A * indicates the value that is recommended in the database.

COMPOUND	CAS-Number	Log Kow	Reference
Chlorinated benzyltoluenes (ugilecs)			
chloro-methyl-diphenylmethanes			
2,2',4,4'-chloro-3-methyl-		7.20	Van Haelst (1992)
2,2',4,4'-chloro-5-methyl-		7.76	Van Haelst (1992)
2,2',4,5'-chloro-5-methyl-		7.54	Van Haelst (1992)
2,2',4,6'-chloro-3-methyl-		7.33	Van Haelst (1992)
2,2',4,6'-chloro-5-methyl-		7.03	Van Haelst (1992)
2,2',5,5'-chloro-4-methyl-		7.49	Van Haelst (1992)
2,3',4,4'-chloro-5-methyl-		7.39	Van Haelst (1992)
2,3',4,4'-chloro-6-methyl-		7.48	Van Haelst (1992)
2,3',4,6'-chloro-6-methyl-		7.08	Van Haelst (1992)
Bromine ugilecs (DBBTs)			
Chloroanilines			
chloroaniline			
2-chloroaniline	95-51-2	1.93	De Bruijn et al. (1989)
3-chloroaniline	108-42-9	1.91	De Bruijn et al. (1989)
4-chloroaniline	106-47-8	1.88 *	De Bruijn et al. (1989)
2,3-dichloroaniline	608-27-5	2.86 *	De Bruijn et al. (1989)
2,4-dichloroaniline	554-00-7	2.91 *	De Bruijn et al. (1989)
2,5-dichloroaniline	95-82-9	2.92 *	De Bruijn et al. (1989)
2,6-dichloroaniline	608-31-1	2.82 *	De Bruijn et al. (1989)
3,4-dichloroaniline	95-76-1	2.72	McCrady et al. (1987)
3,5-dichloroaniline	626-43-7	2.90 *	Hammers et al. (1982)
2,3,4-trichloroaniline	634-67-3	3.68 *	De Bruijn et al. (1989)
2,3,5-trichloroaniline	18487-39-3		
2,4,5-trichloroaniline	636-30-6	3.69 *	De Bruijn et al. (1989)
2,4,6-trichloroaniline	634-93-5	3.69 *	De Bruijn et al. (1989)
3,4,5-trichloroaniline	634-91-3	3.32 *	Hammers et al. (1982)
2,3,4,5-tetrachloroaniline	634-83-3	4.57 *	De Bruijn et al. (1989)
2,3,5,6-tetrachloroaniline	3481-20-7	4.46 *	De Bruijn et al. (1989)
pentachloroaniline	527-20-8	5.08 *	De Bruijn et al. (1989)
Chloronitrobenzenes			
2-chloronitrobenzene	88-73-3	3.31	Opperhuizen et al. (1991)
3-chloronitrobenzene	121-73-3	3.39	Opperhuizen et al. (1991)
4-chloronitrobenzene	100-00-5	2.39 *	Fujita et al. (1964)
2,3-dichloronitrobenzene	3209-22-1	3.87	Opperhuizen et al. (1991)
3,4-dichloronitrobenzene	99-54-7	3.05 *	Kaiser (1983)
2,6-dichloronitrobenzene	601-88-7		
2,4-dichloronitrobenzene	611-06-3		
3,5-dichloronitrobenzene	618-62-2	3.79	Opperhuizen et al. (1991)
2,5-dichloronitrobenzene	89-61-2	3.74	Opperhuizen et al. (1991)

Appendix B K_{ow}'s (and CAS regsitration numbers) for the b and c compounds selected from the MEDCHEM database and the literature. A * indicates the value that is recommended in the database.

COMPOUND	CAS-Number	Log Kow	Reference
2,3,4-trichloronitrobenzene	17700-09-3	3.61 *	Kaiser (1983)
3,4,5-trichloronitrobenzene	20098-48-0	3.78	ClogP
2,3,6-trichloronitrobenzene	89-69-0	3.48 *	Kaiser (1983)
2,4,5-trichloronitrobenzene	89-69-0	3.48 *	Kaiser (1983)
2,3,5-trichloronitrobenzene	89-69-0	4.11	Opperhuizen et al. (1991)
2,4,6-trichloronitrobenzene	18708-70-8	3.62	ClogP
2,3,4,5-tetrachloronitrobenz	879-39-0	4.74	Opperhuizen et al. (1991)
2,3,5,6-tetrachloronitrobenz	117-18-0	5.15	Opperhuizen et al. (1991)
2,3,4,6-tetrachloronitrobenz	3714-62-3	4.09	ClogP
pentachloronitrobenzene	82-68-8	5.50	Opperhuizen et al. (1991)
ORGANOPHOSPHATE PESTICIDES			
azinphos-ethyl	2642-71-9	3.40 *	Bowman and Sans (1983)
chlorfenvinphos	470-90-6	3.82 *	Eadsforth and Moser (1983)
chlorpyrifos	2921-88-2	5.27 *	De Bruijn et al. (1989)
coumaphos	56-72-4	3.98	ClogP method (unreliable for OP pestic.)
demeton	8065-48-3		
dichlorvos	62-73-7	1.47	Bowman and Sans (1983)
disulfoton	298-04-4	4.02 *	Bowman and Sans (1983)
fenitrothion	122-14-5	3.47	De Bruijn and Hermens (1991)
fenthion	55-38-9	4.09 *	Bowman and Sans (1983)
mevinphos	7786-34-7	1.20 *	Briggs Private communication
oxydemeton-methyl	301-12-2	-0.12	ClogP method (unreliable for OP pestic.)
parathion-methyl	298-00-0	3.04	De Bruijn and Hermens (1991)
phoxim	14816-18-3	4.39	Bowman and Sans (1983)
pyrazophos	13457-18-6	3.62	ClogP method (unreliable for OP pestic.)
triazophos	24017-47-8	3.55 *	Edelist et al. (1964)
trichlorfon	52-68-6	0.51 *	Dedek (1962)
UREAS			
linuron	330-55-2	3.11 *	Mitsutake et al. (1986)
TRIAZINES			
simazine	122-34-9	2.14 *	Mitsutake et al. (1986)
ACIDS			
2,4,5-T	93-76-5	3.31 *	Jafvert et al. (1990)
2,4-D	94-75-7	2.81 *	Fujita et al. (1964)
bentazone	25057-89-0	2.80 *	Gould and Hansch (unpublished)
dichlorprop	120-36-5	3.13	ClogP method
dinoseb	88-85-7	3.14	De Bruijn et al. (1989)
DNOC	534-52-1	2.14	Jafvert et al. (1990)
MCPA	94-74-6	2.68	ClogP method
mecoprop	7085-19-0	2.99	ClogP method

Appendix B K_{ow}'s (and CAS regsitration numbers) for the b and c compounds selected from the MEDCHEM database and the literature. A * indicates the value that is recommended in the database.

COMPOUND	CAS-Number	Log Kow	Reference
NON AROMATIC HC HALOGENATED			
hexachlorobutadiene	87-68-3	4.78 *	Banerjee et al. (1980)
AROMATIC HC NON-HALOGENATED			
phenol	108-95-2	1.46 *	Fujita et al. (1964)
PHTHALATE ESTERS			
benzylbutyl PA (BBP)	85-68-7	4.91 *	Leyder and Boulanger (1983)
dibutyl PA	84-74-2		
diethyl PA (DEP)	84-66-2	2.47 *	Chan and Hansch (unpublished)
diisobutyl PA (DBP)	84-69-5	4.11 *	Leyder and Boulanger (1983)
diisooctyl PA	27554-26-3		
dimethyl PA	131-11-3	1.53 *	Jow and Hansch (1983) (unpublished)
dioctyl PA	117-84-0		
di(2-ethyl-hexyl) PA (DEHP	117-81-7		
dihexyl phthalate (DHP)			
diisodecyl phthalate (DIDP)			
ditridecyl phthalate (DTDP)			
ORGANOTIN COMPOUNDS			
tetrabutyltin	1461-25-2		
tributyltin	688-73-3/36643-28-4	3.64	Average of data from Maguire et al. (1983), Laughin et al. (1986), and Tas (1993)
triphenyltin	892-20-6	3.28	Average of data from Tsuda et al. (1989), Wulf and Byington (1973), and Tas (1993)
MISCELANEOUS COMPOUNDS			
phthalateacid-anhydride	85-44-9	1.60 *	
Pyrethoides			
bifenthrin	82657-04-3/83322-02-5	6.00 *	
cypermethrin	52315-07-8	6.05 *	Briggs private communication
deltamethrin	52918-63-5	6.20 *	Briggs private communication
permethrin	52645-53-1	6.50 *	Schimmel et al. (1983)

Appendix B Kow's and (CAS registration numbers) for b3 and c compounds selected from the MEDCHEM database.

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Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
ACETANILIDES		
2-chloroacetanilide	1.58	320
3,4-dichloroacetanilide (3,4-dicl)	2.17	524
3,4-dichloroacetanilide (3,4-dicl)	2.34	320
3,4-dichloroacetanilide (3,4-dicl)	2.34	524
3,4-dichloroacetanilide (3,4-dicl)	2.39	524
3,4-dichloroacetanilide (3,4-dicl)	2.42	524
3,4-dichloroacetanilide (3,4-dicl)	2.45	524
3,4-dichloroacetanilide (3,4-dicl)	2.49	524
3,4-dichloroacetanilide (3,4-dicl)	2.49	524
3,4-dichloroacetanilide (3,4-dicl)	2.53	524
3-bromoacetanilide	2.01	320
3-chloroacetanilide	1.63	524
3-chloroacetanilide	1.82	524
3-chloroacetanilide	1.86	320
3-chloroacetanilide	1.89	524
3-chloroacetanilide	1.92	524
3-chloroacetanilide	1.92	524
3-chloroacetanilide	2.01	524
3-chloroacetanilide	2.05	524
3-chloroacetanilide	2.10	524
3-chloro-4-methoxyacetanilide	1.78	524
3-chloro-4-methoxyacetanilide	1.83	524
3-chloro-4-methoxyacetanilide	1.92	320
3-chloro-4-methoxyacetanilide	1.98	524
3-chloro-4-methoxyacetanilide	2.02	524
3-chloro-4-methoxyacetanilide	2.14	524
3-fluoroacetanilide	1.57	320
3-methylacetanilide (3-ch3)	1.45	320
3-methylacetanilide (3-ch3)	1.46	524
3-methylacetanilide (3-ch3)	1.52	524
3-methylacetanilide (3-ch3)	1.63	524
3-methylacetanilide (3-ch3)	1.70	524
3-methylacetanilide (3-ch3)	1.72	524
3-methylacetanilide (3-ch3)	1.81	524
3-methylacetanilide (3-ch3)	1.84	524
3-methylacetanilide (3-ch3)	2.01	524
3-nitroacetanilide (3-no2)	1.94	320
3-(trifluoromethyl)acetanilide (3-cf3)	1.75	320
4-bromoacetanilide	1.95	320
4-fluoroacetanilide	1.48	320
4-methoxyacetanilide (4-och3)	1.34	524
4-methoxyacetanilide (4-och3)	1.40	320
4-methoxyacetanilide (4-och3)	1.41	524
4-methoxyacetanilide (4-och3)	1.49	524
4-methoxyacetanilide (4-och3)	1.49	524
4-methoxyacetanilide (4-och3)	1.53	524
4-methoxyacetanilide (4-och3)	1.74	524
4-methoxyacetanilide (4-och3)	1.74	524
4-methoxyacetanilide (4-och3)	1.85	524
acetanilide	1.43	320
acetochlor	2.10	238
acetochlor	2.17	238
acetochlor	2.22	238
acetochlor	2.36	238
acetochlor	2.38	238
acetochlor	2.42	238
acetochlor	2.57	238
alachlor	1.78	685
alachlor	1.80	238
alachlor	1.83	238
alachlor	1.87	543
alachlor	2.01	246
alachlor	2.06	246
alachlor	2.07	704
alachlor	2.09	238
alachlor	2.15	238
alachlor	2.19	698
alachlor	2.22	246
alachlor	2.25	238
alachlor	2.25	246
alachlor	2.26	246
alachlor	2.26	704
alachlor	2.28	525
alachlor	2.31	246
alachlor	2.35	698
alachlor	2.35	246

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
alachlor	2.37	238
alachlor	2.41	246
alachlor	2.42	704
alachlor	2.42	698
alachlor	2.43	246
alachlor	2.43	738
alachlor	2.43	685
alachlor	2.47	738
alachlor	2.55	698
alachlor	2.57	698
alachlor	2.64	698
alachlor	2.72	698
butachlor	2.63	738
butachlor	2.80	738
butachlor	2.90	738
butachlor	3.10	738
butyranilide	1.63	524
butyranilide	1.65	524
butyranilide	1.67	524
butyranilide	1.71	320
butyranilide	1.83	524
butyranilide	1.85	524
butyranilide	2.04	524
diphenamid	1.80	24
metazachlor	1.90	721
metazachlor	1.95	721
metazachlor	2.04	721
metazachlor	2.04	721
metazachlor	2.05	721
metazachlor	2.06	721
metazachlor	2.10	721
metazachlor	2.15	721
metazachlor	2.15	721
metazachlor	2.17	721
metazachlor	2.18	721
metazachlor	2.19	721
metazachlor	2.20	721
metazachlor	2.22	721
metazachlor	2.24	721
metazachlor	2.24	721
metazachlor	2.32	721
metazachlor	2.34	721
metolachlor	1.59	238
metolachlor	1.67	238
metolachlor	1.73	238
metolachlor	1.91	543
metolachlor	2.00	246
metolachlor	2.04	704
metolachlor	2.06	238
metolachlor	2.08	662
metolachlor	2.09	704
metolachlor	2.11	246
metolachlor	2.12	246
metolachlor	2.14	667
metolachlor	2.18	662
metolachlor	2.20	94
metolachlor	2.22	246
metolachlor	2.23	246
metolachlor	2.26	246
metolachlor	2.30	246
metolachlor	2.32	704
metolachlor	2.32	747
metolachlor	2.33	735
metolachlor	2.33	735
metolachlor	2.34	94
metolachlor	2.34	246
metolachlor	2.35	94
metolachlor	2.35	238
metolachlor	2.38	246
metolachlor	2.41	687
metolachlor	2.42	238
metolachlor	2.42	687
metolachlor	2.42	735
metolachlor	2.49	367
metolachlor	2.50	735
metolachlor	2.50	747
metolachlor	2.52	735
metolachlor	2.57	735

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
metolachlor	2.60	236
metolachlor	2.65	236
metolachlor	2.65	236
metolachlor	2.66	367
metolachlor	2.67	747
metolachlor	2.72	367
metolachlor	2.79	735
metolachlor	2.82	367
metolachlor	2.84	367
propachlor	1.31	685
propachlor	2.29	685
propachlor	2.42	525
propachlor	2.66	746
propachlor	1.96	1052
propachlor	1.93	1052
propachlor	1.52	1052
propachlor	1.91	1052
propachlor	1.74	1053
propachlor	1.52	1053
propachlor	1.81	1053
CARBAMATES		
4cl−benzaldoxime n−methylcarbamate	1.95	803
aldicarb	0.50	320
aldicarb	0.63	758
aldicarb	0.72	758
aldicarb	0.78	758
aldicarb	0.81	758
aldicarb	0.91	170
aldicarb	0.92	170
aldicarb	1.02	170
aldicarb	1.18	459
aldicarb	1.21	170
aldicarb	1.21	170
aldicarb	1.29	459
aldicarb	1.30	459
aldicarb	1.30	459
aldicarb	1.31	318
aldicarb	1.31	459
aldicarb	1.35	170
aldicarb	1.36	318
aldicarb	1.40	459
aldicarb	1.41	459
aldicarb	1.47	318
aldicarb	1.47	318
aldicarb	1.57	318
aldicarb	1.60	166
aldicarb	1.63	320
aldicarb	1.63	320
aldicarb	1.64	1022
aldicarb sulfone	0.01	170
aldicarb sulfone	0.01	170
aldicarb sulfone	0.23	758
aldicarb sulfone	0.34	758
aldicarb sulfone	0.50	320
aldicarb sulfone	0.50	320
aldicarb sulfone	0.67	170
aldicarb sulfone	0.73	170
aldicarb sulfone	0.74	170
aldicarb sulfone	0.95	170
aldicarb sulfoxide	<1.85	170
aldicarb sulfoxide	0.23	758
aldicarb sulfoxide	0.37	170
aldicarb sulfoxide	0.67	170
aldicarb sulfoxide	0.67	170
aldicarb sulfoxide	0.86	170
aldicarb sulfoxide	1.68	1023
aldicarb sulfoxide	2.66	1023
asulam	2.48	525
benzaldoxime n − methylcarbamate	1.56	803
bromo−3−phenylcarbamate	1.82	792
bromo−3−phenylcarbamate	1.86	792
bromo−3−phenylcarbamate	1.87	792
bromo−3−phenylcarbamate	1.94	792
bromo−3−phenylcarbamate	2.01	792
butylate	2.11	543
carbaryl	1.88	343

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
carbaryl	1.93	524
carbaryl	1.97	524
carbaryl	1.97	524
carbaryl	2.01	166
carbaryl	2.02	320
carbaryl	2.02	792
carbaryl	2.02	792
carbaryl	2.06	524
carbaryl	2.09	524
carbaryl	2.15	792
carbaryl	2.16	792
carbaryl	2.19	792
carbaryl	2.34	524
carbaryl	2.36	525
carbaryl	2.39	184
carbaryl	2.43	184
carbaryl	2.47	746
carbaryl	2.49	406
carbaryl	2.55	184
carbaryl	2.57	361
carbaryl	2.59	361
carbaryl	2.60	184
carbaryl	2.62	45
carbaryl	2.69	184
carbendazim	2.29	164
carbendazim	2.35	166
carbendazim	2.39	164
carbendazim	2.47	164
carbendazim	2.49	164
carbendazim	2.57	164
carbendazim	2.66	164
carbendazim	2.66	164
carbendazim	2.79	164
carbendazim	2.88	164
carbendazim	2.89	164
carbendazim	2.92	164
carbofuran	1.13	710
carbofuran	1.21	692
carbofuran	1.26	552
carbofuran	1.28	792
carbofuran	1.34	692
carbofuran	1.36	692
carbofuran	1.36	546
carbofuran	1.36	792
carbofuran	1.36	792
carbofuran	1.39	184
carbofuran	1.43	792
carbofuran	1.45	661
carbofuran	1.46	710
carbofuran	1.46	792
carbofuran	1.46	437
carbofuran	1.47	722
carbofuran	1.47	401
carbofuran	1.49	710
carbofuran	1.49	552
carbofuran	1.50	692
carbofuran	1.54	443
carbofuran	1.54	692
carbofuran	1.54	443
carbofuran	1.55	783
carbofuran	1.55	710
carbofuran	1.55	784
carbofuran	1.56	401
carbofuran	1.57	546
carbofuran	1.57	692
carbofuran	1.58	552
carbofuran	1.60	692
carbofuran	1.60	546
carbofuran	1.60	401
carbofuran	1.61	552
carbofuran	1.62	784
carbofuran	1.63	1038
carbofuran	1.64	1038
carbofuran	1.64	783
carbofuran	1.64	784
carbofuran	1.71	401
carbofuran	1.72	401
carbofuran	1.75	784

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
carbofuran	1.79	401
carbofuran	1.79	184
carbofuran	1.80	401
carbofuran	1.81	784
carbofuran	1.82	692
carbofuran	1.90	184
carbofuran	2.00	361
carbofuran	2.02	406
carbofuran	2.03	184
carbofuran	2.09	184
carbofuran	2.90	692
carbofuran	3.04	552
chlorbufam	2.04	678
chlorbufam	2.16	678
chlorbufam	2.17	678
chlorbufam	2.30	678
chlorbufam	2.39	678
chlorpropham (cipc)	1.56	251
chlorpropham (cipc)	2.05	251
chlorpropham (cipc)	2.23	251
chlorpropham (cipc)	2.32	658
chlorpropham (cipc)	2.32	251
chlorpropham (cipc)	2.33	251
chlorpropham (cipc)	2.33	251
chlorpropham (cipc)	2.34	251
chlorpropham (cipc)	2.35	251
chlorpropham (cipc)	2.35	251
chlorpropham (cipc)	2.35	251
chlorpropham (cipc)	2.37	251
chlorpropham (cipc)	2.39	616
chlorpropham (cipc)	2.39	251
chlorpropham (cipc)	2.39	251
chlorpropham (cipc)	2.40	251
chlorpropham (cipc)	2.40	251
chlorpropham (cipc)	2.41	251
chlorpropham (cipc)	2.42	251
chlorpropham (cipc)	2.42	251
chlorpropham (cipc)	2.47	251
chlorpropham (cipc)	2.49	251
chlorpropham (cipc)	2.50	251
chlorpropham (cipc)	2.50	251
chlorpropham (cipc)	2.50	251
chlorpropham (cipc)	2.50	251
chlorpropham (cipc)	2.51	658
chlorpropham (cipc)	2.51	658
chlorpropham (cipc)	2.51	658
chlorpropham (cipc)	2.51	24
chlorpropham (cipc)	2.52	251
chlorpropham (cipc)	2.53	251
chlorpropham (cipc)	2.58	658
chlorpropham (cipc)	2.58	251
chlorpropham (cipc)	2.59	251
chlorpropham (cipc)	2.60	658
chlorpropham (cipc)	2.61	251
chlorpropham (cipc)	2.61	658
chlorpropham (cipc)	2.62	251
chlorpropham (cipc)	2.63	658
chlorpropham (cipc)	2.64	658
chlorpropham (cipc)	2.64	658
chlorpropham (cipc)	2.67	251
chlorpropham (cipc)	2.68	251
chlorpropham (cipc)	2.69	658
chlorpropham (cipc)	2.73	658
chlorpropham (cipc)	2.73	658
chlorpropham (cipc)	2.77	525
chlorpropham (cipc)	2.80	283
chlorpropham (cipc)	2.84	658
chlorpropham (cipc)	2.88	283
chlorpropham (cipc)	2.91	722
chlorpropham (cipc)	2.97	283
chlorpropham (cipc)	2.98	283
chlorpropham (cipc)	3.04	263
chlorpropham (cipc)	3.04	263
chlorpropham (cipc)	3.05	263
cycloate (r-2063)	2.26	775
cycloate (r-2063)	2.35	208
cycloate (r-2063)	2.35	208
cycloate (r-2063)	2.44	775

