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Quantitative Structure-Activity Relationships (QSAR) and Pesticides

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Contents

Foreword

The concept of similar structures having similar properties is not new. Already in the 1890's it was discovered, for example, that the anaesthetic potency of substances to aquatic organisms was related to their oil/water solubility ratios, a relationship which led to the use of LogP octanol/water as an estimate of this effect. Today it is known that all chemicals will exhibit a minimum or "basal" narcotic effect which is related to their absorption to cell membranes, and which is well predicted by their lipophilic profile.

The use of logP alone can thus explain about half of the toxicity (R^2=0.5) of unrelated industrial chemicals to fish, and with closely related substances (such as linear alcohols or ketones) such simple models are highly predictive. More reactive chemicals ("polar narcotics" such as phenols and amines) can also be modelled successfully in this manner. In all, approximately 70% of industrial chemicals fall into one of these two general categories where aquatic toxicity estimates can be expected to be within an order of magnitude.

Other parameters such as molecular indices, quantum mechanical properties, shape, size, charge distributions, etc., can greatly improve estimates, particularly for substances which also act via highly reactive toxic mechanisms (such as allylics, or acrylates).

The case is not quite as simple for substances with "specific" activities (pesticides or drugs). While simple narcosis will also be present for such chemicals, this may be of little interest compared with intense activity induced by binding to a critical receptor site. This and other factors has resulted in considerable effort by, among others, the drug industry to develop tools which can better predict effects based on structural information.

Today numerous computerised systems exist for predicting a large range of effects stretching from biodegradability to cancer. These include fragment based statistical systems such as TOPKAT and MCASE, as well as three-dimensional modelling of ligand docking (COMFA). Some are well suited for screening of large numbers of chemicals, while others are very labour-intensive and best confined to small closely related data sets.

Predictive ability will vary depending on both the method used, and the endpoint in question. In general, estimates of environmental effects have been more readily accepted than estimates of mammalian effects. This may be changing rapidly. In general, predictive ability of sophisticated contemporary QSAR systems can often correctly predict the activity of about 80% of the chemicals examined, provided that sufficient biological data exists to cover the domain of the structures. While this may not be good enough for some regulatory purposes, in others it may be sufficient. Even today a great number of chemicals are never synthesised because the potential producer has already determined that they are likely to have harmful properties according to a QSAR estimate.

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Preface

This study considers the current available knowledge on the use of Quantitative Structure-Activity Relationship (QSAR) models relating to the use on pesticides.

The use is based on evaluation of the correlations between experimental values and QSAR estimates from the selected QSAR models. The experimental values are obtained from Pesticide Manual (Tomlin 1994, 1997), Linders ***et al.*** (1994), and from letters of approval for plant protection preparations containing data from studies submitted by manufacturers to the Danish Environmental Protection Agency (Danish EPA) and evaluated in internal reports (Clausen 1998).

QSARs are quantitative models seeking to predict activity such as environmental toxicity derived from the molecular structure. Most often this is accomplished by first correlating properties such as physico-chemical parameters with molecular structure and then correlating toxicity with these parameters. The central paradigm underlying such QSAR modelling is the structure-property similarity principle. This paradigm states that analogous structures have generally similar properties. Since chemicals with similar properties tend to have similar biological activities, toxicity may be predicted from structure alone. More than six million chemical substances are known and humans are exposed to 50,000 to 100,000 of them. As it is impossible to test each substance in a time and cost effective manner, this “guilt by association” approach provides a powerful alternative to direct testing for predicting toxicity for untested substances. While QSARs in environmental toxicology were reported as early as 1869, modern efforts have their roots in the classic turn of the century work of Meyer and Overton on narcotics.

Narcosis is the reversible state of arrested protoplasmic activity. It is a physical phenomenon, which is mostly independent of specific molecular structure. It is considered the most common mode of toxic action, at least in short term exposure of aquatic organisms, and the mode of action for about 70% of the industrial organic chemicals. Narcosis is subdivided into several non-specific and specific mechanisms (e.g. non-polar narcosis, polar narcosis etc.).

However, pesticides are developed specifically based on their specific mode of action mechanisms and this may affect the predictability of QSARs.

Based on the work already performed, the present report uses the most promising descriptors. As most of the preliminary work has been done on simpler molecules an evaluation at this stage may result in a less promising result. However, it has been found reasonable to perform such an analysis to assess the current stage of the use of QSARs on pesticides.

Summary

In environmental risk assessment, information of environmental fate, behaviour and the toxicity of a chemical substance are of basic need. Quantitative Structure-Activity Relationships (QSAR) is a method to derive certain effects or properties of chemical substances in the absence of experimental data.