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
cycloate (r−2063)	2.46	775
cycloate (r−2063)	2.48	775
cycloate (r−2063)	2.54	525
cycloate (r−2063)	2.59	208
cycloate (r−2063)	2.61	775
cycloate (r−2063)	2.62	208
cycloate (r−2063)	2.76	775
diallate	1.94	267
diallate	2.07	267
diallate	2.24	267
diallate	2.36	267
diallate	2.47	280
diallate	2.47	280
diallate	2.57	280
diallate	2.68	280
diallate	2.96	280
diallate	3.28	525
eptc	1.68	775
eptc	1.96	775
eptc	2.03	775
eptc	2.04	775
eptc	2.04	775
eptc	2.24	775
eptc	2.24	208
eptc	2.25	208
eptc	2.38	525
eptc	2.45	667
eptc	2.45	566
eptc	2.49	208
eptc	2.55	208
ethyl n−phenylcarbamate	1.82	320
ethyl−3−phenylcarbamate	1.62	792
ethyl−3−phenylcarbamate	1.62	792
ethyl−3−phenylcarbamate	1.65	792
ethyl−3−phenylcarbamate	1.71	792
ethyl−3−phenylcarbamate	1.80	792
isopropyl−4−phenylcarbamate	1.89	792
isopropyl−4−phenylcarbamate	1.90	792
isopropyl−4−phenylcarbamate	1.95	792
isopropyl−4−phenylcarbamate	1.98	792
isopropyl−4−phenylcarbamate	1.98	792
metam−sodium	2.27	1057
metam−sodium	2.59	1057
methiocarb	2.32	320
methomyl	1.30	1040
methomyl	1.37	1040
methomyl	1.41	1040
methoxy−3−phenylcarbamate	1.36	792
methoxy−3−phenylcarbamate	1.37	792
methoxy−3−phenylcarbamate	1.43	792
methoxy−3−phenylcarbamate	1.53	792
methoxy−3−phenylcarbamate	1.56	792
methoxy−4−phenylcarbamate	1.28	792
methoxy−4−phenylcarbamate	1.30	792
methoxy−4−phenylcarbamate	1.36	792
methoxy−4−phenylcarbamate	1.54	792
methoxy−4−phenylcarbamate	1.64	792
methyl n − (3,4−dichlorophenyl)	2.74	320
methyl n − (3−chlorophenyl)carbamate	2.15	320
methyl n−phenylcarbamate	1.73	320
methyl−3−phenylcarbamate	1.40	792
methyl−3−phenylcarbamate	1.42	792
methyl−3−phenylcarbamate	1.49	792
methyl−3−phenylcarbamate	1.53	792
methyl−3−phenylcarbamate	1.61	792
n−butyl n−phenylcarbamate	2.26	320
n−pentyl n−phenylcarbamate	2.61	320
n−propyl n−phenylcarbamate	2.06	320
oxamyl	0.41	691
oxamyl	0.43	691
oxamyl	0.59	691
oxamyl	0.71	320
oxamyl	0.73	691
oxamyl	0.76	172
oxamyl	0.78	459
oxamyl	0.85	458
oxamyl	0.89	459
oxamyl	0.89	691

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
oxamyl	0.90	459
oxamyl	0.94	172
oxamyl	0.94	691
oxamyl	0.95	458
oxamyl	0.98	458
oxamyl	1.00	459
oxamyl	1.08	172
oxamyl	1.30	458
oxamyl	1.31	458
oxamyl	1.41	172
oxamyl	1.42	458
oxamyl	1.44	458
oxamyl	1.51	458
oxamyl	1.53	458
oxamyl	1.56	458
oxamyl	1.92	458
pebulate	2.56	208
pebulate	2.61	208
pebulate	2.80	525
pebulate	2.93	208
pebulate	2.95	208
pebulate	3.23	208
phenylcarbamate	1.04	792
phenylcarbamate	1.19	792
phenylcarbamate	1.22	792
phenylcarbamate	1.29	792
phenylcarbamate	1.33	792
propham	1.95	320
propoxur	1.30	792
propoxur	1.33	792
propoxur	1.36	792
propoxur	1.36	792
propoxur	1.39	792
ter-butyl-4-phenylcarbamate	1.96	792
ter-butyl-4-phenylcarbamate	2.06	792
ter-butyl-4-phenylcarbamate	2.08	792
ter-butyl-4-phenylcarbamate	2.10	792
ter-butyl-4-phenylcarbamate	2.17	792
thiram	2.36	1039
thiram	2.42	1039
thiram	2.58	1039
thiram	2.61	1039
thiram	2.74	1039
thiram	2.82	1039
thiram	2.85	1039
thiram	3.11	1039
triallate	3.06	685
triallate	3.23	280
triallate	3.33	717
triallate	3.33	280
triallate	3.34	280
triallate	3.35	525
triallate	3.36	280
triallate	3.38	280
triallate	3.44	192
triallate	3.52	267
triallate	3.56	267
triallate	3.56	267
triallate	3.60	661
triallate	3.61	668
triallate	3.63	685
triallate	3.65	192
triallate	3.66	662
triallate	3.67	267
triallate	3.77	668
vernolate	1.91	775
vernolate	2.21	775
vernolate	2.32	775
vernolate	2.39	775
vernolate	2.51	775
vernolate	2.62	775
xylylcarb (meobal)	1.65	792
xylylcarb (meobal)	1.67	792
xylylcarb (meobal)	1.70	792
xylylcarb (meobal)	1.76	792
xylylcarb (meobal)	1.90	792
zectran (mexacarbate)	2.64	454
zectran (mexacarbate)	2.97	454

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
zectran (mexacarbate)	3.28	454
DINITROANILINES		
2,6-dinitro-n-n-propyl-trifluoro-p-toluidine	3.61	123
2,6-dinitro-trifluoro-p-toluidine	2.56	123
benefin (benfluralin)	3.94	220
benefin (benfluralin)	4.03	525
butralin (aa-820)	3.91	525
butralin (aa-820)	4.04	220
chlornidine	3.94	220
dinitramine	3.60	525
dinitramine	3.66	220
fluchloralin	3.53	220
fluchloralin	3.56	525
gs - 38946	3.17	220
gs - 39985	3.23	220
isopropalin	4.72	220
isopropalin	4.88	525
nitralin (sd 11831)	2.70	308
nitralin (sd 11831)	2.79	308
nitralin (sd 11831)	2.84	796
nitralin (sd 11831)	2.93	306
nitralin (sd 11831)	2.93	796
nitralin (sd 11831)	2.95	306
nitralin (sd 11831)	2.98	525
nitralin (sd 11831)	3.26	220
oryzalin	3.40	220
profluralin (cga - 108320)	3.93	525
profluralin (cga - 108320)	4.09	220
sd 13207	2.67	306
sd 13207	2.74	306
sd 11830	2.33	306
sd 11830	2.40	306
sd 12030	3.08	306
sd 12030	3.11	306
sd 12346	3.30	306
sd 12400	2.58	306
sd 12639	2.52	306
sd 12639	2.60	306
trifluralin	3.59	731
trifluralin	3.61	123
trifluralin	3.63	361
trifluralin	3.64	406
trifluralin	3.70	280
trifluralin	3.71	280
trifluralin	3.85	717
trifluralin	3.86	431
trifluralin	3.87	320
trifluralin	3.89	280
trifluralin	3.90	220
trifluralin	3.91	458
trifluralin	3.93	458
trifluralin	3.97	280
trifluralin	3.97	280
trifluralin	4.10	458
trifluralin	4.14	320
trifluralin	4.14	525
trifluralin	4.18	458
trifluralin	4.44	458
trifluralin	4.47	458
trifluralin	4.49	123
trifluralin	3.71	1055
trifluralin	3.89	1055
trifluralin	3.97	1055
trifluralin	3.69	1055
trifluralin	3.96	1055
AROMATIC HALOGENATED HYDROCARBONS		
2-methoxy-3,5,6-trichloropyridine	2.96	525
captafol	3.32	320
captan	2.30	320
chloroneb	3.07	566
chloroneb	3.08	525
chloroneb	3.21	327
chloroneb	3.22	722
dde	4.70	529

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
dde	4.94	321
ddt	4.30	431
ddt	4.38	608
ddt	4.80	652
ddt	5.12	311
ddt	5.12	112
ddt	5.14	396
ddt	5.15	566
ddt	5.18	361
ddt	5.30	652
ddt	5.36	311
ddt	5.38	595
ddt	5.38	437
ddt	5.39	667
ddt	5.45	458
ddt	5.55	311
ddt	5.62	321
ddt	5.65	112
ddt	5.70	652
ddt	5.77	458
ddt	5.84	458
ddt	5.85	662
ddt	5.88	458
ddt	5.95	430
ddt	6.07	458
ddt	6.14	431
ddt	6.25	431
ddt	6.26	431
ddt	6.30	431
ddt	6.63	431
ddt	6.72	431
ddt	6.88	458
dichlobenil	1.77	440
dichlobenil	1.96	440
dichlobenil	1.98	440
dichlobenil	2.01	440
dichlobenil	2.03	440
dichlobenil	2.10	440
dichlobenil	2.14	440
dichlobenil	2.14	440
dichlobenil	2.14	440
dichlobenil	2.15	440
dichlobenil	2.16	440
dichlobenil	2.17	440
dichlobenil	2.19	440
dichlobenil	2.20	440
dichlobenil	2.20	440
dichlobenil	2.21	667
dichlobenil	2.21	440
dichlobenil	2.21	440
dichlobenil	2.21	440
dichlobenil	2.22	566
dichlobenil	2.23	440
dichlobenil	2.23	440
dichlobenil	2.23	440
dichlobenil	2.23	440
dichlobenil	2.24	440
dichlobenil	2.24	440
dichlobenil	2.31	440
dichlobenil	2.32	680
dichlobenil	2.35	440
dichlobenil	2.37	525
dichlobenil	2.39	722
dichlobenil	2.40	440
dichlobenil	2.46	562
dichlobenil	2.50	440
dichlobenil	2.62	440
dichlobenil	2.70	440
dichlobenil	2.72	440
dichlobenil	2.75	440
dichlobenil	2.82	440
dichlobenil	2.92	440
dichlobenil	3.15	680
endosulfan	4.13	1029
endrin	4.29	1029
a-hch	3.01	408
a-hch	3.10	408
a-hch	3.12	408

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
a-hch	3.14	408
a-hch	3.18	408
a-hch	3.20	431
a-hch	3.30	408
a-hch	3.30	437
a-hch	3.31	408
a-hch	3.32	408
a-hch	3.33	408
a-hch	3.33	408
a-hch	3.35	408
a-hch	3.46	408
b-hch	3.06	408
b-hch	3.17	408
b-hch	3.25	408
b-hch	3.26	408
b-hch	3.26	10
b-hch	3.27	408
b-hch	3.29	408
b-hch	3.30	437
b-hch	3.32	408
b-hch	3.38	408
b-hch	3.40	408
b-hch	3.43	408
b-hch	3.46	396
b-hch	3.50	408
b-hch	3.50	408
b-hch	3.55	10
b-hch	3.70	595
y-hch (lindane)	2.15	17
y-hch (lindane)	2.26	17
y-hch (lindane)	2.41	522
y-hch (lindane)	2.44	17
y-hch (lindane)	2.48	17
y-hch (lindane)	2.50	17
y-hch (lindane)	2.56	557
y-hch (lindane)	2.56	17
y-hch (lindane)	2.58	17
y-hch (lindane)	2.59	17
y-hch (lindane)	2.59	17
y-hch (lindane)	2.60	17
y-hch (lindane)	2.61	17
y-hch (lindane)	2.63	522
y-hch (lindane)	2.66	17
y-hch (lindane)	2.67	81
y-hch (lindane)	2.69	17
y-hch (lindane)	2.72	17
y-hch (lindane)	2.73	17
y-hch (lindane)	2.74	81
y-hch (lindane)	2.76	17
y-hch (lindane)	2.76	17
y-hch (lindane)	2.78	17
y-hch (lindane)	2.81	17
y-hch (lindane)	2.81	724
y-hch (lindane)	2.84	17
y-hch (lindane)	2.86	17
y-hch (lindane)	2.86	17
y-hch (lindane)	2.86	176
y-hch (lindane)	2.87	17
y-hch (lindane)	2.87	406
y-hch (lindane)	2.89	17
y-hch (lindane)	2.89	81
y-hch (lindane)	2.91	81
y-hch (lindane)	2.92	506
y-hch (lindane)	2.93	637
y-hch (lindane)	2.93	330
y-hch (lindane)	2.95	17
y-hch (lindane)	2.95	349
y-hch (lindane)	2.96	525
y-hch (lindane)	2.97	409
y-hch (lindane)	2.97	409
y-hch (lindane)	2.98	61
y-hch (lindane)	3.00	61
y-hch (lindane)	3.01	61
y-hch (lindane)	3.01	17
y-hch (lindane)	3.01	81
y-hch (lindane)	3.01	506
y-hch (lindane)	3.02	17
y-hch (lindane)	3.03	81

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
y−hch (lindane)	3.03	184
y−hch (lindane)	3.04	408
y−hch (lindane)	3.05	506
y−hch (lindane)	3.06	637
y−hch (lindane)	3.08	408
y−hch (lindane)	3.08	637
y−hch (lindane)	3.09	61
y−hch (lindane)	3.09	17
y−hch (lindane)	3.11	441
y−hch (lindane)	3.12	10
y−hch (lindane)	3.12	557
y−hch (lindane)	3.12	522
y−hch (lindane)	3.13	566
y−hch (lindane)	3.13	667
y−hch (lindane)	3.14	522
y−hch (lindane)	3.16	330
y−hch (lindane)	3.16	557
y−hch (lindane)	3.17	184
y−hch (lindane)	3.18	81
y−hch (lindane)	3.20	522
y−hch (lindane)	3.21	81
y−hch (lindane)	3.22	409
y−hch (lindane)	3.23	408
y−hch (lindane)	3.23	17
y−hch (lindane)	3.24	408
y−hch (lindane)	3.27	430
y−hch (lindane)	3.28	408
y−hch (lindane)	3.28	408
y−hch (lindane)	3.29	184
y−hch (lindane)	3.30	408
y−hch (lindane)	3.30	437
y−hch (lindane)	3.31	184
y−hch (lindane)	3.31	408
y−hch (lindane)	3.32	408
y−hch (lindane)	3.32	408
y−hch (lindane)	3.33	408
y−hch (lindane)	3.34	17
y−hch (lindane)	3.35	15
y−hch (lindane)	3.36	408
y−hch (lindane)	3.39	408
y−hch (lindane)	3.41	10
y−hch (lindane)	3.41	330
y−hch (lindane)	3.42	557
y−hch (lindane)	3.47	595
mboca	3.90	619
methoxychlor	3.98	181
methoxychlor	4.22	181
methoxychlor	4.61	181
methoxychlor	4.86	181
methoxychlor	4.86	181
methoxychlor	4.90	525
methoxychlor	4.90	181
methoxychlor	4.90	181
methoxychlor	4.91	181
methoxychlor	4.93	181
methoxychlor	4.96	181
methoxychlor	4.96	181
methoxychlor	4.97	181
methoxychlor	5.00	181
methoxychlor	5.02	181
n − serve (nitrpyrin, dowco 163)	2.17	350
n − serve (nitrpyrin, dowco 163)	2.24	320
n − serve (nitrpyrin, dowco 163)	2.27	350
n − serve (nitrpyrin, dowco 163)	2.29	350
n − serve (nitrpyrin, dowco 163)	2.37	350
n − serve (nitrpyrin, dowco 163)	2.37	350
n − serve (nitrpyrin, dowco 163)	2.43	320
n − serve (nitrpyrin, dowco 163)	2.43	566
n − serve (nitrpyrin, dowco 163)	2.45	350
n − serve (nitrpyrin, dowco 163)	2.49	350
n − serve (nitrpyrin, dowco 163)	2.50	350
n − serve (nitrpyrin, dowco 163)	2.51	350
n − serve (nitrpyrin, dowco 163)	2.55	746
n − serve (nitrpyrin, dowco 163)	2.62	731
n − serve (nitrpyrin, dowco 163)	2.62	525
n − serve (nitrpyrin, dowco 163)	2.65	350
n − serve (nitrpyrin, dowco 163)	2.66	361
n − serve (nitrpyrin, dowco 163)	2.66	731

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
n – serve (nitrpyrin, dowco 163)	2.69	731
n – serve (nitrpyrin, dowco 163)	2.71	731
n – serve (nitrpyrin, dowco 163)	2.75	576
n – serve (nitrpyrin, dowco 163)	2.75	731
n – serve (nitrpyrin, dowco 163)	2.79	731
n – serve (nitrpyrin, dowco 163)	2.80	731
n – serve (nitrpyrin, dowco 163)	2.80	731
n – serve (nitrpyrin, dowco 163)	2.87	361
n – serve (nitrpyrin, dowco 163)	2.88	731
nitrofen	4.18	293
2 – pcb (1)	3.47	392
2,2' – dichlorobiphenyl (1)	3.92	321
2,4' – dichlorobiphenyl (8)	2.59	744
2,4' – dichlorobiphenyl (8)	2.72	614
2,4' – dichlorobiphenyl (8)	3.84	744
2,4' – dichlorobiphenyl (8)	4.13	392
2,4' – dichlorobiphenyl (8)	4.14	595
2,2',5 – trichlorobiphenyl (18)	3.93	744
2,2',5 – trichlorobiphenyl (18)	4.03	744
2,2',5 – trichlorobiphenyl (18)	4.05	744
2,2',5 – trichlorobiphenyl (18)	4.11	744
2,2',5 – trichlorobiphenyl (18)	4.20	744
2,2',5 – trichlorobiphenyl (18)	4.27	744
2,2',5 – trichlorobiphenyl (18)	5.04	744
2,4,4' – trichlorobiphenyl (28)	3.74	321
2,4,4' – trichlorobiphenyl (28)	4.62	392
2,4,4' – trichlorobiphenyl (28)	5.50	1032
2,2',4,4' – tetrachlorobiphenyl (47)	3.43	615
2,2',5,5' – tetrachlorobiphenyl (52)	3.43	744
2,2',5,5' – tetrachlorobiphenyl (52)	3.57	614
2,2',5,5' – tetrachlorobiphenyl (52)	4.91	321
2,2',5,5' – tetrachlorobiphenyl (52)	5.58	1032
2,2',5,5' – tetrachlorobiphenyl (52)	6.15	550
2,2',6,6' – tetrachlorobiphenyl (54)	4.72	665
2,2',6,6' – tetrachlorobiphenyl (54)	4.79	744
2,2',6,6' – tetrachlorobiphenyl (54)	4.89	665
2,2',6,6' – tetrachlorobiphenyl (54)	4.91	665
2,2',6,6' – tetrachlorobiphenyl (54)	5.11	665
2,2',6,6' – tetrachlorobiphenyl (54)	5.63	555
2,3',4',5 – tetrachlorobiphenyl (70)	4.69	665
2,3',4',5 – tetrachlorobiphenyl (70)	4.76	744
2,3',4',5 – tetrachlorobiphenyl (70)	4.85	665
2,3',4',5 – tetrachlorobiphenyl (70)	4.86	665
2,3',4',5 – tetrachlorobiphenyl (70)	5.02	665
2,2',3,4,5' – pentachlorobiphenyl (87)	4.50	529
2,2',3,4,5' – pentachlorobiphenyl (87)	4.74	321
2,4,5,2',5' – pentachlorobiphenyl (101)	4.87	321
2,4,5,2',5' – pentachlorobiphenyl (101)	5.45	361
2,4,5,2',5' – pentachlorobiphenyl (101)	5.70	361
2,4,5,2',5' – pentachlorobiphenyl (101)	5.80	652
2,4,5,2',5' – pentachlorobiphenyl (101)	5.90	550
2,4,5,2',5' – pentachlorobiphenyl (101)	6.04	652
2,4,5,2',5' – pentachlorobiphenyl (101)	6.30	550
2,4,5,2',5' – pentachlorobiphenyl (101)	6.40	550
2,4,5,2',5' – pentachlorobiphenyl (101)	6.41	550
2,2',3,3',4,4' – hexachlorobiphenyl (128)	5.29	321
2,2',4,4',5,5' – hexachlorobiphenyl (153)	4.25	744
2,2',4,4',5,5' – hexachlorobiphenyl (153)	4.28	550
2,2',4,4',5,5' – hexachlorobiphenyl (153)	4.32	431
2,2',4,4',5,5' – hexachlorobiphenyl (153)	4.38	614
2,2',4,4',5,5' – hexachlorobiphenyl (153)	4.78	744
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.05	550
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.20	431
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.20	431
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.22	550
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.23	431
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.24	431
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.30	431
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.33	431
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.34	550
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.35	431
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.41	744
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.54	744
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.58	744
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.58	396
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.58	529
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.60	744
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.62	614

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.65	393
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.80	393
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.82	595
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.83	393
2,2',4,4',5,5' – hexachlorobiphenyl (153)	5.86	431
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.07	744
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.08	525
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.08	622
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.10	431
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.20	744
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.22	550
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.30	1032
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.32	321
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.80	550
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.86	651
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.86	550
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.87	744
2,2',4,4',5,5' – hexachlorobiphenyl (153)	6.90	550
2,2',4,4',6,6' – hexachlorobiphenyl (155)	6.08	181
2,2',3,4,5,5',6 – heptachlorobiphenyl (185)	6.19	321
2,2',3,4,5,5',6 – heptachlorobiphenyl (185)	6.34	652
2,2',3,4,5,5',6 – heptachlorobiphenyl (185)	7.15	652
chloroaniline	1.96	99
chloroaniline	2.59	577
chloroaniline	2.82	577
chloroaniline	1.98	99
chloroaniline	2.60	155
chloroaniline	2.85	155
chloroaniline	2.03	99
chloroaniline	2.70	155
chloroaniline	2.89	577
chloroaniline	2.25	342
chloroaniline	2.71	577
chloroaniline	2.91	155
chloroaniline	2.25	342
chloroaniline	2.75	722
chloroaniline	2.98	577
chloroaniline	2.58	155
3,5 – dichloroaniline	2.38	99
3,5 – dichloroaniline	2.49	99
2,6 – dichloroaniline	3.25	1032
2,4 – dichloroaniline	2.88	1044
2,4 – dichloroaniline	2.69	1044
2,4 – dichloroaniline	2.48	1044
2,4 – dichloroaniline	2.85	1044
3,4 – dichloroaniline	3.56	1033
3,4 – dichloroaniline	3.53	1033
3,4 – dichloroaniline	3.42	1033
3,4 – dichloroaniline	2.17	1035
3,4 – dichloroaniline	2.29	320
2,3,4–trichloroaniline	2.60	99
2,3,4–trichloroaniline	2.65	99
2,3,4–trichloroaniline	3.66	1032
2,3,4,5–tetrachloroaniline	3.04	99
2,3,4,5–tetrachloroaniline	3.98	1032
2,3,5,6–tetrachloroaniline	3.94	1032
pentachloroaniline	4.62	1032
3–cf3 aniline	2.36	320
4–bromoaniline	1.96	320
3–chloro–4–methoxyaniline (3–cl–4–och3)	1.93	320
3–ch3–4–bromoaniline	2.26	320
4–bromonitrobenzene	2.42	320
3,4–dichloronitrobenzene	2.53	320
2,3–dichloronitrobenzene	3.97	1032
3,5–dichloronitrobenzene	4.19	1032
2,3,4,5–tetrachloronitrobenzene	4.23	1032
2,3,5,6–tetrachloronitrobenzene	4.05	1032
pentachloronitrobenzene	4.60	1032
pentachloronitrobenzene	4.40	1028
pentachloronitrobenzene	4.22	1028
pentachloronitrobenzene	4.21	1028
3–chloro–4–bromonitrobenzene	2.60	320
chlorobenzene	1.92	392
chlorobenzene	2.30	734
chlorobenzene	2.59	396
chlorobenzene	2.10	529
chlorobenzene	2.34	734
chlorobenzene	2.61	734

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
chlorobenzene	2.18	109
chlorobenzene	2.34	321
chlorobenzene	2.70	396
chlorobenzene	2.22	396
chlorobenzene	2.41	396
iodobenzene	3.10	529
bromobenzene	2.18	525
bromobenzene	2.42	321
bromobenzene	3.04	321
1,2 – dichlorobenzene	2.40	529
1,2 – dichlorobenzene	2.50	321
1,2 – dichlorobenzene	2.54	521
1,2 – dichlorobenzene	2.49	521
1,2 – dichlorobenzene	2.51	392
1,2 – dichlorobenzene	2.60	109
1,2 – dichlorobenzene	2.49	595
1,3 – dichlorobenzene	2.47	392
1,3 – dichlorobenzene	2.47	321
1,3 – dichlorobenzene	2.49	595
1,4 – dichlorobenzene	2.44	392
1,4 – dichlorobenzene	2.75	734
1,4 – dichlorobenzene	2.86	734
1,4 – dichlorobenzene	2.60	109
1,4 – dichlorobenzene	2.78	396
1,4 – dichlorobenzene	3.10	734
1,4 – dichlorobenzene	2.64	321
1,4 – dichlorobenzene	2.86	396
1,4 – dichlorobenzene	3.14	396
1,2,3 –trichlorobenzene	3.00	109
1,2,3 –trichlorobenzene	3.42	396
1,2,3 –trichlorobenzene	3.61	746
1,2,3 –trichlorobenzene	3.12	109
1,2,4 – trichlorobenzene	2.94	392
1,2,4 – trichlorobenzene	3.37	396
1,2,4 – trichlorobenzene	3.49	396
1,2,4 – trichlorobenzene	3.30	734
1,2,4 – trichlorobenzene	3.41	734
1,2,4 – trichlorobenzene	3.61	734
1,2,4 – trichlorobenzene	3.30	396
1,3,5 – trichlorobenzene	3.09	746
1,2,3,4 – tetrachlorobenzene	3.84	396
1,2,3,4 – tetrachlorobenzene	4.07	746
1,2,3,5 tetrachlorobenzene	3.20	529
1,2,3,5 tetrachlorobenzene	3.44	321
1,2,3,5 tetrachlorobenzene	3.49	166
1,2,4,5 – tetrachlorobenzene	3.72	396
1,2,4,5 – tetrachlorobenzene	3.89	396
1,2,4,5 – tetrachlorobenzene	4.09	734
1,2,4,5 – tetrachlorobenzene	3.80	734
1,2,4,5 – tetrachlorobenzene	3.93	396
1,2,4,5 – tetrachlorobenzene	4.10	746
1,2,4,5 – tetrachlorobenzene	3.81	734
pentachlorobenzene	3.50	529
pentachlorobenzene	3.74	321
hexachlorobenzene	3.59	525
hexachlorobenzene	3.90	529
hexachlorobenzene	4.40	726
hexachlorobenzene	3.77	726
hexachlorobenzene	4.06	726
hexachlorobenzene	4.49	166
o–chlorophenol	1.67	93
m–chlorophenol	1.78	93
p–chlorophenol	1.80	93
2,3 – dichlorophenol	2.27	353
2,3 – dichlorophenol	2.66	611
2,3 – dichlorophenol	2.77	611
2,3 – dichlorophenol	2.35	611
2,4 – dichlorophenol	2.06	93
2,4 – dichlorophenol	2.42	611
2,4 – dichlorophenol	2.85	611
2,4 – dichlorophenol	2.22	353
2,4 – dichlorophenol	2.82	611
2,4,5 – trichlorophenol	2.52	93
2,4,5 – trichlorophenol	3.45	611
2,4,5 – trichlorophenol	3.38	611
2,4,5 – trichlorophenol	3.25	611
2,4,6 – trichlorophenol	2.92	611
2,4,6 – trichlorophenol	3.03	611

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
2,4,6 – trichlorophenol	3.12	611
3,4,5 – trichlorophenol	3.47	611
3,4,5 – trichlorophenol	3.57	611
3,4,5 – trichlorophenol	3.65	611
2,3,4,5 – tetrachlorophenol	4.10	611
2,3,4,5 – tetrachlorophenol	4.12	611
2,3,4,5 – tetrachlorophenol	4.14	611
pentachlorophenol	4.38	611
pentachlorophenol	4.55	611
pentachlorophenol	4.59	611
4–bromophenol	2.41	320
o–benzyl–p–chlorophenol	3.07	805
o–benzyl–p–chlorophenol	3.31	805
o–benzyl–p–chlorophenol	3.84	805
ORGANOPHOSPHATES		
3,5,6–trichloro–2–pyridinol (chlorpyrifos metabolite)	2.30	1021
3,5,6–trichloro–2–pyridinol (chlorpyrifos metabolite)	2.34	1021
3,5,6–trichloro–2–pyridinol (chlorpyrifos metabolite)	2.44	1021
azinphos methyl	2.61	787
azinphos methyl	2.70	787
azinphos methyl	3.70	787
azinphos methyl	3.72	787
azinphos methyl	2.67	1056
azinphos methyl	2.76	1056
azinphos methyl	3.53	1056
carbophenothion (trithion)	4.28	64
carbophenothion (trithion)	4.66	525
carbophenothion (trithion)	4.68	64
carbophenothion (trithion)	4.82	64
carbophenothion (trithion)	4.96	64
carbophenothion – methyl	4.67	184
chlorfenvinphos	2.47	166
chlorfenvinphos	2.79	308
chlorfenvinphos	2.79	308
chlorpyrifos	3.00	1017
chlorpyrifos	3.18	1017
chlorpyrifos	3.30	318
chlorpyrifos	3.54	318
chlorpyrifos	3.63	184
chlorpyrifos	3.64	184
chlorpyrifos	3.64	318
chlorpyrifos	3.65	318
chlorpyrifos	3.66	320
chlorpyrifos	3.70	1020
chlorpyrifos	3.75	318
chlorpyrifos	3.77	1020
chlorpyrifos	3.78	406
chlorpyrifos	3.79	576
chlorpyrifos	3.79	318
chlorpyrifos	3.79	361
chlorpyrifos	3.87	1020
chlorpyrifos	3.90	184
chlorpyrifos	3.93	184
chlorpyrifos	3.99	318
chlorpyrifos	4.02	318
chlorpyrifos	4.11	414
chlorpyrifos	4.13	320
chlorpyrifos	4.13	525
chlorpyrifos	4.13	608
chlorpyrifos	4.15	731
chlorpyrifos	4.19	414
chlorpyrifos	4.21	414
chlorpyrifos	4.23	414
chlorpyrifos	4.23	736
chlorpyrifos	4.24	736
chlorpyrifos	4.28	414
chlorpyrifos	4.28	414
chlorpyrifos	4.32	736
chlorpyrifos – methyl	3.52	525
ciodrin (crotoxiphos)	1.87	722
ciodrin (crotoxiphos)	2.13	420
ciodrin (crotoxiphos)	2.23	525
ciodrin (crotoxiphos)	2.24	564
ciodrin (crotoxiphos)	2.44	420
ciodrin (crotoxiphos)	2.69	420
diamidaphos (nellite)	1.49	564

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
diamidaphos (nellite)	1.51	525
diamidaphos (nellite)	1.52	564
diamidaphos (nellite)	1.64	564
diazinon	2.36	661
diazinon	2.36	166
diazinon	2.60	184
diazinon	2.64	667
diazinon	2.64	184
diazinon	2.69	184
diazinon	2.70	667
diazinon	2.75	667
diazinon	2.75	714
diazinon	2.87	184
dichlorvos	1.55	1028
dichlorvos	1.55	1028
dichlorvos	1.64	1028
dichlorvos	2.23	1059
dichlorvos	2.17	1059
dimefox	1.76	707
dimefox	1.82	707
dimethoate	0.71	542
dimethoate	0.93	320
dimethoate	0.96	320
dimethoate	1.21	592
dimethoate	1.46	1039
dimethoate	1.63	1039
dimethoate	1.67	1039
dimethoate	1.68	1039
dimethoate	1.77	1039
dimethoate	1.87	1039
dimethoate	1.97	1039
dimethoate	2.26	1039
disulfoton (disyston)	2.64	561
disulfoton (disyston)	2.75	320
disulfoton (disyston)	2.81	561
disulfoton (disyston)	2.81	561
disulfoton (disyston)	2.81	561
disulfoton (disyston)	2.82	561
disulfoton (disyston)	2.83	561
disulfoton (disyston)	2.88	561
disulfoton (disyston)	2.90	542
disulfoton (disyston)	2.90	561
disulfoton (disyston)	2.90	561
disulfoton (disyston)	2.93	320
disulfoton (disyston)	2.95	561
disulfoton (disyston)	3.02	561
disulfoton (disyston)	3.04	561
disulfoton (disyston)	3.08	561
disulfoton (disyston)	3.09	561
disulfoton (disyston)	3.13	561
disulfoton (disyston)	3.15	592
disulfoton (disyston)	3.20	722
disulfoton (disyston)	3.20	561
disulfoton (disyston)	3.25	525
disulfoton (disyston)	3.30	561
disulfoton (disyston)	3.31	64
disulfoton (disyston)	3.58	64
disulfoton (disyston)	3.89	64
disulfoton (disyston)	3.93	64
disulfoton (disyston)	4.29	566
dowco 275	2.41	320
dyfonate (fonofos)	3.44	339
ethion	3.81	184
ethion	3.92	184
ethion	3.94	64
ethion	3.99	184
ethion	4.00	184
ethion	4.16	64
ethion	4.19	525
ethion	4.35	64
ethion	4.53	64
ethoprophos	1.61	742
ethoprophos	1.63	742
ethoprophos	1.64	742
ethoprophos	1.64	742
ethoprophos	1.64	742
ethoprophos	1.68	742
ethoprophos	1.69	742

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
ethoprophos	1.69	742
ethoprophos	1.69	742
ethoprophos	1.72	742
ethoprophos	1.72	742
ethoprophos	1.74	742
ethoprophos	1.74	742
ethoprophos	1.75	742
ethoprophos	1.75	742
ethoprophos	1.76	742
ethoprophos	1.76	742
ethoprophos	1.76	742
ethoprophos	1.76	742
ethoprophos	1.76	742
ethoprophos	1.77	742
ethoprophos	1.77	742
ethoprophos	1.78	742
ethoprophos	1.80	742
ethoprophos	1.81	742
ethoprophos	1.86	348
ethoprophos	1.86	347
ethoprophos	1.87	347
ethoprophos	1.87	348
ethoprophos	1.88	346
ethoprophos	1.97	348
ethoprophos	1.99	347
ethoprophos	2.02	346
ethoprophos	2.08	661
ethoprophos	2.10	346
ethoprophos	2.24	346
fenamiphos	2.17	459
fenamiphos	2.29	459
fenamiphos	2.38	556
fenamiphos	2.40	459
fenamiphos	2.48	735
fenamiphos	2.51	735
fenamiphos	2.52	735
fenamiphos	2.52	459
fenamiphos	2.52	166
fenamiphos	2.63	735
fenamiphos	2.63	735
fenamiphos	2.69	735
fenamiphos	2.89	735
fenamiphos sulfoxide	1.57	556
fenamiphos sulfone	1.64	556
fenitrothion	2.42	1017
fenitrothion	2.68	1017
fenitrothion	3.11	1037
fenitrothion	3.14	1037
fenitrothion	3.17	1038
fenitrothion	3.24	1037
fenitrothion	3.28	1038
fenitrothion	3.32	1038
fenitrothion	3.43	1038
fenitrothion	3.50	1037
fensulfothion	2.40	411
fensulfothion	2.40	411
fensulfothion	2.59	411
fensulfothion	2.68	411
fensulfothion sulfide	2.99	411
fensulfothion sulfide	3.17	411
fensulfothion sulfide	3.24	411
fensulfothion sulfide	3.33	411
fensulfothion sulfone	1.88	455
fensulfothion sulfone	2.10	455
fensulfothion sulfone	2.33	455
fensulfothion sulfone	2.35	455
isazophos	1.99	662
isazophos	2.01	667
isazophos	2.03	662
leptophos	3.95	431
leptophos	3.97	525
leptophos	4.97	184
leptophos	5.07	184
leptophos	5.09	184
malathion	2.36	728
malathion	2.63	66
malathion	2.64	66
malathion	2.67	66

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
malathion	2.76	66
malathion	2.87	66
malathion	2.91	66
malathion	2.93	66
malathion	2.94	66
malathion	3.09	66
malathion	3.13	66
malathion	3.16	66
malathion	3.16	66
malathion	3.22	66
malathion	3.25	722
malathion	3.29	66
malathion	3.32	66
malathion	3.34	66
malathion	3.36	66
malathion	3.41	66
malathion	3.58	66
malathion	3.62	66
methidathion	2.26	662
methidathion	2.27	667
methyl parathion	2.17	1038
methyl parathion	2.54	182
methyl parathion	2.55	431
methyl parathion	2.64	182
methyl parathion	2.69	182
methyl parathion	2.78	1038
methyl parathion	2.90	1038
methyl parathion	2.98	1038
methyl parathion	3.33	722
methyl parathion	3.39	64
methyl parathion	3.55	431
methyl parathion	3.71	437
methyl parathion	3.71	64
methyl parathion	3.78	64
methyl parathion	3.99	525
methyl parathion	4.06	64
mevinphos	1.64	184
mevinphos	1.99	1036
mevinphos	2.01	1036
mevinphos	2.14	1036
mevinphos	2.18	1036
mevinphos	2.32	1036
mevinphos	2.34	1036
mevinphos	2.36	1036
mevinphos	2.43	1036
mevinphos	2.51	1036
mevinphos	2.60	1036
mevinphos	2.98	1036
mevinphos	3.01	1036
mevinphos	3.10	1036
mevinphos	3.18	1036
mevinphos	3.19	1036
mevinphos	3.28	1036
mevinphos	3.50	1036
mevinphos	3.62	1036
mevinphos	3.64	1036
mevinphos	4.74	1036
parathion	2.41	81
parathion	2.42	540
parathion	2.48	540
parathion	2.51	81
parathion	2.53	81
parathion	2.54	540
parathion	2.56	540
parathion	2.58	540
parathion	2.63	540
parathion	2.66	540
parathion	2.71	540
parathion	2.72	458
parathion	2.73	458
parathion	2.74	540
parathion	2.76	540
parathion	2.78	458
parathion	2.79	458
parathion	2.80	81
parathion	2.81	81
parathion	2.86	81
parathion	2.87	559

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
parathion	2.87	458
parathion	2.88	559
parathion	2.88	458
parathion	2.89	458
parathion	2.89	662
parathion	2.92	458
parathion	2.92	81
parathion	2.97	662
parathion	2.97	184
parathion	2.99	316
parathion	2.99	326
parathion	3.01	318
parathion	3.02	326
parathion	3.02	166
parathion	3.02	320
parathion	3.03	318
parathion	3.05	318
parathion	3.06	731
parathion	3.06	396
parathion	3.09	317
parathion	3.11	318
parathion	3.11	724
parathion	3.11	317
parathion	3.12	340
parathion	3.12	521
parathion	3.13	317
parathion	3.13	184
parathion	3.14	318
parathion	3.15	458
parathion	3.18	317
parathion	3.18	458
parathion	3.20	312
parathion	3.20	458
parathion	3.22	458
parathion	3.23	184
parathion	3.23	184
parathion	3.23	317
parathion	3.24	521
parathion	3.25	312
parathion	3.25	326
parathion	3.26	316
parathion	3.27	317
parathion	3.30	595
parathion	3.30	317
parathion	3.36	521
parathion	3.37	317
parathion	3.43	312
parathion	3.44	317
parathion	3.45	431
parathion	3.47	64
parathion	3.49	317
parathion	3.50	521
parathion	3.51	317
parathion	3.52	317
parathion	3.59	521
parathion	3.65	521
parathion	3.68	437
parathion	3.68	525
parathion	3.76	64
parathion	3.79	312
parathion	3.90	64
parathion	4.00	731
parathion	4.02	667
parathion	4.03	722
parathion	4.04	661
parathion	4.19	64
parathion	4.73	27
parathion	4.81	27
phorate (thimet)	2.56	318
phorate (thimet)	2.60	318
phorate (thimet)	2.63	318
phorate (thimet)	2.66	318
phorate (thimet)	2.71	318
phorate (thimet)	2.81	166
phorate (thimet)	2.82	320
phorate (thimet)	3.29	64
phorate (thimet)	3.39	64
phorate (thimet)	3.51	525

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
phorate (thimet)	3.66	64
phorate (thimet)	3.82	64
piperophos	2.72	548
piperophos	2.74	548
piperophos	2.80	548
piperophos	2.80	548
piperophos	2.83	548
piperophos	2.86	548
piperophos	2.94	548
piperophos	3.03	548
piperophos	3.07	548
piperophos	3.23	548
piperophos	3.23	548
piperophos	3.33	548
piperophos	3.41	548
piperophos	3.67	548
piperophos	4.12	548
profenophos	3.03	714
terbufos	2.46	318
terbufos	2.50	318
terbufos	2.59	546
terbufos	2.75	318
terbufos	2.82	318
terbufos	2.87	546
terbufos	2.89	546
terbufos	3.03	318
terbufos	3.28	456
terbufos	3.41	456
terbufos	3.50	456
terbufos	3.59	456
terbufos sulfone	1.83	456
terbufos sulfone	2.00	456
terbufos sulfone	2.17	456
terbufos sulfone	2.70	456
terbufos sulfoxide	1.84	456
terbufos sulfoxide	1.94	456
terbufos sulfoxide	2.08	456
terbufos sulfoxide	2.87	456
triazofos	2.62	1058
triazofos	2.51	1058
triazofos	2.52	1058
trichlorfon	1.61	1028
trichlorfon	1.71	1028
trichlorfon	1.82	1028
trichlorfon	1.49	1054
trichlorfon	1.58	1054
trichlorfon	1.28	1054
UREAS		
cga-15646	2.16	240
cga-15646	2.31	240
cga-15646	2.52	240
cga-15646	2.17	240
cga-15646	2.39	240
cga-15646	2.54	240
cga-15646	2.18	240
cga-15646	2.40	240
chlorbromuron	2.19	524
chlorbromuron	2.59	524
chlorbromuron	2.87	337
chlorbromuron	2.23	524
chlorbromuron	2.64	218
chlorbromuron	2.88	337
chlorbromuron	2.34	501
chlorbromuron	2.64	242
chlorbromuron	2.91	218
chlorbromuron	2.35	524
chlorbromuron	2.65	524
chlorbromuron	2.99	240
chlorbromuron	2.43	524
chlorbromuron	2.66	525
chlorbromuron	2.99	337
chlorbromuron	2.50	254
chlorbromuron	2.67	218
chlorbromuron	3.00	722
chlorbromuron	2.50	524
chlorbromuron	2.68	524

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
chlorbromuron	3.02	218
chlorbromuron	2.53	524
chlorbromuron	2.71	524
chlorbromuron	3.07	240
chlorbromuron	2.53	254
chlorbromuron	2.72	524
chlorbromuron	3.18	240
chlorbromuron	2.56	524
chlorbromuron	2.73	337
chlorbromuron	3.19	240
chlorbromuron	2.56	218
chlorbromuron	2.75	240
chlorbromuron	3.29	337
chlorbromuron	2.57	524
chlorbromuron	2.78	524
chlorbromuron	3.44	240
chlorbromuron	2.58	320
chlorbromuron	2.82	218
chlorbromuron	3.51	240
chlorbromuron	2.58	524
chlorbromuron	2.84	240
chlorbromuron	3.61	218
chloroxuron	3.12	285
chloroxuron	3.51	525
chloroxuron	3.68	261
chloroxuron	3.20	285
chloroxuron	3.60	261
chloroxuron	3.70	616
chloroxuron	3.27	285
chloroxuron	3.60	261
chloroxuron	3.79	261
chloroxuron	3.45	261
chloroxuron	3.64	535
chlorsulfuron	0.96	247
chlorsulfuron	2.00	705
chlorsulfuron	2.48	705
chlorsulfuron	0.98	705
chlorsulfuron	2.04	249
chlorsulfuron	2.55	249
chlorsulfuron	1.17	247
chlorsulfuron	2.04	249
chlorsulfuron	2.59	249
chlorsulfuron	1.38	247
chlorsulfuron	2.23	407
chlorsulfuron	2.66	407
chlorsulfuron	1.39	705
chlorsulfuron	2.33	249
chlorsulfuron	2.76	407
chlorsulfuron	1.47	247
chlorsulfuron	2.35	249
chlorsulfuron	2.80	407
chlorsulfuron	1.81	249
chlortoluron	1.63	524
chlortoluron	2.10	589
chlortoluron	2.26	589
chlortoluron	1.67	524
chlortoluron	2.12	524
chlortoluron	2.27	589
chlortoluron	1.81	292
chlortoluron	2.12	589
chlortoluron	2.27	589
chlortoluron	1.83	589
chlortoluron	2.13	589
chlortoluron	2.27	589
chlortoluron	1.88	589
chlortoluron	2.13	524
chlortoluron	2.28	589
chlortoluron	1.89	293
chlortoluron	2.13	589
chlortoluron	2.29	776
chlortoluron	1.91	589
chlortoluron	2.14	589
chlortoluron	2.30	589
chlortoluron	1.92	524
chlortoluron	2.14	524
chlortoluron	2.31	589
chlortoluron	1.94	524
chlortoluron	2.14	589