For pesticides, the data requirements demanded for their authorisation normally means that sufficient data for a risk assessment exist. This is rarely the case for additives, impurities, degradation or transformation products. Most QSAR models are developed from simple industrial chemicals and usually only a few pesticides are included. Especially, new pesticides consist of complicated molecular structures acting with specific modes of action and their physico-chemical properties and ecotoxicological effect concentrations may not be estimated sufficiently close to the correct effect value by QSAR.

The current document presents the general framework in which QSARs can be used within the risk assessment procedure. Furthermore, it presents recommended QSARs for physico-chemical parameters and ecotoxicological effect concentrations and performs an evaluation of their correlation with approximately 400 selected pesticides including salts and esters.

Of physico-chemical properties, the recommended QSARs to estimate the boiling point could not be evaluated due to lack of experimental values. Estimations of the melting point were inaccurate and mainly overestimated by the presented QSAR. The solubility in water was reasonably well correlated with the recommended QSAR and a QSAR based on 322 pesticides was developed. The vapour pressure QSAR based on suggested values from a computer model showed low correlation with the pesticides used. The Henry's Law constant was evaluated by comparing calculated values with QSAR predicted values. A low correlation was observed. The octanol/water partition coefficient Kow derived by structure fragment analysis demonstrated acceptable agreement with the measured values. As the model was a computerised version, a QSAR based on water solubility was suggested. Several QSARs have been developed to derive the adsorption coefficient Koc. Four recommended QSARs were selected for comparison. The correlations between estimated and experimental Koc were acceptable for one of the QSARs. The QSAR for bioaccumulation was in reasonably good agreement with the experimental values for pesticides.

For aquatic toxicity, QSARs have been developed for acute toxicity estimations for fish, daphnia and algae. The correlations between estimated and experimental EC_{50}-values were low for fish, daphnia and algae. New QSARs, based on experimental toxicity values and log Kow, were suggested following a grouping of pesticides into modes of action. It was observed that improvements of the predictability could be obtained in some of the groups. However in other groups, the correlation coefficients were low and they could not be recommended except perhaps for screening procedures.

QSAR should not replace experimental values for pesticides. However, QSARs proved to have a reasonable predictive value and might be usable if no data were available.

Dansk sammendrag

Til risikovurdering er oplysninger om stoffernes opførsel og skæbne samt deres toksicitet nødvendige. Quantitative Structure-Activity Relationship (QSAR) er en metode til at skønne størrelsen af visse fysisk/kemiske og toksiske værdier.

De dokumentationskrav, der forlanges ved godkendelse af bekæmpelsesmidler, betyder normalt, at tilstrækkelige data er til stede til en risikovurdering. Det samme er sjældent tilfældet for additiver, urenheder, nedbrydnings- eller omdannelsesprodukter. De fleste QSAR modeller er udviklet ud fra simple industrikemikalier, og ofte er kun få pesticider medtaget. Da moderne pesticider ofte består af komplicerede kemiske strukturer og er udviklet på basis af deres specifikke effekt, kan det medføre, at deres fysisk/kemiske egenskaber og toksiske effektkoncentrationer ikke kan skønnes tilstrækkeligt præcist med QSAR modeller.

I projektet præsenteres områder for QSARs anvendelse, anbefalede QSAR modeller for fysisk/kemiske parametre og økotoksikologiske effekt-koncentrationer samt en vurdering af de anbefalede QSAR modeller ved korrelationsanalyse med eksperimentelle værdier fra cirka 400 pesticider (inkl. salte og estere).

For fysisk/kemiske egenskaber blev det fundet, at den anbefalede QSAR model til skøn af kogepunktet ikke kunne vurderes på grund af manglende eksperimentelle data. Skøn af smeltepunktet var upræcise og som regel over-estimerede med den anvendte QSAR. Opløseligheden i vand var til gengæld i god overensstemmelse med de målte data fra de anvendte pesticider. Damptrykket kunne ikke estimeres særligt godt med den anvendte QSAR computer model. Henrys lovkonstant (H) vurderedes ved sammenligning med beregnede H fra eksperimentelle data og modelberegninger. Overensstemmelsen var lille. Oktanol/vand koefficienten Kow beregnet ud fra en struktur analyse viste en rimelig overensstemmelse med de målte værdier. Da modellen kræver anvendelse af computer, anbefales en QSAR model baseret på vandopløselighed. Der findes mange modeller til skøn af adsorptionskoefficienten Koc. Fire anbefalede modeller er anvendt i projektet, og den ene viste en acceptabel korrelation til de eksperimentelle værdier. QSAR modeller for bioakkumulering i fisk viste god overensstemmelse med eksperimentelle data.