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
chlortoluron	2.32	589
chlortoluron	1.95	292
chlortoluron	2.14	589
chlortoluron	2.33	589
chlortoluron	1.97	524
chlortoluron	2.15	589
chlortoluron	2.33	292
chlortoluron	1.98	589
chlortoluron	2.15	589
chlortoluron	2.36	589
chlortoluron	1.98	589
chlortoluron	2.15	589
chlortoluron	2.38	589
chlortoluron	1.98	589
chlortoluron	2.16	589
chlortoluron	2.39	589
chlortoluron	1.98	524
chlortoluron	2.16	589
chlortoluron	2.40	589
chlortoluron	1.98	776
chlortoluron	2.17	524
chlortoluron	2.40	589
chlortoluron	1.99	589
chlortoluron	2.18	589
chlortoluron	2.40	589
chlortoluron	2.00	524
chlortoluron	2.18	589
chlortoluron	2.43	808
chlortoluron	2.02	524
chlortoluron	2.18	589
chlortoluron	2.48	776
chlortoluron	2.02	524
chlortoluron	2.19	776
chlortoluron	2.50	589
chlortoluron	2.02	524
chlortoluron	2.20	589
chlortoluron	2.51	776
chlortoluron	2.02	320
chlortoluron	2.21	589
chlortoluron	2.52	589
chlortoluron	2.02	776
chlortoluron	2.23	589
chlortoluron	2.62	808
chlortoluron	2.03	294
chlortoluron	2.23	589
chlortoluron	2.65	772
chlortoluron	2.04	524
chlortoluron	2.23	589
chlortoluron	2.67	772
chlortoluron	2.08	524
chlortoluron	2.24	776
chlortoluron	2.77	776
chlortoluron	2.08	524
chlortoluron	2.26	589
chlortoluron	2.80	589
chlortoluron	2.08	524
chlortoluron	2.26	589
chlortoluron	3.03	772
chlortoluron	2.09	589
3,4 – dichlorophenylurea	2.62	166
diflubenzuron	3.83	525
diuron	1.38	251
diuron	2.30	524
diuron	2.65	212
diuron	1.76	251
diuron	2.31	524
diuron	2.66	261
diuron	1.80	658
diuron	2.31	524
diuron	2.67	284
diuron	1.80	658
diuron	2.32	524
diuron	2.68	431
diuron	1.80	720
diuron	2.32	658
diuron	2.68	808
diuron	1.84	524
diuron	2.33	251

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
diuron	2.69	212
diuron	1.90	658
diuron	2.33	251
diuron	2.69	616
diuron	1.93	658
diuron	2.33	658
diuron	2.70	212
diuron	1.97	320
diuron	2.33	212
diuron	2.73	20
diuron	1.98	524
diuron	2.34	251
diuron	2.73	108
diuron	1.99	658
diuron	2.35	251
diuron	2.74	212
diuron	2.02	658
diuron	2.35	251
diuron	2.75	337
diuron	2.03	658
diuron	2.36	212
diuron	2.75	337
diuron	2.04	251
diuron	2.36	524
diuron	2.75	212
diuron	2.06	251
diuron	2.36	251
diuron	2.76	212
diuron	2.08	251
diuron	2.39	20
diuron	2.76	261
diuron	2.09	658
diuron	2.40	212
diuron	2.77	327
diuron	2.10	251
diuron	2.40	212
diuron	2.77	562
diuron	2.10	251
diuron	2.41	212
diuron	2.78	108
diuron	2.10	251
diuron	2.41	524
diuron	2.78	108
diuron	2.11	658
diuron	2.45	251
diuron	2.79	535
diuron	2.13	251
diuron	2.46	506
diuron	2.79	535
diuron	2.13	251
diuron	2.46	212
diuron	2.80	212
diuron	2.13	658
diuron	2.47	212
diuron	2.80	261
diuron	2.15	251
diuron	2.48	524
diuron	2.81	212
diuron	2.15	20
diuron	2.49	361
diuron	2.81	212
diuron	2.15	341
diuron	2.49	212
diuron	2.81	212
diuron	2.16	658
diuron	2.49	212
diuron	2.81	108
diuron	2.16	251
diuron	2.50	212
diuron	2.82	261
diuron	2.17	251
diuron	2.51	212
diuron	2.83	337
diuron	2.18	524
diuron	2.51	524
diuron	2.85	212
diuron	2.19	251
diuron	2.52	212

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
diuron	2.85	535
diuron	2.19	251
diuron	2.52	506
diuron	2.85	261
diuron	2.19	251
diuron	2.52	327
diuron	2.86	261
diuron	2.20	524
diuron	2.53	212
diuron	2.86	261
diuron	2.21	320
diuron	2.56	108
diuron	2.86	337
diuron	2.21	251
diuron	2.56	506
diuron	2.87	110
diuron	2.21	251
diuron	2.56	212
diuron	2.87	261
diuron	2.21	524
diuron	2.56	212
diuron	2.87	262
diuron	2.22	251
diuron	2.58	611
diuron	2.88	108
diuron	2.22	524
diuron	2.58	242
diuron	2.90	229
diuron	2.22	524
diuron	2.59	261
diuron	2.93	229
diuron	2.22	251
diuron	2.59	212
diuron	2.93	165
diuron	2.23	251
diuron	2.59	406
diuron	2.94	165
diuron	2.23	212
diuron	2.59	212
diuron	2.94	808
diuron	2.23	251
diuron	2.60	525
diuron	2.96	261
diuron	2.25	212
diuron	2.61	212
diuron	3.00	108
diuron	2.26	251
diuron	2.63	535
diuron	3.00	212
diuron	2.27	524
diuron	2.63	448
diuron	3.06	798
diuron	2.27	524
diuron	2.64	212
diuron	3.08	108
diuron	2.27	658
diuron	2.64	261
diuron	3.14	337
diuron	2.30	251
diuron	2.65	535
diuron	3.24	212
ethylenethiurea (etu)	2.07	631
fenuron	1.09	166
fenuron	1.35	524
fenuron	1.52	261
fenuron	1.12	320
fenuron	1.35	524
fenuron	1.52	524
fenuron	1.14	524
fenuron	1.36	535
fenuron	1.52	524
fenuron	1.19	524
fenuron	1.36	261
fenuron	1.52	535
fenuron	1.24	524
fenuron	1.39	448
fenuron	1.52	337
fenuron	1.24	524

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
fenuron	1.39	261
fenuron	1.59	261
fenuron	1.24	524
fenuron	1.41	524
fenuron	1.59	535
fenuron	1.29	261
fenuron	1.43	437
fenuron	1.62	524
fenuron	1.29	535
fenuron	1.43	525
fenuron	1.63	437
fenuron	1.29	535
fenuron	1.46	337
fenuron	1.63	524
fenuron	1.30	261
fenuron	1.47	337
fenuron	1.65	524
fenuron	1.32	524
fenuron	1.49	524
fenuron	1.83	337
fenuron	1.32	524
fenuron	1.49	524
fenuron	2.13	337
fluometuron	1.08	242
fluometuron	1.82	253
fluometuron	2.04	699
fluometuron	1.50	785
fluometuron	1.84	778
fluometuron	2.05	253
fluometuron	1.50	101
fluometuron	1.85	785
fluometuron	2.09	629
fluometuron	1.56	785
fluometuron	1.88	366
fluometuron	2.14	221
fluometuron	1.60	785
fluometuron	1.88	699
fluometuron	2.16	221
fluometuron	1.61	30
fluometuron	1.90	366
fluometuron	2.20	699
fluometuron	1.66	785
fluometuron	1.90	699
fluometuron	2.24	221
fluometuron	1.67	785
fluometuron	1.92	289
fluometuron	2.24	525
fluometuron	1.70	785
fluometuron	1.93	778
fluometuron	2.26	366
fluometuron	1.71	785
fluometuron	1.96	289
fluometuron	2.30	687
fluometuron	1.72	24
fluometuron	1.98	221
fluometuron	2.43	687
fluometuron	1.74	785
fluometuron	1.99	778
fluometuron	2.48	72
fluometuron	1.74	699
fluometuron	2.00	221
fluometuron	2.48	699
fluometuron	1.77	699
fluometuron	2.02	377
fluometuron	2.56	221
fluometuron	1.82	320
fluometuron	2.04	221
isouron	0.64	572
isouron	2.79	572
isouron	2.78	572
isouron	1.85	572
isouron	2.77	572
linuron	1.99	524
linuron	2.72	162
linuron	2.87	708
linuron	2.09	524
linuron	2.73	162
linuron	2.88	337

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
linuron	2.14	65
linuron	2.73	261
linuron	2.88	711
linuron	2.16	524
linuron	2.73	162
linuron	2.88	337
linuron	2.19	501
linuron	2.73	162
linuron	2.88	711
linuron	2.26	524
linuron	2.74	162
linuron	2.88	66
linuron	2.32	524
linuron	2.74	124
linuron	2.89	711
linuron	2.32	524
linuron	2.74	711
linuron	2.89	708
linuron	2.36	524
linuron	2.74	66
linuron	2.90	162
linuron	2.36	524
linuron	2.75	162
linuron	2.91	66
linuron	2.36	65
linuron	2.75	284
linuron	2.91	437
linuron	2.38	524
linuron	2.75	341
linuron	2.91	525
linuron	2.38	524
linuron	2.75	711
linuron	2.93	124
linuron	2.38	524
linuron	2.76	162
linuron	2.94	124
linuron	2.39	732
linuron	2.76	708
linuron	2.94	66
linuron	2.40	524
linuron	2.76	711
linuron	2.94	437
linuron	2.41	524
linuron	2.77	717
linuron	2.94	124
linuron	2.41	269
linuron	2.77	162
linuron	2.94	261
linuron	2.43	320
linuron	2.78	66
linuron	2.95	66
linuron	2.43	524
linuron	2.78	261
linuron	2.95	162
linuron	2.48	524
linuron	2.78	711
linuron	2.96	711
linuron	2.51	524
linuron	2.78	708
linuron	2.97	711
linuron	2.54	240
linuron	2.79	717
linuron	2.98	66
linuron	2.55	524
linuron	2.79	711
linuron	2.99	66
linuron	2.56	124
linuron	2.79	711
linuron	2.99	240
linuron	2.57	162
linuron	2.80	711
linuron	3.02	708
linuron	2.62	162
linuron	2.80	162
linuron	3.02	240
linuron	2.63	162
linuron	2.80	65
linuron	3.04	66

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
linuron	2.65	124
linuron	2.81	708
linuron	3.04	66
linuron	2.65	263
linuron	2.81	711
linuron	3.04	711
linuron	2.65	448
linuron	2.81	162
linuron	3.08	66
linuron	2.65	124
linuron	2.81	717
linuron	3.13	261
linuron	2.66	124
linuron	2.81	124
linuron	3.19	717
linuron	2.66	717
linuron	2.81	124
linuron	3.21	337
linuron	2.66	162
linuron	2.81	66
linuron	3.22	66
linuron	2.66	66
linuron	2.82	124
linuron	3.24	66
linuron	2.67	682
linuron	2.82	708
linuron	3.26	66
linuron	2.67	240
linuron	2.82	240
linuron	3.27	263
linuron	2.68	162
linuron	2.83	711
linuron	3.28	240
linuron	2.69	240
linuron	2.83	337
linuron	3.30	261
linuron	2.70	682
linuron	2.84	711
linuron	3.31	549
linuron	2.70	708
linuron	2.84	162
linuron	3.39	261
linuron	2.70	240
linuron	2.85	711
linuron	3.45	66
linuron	2.71	162
linuron	2.86	708
linuron	3.49	66
linuron	2.71	708
linuron	2.86	66
linuron	4.09	66
linuron	2.71	337
linuron	2.87	711
methabenzthiazuron	2.42	578
methabenzthiazuron	2.78	578
methabenzthiazuron	2.94	578
methabenzthiazuron	2.64	578
methabenzthiazuron	2.82	578
methabenzthiazuron	2.95	578
methabenzthiazuron	2.64	578
methabenzthiazuron	2.82	578
methabenzthiazuron	2.99	578
methabenzthiazuron	2.67	578
methabenzthiazuron	2.82	578
methabenzthiazuron	3.08	578
methabenzthiazuron	2.76	578
methabenzthiazuron	2.91	578
methylurea	1.68	261
methylurea	1.77	722
methylurea	1.85	261
methylurea	1.75	261
methylurea	1.78	261
methylurea	1.86	261
methylurea	1.76	261
metobromuron	1.67	524
metobromuron	2.01	524
metobromuron	2.31	240
metobromuron	1.75	524

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
metobromuron	2.02	320
metobromuron	2.34	240
metobromuron	1.78	501
metobromuron	2.06	524
metobromuron	2.43	722
metobromuron	1.78	525
metobromuron	2.09	524
metobromuron	2.45	240
metobromuron	1.80	524
metobromuron	2.10	524
metobromuron	2.47	337
metobromuron	1.93	524
metobromuron	2.11	524
metobromuron	2.52	240
metobromuron	1.93	524
metobromuron	2.12	524
metobromuron	2.60	337
metobromuron	1.95	524
metobromuron	2.13	240
metobromuron	2.70	240
metobromuron	1.98	524
metobromuron	2.15	524
metobromuron	3.00	337
metobromuron	2.00	524
metobromuron	2.19	240
metobromuron	3.32	240
metobromuron	2.01	524
metobromuron	2.25	337
metobromuron	2.01	524
metobromuron	2.31	337
metoxuron	1.47	524
metoxuron	1.74	320
metoxuron	1.88	524
metoxuron	1.58	524
metoxuron	1.82	524
metoxuron	1.90	524
metoxuron	1.58	524
metoxuron	1.82	524
metoxuron	1.93	524
metoxuron	1.62	524
metoxuron	1.85	524
metoxuron	1.94	524
metoxuron	1.73	524
metoxuron	1.86	524
metoxuron	1.96	524
metoxuron	1.74	524
metoxuron	1.87	524
metoxuron	2.18	524
monolinuron	1.41	524
monolinuron	1.93	524
monolinuron	2.35	240
monolinuron	1.49	524
monolinuron	1.97	524
monolinuron	2.39	337
monolinuron	1.60	501
monolinuron	1.97	524
monolinuron	2.40	580
monolinuron	1.67	524
monolinuron	1.98	524
monolinuron	2.44	240
monolinuron	1.71	524
monolinuron	1.99	524
monolinuron	2.45	437
monolinuron	1.73	524
monolinuron	2.07	337
monolinuron	2.47	261
monolinuron	1.73	524
monolinuron	2.17	337
monolinuron	2.51	240
monolinuron	1.75	524
monolinuron	2.17	337
monolinuron	2.52	240
monolinuron	1.78	524
monolinuron	2.25	261
monolinuron	2.66	261
monolinuron	1.79	524
monolinuron	2.30	437
monolinuron	2.70	261

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
monolinuron	1.82	524
monolinuron	2.30	525
monolinuron	2.72	240
monolinuron	1.84	320
monolinuron	2.32	261
monolinuron	2.73	337
monolinuron	1.86	580
monolinuron	2.32	240
monolinuron	2.96	580
monolinuron	1.87	524
monolinuron	2.35	261
monolinuron	3.31	240
monolinuron	1.92	524
monolinuron	2.35	240
monuron	0.66	419
monuron	1.77	524
monuron	2.19	337
monuron	0.94	419
monuron	1.78	524
monuron	2.20	263
monuron	1.02	419
monuron	1.82	524
monuron	2.24	263
monuron	1.04	419
monuron	1.82	368
monuron	2.26	437
monuron	1.06	419
monuron	1.85	524
monuron	2.27	204
monuron	1.09	419
monuron	1.85	524
monuron	2.27	261
monuron	1.10	419
monuron	1.86	524
monuron	2.29	261
monuron	1.10	419
monuron	1.86	419
monuron	2.31	261
monuron	1.37	419
monuron	1.89	524
monuron	2.33	337
monuron	1.38	524
monuron	1.90	524
monuron	2.33	448
monuron	1.44	524
monuron	1.92	667
monuron	2.33	327
monuron	1.46	501
monuron	1.92	616
monuron	2.34	261
monuron	1.58	524
monuron	1.99	337
monuron	2.36	562
monuron	1.63	524
monuron	1.99	327
monuron	2.41	263
monuron	1.65	524
monuron	2.00	524
monuron	2.44	261
monuron	1.67	524
monuron	2.00	525
monuron	2.45	204
monuron	1.68	419
monuron	2.05	419
monuron	2.45	261
monuron	1.70	320
monuron	2.08	204
monuron	2.54	204
monuron	1.73	524
monuron	2.12	337
monuron	2.73	337
monuron	1.77	524
neburon	3.12	448
neburon	3.43	261
neburon	3.52	261
neburon	3.26	261
neburon	3.46	562
neburon	3.57	261

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
neburon	3.31	261
neburon	3.49	722
neburon	3.58	261
neburon	3.36	525
siduron	2.31	448
tebuthiuron	1.72	226
tebuthiuron	1.83	226
tebuthiuron	2.79	525
tebuthiuron	1.79	226
tebuthiuron	1.97	226
tebuthiuron	2.79	235
urea	0.90	261
urea	1.15	525
urea	1.21	198
vel 3510	2.51	235
3-(3-chlorophenyl)-1,1-dimethylurea	1.79	320
3-(3-methoxyphenyl)-1,1-dimethylurea	1.72	320
3-(3-fluorophenyl)-1,1-dimethylurea	1.73	320
3-(4-fluorophenyl)-1,1-dimethylurea	1.43	320
3-(4-methylphenyl)-1,1-dimethylurea	1.51	320
3-(4-methoxyphenyl)-1,1-dimethylurea	1.40	320
3-(3,5-dimethylphenyl)-1,1-dimethylurea	1.41	524
3-(3,5-dimethylphenyl)-1,1-dimethylurea	1.75	524
3-(3,5-dimethylphenyl)-1,1-dimethylurea	1.82	524
3-(3,5-dimethylphenyl)-1,1-dimethylurea	1.65	524
3-(3,5-dimethylphenyl)-1,1-dimethylurea	1.82	524
3-(3,5-dimethylphenyl)-1,1-dimethylurea	1.90	524
3-(3,5-dimethylphenyl)-1,1-dimethylurea	1.67	524
3-(3,5-dimethyl-4-bromophenyl)-1,1-dimethylure	2.53	320
h-(n-methyl-n'-phenylurea)	1.35	524
h-(n-methyl-n'-phenylurea)	1.58	524
h-(n-methyl-n'-phenylurea)	1.78	524
h-(n-methyl-n'-phenylurea)	1.35	524
h-(n-methyl-n'-phenylurea)	1.58	524
h-(n-methyl-n'-phenylurea)	1.79	524
h-(n-methyl-n'-phenylurea)	1.49	524
h-(n-methyl-n'-phenylurea)	1.70	524
h-(n-methyl-n'-phenylurea)	1.79	524
h-(n-methyl-n'-phenylurea)	1.49	524
h-(n-methyl-n'-phenylurea)	1.74	524
h-(n-methyl-n'-phenylurea)	1.93	524
h-(n-methyl-n'-phenylurea)	1.56	524
h-(n-methyl-n'-phenylurea)	1.77	524
3-(3-chlorophenyl)-1-methylurea	1.93	320
3,4-cl2 (dmu)	2.06	524
3,4-cl2 (dmu)	2.46	320
3,4-cl2 (dmu)	2.54	524
3,4-cl2 (dmu)	2.16	524
3,4-cl2 (dmu)	2.49	524
3,4-cl2 (dmu)	2.55	524
3,4-cl2 (dmu)	2.19	524
3,4-cl2 (dmu)	2.51	524
3,4-cl2 (dmu)	2.59	524
3,4-cl2 (dmu)	2.39	524
3,4-cl2 (dmu)	2.53	524
3,4-cl2 (dmu)	2.67	524
3,4-cl2 (dmu)	2.41	524
3,4-cl2 (dmu)	2.53	524
3,4-cl2 (dmu)	2.70	524
3,4-cl2 (dmu)	2.44	524
3,4-cl2 (dmu)	2.53	524
3,4-cl2 (dmu)	2.71	524
3-(3-chloro-4-methoxyphenyl)-1-methylurea	1.84	320
3-(3-chloro-4-methoxyphenyl)-1-methylurea	1.96	501
3-(3-chloro-4-methylphenyl)-1-methylurea	2.10	320
3-phenyl-1-cyclopropylurea	1.74	320
3-phenyl-1-ciclopentylurea	1.93	320
3-phenyl-1-ciclohexylurea	2.07	320
3-phenyl-1-cicloheptylurea	2.37	320
2-fluorophenylurea	1.32	320
2-chlorophenylurea)	1.61	320
3-fluorophenylurea	1.77	320
3-chlorophenylurea	2.01	320
3-bromophenylurea	2.06	320
3-methylphenylurea	1.56	320
4-bromophenylurea	2.12	320
4-phenoxymethylurea	2.56	320
3-chloro-4-methoxyphenylurea	2.00	320

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
3-methyl-4-bromophenylurea	2.37	320
3-cf3-phenylurea	1.71	524
3-cf3-phenylurea	1.96	320
3-cf3-phenylurea	2.05	524
3-cf3-phenylurea	1.85	524
3-cf3-phenylurea	1.99	524
3-cf3-phenylurea	2.12	524
3-cf3-phenylurea	1.90	524
3-cf3-phenylurea	2.04	524
3-cf3-phenylurea	2.14	524
3-cf3-phenylurea	1.95	524
4-f-phenylurea	1.19	524
4-f-phenylurea	1.49	524
4-f-phenylurea	1.77	524
4-f-phenylurea	1.24	524
4-f-phenylurea	1.52	320
4-f-phenylurea	1.77	524
4-f-phenylurea	1.32	524
4-f-phenylurea	1.54	524
4-f-phenylurea	1.88	524
4-f-phenylurea	1.41	524
4-so3-phenylurea	1.14	501
h-phenylurea	1.35	501
h-phenylurea	1.87	261
h-phenylurea	1.97	261
h-phenylurea	1.78	261
h-phenylurea	1.88	722
h-phenylurea	2.07	261
h-phenylurea	1.86	261
h-phenylurea	1.92	261
3-ch3,4-f-phenylurea	1.54	524
3-ch3,4-f-phenylurea	1.68	524
3-ch3,4-f-phenylurea	1.96	524
3-ch3,4-f-phenylurea	1.54	524
3-ch3,4-f-phenylurea	1.78	320
3-ch3,4-f-phenylurea	2.03	524
3-ch3,4-f-phenylurea	1.63	524
3-ch3,4-f-phenylurea	1.88	524
3,4-di-cl-phenylurea	2.27	524
3,4-di-cl-phenylurea	2.49	320
3,4-di-cl-phenylurea	2.49	501
3,4-di-cl-phenylurea	2.63	524
3,4-di-cl-phenylurea	2.30	524
3,4-di-cl-phenylurea	2.53	524
3,4-di-cl-phenylurea	2.64	524
3,4-di-cl-phenylurea	2.36	524
3,4-di-cl-phenylurea	2.56	524
3,4-di-cl-phenylurea	2.69	524
3,4-di-cl-phenylurea	2.39	524
3,4-di-cl-phenylurea	2.57	524
3,4-di-cl-phenylurea	2.70	524
3,4-di-cl-phenylurea	2.41	524
3,4-di-cl-phenylurea	2.58	524
3,4-di-cl-phenylurea	2.80	524
3,4-di-cl-phenylurea	2.48	524
3,4-di-cl-phenylurea	2.59	524
TRIAZINES		
2-hydroxy-4,6-bis(ethylamino)-1,3,5-triazine	2.11	1016
2-hydroxy-4,6-bis(ethylamino)-1,3,5-triazine	2.25	1016
ametryn	1.97	633
ametryn	2.00	26
ametryn	2.06	633
ametryn	2.07	212
ametryn	2.13	212
ametryn	2.16	212
ametryn	2.20	212
ametryn	2.23	212
ametryn	2.23	212
ametryn	2.28	212
ametryn	2.29	212
ametryn	2.33	212
ametryn	2.40	212
ametryn	2.40	212
ametryn	2.44	212
ametryn	2.44	212
ametryn	2.46	212

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
ametryn	2.49	212
ametryn	2.50	212
ametryn	2.50	26
ametryn	2.51	212
ametryn	2.52	212
ametryn	2.53	212
ametryn	2.57	212
ametryn	2.57	212
ametryn	2.58	212
ametryn	2.58	616
ametryn	2.59	525
ametryn	2.63	212
ametryn	2.67	212
ametryn	2.68	212
ametryn	2.74	26
ametryn	2.74	212
ametryn	2.77	212
ametryn	2.79	212
ametryn	2.81	212
ametryn	2.84	212
ametryn	2.88	212
ametryn	2.90	212
ametryn	2.92	212
ametryn	2.98	212
amitrole	1.25	745
atrazine	1.30	647
atrazine	1.40	207
atrazine	1.41	647
atrazine	1.51	207
atrazine	1.57	647
atrazine	1.57	520
atrazine	1.62	65
atrazine	1.63	124
atrazine	1.69	207
atrazine	1.69	765
atrazine	1.70	373
atrazine	1.71	341
atrazine	1.71	210
atrazine	1.71	125
atrazine	1.72	520
atrazine	1.74	62
atrazine	1.74	26
atrazine	1.76	520
atrazine	1.78	255
atrazine	1.79	24
atrazine	1.81	125
atrazine	1.82	524
atrazine	1.83	167
atrazine	1.83	591
atrazine	1.84	520
atrazine	1.84	444
atrazine	1.84	591
atrazine	1.85	255
atrazine	1.86	511
atrazine	1.87	210
atrazine	1.87	204
atrazine	1.88	255
atrazine	1.88	171
atrazine	1.89	591
atrazine	1.89	520
atrazine	1.91	194
atrazine	1.91	292
atrazine	1.92	255
atrazine	1.92	520
atrazine	1.94	520
atrazine	1.94	98
atrazine	1.94	520
atrazine	1.95	549
atrazine	1.95	520
atrazine	1.95	255
atrazine	1.95	167
atrazine	1.95	520
atrazine	1.96	520
atrazine	1.96	520
atrazine	1.96	591
atrazine	1.96	591
atrazine	1.97	520
atrazine	1.98	765

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
atrazine	1.98	242
atrazine	1.98	167
atrazine	1.99	520
atrazine	1.99	650
atrazine	1.99	520
atrazine	1.99	203
atrazine	2.00	520
atrazine	2.00	182
atrazine	2.00	520
atrazine	2.00	520
atrazine	2.00	520
atrazine	2.00	373
atrazine	2.00	520
atrazine	2.00	210
atrazine	2.01	255
atrazine	2.01	650
atrazine	2.02	520
atrazine	2.02	263
atrazine	2.02	520
atrazine	2.02	230
atrazine	2.03	520
atrazine	2.03	520
atrazine	2.04	60
atrazine	2.04	520
atrazine	2.04	255
atrazine	2.04	182
atrazine	2.04	65
atrazine	2.05	520
atrazine	2.05	210
atrazine	2.05	230
atrazine	2.06	26
atrazine	2.06	98
atrazine	2.06	650
atrazine	2.06	520
atrazine	2.07	520
atrazine	2.07	524
atrazine	2.07	520
atrazine	2.07	520
atrazine	2.09	203
atrazine	2.09	765
atrazine	2.09	284
atrazine	2.11	255
atrazine	2.13	230
atrazine	2.13	26
atrazine	2.13	520
atrazine	2.15	650
atrazine	2.15	591
atrazine	2.15	263
atrazine	2.15	266
atrazine	2.15	520
atrazine	2.16	203
atrazine	2.16	399
atrazine	2.16	520
atrazine	2.17	525
atrazine	2.19	182
atrazine	2.19	708
atrazine	2.19	203
atrazine	2.19	669
atrazine	2.20	368
atrazine	2.20	661
atrazine	2.21	669
atrazine	2.21	203
atrazine	2.21	722
atrazine	2.21	591
atrazine	2.21	437
atrazine	2.21	292
atrazine	2.22	520
atrazine	2.22	20
atrazine	2.23	203
atrazine	2.23	669
atrazine	2.23	437
atrazine	2.23	708
atrazine	2.24	443
atrazine	2.24	616
atrazine	2.24	205
atrazine	2.24	203
atrazine	2.24	443
atrazine	2.24	194

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
atrazine	2.25	669
atrazine	2.25	520
atrazine	2.26	708
atrazine	2.26	669
atrazine	2.27	203
atrazine	2.27	708
atrazine	2.27	669
atrazine	2.28	203
atrazine	2.28	203
atrazine	2.29	203
atrazine	2.29	765
atrazine	2.30	203
atrazine	2.30	204
atrazine	2.30	506
atrazine	2.31	669
atrazine	2.31	203
atrazine	2.31	708
atrazine	2.32	230
atrazine	2.32	117
atrazine	2.32	203
atrazine	2.33	123
atrazine	2.33	203
atrazine	2.33	204
atrazine	2.33	203
atrazine	2.33	203
atrazine	2.34	524
atrazine	2.34	591
atrazine	2.35	708
atrazine	2.35	669
atrazine	2.35	117
atrazine	2.36	204
atrazine	2.36	669
atrazine	2.36	203
atrazine	2.36	708
atrazine	2.37	20
atrazine	2.37	708
atrazine	2.37	124
atrazine	2.37	117
atrazine	2.37	669
atrazine	2.37	669
atrazine	2.37	263
atrazine	2.37	399
atrazine	2.37	708
atrazine	2.38	650
atrazine	2.39	708
atrazine	2.39	669
atrazine	2.41	203
atrazine	2.42	117
atrazine	2.42	124
atrazine	2.43	117
atrazine	2.43	591
atrazine	2.43	203
atrazine	2.46	203
atrazine	2.47	203
atrazine	2.48	203
atrazine	2.49	203
atrazine	2.50	98
atrazine	2.50	117
atrazine	2.50	124
atrazine	2.55	62
atrazine	2.58	62
atrazine	2.59	650
atrazine	2.60	203
atrazine	2.60	117
atrazine	2.60	98
atrazine	2.62	124
atrazine	2.62	124
atrazine	2.67	124
atrazine	2.68	62
atrazine	2.68	62
atrazine	2.69	399
atrazine	2.73	124
atrazine	2.73	124
atrazine	2.76	765
atrazine	2.77	117
atrazine	2.81	525
atrazine	2.81	124
atrazine	2.86	214

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
atrazine	2.92	124
atrazine	2.92	214
atrazine	3.06	26
atrazine	3.06	292
atrazine	3.08	520
atrazine	3.09	255
atrazine	3.28	124
atrazine	3.64	255
cyanazine	1.75	591
cyanazine	1.85	591
cyanazine	1.93	591
cyanazine	1.96	591
cyanazine	2.04	591
cyanazine	2.14	591
cyanazine	2.23	591
cyanazine	2.26	123
cyanazine	2.30	525
cyanazine	2.35	591
cyanazine	2.40	591
cyanazine	2.44	229
cyanazine	2.57	229
dipropetryn	2.58	315
dipropetryn	2.69	242
dipropetryn	2.81	315
dipropetryn	2.92	315
dipropetryn	2.93	315
dipropetryn	3.06	315
dipropetryn	3.07	722
dipropetryn	3.07	525
dipropetryn	3.43	315
hexazinone	1.31	125
hexazinone	1.37	125
hexazinone	1.42	125
hexazinone	1.43	125
hexazinone	1.46	770
ipazine	2.91	123
ipazine	3.22	525
ipazine	3.39	341
metamitron	1.83	578
metamitron	1.85	721
metamitron	1.85	578
metamitron	1.88	721
metamitron	1.94	578
metamitron	1.95	578
metamitron	1.98	578
metamitron	2.00	588
metamitron	2.03	578
metamitron	2.03	721
metamitron	2.04	721
metamitron	2.07	721
metamitron	2.07	578
metamitron	2.08	578
metamitron	2.08	721
metamitron	2.10	721
metamitron	2.14	578
metamitron	2.17	721
metamitron	2.22	578
metamitron	2.23	721
metamitron	2.24	721
metamitron	2.30	588
metamitron	2.31	721
metamitron	2.34	721
metamitron	2.35	588
metamitron	2.40	721
metamitron	2.40	721
metamitron	2.40	721
metamitron	2.48	721
metamitron	2.53	721
metamitron	2.58	721
metamitron	2.74	588
metamitron	2.93	588
metribuzin	0.46	765
metribuzin	0.84	765
metribuzin	0.94	765
metribuzin	1.01	765
metribuzin	1.01	765
metribuzin	1.24	578
metribuzin	1.32	578

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
metribuzin	1.50	721
metribuzin	1.51	635
metribuzin	1.56	721
metribuzin	1.56	171
metribuzin	1.57	578
metribuzin	1.57	578
metribuzin	1.58	225
metribuzin	1.58	578
metribuzin	1.59	721
metribuzin	1.60	682
metribuzin	1.60	635
metribuzin	1.61	578
metribuzin	1.61	259
metribuzin	1.62	578
metribuzin	1.63	578
metribuzin	1.63	578
metribuzin	1.63	578
metribuzin	1.64	225
metribuzin	1.64	721
metribuzin	1.65	578
metribuzin	1.65	721
metribuzin	1.66	721
metribuzin	1.66	225
metribuzin	1.67	721
metribuzin	1.67	721
metribuzin	1.69	721
metribuzin	1.70	721
metribuzin	1.70	721
metribuzin	1.72	225
metribuzin	1.72	632
metribuzin	1.72	193
metribuzin	1.75	225
metribuzin	1.78	721
metribuzin	1.79	259
metribuzin	1.80	721
metribuzin	1.80	225
metribuzin	1.80	721
metribuzin	1.81	721
metribuzin	1.82	259
metribuzin	1.87	578
metribuzin	1.87	259
metribuzin	1.88	721
metribuzin	1.88	257
metribuzin	1.89	259
metribuzin	1.90	259
metribuzin	1.90	259
metribuzin	1.94	721
metribuzin	1.94	225
metribuzin	1.94	721
metribuzin	1.94	259
metribuzin	1.98	525
metribuzin	1.98	225
metribuzin	1.99	780
metribuzin	2.00	259
metribuzin	2.02	259
metribuzin	2.03	259
metribuzin	2.05	259
metribuzin	2.14	259
metribuzin	2.14	259
metribuzin	2.18	780
metribuzin	2.24	259
metribuzin	2.29	780
metribuzin	2.30	780
metribuzin	2.31	780
metribuzin	2.42	780
prometon	1.49	520
prometon	1.62	520
prometon	1.67	520
prometon	1.67	520
prometon	1.73	520
prometon	1.73	24
prometon	1.74	520
prometon	1.76	520
prometon	1.77	520
prometon	1.79	520
prometon	1.82	520
prometon	1.83	520
prometon	1.85	203

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
prometon	1.85	520
prometon	1.85	520
prometon	1.87	203
prometon	1.87	520
prometon	1.87	520
prometon	1.87	203
prometon	1.88	520
prometon	1.88	520
prometon	1.88	520
prometon	1.89	520
prometon	1.90	520
prometon	1.90	520
prometon	1.92	520
prometon	1.92	204
prometon	1.94	203
prometon	1.94	520
prometon	1.97	520
prometon	1.97	520
prometon	1.97	520
prometon	2.00	520
prometon	2.00	520
prometon	2.00	520
prometon	2.02	520
prometon	2.03	520
prometon	2.03	520
prometon	2.04	520
prometon	2.06	520
prometon	2.09	520
prometon	2.14	203
prometon	2.30	203
prometon	2.30	203
prometon	2.31	242
prometon	2.31	203
prometon	2.40	204
prometon	2.41	203
prometon	2.43	203
prometon	2.47	204
prometon	2.48	616
prometon	2.48	203
prometon	2.52	203
prometon	2.54	525
prometon	2.56	203
prometon	2.58	203
prometon	2.58	203
prometon	2.58	203
prometon	2.61	203
prometon	2.62	203
prometon	2.72	722
prometon	2.73	203
prometon	2.77	203
prometon	2.78	204
prometon	2.88	203
prometon	3.03	203
prometon	3.12	203
prometon	3.15	520
prometon	3.26	203
prometon	3.58	203
prometryn	1.51	242
prometryn	1.69	253
prometryn	1.82	253
prometryn	1.84	24
prometryn	1.95	253
prometryn	2.05	253
prometryn	2.06	568
prometryn	2.12	204
prometryn	2.17	101
prometryn	2.26	520
prometryn	2.27	238
prometryn	2.27	520
prometryn	2.28	315
prometryn	2.30	203
prometryn	2.30	203
prometryn	2.32	520
prometryn	2.32	203
prometryn	2.33	520
prometryn	2.36	520
prometryn	2.38	520
prometryn	2.38	203

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
prometryn	2.39	446
prometryn	2.39	568
prometryn	2.40	520
prometryn	2.41	520
prometryn	2.41	203
prometryn	2.42	520
prometryn	2.43	520
prometryn	2.43	288
prometryn	2.44	520
prometryn	2.45	520
prometryn	2.46	520
prometryn	2.47	203
prometryn	2.47	288
prometryn	2.48	520
prometryn	2.48	520
prometryn	2.48	520
prometryn	2.48	520
prometryn	2.48	238
prometryn	2.49	520
prometryn	2.50	520
prometryn	2.50	520
prometryn	2.50	520
prometryn	2.51	288
prometryn	2.51	288
prometryn	2.51	288
prometryn	2.52	520
prometryn	2.52	520
prometryn	2.52	520
prometryn	2.54	238
prometryn	2.54	520
prometryn	2.54	203
prometryn	2.55	203
prometryn	2.56	520
prometryn	2.58	76
prometryn	2.58	568
prometryn	2.59	203
prometryn	2.60	520
prometryn	2.60	76
prometryn	2.61	520
prometryn	2.61	644
prometryn	2.61	520
prometryn	2.62	520
prometryn	2.64	203
prometryn	2.64	446
prometryn	2.65	520
prometryn	2.67	315
prometryn	2.67	238
prometryn	2.67	76
prometryn	2.67	315
prometryn	2.69	446
prometryn	2.70	203
prometryn	2.70	203
prometryn	2.70	568
prometryn	2.70	203
prometryn	2.71	759
prometryn	2.71	616
prometryn	2.72	520
prometryn	2.72	203
prometryn	2.73	238
prometryn	2.74	520
prometryn	2.75	446
prometryn	2.76	644
prometryn	2.77	204
prometryn	2.77	412
prometryn	2.78	203
prometryn	2.78	203
prometryn	2.78	288
prometryn	2.79	759
prometryn	2.79	722
prometryn	2.79	315
prometryn	2.79	520
prometryn	2.79	203
prometryn	2.79	238
prometryn	2.80	203
prometryn	2.81	76
prometryn	2.84	204
prometryn	2.84	520
prometryn	2.89	76

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
prometryn	2.90	644
prometryn	2.91	705
prometryn	2.91	525
prometryn	2.91	759
prometryn	2.91	204
prometryn	2.92	203
prometryn	2.94	203
prometryn	2.95	446
prometryn	2.96	203
prometryn	2.97	644
prometryn	2.97	705
prometryn	3.02	203
prometryn	3.03	705
prometryn	3.04	94
prometryn	3.13	203
prometryn	3.20	644
prometryn	3.24	203
prometryn	3.37	315
prometryn	3.40	238
prometryn	3.48	203
prometryn	3.52	520
prometryn	3.55	94
prometryn	3.57	76
prometryn	3.57	644
prometryn	3.73	705
prometryn	3.89	705
propazine	1.44	647
propazine	1.46	203
propazine	1.61	647
propazine	1.72	204
propazine	1.80	520
propazine	1.82	647
propazine	1.90	520
propazine	1.92	242
propazine	1.94	520
propazine	1.94	203
propazine	1.96	288
propazine	2.00	203
propazine	2.00	203
propazine	2.00	520
propazine	2.01	520
propazine	2.01	288
propazine	2.01	520
propazine	2.01	203
propazine	2.04	167
propazine	2.05	520
propazine	2.05	203
propazine	2.06	203
propazine	2.08	203
propazine	2.09	203
propazine	2.10	520
propazine	2.10	520
propazine	2.10	520
propazine	2.11	520
propazine	2.11	203
propazine	2.12	520
propazine	2.12	520
propazine	2.13	203
propazine	2.13	203
propazine	2.13	520
propazine	2.14	520
propazine	2.15	520
propazine	2.16	520
propazine	2.16	288
propazine	2.16	167
propazine	2.16	204
propazine	2.17	520
propazine	2.17	520
propazine	2.18	616
propazine	2.18	520
propazine	2.19	203
propazine	2.19	203
propazine	2.19	520
propazine	2.19	722
propazine	2.19	520
propazine	2.20	525
propazine	2.20	520
propazine	2.20	203

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
propazine	2.21	520
propazine	2.21	203
propazine	2.21	520
propazine	2.22	520
propazine	2.22	520
propazine	2.22	520
propazine	2.23	288
propazine	2.23	204
propazine	2.24	203
propazine	2.25	288
propazine	2.26	520
propazine	2.26	520
propazine	2.26	520
propazine	2.27	520
propazine	2.27	520
propazine	2.28	520
propazine	2.28	203
propazine	2.28	288
propazine	2.29	520
propazine	2.30	204
propazine	2.32	203
propazine	2.36	203
propazine	2.38	203
propazine	2.38	203
propazine	2.40	203
propazine	2.41	203
propazine	2.41	203
propazine	2.56	123
propazine	3.04	520
secbumeton (gs 14254)	2.10	255
secbumeton (gs 14254)	2.11	525
secbumeton (gs 14254)	2.13	255
secbumeton (gs 14254)	2.15	255
secbumeton (gs 14254)	2.18	255
secbumeton (gs 14254)	2.48	255
secbumeton (gs 14254)	2.54	746
secbumeton (gs 14254)	2.77	255
secbumeton (gs 14254)	2.82	255
secbumeton (gs 14254)	3.11	255
secbumeton (gs 14254)	3.39	255
secbumeton (gs 14254)	3.84	255
simazine	1.25	291
simazine	1.42	291
simazine	1.46	711
simazine	1.48	291
simazine	1.50	291
simazine	1.50	711
simazine	1.52	206
simazine	1.55	645
simazine	1.56	251
simazine	1.56	206
simazine	1.56	251
simazine	1.56	251
simazine	1.57	264
simazine	1.58	711
simazine	1.59	264
simazine	1.60	711
simazine	1.61	291
simazine	1.62	711
simazine	1.62	206
simazine	1.63	206
simazine	1.63	264
simazine	1.64	206
simazine	1.65	647
simazine	1.65	264
simazine	1.66	264
simazine	1.67	264
simazine	1.67	206
simazine	1.67	206
simazine	1.68	166
simazine	1.68	264
simazine	1.68	206
simazine	1.68	264
simazine	1.69	264
simazine	1.70	264
simazine	1.70	647
simazine	1.70	206
simazine	1.70	682