For toksisk effekt på vandlevende organismer er der udviklet QSAR modeller for fisk, dafnier og alger. Korrelationen mellem skønnede og eksperimentelle værdier var lav for både fisk, dafnier og alger. Projektet har beregnet nye QSAR modeller baseret på pesticider opdelt efter deres virkningsmekanisme. Denne opdeling medførte væsentligt forbedrede korrelationer for nogle af de dannede grupper, mens korrelationerne stadig var lave i andre. Der kan således ikke fremføres en generel anbefaling undtagen måske med forsigtighed i en “screening” fase. Studiet viste dog, at en opdeling efter stoffernes specifikke virkning var en væsentlig forbedring fremfor anvendelsen af de mere generelle QSAR modeller.

QSAR modeller skal ikke erstatte eksperimentelle værdier for pesticider. QSAR modeller viste dog en rimelig skønnet niveau, hvis der ikke findes eksperimentelle data.

1 Introduction

The study on the relationships between molecular structure and physico-chemical and biological response, collectively known as Structure-Activity Relationships (SAR), is a rapidly growing field of research in chemistry and biology. Some areas of the application of SAR include the design of more active and less toxic agricultural products (Martin 1978).

Basically, a SAR analysis consists of comparison between experimental values by mathematical variance analysis (e.g. regression analysis, discriminant analysis, factorial analysis and pattern recognition techniques) and a selection of the best correlation values. The best-fitted correlations are then used to develop a mathematical expression to estimate end-values from known substances to unknown substances.

When performing a SAR analysis, it is assumed that the chemical or biological response produced by a substance (usually an organic compound) is a direct function of its chemical structure, and that the same substance will always produce the same response, under a given set of experimental conditions.

However, ”chemical structure” cannot be dealt with directly. Instead quantities, usually of a numerical nature, which are derived from and represent the chemical structures, are used. These quantities are called molecular descriptors. The molecular descriptors are of various types:

- fragments (e.g. counts of atoms, bonds of various types, rings, ring atoms, molecular weight)
- topological (e.g. molecular connectivity, molecular symmetry)
- geometrical (e.g. molecular surface area and volume)
- physico-chemical (e.g. molar refraction, log Kow) or substructural (e.g. topological
- physico-chemical properties of substructures as embedded in the structure).

The more relevant to the chemical and to the observed responses the molecular descriptors become, the more exact the approximation will be and the more valid and useful the relationship will be.

Based on the work already performed on these initial analyses, this report uses the most promising descriptors. As most of the preliminary work has been done on simpler molecules, an evaluation at this stage may result in a less promising result. However, it has been found reasonable to perform such an analysis to assess the current stage of the use of QSARs on pesticides.

The fast development in models (i.e. mathematical expressions) has resulted in a constant rewriting to include the most recent relationships during the processing of this report. The inclusion of QSAR in the formal EU technical guidance document on risk assessment (TGD 1996) has made it imperative to present a report on QSARs and pesticides at this stage.

The statistical procedure used to derive QSAR models is linear regression analysis and it can be either single or multivariable depending on the number of structural descriptors used in a particular analysis. The regression method affords transparent relations and simple mathematical equations and leads to quantitative correlations. However, for a successful and meaningful regression analysis, precise and accurate input data are required (Karcher and Devilliers 1990).

It is important to keep in mind that the values used may be averages or otherwise selected data and do not demonstrate the variation inherent in biological systems in contradiction to the precise estimates made from mathematical expressions. It is easy to become mesmerised by the string of precise numbers being churned out by computers and to forget that the biological data going in are not anywhere near so precise (Dagani 1981).

It is important not to exaggerate the predictive accuracy of models, especially where the experimental data are either limited or controversial (Hart 1991). The weight in evaluation of QSAR results should be placed on the level of magnitude and not the exact value which can only be established by experimental studies performed by internationally accepted guidelines. Different methods or guidelines for physical, chemical and ecotoxicological tests can be used but priority to EU recommended methods is given in Commission Directive 92/69/EEC and 87/302/EEC (revision of Annex V in 67/548/EEC) or revised versions e.g. OECD technical guidelines (OECD 1993),

Thus, QSARs can be used to assist data evaluation to contribute to the decision on whether further testing is necessary to clarify an endpoint of concern and to establish input parameters which are necessary to conduct the exposure or effect assessment.