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
simazine	1.70	264
simazine	1.70	264
simazine	1.70	167
simazine	1.71	206
simazine	1.71	264
simazine	1.72	206
simazine	1.72	264
simazine	1.72	264
simazine	1.72	206
simazine	1.73	711
simazine	1.73	206
simazine	1.74	206
simazine	1.74	202
simazine	1.75	206
simazine	1.75	206
simazine	1.76	206
simazine	1.76	264
simazine	1.76	206
simazine	1.77	206
simazine	1.77	251
simazine	1.77	206
simazine	1.77	251
simazine	1.77	206
simazine	1.78	291
simazine	1.78	202
simazine	1.78	320
simazine	1.79	711
simazine	1.79	24
simazine	1.80	202
simazine	1.80	251
simazine	1.81	206
simazine	1.81	291
simazine	1.82	694
simazine	1.82	251
simazine	1.82	291
simazine	1.82	658
simazine	1.82	264
simazine	1.82	206
simazine	1.83	202
simazine	1.83	711
simazine	1.83	202
simazine	1.83	206
simazine	1.83	251
simazine	1.83	251
simazine	1.83	206
simazine	1.83	645
simazine	1.84	206
simazine	1.84	206
simazine	1.84	711
simazine	1.84	206
simazine	1.85	206
simazine	1.85	264
simazine	1.85	206
simazine	1.85	711
simazine	1.86	206
simazine	1.86	264
simazine	1.87	711
simazine	1.88	206
simazine	1.88	202
simazine	1.89	251
simazine	1.90	206
simazine	1.90	694
simazine	1.91	206
simazine	1.91	202
simazine	1.91	251
simazine	1.91	206
simazine	1.91	202
simazine	1.92	658
simazine	1.92	647
simazine	1.92	289
simazine	1.92	206
simazine	1.92	251
simazine	1.92	204
simazine	1.93	264
simazine	1.93	251
simazine	1.93	167
simazine	1.93	202
simazine	1.94	251

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
simazine	1.94	206
simazine	1.94	658
simazine	1.94	658
simazine	1.95	711
simazine	1.95	711
simazine	1.95	167
simazine	1.95	206
simazine	1.96	251
simazine	1.96	206
simazine	1.96	206
simazine	1.97	658
simazine	1.97	658
simazine	1.97	682
simazine	1.97	251
simazine	1.97	251
simazine	1.97	264
simazine	2.00	206
simazine	2.00	251
simazine	2.00	251
simazine	2.00	206
simazine	2.00	645
simazine	2.01	206
simazine	2.01	206
simazine	2.01	251
simazine	2.01	711
simazine	2.02	206
simazine	2.02	658
simazine	2.02	202
simazine	2.03	206
simazine	2.03	711
simazine	2.04	202
simazine	2.04	206
simazine	2.04	251
simazine	2.05	251
simazine	2.06	251
simazine	2.06	711
simazine	2.06	645
simazine	2.06	206
simazine	2.07	206
simazine	2.07	206
simazine	2.07	658
simazine	2.09	203
simazine	2.09	202
simazine	2.09	284
simazine	2.10	206
simazine	2.11	206
simazine	2.11	206
simazine	2.12	206
simazine	2.12	202
simazine	2.13	320
simazine	2.13	525
simazine	2.13	658
simazine	2.13	202
simazine	2.14	206
simazine	2.14	251
simazine	2.14	722
simazine	2.15	284
simazine	2.15	661
simazine	2.15	242
simazine	2.17	658
simazine	2.17	251
simazine	2.17	206
simazine	2.18	658
simazine	2.18	206
simazine	2.20	206
simazine	2.20	711
simazine	2.22	203
simazine	2.23	203
simazine	2.24	203
simazine	2.25	203
simazine	2.26	202
simazine	2.26	206
simazine	2.27	711
simazine	2.27	204
simazine	2.28	203
simazine	2.28	251
simazine	2.30	203
simazine	2.30	284

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
simazine	2.33	206
simazine	2.33	123
simazine	2.33	537
simazine	2.34	658
simazine	2.34	204
simazine	2.34	251
simazine	2.36	206
simazine	2.36	206
simazine	2.37	203
simazine	2.37	206
simazine	2.37	284
simazine	2.39	206
simazine	2.39	203
simazine	2.41	202
simazine	2.41	645
simazine	2.41	251
simazine	2.41	251
simazine	2.42	251
simazine	2.43	203
simazine	2.43	203
simazine	2.43	203
simazine	2.43	203
simazine	2.44	203
simazine	2.45	117
simazine	2.46	203
simazine	2.46	203
simazine	2.47	203
simazine	2.48	203
simazine	2.48	203
simazine	2.49	203
simazine	2.49	251
simazine	2.52	658
simazine	2.56	203
simazine	2.59	694
simazine	2.63	204
simazine	2.64	203
simazine	2.67	203
simazine	2.68	203
simazine	2.71	658
simazine	2.71	202
simazine	2.71	203
simazine	2.83	251
simazine	3.18	206
simazine	3.30	62
simazine	3.33	62
simazine	3.35	62
simazine	3.35	62
simazine	2.46	1001
simazine	1.74	1006
simazine	1.89	1007
simazine	1.72	1008
simazine	1.79	1008
simazine	1.94	1008
simazine	2.00	1008
simazine	2.11	1008
simazine	2.22	1008
simazine	2.35	1008
simazine	2.36	1008
simazine	2.68	1008
simazine	2.14	1009
simazine	2.27	1009
simazine	2.27	1009
simazine	2.30	1009
simazine	2.46	1009
simazine	2.02	1010
simazine	2.19	1010
simazine	2.38	1010
simazine	3.11	1010
simazine	2.33	1015
simazine	2.51	1015
simazine	2.81	1015
simazine	2.95	1015
terbutryn	2.63	255
terbutryn	2.65	255
terbutryn	2.69	650
terbutryn	2.70	255
terbutryn	2.77	255
terbutryn	2.79	255

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
terbutryn	2.85	525
terbutryn	2.91	650
terbutryn	3.04	255
terbutryn	3.07	255
terbutryn	3.11	293
terbutryn	3.28	650
terbutryn	3.34	255
terbutryn	3.52	255
terbutryn	3.58	650
terbutryn	3.77	650
terbutryn	3.95	650
terbutryn	4.33	255
terbutylazine	2.24	167
terbutylazine	2.65	167
terbutylazine	2.65	167
trietazine	2.74	123
trietazine	2.78	525
TRIAZOLES		
benzyltriazole cl cl	2.33	789
benzyltriazole h c4h9	2.16	789
benzyltriazole h cf3	1.77	789
benzyltriazole h ch3o	1.80	789
benzyltriazole h cl	1.98	789
benzyltriazole h f	1.69	789
benzyltriazole pp450	1.88	789
buthidazole	2.01	235
buthidazole	2.37	237
imazalil	3.62	799
imazalil	3.84	799
methazole	3.42	525
methazole	3.66	244
methazole	3.90	244
nia 23486	1.48	762
nia 23486	1.58	762
nia 23486	1.64	762
nia 23486	1.68	762
nia 23486	1.72	762
nia 23486	1.76	762
nia 23486	1.83	762
nia 23486	1.84	762
oxadiazon	3.51	525
propiconazole	3.21	706
propiconazole	3.39	706
propiconazole	3.47	706
propiconazole	4.20	706
propiconazole	4.21	706
thiabendazole	3.03	554
thiabendazole	3.19	554
thiabendazole	3.24	525
thiabendazole	3.24	554
thiabendazole	3.28	554
thiabendazole	3.33	554
thiabendazole	3.40	554
thiabendazole	3.43	554
thiabendazole	3.47	554
thiabendazole	3.49	554
thiabendazole	3.56	554
thiabendazole	3.56	554
thiabendazole	3.57	554
triadimefon	2.71	789
tricyclazole	3.02	412
tricyclazole	3.07	412
tricyclazole	3.10	412
tricyclazole	3.10	412
tricyclazole	3.21	412
ACIDS		
2,3,6-tba	0.25	782
2,3,6-tba	1.12	782
2,3,6-tba	1.13	782
2,4,5-t	1.13	516
2,4,5-t	1.37	516
2,4,5-t	1.56	516
2,4,5-t	1.59	32
2,4,5-t	1.62	516

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
2,4,5–t	1.64	516
2,4,5–t	1.72	608
2,4,5–t	1.73	516
2,4,5–t	1.76	516
2,4,5–t	1.77	1030
2,4,5–t	1.78	113
2,4,5–t	1.82	32
2,4,5–t	1.86	113
2,4,5–t	1.94	1030
2,4,5–t	1.95	113
2,4,5–t	1.96	85
2,4,5–t	1.97	32
2,4,5–t	2.03	113
2,4,5–t	2.06	40
2,4,5–t	2.06	44
2,4,5–t	2.07	783
2,4,5–t	2.08	113
2,4,5–t	2.09	783
2,4,5–t	2.09	32
2,4,5–t	2.12	113
2,4,5–t	2.13	393
2,4,5–t	2.30	44
2,4,5–t	2.34	110
2,4,5–t	2.57	50
2,4,5–t	2.57	44
2,4,5–t	2.63	111
2,4,5–t	2.63	1030
2,4,5–t	2.85	516
2,4–d	0.67	104
2,4–d	0.73	272
2,4–d	0.94	272
2,4–d	0.97	104
2,4–d	0.98	1030
2,4–d	1.03	272
2,4–d	1.10	272
2,4–d	1.12	272
2,4–d	1.14	104
2,4–d	1.16	104
2,4–d	1.16	272
2,4–d	1.19	104
2,4–d	1.21	24
2,4–d	1.21	516
2,4–d	1.22	113
2,4–d	1.24	516
2,4–d	1.25	1030
2,4–d	1.29	722
2,4–d	1.30	608
2,4–d	1.30	113
2,4–d	1.33	272
2,4–d	1.35	516
2,4–d	1.38	113
2,4–d	1.40	516
2,4–d	1.40	516
2,4–d	1.41	113
2,4–d	1.50	113
2,4–d	1.51	113
2,4–d	1.51	616
2,4–d	1.56	516
2,4–d	1.66	46
2,4–d	1.72	516
2,4–d	1.73	106
2,4–d	1.76	406
2,4–d	1.76	106
2,4–d	1.77	106
2,4–d	1.77	106
2,4–d	1.78	361
2,4–d	1.78	576
2,4–d	1.80	106
2,4–d	1.82	106
2,4–d	1.83	106
2,4–d	2.01	516
2,4–d	2.04	46
2,4–d	2.11	106
2,4–d	2.18	78
2,4–d	2.23	106
2,4–d	2.29	1030
2,4–d	2.29	106
2,4–d	2.40	106

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
2,4-d	2.42	516
2,4-d	2.48	106
2,4-d	2.52	106
2,4-d	2.74	106
2,4-d	2.75	106
2,4-d	2.77	106
2,4-d	2.78	106
2,4-d	2.79	106
2,4-d-amine	0.90	334
2,4-d-amine	1.08	334
2,4-d-amine	1.21	334
2,4-d-amine	1.35	334
2,4-d-amine	1.86	182
2,4-d-amine	1.87	60
2,4-d-amine	2.04	722
2,4-d-amine	2.08	182
2,4-d-amine	2.08	60
2,4-d-amine	2.13	182
3,6-dichloropicolinic acid	0.30	525
anthracene-9-carboxylic acid	2.42	521
anthracene-9-carboxylic acid	2.43	521
anthracene-9-carboxylic acid	2.45	521
anthracene-9-carboxylic acid	2.52	521
anthracene-9-carboxylic acid	2.54	521
anthracene-9-carboxylic acid	2.54	521
anthracene-9-carboxylic acid	2.62	521
anthracene-9-carboxylic acid	2.63	521
anthracene-9-carboxylic acid	2.64	521
anthracene-9-carboxylic acid	2.70	521
anthracene-9-carboxylic acid	2.71	746
anthracene-9-carboxylic acid	2.88	521
anthracene-9-carboxylic acid	3.01	521
anthracene-9-carboxylic acid	3.09	521
anthracene-9-carboxylic acid	3.32	521
anthracene-9-carboxylic acid	3.41	521
bentazon	1.65	217
bentazon	2.04	217
bentazon	1.58	1048
bentazon	1.12	1048
bentazon	1.68	1048
bentazon	1.04	1049
chloramben (amiben)	0.68	374
chloramben (amiben)	1.00	374
chloramben (amiben)	1.11	616
chloramben (amiben)	1.24	374
chloramben (amiben)	1.25	209
chloramben (amiben)	1.25	374
chloramben (amiben)	1.31	374
chloramben (amiben)	1.32	525
chloramben (amiben)	1.48	209
chloramben (amiben)	1.59	374
chloramben (amiben)	1.60	209
chloramben (amiben)	1.60	209
chloramben (amiben)	1.76	371
chloramben (amiben)	2.28	722
chloramben (amiben)	2.66	209
chloramben (methyl esther)	2.40	209
chloramben (methyl esther)	2.50	371
chloramben (methyl esther)	2.53	209
chloramben (methyl esther)	2.56	371
chloramben (methyl esther)	2.66	209
chloramben (methyl esther)	2.68	371
chloramben (methyl esther)	2.71	525
chloramben (methyl esther)	2.73	209
chloramben (methyl esther)	2.92	209
chloramben (methyl esther)	2.94	371
chloramben (methyl esther)	3.54	209
chloropicolinic acid	0.95	525
dalapon	0.40	694
dicamba	−0.40	525
dicamba	0.10	228
dicamba	0.11	334
dicamba	0.12	228
dicamba	0.26	726
dicamba	0.26	334
dicamba	0.27	334
dicamba	0.34	722
dicamba	0.46	228

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
dicamba	0.58	369
dicamba	0.69	228
dicamba	0.76	228
dinoseb (dnbp)	2.09	525
dinoseb	1.86	1050
dinoseb	2.11	1050
dinoseb	2.22	1050
dinoseb	1.71	1050
dinoseb	3.46	1051
dinoseb	2.16	1051
dinoseb	2.48	1051
DNOC	2.25	1046
DNOC	2.40	1046
DNOC	2.38	1046
DNOC	2.35	1046
DNOC	2.19	1046
DNOC	2.78	1046
DNOC	2.39	1046
DNOC	2.00	1046
DNOC	2.20	1046
DNOC	2.34	1046
DNOC	2.80	1046
DNOC	1.95	1046
endothall	2.04	745
endothall	2.14	745
fenac	0.78	745
fenac	2.82	745
imazaquin	1.23	737
imazaquin	1.24	737
imazaquin	1.35	737
imazaquin	1.56	375
mcpa	1.70	741
mcpa	1.71	783
mcpa	1.71	741
mcpa	1.76	783
mcpa	1.77	741
mecoprop	0.92	1045
mecoprop	1.12	1045
mecoprop	0.72	1045
picloram	0.83	224
picloram	0.85	231
picloram	0.91	658
picloram	0.91	215
picloram	0.92	215
picloram	0.93	215
picloram	0.94	215
picloram	0.98	215
picloram	1.00	215
picloram	1.02	215
picloram	1.03	658
picloram	1.07	516
picloram	1.13	224
picloram	1.14	231
picloram	1.14	516
picloram	1.16	674
picloram	1.18	231
picloram	1.19	224
picloram	1.19	658
picloram	1.21	658
picloram	1.23	525
picloram	1.24	516
picloram	1.26	195
picloram	1.26	23
picloram	1.26	623
picloram	1.26	101
picloram	1.29	658
picloram	1.33	516
picloram	1.35	31
picloram	1.35	516
picloram	1.36	516
picloram	1.38	224
picloram	1.39	658
picloram	1.40	31
picloram	1.41	722
picloram	1.43	31
picloram	1.52	516
picloram	1.52	658
picloram	1.53	658

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
picloram	1.54	516
picloram	1.57	658
picloram	1.60	658
picloram	1.61	28
picloram	1.62	28
picloram	1.63	224
picloram	1.64	658
picloram	1.82	658
picloram	1.94	658
picloram	2.00	28
picloram	2.03	224
picloram	2.14	231
picloram	2.20	224
picloram	2.30	316
picloram	2.47	231
picloram	2.54	224
picloram	2.66	231
picloram	2.68	516
picloram	2.74	658
picloram	2.74	231
silvex (fenoprop)	2.59	372
silvex (fenoprop)	3.41	608
silvex (fenoprop)	3.43	372
silvex (fenoprop)	3.70	372
sulfometuron methyl	0.84	765
sulfometuron methyl	0.99	765
sulfometuron methyl	1.49	765
sulfometuron methyl	1.52	765
sulfometuron methyl	1.78	323
sulfometuron methyl	1.85	323
sulfometuron methyl	1.94	323
sulfometuron methyl	2.07	765
sulfometuron methyl	2.09	323
POLYAROMATIC HYDROCARBONS		
1 – naphthol	2.52	47
1 – naphthol	2.55	47
1 – naphthol	2.65	47
1 – naphthol	2.72	47
1 – naphthol	2.77	47
1 – naphthol	2.77	47
1 – naphthol	2.84	47
1 – naphthol	2.89	47
1 – naphthol	2.92	47
1 – naphthol	2.96	47
1 – naphthol	3.22	47
1 – naphthol	3.24	47
1 – naphthol	3.32	47
1 – naphthol	3.43	47
1 – naphthol	3.57	746
1 – naphthol	3.62	47
1 – naphthol	4.19	47
13h – dibenzo (a,i) carbazole	5.77	521
13h – dibenzo (a,i) carbazole	5.81	521
13h – dibenzo (a,i) carbazole	5.95	521
13h – dibenzo (a,i) carbazole	5.96	521
13h – dibenzo (a,i) carbazole	6.02	521
13h – dibenzo (a,i) carbazole	6.03	521
13h – dibenzo (a,i) carbazole	6.08	521
13h – dibenzo (a,i) carbazole	6.10	521
13h – dibenzo (a,i) carbazole	6.15	521
13h – dibenzo (a,i) carbazole	6.16	521
13h – dibenzo (a,i) carbazole	6.23	521
13h – dibenzo (a,i) carbazole	6.24	521
13h – dibenzo (a,i) carbazole	6.31	521
13h – dibenzo (a,i) carbazole	6.33	521
13h – dibenzo (a,i) carbazole	6.39	521
2,2' – biquinoline	3.85	521
2,2' – biquinoline	3.86	521
2,2' – biquinoline	3.94	521
2,2' – biquinoline	4.01	521
2,2' – biquinoline	4.03	521
2,2' – biquinoline	4.03	521
2,2' – biquinoline	4.06	521
2,2' – biquinoline	4.09	521
2,2' – biquinoline	4.15	521
2,2' – biquinoline	4.21	521

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
2,2' – biquinoline	4.26	521
2,2' – biquinoline	4.38	521
2,2' – biquinoline	4.58	521
2,2' – biquinoline	4.74	521
2 – aminoanthracene	4.13	521
2 – aminoanthracene	4.20	521
2 – aminoanthracene	4.42	521
2 – aminoanthracene	4.45	521
2 – aminoanthracene	4.45	521
2 – aminoanthracene	4.48	521
2 – aminoanthracene	4.48	521
2 – aminoanthracene	4.55	521
2 – aminoanthracene	4.56	521
2 – aminoanthracene	4.57	521
2 – aminoanthracene	4.62	521
2 – aminoanthracene	4.63	521
2 – aminoanthracene	4.67	521
2 – aminoanthracene	4.72	521
2 – aminoanthracene	4.97	521
2 – methylnaphtalene	3.93	404
2 – methylnaphtalene	4.17	321
3 – methylcholanthrene	5.56	394
3 – methylcholanthrene	5.86	394
3 – methylcholanthrene	6.09	437
3 – methylcholanthrene	6.10	394
3 – methylcholanthrene	6.10	394
3 – methylcholanthrene	6.10	394
3 – methylcholanthrene	6.12	394
3 – methylcholanthrene	6.16	394
3 – methylcholanthrene	6.18	394
3 – methylcholanthrene	6.34	394
3 – methylcholanthrene	6.39	394
3 – methylcholanthrene	6.39	394
3 – methylcholanthrene	6.40	394
3 – methylcholanthrene	6.50	394
3 – methylcholanthrene	6.80	394
6 – aminochrysene	4.83	521
6 – aminochrysene	4.94	521
6 – aminochrysene	5.06	521
6 – aminochrysene	5.13	521
6 – aminochrysene	5.14	521
6 – aminochrysene	5.16	521
6 – aminochrysene	5.16	521
6 – aminochrysene	5.18	521
6 – aminochrysene	5.18	521
6 – aminochrysene	5.22	521
6 – aminochrysene	5.24	521
6 – aminochrysene	5.28	521
6 – aminochrysene	5.33	521
6 – aminochrysene	5.58	521
6 – aminochrysene	5.79	521
7,12 – dimethylbenz (a) anthracene	5.07	521
7,12 – dimethylbenz (a) anthracene	5.09	521
7,12 – dimethylbenz (a) anthracene	5.11	521
7,12 – dimethylbenz (a) anthracene	5.21	521
7,12 – dimethylbenz (a) anthracene	5.27	521
7,12 – dimethylbenz (a) anthracene	5.29	521
7,12 – dimethylbenz (a) anthracene	5.35	437
7,12 – dimethylbenz (a) anthracene	5.36	521
7,12 – dimethylbenz (a) anthracene	5.40	521
7,12 – dimethylbenz (a) anthracene	5.45	521
7,12 – dimethylbenz (a) anthracene	5.46	521
7,12 – dimethylbenz (a) anthracene	5.47	521
7,12 – dimethylbenz (a) anthracene	5.60	521
7,12 – dimethylbenz (a) anthracene	5.61	521
7,12 – dimethylbenz (a) anthracene	5.73	734
7,12 – dimethylbenz (a) anthracene	5.97	521
9 – methylanthracene	4.71	437
9 – methylanthracene	4.81	181
9 – methylanthracene	4.81	404
9 – methylanthracene	5.05	321
acridine	3.74	92
acridine	4.04	92
acridine	4.08	92
acridine	4.09	92
acridine	4.11	521
acridine	4.16	92
acridine	4.17	92

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
acridine	4.18	92
acridine	4.18	92
acridine	4.21	92
acridine	4.24	92
acridine	4.26	92
acridine	4.34	92
acridine	4.46	746
acridine	4.47	92
acridine	4.49	92
anthracene	4.20	437
anthracene	4.24	757
anthracene	4.41	181
anthracene	4.66	321
benzo(a)pyrene	4.89	431
benzo(a)pyrene	5.68	431
benz(a)anthracene	5.92	431
dibenz (a,h) anthracene	5.75	521
dibenz (a,h) anthracene	5.91	521
dibenz (a,h) anthracene	5.91	521
dibenz (a,h) anthracene	6.07	521
dibenz (a,h) anthracene	6.22	521
dibenz (a,h) anthracene	6.23	521
dibenz (a,h) anthracene	6.23	521
dibenz (a,h) anthracene	6.31	743
dibenz (a,h) anthracene	6.36	521
dibenz (a,h) anthracene	6.38	521
dibenz (a,h) anthracene	6.42	521
dibenz (a,h) anthracene	6.43	521
dibenz (a,h) anthracene	6.43	521
dibenz (a,h) anthracene	6.47	521
dibenz (a,h) anthracene	6.48	521
dibenz (a,h) anthracene	6.49	521
dibenzothiophene	3.72	521
dibenzothiophene	3.80	521
dibenzothiophene	3.87	521
dibenzothiophene	3.89	521
dibenzothiophene	3.93	521
dibenzothiophene	3.94	521
dibenzothiophene	3.96	521
dibenzothiophene	3.99	521
dibenzothiophene	3.99	521
dibenzothiophene	4.02	521
dibenzothiophene	4.02	521
dibenzothiophene	4.17	521
dibenzothiophene	4.21	521
dibenzothiophene	4.28	521
naphtalene	2.62	320
naphtalene	2.63	243
naphtalene	2.78	243
naphtalene	2.94	437
naphtalene	3.11	404
naphtalene	3.35	321
naphtalene	3.36	181
phenanthrene	4.08	437
phenanthrene	4.36	404
phenanthrene	4.60	321
pyrene	4.04	181
pyrene	4.08	181
pyrene	4.51	181
pyrene	4.64	521
pyrene	4.68	521
pyrene	4.70	521
pyrene	4.71	521
pyrene	4.75	521
pyrene	4.76	521
pyrene	4.77	521
pyrene	4.80	731
pyrene	4.80	521
pyrene	4.81	521
pyrene	4.83	521
pyrene	4.83	521
pyrene	4.83	437
pyrene	4.88	181
pyrene	4.88	521
pyrene	4.92	521
pyrene	4.92	404
pyrene	4.93	521
pyrene	4.96	181

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
pyrene	5.04	181
pyrene	5.04	181
pyrene	5.05	181
pyrene	5.06	181
pyrene	5.06	181
pyrene	5.07	181
pyrene	5.10	181
pyrene	5.10	181
pyrene	5.11	181
pyrene	5.16	321
pyrene	5.18	387
quinoline	1.92	801
quinoline	1.93	400
quinoline	2.17	400
quinoline	2.29	400
quinoline	2.92	400
quinoline	3.09	400
quinoline	3.12	801
quinoline	3.14	400
quinoline	3.31	400
quinoline	3.33	801
quinoline	3.38	400
quinoline	3.42	400
tetracene (2,3-benzanthracene)	5.81	404
tetracene (2,3-benzanthracene)	6.05	321
NONAROMATIC HALOGENATED HYDROCARBONS		
1,1,1 - trichloroethane	0.97	435
1,1,1 - trichloroethane	1.01	435
1,1,1 - trichloroethane	2.11	746
1,1,1 - trichloroethane	2.25	595
1,1,1 - trichloroethane	2.26	321
1,1,1 - trichloroethane	2.30	521
1,1,2,2 - tetrachloroethane	1.90	595
1,1,2,2 - tetrachloroethane	1.94	521
1,1,2 - trichloroethane	1.88	109
1,1,2 - trichloroethane	2.11	746
1,2 - dibromo - 3 - chloropropane (dbcp)	1.60	728
1,2 - dibromo - 3 - chloropropane (dbcp)	1.94	676
1,2 - dibromo - 3 - chloropropane (dbcp)	1.99	676
1,2 - dibromo - 3 - chloropropane (dbcp)	2.01	676
1,2 - dibromo - 3 - chloropropane (dbcp)	2.11	295
1,2 - dibromo - 3 - chloropropane (dbcp)	2.11	525
1,2 - dibromo - 3 - chloropropane (dbcp)	2.12	566
1,2 - dibromo - 3 - chloropropane (dbcp)	2.16	521
1,2 - dibromo - 3 - chloropropane (dbcp)	2.18	109
1,2 - dibromo - 3 - chloropropane (dbcp)	2.35	321
1,2 - dibromoethene	1.89	321
1,2 - dichloroethane	1.51	595
1,2 - dichloroethane	1.52	321
1,2 - dichloroethane	1.56	521
1,2 - dichloroethane	1.88	109
1,2 - dichloropropane	1.66	521
1,2 - dichloropropane	1.67	595
1,2 - dichloropropane	1.71	521
1,3 - dichloropropene (telone)	1.36	525
1,3 - dichloropropene (telone)	1.38	418
1,3 - dichloropropene (telone)	1.41	525
1,3 - dichloropropene (telone)	1.66	321
1,3 - dichloropropene (telone)	1.83	576
bis (2 - chloroethyl) ether	1.88	109
bromoform	2.10	621
carbon tetrachloride	1.10	435
carbon tetrachloride	1.15	435
carbon tetrachloride	1.30	435
carbon tetrachloride	1.38	726
carbon tetrachloride	1.82	726
carbon tetrachloride	1.85	529
carbon tetrachloride	2.09	321
chloroform (trichloromethane)	1.65	529
chloroform (trichloromethane)	1.88	109
chloroform (trichloromethane)	1.89	321
dichloromethane	1.44	529
dichloromethane	1.68	321
ethylene dibromide (edb;1,2-dibromoethane)	1.06	573
ethylene dibromide (edb;1,2-dibromoethane)	1.23	573
ethylene dibromide (edb;1,2-dibromoethane)	1.24	574

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
ethylene dibromide (edb;1,2-dibromoethane)	1.51	566
ethylene dibromide (edb;1,2-dibromoethane)	1.60	574
ethylene dibromide (edb;1,2-dibromoethane)	1.61	574
ethylene dibromide (edb;1,2-dibromoethane)	1.64	661
ethylene dibromide (edb;1,2-dibromoethane)	1.79	395
ethylene dibromide (edb;1,2-dibromoethane)	1.80	321
ethylene dibromide (edb;1,2-dibromoethane)	1.84	521
hexachloroethane	3.61	733
tetrachloroethylene	2.10	435
tetrachloroethylene	2.14	435
tetrachloroethylene	2.18	435
tetrachloroethylene	2.26	435
tetrachloroethylene	2.30	435
tetrachloroethylene	2.32	396
tetrachloroethylene	2.35	734
tetrachloroethylene	2.56	437
tetrachloroethylene	2.57	396
tetrachloroethylene	2.67	734
tetrachloroethylene	2.78	734
trichloroethylene	1.88	435
trichloroethylene	1.91	435
trichloroethylene	1.91	435
trichloroethylene	1.94	726
trichloroethylene	2.00	435
trichloroethylene	2.02	109
trichloroethylene	2.07	621
trichloroethylene	2.07	621
trichloroethylene	2.08	435
trichloroethylene	2.12	621
trichloroethylene	2.13	620
trichloroethylene	2.17	726
trichloroethylene	2.24	746
AROMATIC NONHALOGENATED HYDROCARBONS		
1,2,3 - trimethylbenzene	3.04	396
1,2,4,5 - tetramethylbenzene	3.53	734
1,2,4,5 - tetramethylbenzene	3.36	396
1,2,4,5 - tetramethylbenzene	3.29	734
1,2,4,5 - tetramethylbenzene	3.17	734
1,3,5 - trimethylbenzene	3.16	734
1,3,5 - trimethylbenzene	3.06	396
1,3,5 - trimethylbenzene	2.95	734
1,3,5 - trimethylbenzene	2.84	734
2,6 - dimethylphenol	1.55	659
2,6 - dimethylphenol	1.55	351
2,6 - dimethylphenol	1.55	351
3-aminonitrobenzene (3-nh2)	1.73	320
3-ch3 aniline	1.65	320
4-aminonitrobenzene (4-nh2)	1.88	320
4-methylaniline (4-ch3)	1.90	320
acetophenone	2.15	458
acetophenone	1.98	82
acetophenone	1.91	82
acetophenone	1.87	746
acetophenone	1.82	524
acetophenone	1.82	320
acetophenone	1.74	458
acetophenone	1.68	82
acetophenone	1.66	82
acetophenone	1.65	82
acetophenone	1.65	82
acetophenone	1.63	396
acetophenone	1.63	82
acetophenone	1.56	82
acetophenone	1.56	82
acetophenone	1.54	437
acetophenone	1.49	82
acetophenone	1.46	82
acetophenone	1.45	82
acetophenone	1.42	458
acetophenone	1.41	458
acetophenone	1.40	82
acetophenone	1.38	82
acetophenone	1.38	458
acetophenone	1.38	458
acetophenone	1.38	458
acetophenone	1.34	82

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
acetophenone	1.31	458
acetophenone	1.28	458
acetophenone	1.19	458
aniline	3.17	96
aniline	2.85	278
aniline	2.66	278
aniline	2.35	720
aniline	2.35	96
aniline	2.32	278
aniline	2.23	96
aniline	2.17	96
aniline	1.88	99
aniline	1.87	342
aniline	1.83	99
aniline	1.78	342
aniline	1.73	99
aniline	1.41	320
aniline	1.25	320
anisole	1.54	392
azobenzene	3.13	320
benzene	2.16	321
benzene	2.00	395
benzene	1.98	396
benzene	1.97	395
benzene	1.92	404
benzene	1.78	437
benzene	1.50	392
benzidine	5.92	118
benzidine	5.91	521
benzidine	5.89	118
benzidine	5.70	521
benzidine	5.66	118
benzidine	5.36	521
benzidine	5.36	118
benzidine	5.25	521
benzidine	5.25	521
benzidine	4.93	521
benzidine	4.76	521
benzidine	4.65	521
benzidine	4.62	521
benzidine	4.44	521
benzidine	4.41	521
benzidine	3.86	521
benzidine	3.65	521
benzidine	3.42	521
benzophenone	2.63	320
benzyl alcohol	1.43	320
catechol	2.03	93
diphenyl ether	3.29	320
ethylbenzene	2.22	392
m - cresol	1.49	93
m - methoxy-phenol	1.50	93
m - nitrophenol	1.68	93
m - xylene	2.50	746
n - butylbenzene	3.69	734
n - butylbenzene	3.63	396
n - butylbenzene	3.47	734
n - butylbenzene	3.31	734
nitrobenzene	2.77	557
nitrobenzene	2.28	109
nitrobenzene	2.15	557
nitrobenzene	1.94	320
nitrobenzene	1.88	109
o - cresol	1.30	93
o - methoxy-phenol	1.56	93
o - nitrophenol	2.01	93
p - cresol	1.65	93
p - cresol	1.62	353
p - cresol	1.59	353
p - cresol	1.58	353
p - cresol	1.56	353
p - cresol	1.51	353
p - cresol	1.44	353
p - methoxy-phenol	1.70	93
p - nitrophenol	1.70	93
p - xylene (1,4 - dimethylbenzene)	2.89	734
p - xylene (1,4 - dimethylbenzene)	2.76	396
p - xylene (1,4 - dimethylbenzene)	2.68	734

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
p - xylene (1,4 - dimethylbenzene)	2.54	734
phenol	2.35	573
phenol	2.09	114
phenol	1.93	599
phenol	1.72	320
phenol	1.63	599
phenol	1.59	114
phenol	1.43	661
phenol	1.21	93
phenol	0.80	573
phenol	0.76	573
pyridine	3.36	801
pyridine	1.60	801
resorcinol	0.98	93
toluene	2.63	396
toluene	2.28	376
toluene	2.21	603
toluene	2.18	109
toluene	1.89	376
toluene	1.67	603
toluene	1.57	603
veratrole	2.03	524
AMIDES		
PHTHALATES		
butylbenzyl phthalate	2.19	1041
butylbenzyl phthalate	4.23	1034
diethyl phthalate (DEP)	2.85	1030
diethyl phthalate (DEP)	3.00	1030
diethyl phthalate (DEP)	3.24	1030
diethyl phthalate (DEP)	1.84	1034
dimethyl phthalate	1.90	1043
dimethyl phthalate	2.56	1043
dimethyl phthalate	2.49	1043
dimethyl phthalate	2.49	1043
dimethyl phthalate	2.23	1043
dihexyl phthalate (DHP)	4.69	1042
dihexyl phthalate (DHP)	4.70	1042
dihexyl phthalate (DHP)	4.76	1042
diisodecyl phthalate (DIDP)	5.05	1042
diisodecyl phthalate (DIDP)	5.16	1042
diisodecyl phthalate (DIDP)	5.78	1042
ditridecyl phthalate (DTDP)	4.28	1042
ditridecyl phthalate (DTDP)	5.87	1042
ditridecyl phthalate (DTDP)	6.45	1042
di(2-ethyl-hexyl) phthalate (DEHP)	4.94	1034
di(2-ethyl-hexyl) phthalate (DEHP)	5.41	1042
di(2-ethyl-hexyl) phthalate (DEHP)	5.48	1042
di(2-ethyl-hexyl) phthalate (DEHP)	5.95	1042
di-n-butyl PA (DBP)	3.14	1034
ORGANOTIN COMPOUNDS		
tributyltin	5.29	1031
tributyltin	4.65	1031
tributyltin	5.25	1031
tributyltin	4.09	1031
tributyltin	3.03	1060
tributyltin	3.85	1060
tributyltin	3.85	1060
tributyltin	3.87	1060
tributyltin	4.04	1060
tributyltin	4.09	1060
tributyltin	4.31	1060
tributyltin	3.65	1060
tributyltin	3.84	1060
tributyltin	4.14	1060
tributyltin	4.06	1060
tributyltin	3.90	1060
tributyltin	3.81	1060
tributyltin	3.61	1060
tributyltin	4.02	1060
tributyltin	4.22	1060
tributyltin	4.25	1060
tributyltin	4.20	1060
tributyltin	4.04	1060

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
tributyltin	4.23	1060
tributyltin	3.78	1060
tributyltin	4.06	1060
tributyltin	4.24	1060
tributyltin	4.00	1060
tributyltin	4.16	1060
tributyltin	4.38	1061
triphenyltin	4.34	1061
MISCELANEOUS COMPOUNDS (NONCLASSIFIED)		
1-naphtylamine		118
1-naphtylamine		118
1-naphtylamine		118
3,5,6 - trichloro - 2 - pyridinol	2.11	525
ac 252,214 (scepter)	0.84	705
ac 252,214 (scepter)	1.29	760
ac 252,214 (scepter)	1.40	705
ac 252,214 (scepter)	1.42	705
ac 252,214 (scepter)	1.47	705
ac 252,214 (scepter)	1.52	705
ac 252,214 (scepter)	1.74	760
acrolein	-0.31	657
benazolin ethyl	2.64	761
benazolin ethyl	2.86	761
bifenthrin	5.12	1047
bifenthrin	5.38	1047
bifenthrin	5.48	1047
bifenthrin	5.44	1047
bromacil		458
bromacil	1.12	458
bromacil	1.25	458
bromacil	1.29	458
bromacil	1.29	327
bromacil	1.36	458
bromacil	1.36	54
bromacil	1.37	458
bromacil	1.39	458
bromacil	1.40	52
bromacil	1.41	458
bromacil	1.41	458
bromacil	1.44	567
bromacil	1.45	610
bromacil	1.46	52
bromacil	1.46	458
bromacil	1.46	610
bromacil	1.48	458
bromacil	1.49	458
bromacil	1.51	52
bromacil		567
bromacil	1.52	52
bromacil	1.52	52
bromacil	1.53	759
bromacil	1.61	759
bromacil	1.64	610
bromacil	1.64	610
bromacil	1.69	610
bromacil	1.69	610
bromacil	1.70	52
bromacil	1.74	115
bromacil	1.81	567
bromacil	1.81	115
bromacil	1.82	115
bromacil	1.84	610
bromacil	1.85	616
bromacil	1.86	759
bromacil	1.86	525
bromacil	1.87	808
bromacil	1.88	808
bromacil	1.96	115
bromacil	2.05	115
bromacil	2.09	448
bromacil	2.09	327
bromacil	2.10	115
butyl ester of fluazifop	1.20	763
butyl ester of fluazifop	1.38	763
butyl ester of fluazifop	1.52	763
butyl ester of fluazifop	1.61	763

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
butyl ester of fluazifop	1.65	763
butyl ester of fluazifop	1.78	763
butyl ester of fluazifop	1.82	763
butyl ester of fluazifop	1.98	763
butyl ester of fluazifop	2.23	763
butyl ester of fluazifop	2.47	763
cinmethylin (sd 95481)	2.35	755
cinmethylin (sd 95481)	2.38	755
cinmethylin (sd 95481)	2.39	755
cinmethylin (sd 95481)	2.41	755
cinmethylin (sd 95481)	2.45	755
cinmethylin (sd 95481)	2.48	755
cinmethylin (sd 95481)	2.48	802
cinmethylin (sd 95481)	2.51	755
cinmethylin (sd 95481)	2.51	755
cinmethylin (sd 95481)	2.52	755
cinmethylin (sd 95481)	2.54	755
cinmethylin (sd 95481)	2.59	755
cinmethylin (sd 95481)	2.60	755
cinmethylin (sd 95481)	2.60	755
cinmethylin (sd 95481)	2.63	755
cinmethylin (sd 95481)	2.78	802
cinmethylin (sd 95481)	2.80	705
cinmethylin (sd 95481)	3.11	705
cinmethylin (sd 95481)	3.34	705
dimethirimol	1.94	596
dimethirimol	2.19	596
dimethirimol	2.24	596
dimethirimol	2.27	596
dimethirimol	2.34	596
dimethirimol	2.38	596
dimethirimol	2.49	596
dimethirimol	2.54	596
dimethylamine	2.49	334
dimethylamine	2.59	334
dimethylamine	2.64	334
dimethylamine	2.64	722
dimethylamine	2.70	334
dimethylamine	2.73	334
diphenyl methanol	2.34	320
diphenylamine	2.78	320
ethirimol	2.49	596
ethirimol	2.56	695
ethirimol	2.56	596
ethirimol	2.62	695
ethirimol	2.66	596
ethirimol	2.68	596
ethirimol	2.73	583
ethirimol	2.83	583
ethirimol	2.87	596
ethirimol	3.04	596
ethirimol	3.09	695
ethirimol	3.09	596
ethirimol	3.16	596
ethirimol	3.26	583
ethirimol	3.37	596
ethofumesate	2.53	798
fenvalerate	3.74	413
fluridone	2.18	191
fluridone	2.34	233
fluridone	2.35	191
fluridone	2.40	191
fluridone	2.54	191
fluridone	2.58	191
fluridone	2.64	191
fluridone	2.66	191
fluridone	2.66	233
fluridone	2.66	191
fluridone	2.68	191
fluridone	2.70	191
fluridone	2.72	191
fluridone	2.73	191
fluridone	2.77	191
fluridone	2.82	233
fluridone	2.82	233
fluridone	2.84	191
fluridone	2.87	233
fluridone	2.90	233

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
fluridone	2.91	233
fluridone	2.92	233
fluridone	2.93	233
fluridone	2.95	107
fluridone	2.95	233
fluridone	2.97	107
fluridone	3.00	235
fluridone	3.00	233
fluridone	3.01	107
fluridone	3.02	233
fluridone	3.02	233
fluridone	3.04	191
fluridone	3.05	191
fluridone	3.09	191
fluridone	3.20	233
fluridone	3.29	191
fluridone	3.34	107
fluridone	3.36	107
fluridone	3.39	107
folpet	3.27	166
isocil	2.11	525
metalaxyl	1.53	662
metalaxyl	1.57	667
metalaxyl	1.62	662
methyl ester of haloxyfop	1.19	763
methyl ester of haloxyfop	1.31	763
methyl ester of haloxyfop	1.38	763
methyl ester of haloxyfop	1.50	763
methyl ester of haloxyfop	1.60	763
methyl ester of haloxyfop	1.89	763
methyl ester of haloxyfop	1.89	763
methyl ester of haloxyfop	1.90	763
methyl ester of haloxyfop	1.92	763
methyl ester of haloxyfop	1.95	763
methyl ester of haloxyfop	2.00	763
methyl ester of haloxyfop	2.03	763
methyl ester of haloxyfop	2.19	763
methyl ester of haloxyfop	2.21	763
methyl ester of haloxyfop	2.23	763
methyl isothiocyanate (mit)	0.51	39
methyl isothiocyanate (mit)	0.66	39
methyl isothiocyanate (mit)	0.78	525
methyl isothiocyanate (mit)	1.14	551
methyl isothiocyanate (mit)	1.15	39
methyl isothiocyanate (mit)	1.19	39
methyl isothiocyanate (mit)	1.38	39
methyl pentafluorophenyl sulfone	1.46	166
norflurazon	2.38	666
norflurazon	2.66	666
norflurazon	2.82	666
norflurazon	3.28	525
norflurazon	3.52	746
p - toluidine	2.49	118
p - toluidine	2.69	118
p - toluidine	2.71	118
permethrin	3.91	524
permethrin	4.05	803
permethrin	4.19	410
permethrin	4.26	524
permethrin	4.36	524
permethrin	4.38	524
permethrin	4.80	320
permethrin	4.80	524
permethrin	4.80	524
propyl ester of cga-82725	1.39	763
propyl ester of cga-82725	1.45	763
propyl ester of cga-82725	1.67	763
propyl ester of cga-82725	1.68	763
propyl ester of cga-82725	1.68	763
propyl ester of cga-82725	1.72	763
propyl ester of cga-82725	1.73	763
propyl ester of cga-82725	1.73	763
propyl ester of cga-82725	1.94	763
propyl ester of cga-82725	1.97	763
propyl ester of cga-82725	2.00	763
propyl ester of cga-82725	2.03	763
propyl ester of cga-82725	2.31	763
propyl ester of cga-82725	2.37	763

Appendix C. Experimental logarithmic K_{oc} values.

compound	log K_{oc}	Ref
propyl ester of cga-82725	2.52	763
pyrazon (chloridazon)	1.66	213
pyrazon (chloridazon)	1.71	274
pyrazon (chloridazon)	1.76	274
pyrazon (chloridazon)	1.77	213
pyrazon (chloridazon)	1.82	686
pyrazon (chloridazon)	1.86	686
pyrazon (chloridazon)	1.88	274
pyrazon (chloridazon)	1.89	546
pyrazon (chloridazon)	1.95	686
pyrazon (chloridazon)	1.97	686
pyrazon (chloridazon)	1.97	213
pyrazon (chloridazon)	1.98	546
pyrazon (chloridazon)	2.00	213
pyrazon (chloridazon)	2.00	213
pyrazon (chloridazon)	2.00	213
pyrazon (chloridazon)	2.01	686
pyrazon (chloridazon)	2.02	213
pyrazon (chloridazon)	2.02	686
pyrazon (chloridazon)	2.05	686
pyrazon (chloridazon)	2.08	525
pyrazon (chloridazon)	2.11	213
pyrazon (chloridazon)	2.12	274
pyrazon (chloridazon)	2.14	213
pyrazon (chloridazon)	2.22	686
pyrazon (chloridazon)	2.22	274
pyrazon (chloridazon)	2.23	274
pyrazon (chloridazon)	2.23	546
pyrazon (chloridazon)	2.23	274
pyrazon (chloridazon)	2.39	274
pyrazon (chloridazon)	2.81	274
pyroxichlor	3.48	525
r-40244	2.55	732
terbacil	1.25	291
terbacil	1.33	182
terbacil	1.38	242
terbacil	1.42	291
terbacil	1.48	291
terbacil	1.56	327
terbacil	1.61	291
terbacil	1.61	722
terbacil	1.63	182
terbacil	1.71	525
terbacil	1.78	291
terbacil	1.78	291
terbacil	1.80	182
terbacil	1.81	291
terbacil	1.82	291
terbacil	2.14	448
terbacil	2.14	327

Appendix D Sources for the K_{oc}s from Appendix C (A numbers below 1000 indicates literature reviewed by Gerstl, 1990)

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Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
ACETANILIDES			
2-chloroacetanilide	1	1.58	
3,4-dichloroacetanilide (3,4-dicl)	9	2.40	0.11
3-bromoacetanilide	1	2.01	
3-chloroacetanilide	9	1.91	0.14
3-chloro-4-methoxyacetanilide	6	1.95	0.13
3-fluoroacetanilide	1	1.57	
3-methylacetanilide (3-ch3)	9	1.68	0.19
3-nitroacetanilide (3-no2)	1	1.94	
3-(trifluoromethyl)acetanilide (3-cf3)	1	1.75	
4-bromoacetanilide	1	1.95	
4-fluoroacetanilide	1	1.48	
4-methoxyacetanilide (4-och3)	9	1.55	0.18
acetanilide	1	1.43	
acetochlor	7	2.32	0.16
alachlor	31	2.27	0.24
butachlor	4	2.86	0.20
butyranilide	7	1.77	0.15
diphenamid	1	1.80	
metazachlor	18	2.14	0.12
metolachlor	45	2.33	0.29
propachlor	11	1.91	0.41
CARBAMATES			
4cl-benzaldoxime n-methylcarbamate	1	1.95	
aldicarb	27	1.22	0.33
aldicarb sulfone	10	0.47	0.32
aldicarb sulfoxide	8	0.89	0.88
asulam	1	2.48	
benzaldoxime n - methylcarbamate	1	1.56	
bromo-3-phenylcarbamate	5	1.90	0.08

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
butylate	1	2.11	
carbaryl	25	2.26	0.26
carbendazim	12	2.61	0.22
carbofuran	54	1.63	0.34
chlorbufam	5	2.21	0.14
chlorpropham (cipc)	57	2.54	0.25
cycloate (r-2063)	11	2.50	0.15
diallate	10	2.50	0.40
eptc	13	2.22	0.25
ethyl n-phenylcarbamate	1	1.82	
ethyl-3-phenylcarbamate	5	1.68	0.08
isopropyl-4-phenylcarbamate	5	1.94	0.04
metam-sodium	2	2.43	0.23
methiocarb	1	2.32	
methomyl	3	1.36	0.05
methoxy-3-phenylcarbamate	5	1.45	0.09
methoxy-4-phenylcarbamate	5	1.42	0.16
methyl n - (3,4-dichlorophenyl)	1	2.74	
methyl n - (3-chlorophenyl)carbamate	1	2.15	
methyl n-phenylcarbamate	1	1.73	
methyl-3-phenylcarbamate	5	1.49	0.09
n-butyl n-phenylcarbamate	1	2.26	
n-pentyl n-phenylcarbamate	1	2.61	
n-propyl n-phenylcarbamate	1	2.06	
oxamyl	26	1.05	0.38
pebulate	6	2.85	0.25
phenylcarbamate	5	1.21	0.11
propham	1	1.95	
propoxur	5	1.35	0.03
ter-butyl-4-phenylcarbamate	5	2.07	0.08

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
thiram	8	2.69	0.25
triallate	19	3.48	0.18
vernolate	6	2.33	0.25
xylylcarb (meobal)	5	1.74	0.10
zectran (mexacarbate)	3	2.96	0.32
DINITROANILINES			
2,6-dinitro-n-n-propyl-trifluoro-p-toluidine	1	3.61	
2,6-dinitro-trifluoro-p-toluidine	1	2.56	
benefin (benfluralin)	2	3.99	0.06
butralin (aa-820)	2	3.98	0.09
chlornidine	1	3.94	
dinitramine	2	3.63	0.04
fluchloralin	2	3.55	0.02
gs - 38946	1	3.17	
gs - 39985	1	3.23	
isopropalin	2	4.80	0.11
nitralin (sd 11831)	8	2.92	0.17
oryzalin	1	3.40	
profluralin (cga - 108320)	2	4.01	0.11
sd 13207	2	2.71	0.05
sd 11830	2	2.37	0.05
sd 12030	2	3.10	0.02
sd 12346	1	3.30	
sd 12400	1	2.58	
sd 12639	2	2.56	0.06
trifluralin	27	3.93	0.25
AROMATIC HALOGENATED HYDROCARBONS			
2-methoxy-3,5,6-trichloropyridine	1	2.96	
captafol	1	3.32	
captan	1	2.30	
chloroneb	4	3.15	0.08

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
dde	2	4.82	0.17
ddt	31	5.63	0.61
dichlobenil	41	2.31	0.28
endosulfan	1	4.13	
endrin	1	4.29	
a-hch	14	3.25	0.12
b-hch	17	3.36	0.15
y-hch (lindane)	94	2.98	0.28
mboca	1	3.90	
methoxychlor	15	4.80	0.30
n - serve (nitrpyrin, dowco 163)	27	2.57	0.20
nitrofen	1	4.18	
2 - pcb (1)	1	3.47	
2,2' - dichlorobiphenyl (1)	1	3.92	
2,4' - dichlorobiphenyl (8)	5	3.48	0.77
2,2',5 - trichlorobiphenyl (18)	7	4.23	0.37
2,4,4' - trichlorobiphenyl (28)	3	4.62	0.88
2,2',4,4' - tetrachlorobiphenyl (47)	1	3.43	
2,2',5,5' - tetrachlorobiphenyl (52)	5	4.73	1.20
2,2',6,6' - tetrachlorobiphenyl (54)	6	5.01	0.33
2,3',4',5 - tetrachlorobiphenyl (70)	5	4.84	0.12
2,2',3,4,5' - pentachlorobiphenyl (87)	2	4.62	0.17
2,4,5,2',5' - pentachlorobiphenyl (101)	9	5.87	0.50
2,2',3,3',4,4' - hexachlorobiphenyl (128)	1	5.29	
2,2',4,4',5,5' - hexachlorobiphenyl (153)	40	5.65	0.71
2,2',4,4',6,6' - hexachlorobiphenyl (155)	1	6.08	
2,2',3,4,5,5',6 - heptachlorobiphenyl (185)	3	6.56	0.52
chloroaniline	16	2.55	0.35
3,5 - dichloroaniline	2	2.44	0.08
2,6 - dichloroaniline	1	3.25	

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
2,4 - dichloroaniline	4	2.72	0.18
3,4 - dichloroaniline	5	2.99	0.70
2,3,4-trichloroaniline	3	2.97	0.60
2,3,4,5-tetrachloroaniline	2	3.51	0.66
2,3,5,6-tetrachloroaniline	1	3.94	
pentachloroaniline	1	4.62	
3-cf3 aniline	1	2.36	
4-bromoaniline	1	1.96	
3-chloro-4-methoxyaniline (3-cl-4-och3)	1	1.93	
3-ch3-4-bromoaniline	1	2.26	
4-bromonitrobenzene	1	2.42	
3,4-dichloronitrobenzene	1	2.53	
2,3-dichloronitrobenzene	1	3.97	
3,5-dichloronitrobenzene	1	4.19	
2,3,4,5-tetrachloronitrobenzene	1	4.23	
2,3,5,6-tetrachloronitrobenzene	1	4.05	
pentachloronitrobenzene	4	4.36	0.18
3-chloro-4-bromonitrobenzene	1	2.60	
chlorobenzene	11	2.34	0.23
iodobenzene	1	3.10	
bromobenzene	3	2.55	0.44
1,2 - dichlorobenzene	7	2.50	0.06
1,3 - dichlorobenzene	3	2.48	0.01
1,4 - dichlorobenzene	9	2.80	0.23
1,2,3 -trichlorobenzene	4	3.29	0.28
1,2,4 - trichlorobenzene	7	3.35	0.21
1,3,5 - trichlorobenzene	1	3.09	
1,2,3,4 - tetrachlorobenzene	2	3.96	0.16
1,2,3,5 tetrachlorobenzene	3	3.38	0.16
1,2,4,5 - tetrachlorobenzene	7	3.91	0.15
pentachlorobenzene	2	3.62	0.17

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
hexachlorobenzene	6	4.04	0.35
o-chlorophenol	1	1.67	
m-chlorophenol	1	1.78	
p-chlorophenol	1	1.80	
2,3 - dichlorophenol	4	2.51	0.24
2,4 - dichlorophenol	5	2.47	0.35
2,4,5 - trichlorophenol	4	3.15	0.43
2,4,6 - trichlorophenol	3	3.02	0.10
3,4,5 - trichlorophenol	3	3.56	0.09
2,3,4,5 - tetrachlorophenol	3	4.12	0.02
pentachlorophenol	3	4.51	0.11
4-bromophenol	1	2.41	
o-benzyl-p-chlorophenol	3	3.41	0.39
ORGANOPHOSPHATES			
3,5,6-trichloro-2-pyridinol (chlorpyrifos metabolite)	3	2.36	0.07
azinphos methyl	7	3.10	0.52
carbophenothion (trithion)	5	4.68	0.25
carbophenothion - methyl	1	4.67	
chlorfenvinphos	3	2.68	0.18
chlorpyrifos	34	3.88	0.33
chlorpyrifos - methyl	1	3.52	
ciodrin (crotoxiphos)	6	2.27	0.28
diamidaphos (nellite)	4	1.54	0.07
diazinon	10	2.64	0.16
dichlorvos	5	1.83	0.34
dimefox	2	1.79	0.04
dimethoate	12	1.51	0.47
disulfoton (disyston)	28	3.12	0.39
dowco 275	1	2.41	
dyfonate (fonofos)	1	3.44	

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
ethion	9	4.10	0.23
ethoprophos	36	1.80	0.14
fenamiphos	13	2.51	0.18
fenamiphos sulfoxide	1	1.57	
fenamiphos sulfone	1	1.64	
fenitrothion	10	3.13	0.33
fensulfothion	4	2.52	0.14
fensulfothion sulfide	4	3.18	0.14
fensulfothion sulfone	4	2.17	0.22
isazophos	3	2.01	0.02
leptophos	5	4.61	0.60
malathion	22	3.07	0.33
methidathion	2	2.27	0.01
methyl parathion	16	3.17	0.59
mevinphos	21	2.80	0.73
parathion	89	3.17	0.46
phorate (thimet)	12	3.04	0.46
piperophos	15	3.12	0.39
profenophos	1	3.03	
terbufos	12	2.97	0.39
terbufos sulfone	4	2.18	0.38
terbufos sulfoxide	4	2.18	0.47
triazofos	3	2.55	0.06
trichlorfon	6	1.58	0.19
UREAS			
cga-15646	8	2.33	0.15
chlorbromuron	42	2.77	0.33
chloroxuron	11	3.51	0.22
chlorsulfuron	19	2.00	0.61
chlortoluron	85	2.19	0.24
3,4 - dichlorophenylurea	1	2.62	

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
diflubenzuron	1	3.83	
diuron	156	2.47	0.33
ethylenethiurea (etu)	1	2.07	
fenuron	39	1.43	0.20
fluometuron	44	1.93	0.30
isouron	5	2.17	0.94
linuron	137	2.78	0.29
methabenzthiazuron	14	2.80	0.17
methylurea	7	1.78	0.06
metobromuron	34	2.18	0.35
metoxuron	18	1.80	0.17
monolinuron	44	2.16	0.41
monuron	58	1.87	0.47
neburon	10	3.41	0.15
siduron	1	2.31	
tebuthiuron	6	2.15	0.50
urea	3	1.09	0.16
vel 3510	1	2.51	
3-(3-chlorophenyl)-1,1-dimethylurea	1	1.79	
3-(3-methoxyphenyl)-1,1-dimethylurea	1	1.72	
3-(3-fluorophenyl)-1,1-dimethylurea	1	1.73	
3-(4-fluorophenyl)-1,1-dimethylurea	1	1.43	
3-(4-methylphenyl)-1,1-dimethylurea	0		
3-(4-methoxyphenyl)-1,1-dimethylurea	1	1.40	
3-(3,5-dimethylphenyl)-1,1-dimethylurea	7	1.72	0.16
3-(3,5-dimethyl-4-bromophenyl)-1,1-dimethylurea	1	2.53	
h-(n-methyl-n'-phenylurea)	14	1.64	0.18
3-(3-chlorophenyl)-1-methylurea	1	1.93	
3,4-cl2 (dmu)	18	2.47	0.18
3-(3-chloro-4-methoxyphenyl)-1-methylurea	2	1.90	0.08

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
3-(3-chloro-4-methylphenyl)-1-methylurea	1	2.10	
3-phenyl-1-cyclopropylurea	1	1.74	
3-phenyl-1-cyclopentylurea	0		
3-phenyl-1-cyclohexylurea	0		
3-phenyl-1-cycloheptylurea	0		
2-fluorophenylurea	1	1.32	
2-chlorophenylurea	0		
3-fluorophenylurea	1	1.77	
3-chlorophenylurea	1	2.01	
3-bromophenylurea	1	2.06	
3-methylphenylurea	1	1.56	
4-bromophenylurea	1	2.12	
4-phenoxymethylurea	1	2.56	
3-chloro-4-methoxyphenylurea	1	2.00	
(3-methyl-4-bromophenylurea	0		
3-cf3-phenylurea)	0		
4-f-phenylurea)	0		
4-so3 phenylurea	0		
h-phenylurea	8	1.84	0.21
3-ch3,4-f-phenylurea	8	1.76	0.19
3,4-di-cl-phenylurea	18	2.53	0.14
TRIAZINES			
2-hydroxy-4,6-bis(ethylamino)-1,3,5-triazine (hydroxy sima	2	2.18	0.10
ametryn	41	2.50	0.27
amitrole	1	1.25	
atrazine	217	2.19	0.34
cyanazine	13	2.17	0.25
dipropetryn	9	2.95	0.25
hexazinone	5	1.40	0.06
ipazine	3	3.17	0.24
metamitron	33	2.20	0.26

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
metribuzin	72	1.73	0.34
prometon	70	2.19	0.45
prometryn	125	2.66	0.38
propazine	81	2.14	0.22
secbumeton (gs 14254)	12	2.64	0.57
simazine	265	2.04	0.36
terbutryn	18	3.17	0.49
terbutylazine	3	2.51	0.24
trietazine	2	2.76	0.03
TRIAZOLES			
benzyltriazole cl cl	1	2.33	
benzyltriazole h c4h9	1	2.16	
benzyltriazole h cf3	1	1.77	
benzyltriazole h ch3o	1	1.80	
benzyltriazole h cl	1	1.98	
benzyltriazole h f	1	1.69	
benzyltriazole pp450	1	1.88	
buthidazole	2	2.19	0.25
imazalil	2	3.73	0.16
methazole	3	3.66	0.24
nia 23486	8	1.69	0.12
oxadiazon	1	3.51	
propiconazole	5	3.70	0.47
thiabendazole	13	3.37	0.17
triadimefon	1	2.71	
tricyclazole	5	3.10	0.07
ACIDS			
2,3,6-tba	3	0.83	0.51
2,4,5-t	33	1.99	0.38
2,4-d	58	1.66	0.56

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
2,4-d-amine	10	1.66	0.47
3,6-dichloropicolinic acid	1	0.30	
anthracene-9-carboxylic acid	16	2.74	0.31
bentazon	6	1.52	0.37
chloramben (amiben)	15	1.48	0.49
chloramben (methyl esther)	11	2.74	0.31
chloropicolinic acid	1	0.95	
dalapon	1	0.40	
dicamba	12	0.30	0.31
dinoseb (dnbp)	1	2.09	
dinoseb	7	2.29	0.58
DNOC	12	2.34	0.26
endothall	2	2.09	0.07
fenac	2	1.80	1.44
imazaquin	4	1.35	0.15
mcpa	5	1.73	0.03
mecoprop	3	0.92	0.20
picloram	59	1.49	0.52
silvex (fenoprop)	4	3.28	0.48
sulfometuron methyl	9	1.62	0.45
POLYAROMATIC HYDROCARBONS			
1 - naphthol	17	3.07	0.45
13h - dibenzo (a,i) carbazole	15	6.10	0.18
2,2' - biquinoline	14	4.16	0.26
2 - aminoanthracene	15	4.53	0.20
2 - methylnaphtalene	2	4.05	0.17
3 - methylcholanthrene	15	6.21	0.29
6 - aminochrysene	15	5.21	0.23
7,12 - dimethylbenz (a) anthracene	16	5.40	0.24
9 - methylanthracene	4	4.85	0.14
acridine	16	4.20	0.19

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
anthracene	4	4.38	0.21
benzo(a)pyrene	2	5.29	0.56
benz(a)anthracene	1	5.92	
dibenz (a,h) anthracene	16	6.26	0.23
dibenzothiophene	14	3.99	0.15
naphtalene	7	2.97	0.31
phenanthrene	3	4.35	0.26
pyrene	33	4.85	0.26
quinoline	12	2.84	0.58
tetracene (2,3-benzanthracene)	2	5.93	0.17
NONAROMATIC HALOGENATED HYDROCARBONS			
1,1,1 - trichloroethane	6	1.82	0.64
1,1,2,2 - tetrachloroethane	2	1.92	0.03
1,1,2 - trichloroethane	2	1.99	0.16
1,2 - dibromo - 3 - chloropropane (dbcp)	10	2.06	0.20
1,2 - dibromoethene	1	1.89	
1,2 - dichloroethane	4	1.62	0.18
1,2 - dichloropropane	3	1.68	0.03
1,3 - dichloropropene (telone)	5	1.53	0.21
bis (2 - chloroethyl) ether	1	1.88	
bromoform	1	2.10	
carbon tetrachloride	7	1.53	0.39
chloroform (trichloromethane)	3	1.81	0.14
dichloromethane	2	1.56	0.17
ethylene dibromide (edb;1,2-dibromoethane)	10	1.53	0.27
hexachloroethane	1	3.61	
tetrachloroethylene	11	2.38	0.23
trichloroethylene	13	2.04	0.11
AROMATIC NONHALOGENATED HYDROCARBONS			
1,2,3 - trimethylbenzene	1	3.04	

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
1,2,4,5 - tetramethylbenzene	4	3.34	0.15
1,3,5 - trimethylbenzene	4	3.00	0.14
2,6 - dimethylphenol	3	1.55	0.00
3-aminonitrobenzene (3-nh2)	1	1.73	
3-ch3 aniline	1	1.65	
4-aminonitrobenzene (4-nh2)	1	1.88	
4-methylaniline (4-ch3)	1	1.90	
acetophenone	30	1.57	0.23
aniline	15	2.12	0.52
anisole	1	1.54	
azobenzene	1	3.13	
benzene	7	1.90	0.21
benzidine	18	4.95	0.78
benzophenone	1	2.63	
benzyl alcohol	1	1.43	
catechol	1	2.03	
diphenyl ether	1	3.29	
ethylbenzene	1	2.22	
m - cresol	1	1.49	
m - methoxy-phenol	1	1.50	
m - nitrophenol	1	1.68	
m - xylene	1	2.50	
n - butylbenzene	4	3.53	0.17
nitrobenzene	5	2.20	0.35
o - cresol	1	1.30	
o - methoxy-phenol	1	1.56	
o - nitrophenol	1	2.01	
p - cresol	7	1.56	0.07
p - methoxy-phenol	1	1.70	
p - nitrophenol	1	1.70	
p - xylene (1,4 - dimethylbenzene)	4	2.72	0.15

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
phenol	10	1.55	0.52
pyridine	2	2.48	1.24
resorcinol	1	0.98	
toluene	7	2.06	0.37
veratrole	1	2.03	
PHTHALATES			
butylbenzyl phthalate	2	3.21	1.44
diethyl phthalate (DEP)	4	2.73	0.62
dimethyl phthalate	5	2.33	0.27
dihexyl phthalate (DHP)	3	4.72	0.04
diisodecyl phthalate (DIDP)	3	5.33	0.39
ditridecyl phthalate (DTDP)	3	5.53	1.13
di(2-ethyl-hexyl) phthalate (DEHP)	4	5.44	0.41
di-n-butyl PA (DBP)	1	3.14	
ORGANOTIN COMPOUNDS			
tributyltin	30	4.10	0.48
triphenyltin	1	4.34	
MISCELANEOUS COMPOUNDS (NONCLASSIFIED)			
1-naphtylamine	3	3.50	0.07
3,5,6 - trichloro - 2 - pyridinol	1	2.11	
ac 252,214 (scepter)	7	1.38	0.28
acrolein	1	-0.31	
benazolin ethyl	2	2.75	0.16
bifenthrin	4	5.35	0.16
bromacil	45	1.60	0.26
butyl ester of fluazifop	10	1.76	0.38
cinmethylin (sd 95481)	19	2.60	0.25
dimethirimol	8	2.30	0.19
dimethylamine	6	2.63	0.09
diphenyl methanol	1	2.34	

Appendix E. Average experimental K_{oc} values.

	N	log K_{oc} average	STD
diphenylamine	1	2.78	
ethirimol	15	2.87	0.28
ethofumesate	1	2.53	
fenvalerate	1	3.74	
fluridone	39	2.85	0.28
folpet	1	3.27	
isocil	1	2.11	
metalaxyl	3	1.57	0.05
methyl ester of haloxyfop	15	1.81	0.34
methyl isothiocyanate (mit)	7	0.97	0.32
methyl pentafluorophenyl sulfone	1	1.46	
norflurazon	5	2.93	0.46
p - toluidine	3	2.63	0.12
permethrin	9	4.39	0.34
propyl ester of cga-82725	15	1.88	0.33
pyrazon (chloridazon)	30	2.04	0.23
pyroxichlor	1	3.48	
r-40244	1	2.55	
terbacil	17	1.66	0.25