2 QSAR

2.1 QSAR method

Risk assessment

In environmental risk assessment, knowledge of the acute toxicity, chronic toxicity and environmental fate and behaviour of a chemical substance is a basic need. Factors affecting the environmental fate and behaviour of a chemical comprise its water solubility, adsorption to soil and sediments, volatilisation, biotic and abiotic degradation, and bioaccumulation. Quantitative knowledge of these processes enables one to model the concentrations of a certain chemical substance in the different environmental compartments (soil, air, water, and sediment). The knowledge of the toxicity of a chemical to aquatic organisms is normally limited to simple effects as lethality, growth or reproduction inhibition. The effect concentration for acute toxicity is expressed as the LC_{50} (EC_{50}), the aqueous concentration that produces 50% lethality (and/or other effects). The effect concentrations for long-term or chronic effects is expressed as the NOEC, the highest test concentration with no observed effect on e.g. reproduction, population growth or other kinds of sublethal toxicity. An approach towards the toxicity of a compound with regard to environmental risk assessment would be to determine a "safe level", a concentration at or below which, no organism or only a certain percentage of organisms in an ecosystem would be affected by the compound. Methods to predict the level of no-effect use the lowest acute or chronic values (TGD 1996) or interpolation of several values (e.g. Straalen & Denneman 1989, Wagner and Løkke 1991) and multiply with a relevant assessment factor.

Pesticides

For pesticides, the comprehensive data requirements demanded for authorisation normally mean that sufficient data for a risk assessment are present. This is not the case for the additives, impurities and substances used in the formulation of the pesticide product and usually not the case for the degradation or transformation products from biocidal active substances. The research devoted to develop reliable estimation procedures for the toxicity of environmental pollutants may therefore have a potential in estimating the needed data for the groups of substances. Today, the most promising technique for estimating the toxicity of pollutants is QSAR. However, it should be noted that QSARs should be applied within its recognised limits of applicability, e.g. validity within a certain range of parameters (Kow-values, pH, etc.), certain groups of chemicals (carbamates, phenylureas, triazines, etc.), or mode of action.

Structure-Activity Relationships

SAR is based on the knowledge that substances with a similar (analogous) chemical structure may have the same biological activity. SAR is a qualitative comparison of the structures of chemical compounds and their effects in the biological system. From this evaluation of the influence of the chemical structure on the biological system, combined with experience in how changes in the chemical structure affect the magnitude and type of biological effect, unknown toxic effects to the biological system of unknown compounds with related chemically structure are predicted.

Quantitative Structure-Activity Relationships

QSAR is a statistical data analytical procedure in which quantitative endpoints of compounds (e.g. toxicity) are correlated with one or more structural parameters of these compounds, normally through uni- or multivariate linear regression (Chapman & Shorter 1978), non-linear regression (Könemann 1981), bilinear (Veith ***et al.*** 1983) or exponential regression. Commonly used structural parameters for inclusion in QSAR correlations are for instance:

- octanol-water partition coefficients (log Kow)
- aqueous solubility (log S)
- Molar Refraction or Parachor (dispersion forces)
- dipole moment
- ionisation potentials
- molar volumes
- molar surface areas (Hermens 1989).

Several variables have been used in attempts to obtain the best-fitted parameter(s).

N-Octanol/water partition coefficient

The parameter n-octanol/water partition coefficient, Kow, is an experimental data describing the lipophilicity of the substance. It has been shown that a non-linear relation between biological activity and lipophilicity exists. Substances of very low lipophilicity may be less able to pass lipidous membranes and substances with a high lipophilicity will accumulate in fat tissue and other lipophile phases and may therefore not release a biological response.

Polarity

The polarity is an expression of the electronic distribution in the substance. The polarity is essential to the binding or release of the substance to an organism's membranes and/or macromolecules and thus determines whether a biological response may take place or not.

Stereochemical structure

The stereochemical structure may influence the possibility of interaction with the macromolecules of an organism. Size and shape should be suitable to fit into the receptor or enzyme before biological action may take place.

Scope

QSARs were originally mathematical models relating biological activity of chemicals to their structures and were developed and used mainly on the drug design area. Today, the scope has been broadened to predict any kind of data related to both toxicity and exposure of chemicals i.e. the two categories of data that integrated together should permit the risk assessment of chemicals.

In ecotoxicology, QSAR models are used in the estimation of physico-chemical and effect related properties of chemicals in non-tested endpoints to assess if testing is needed or not.

QSARs are empirical models indicating that the results of evaluated studies are used in the further development of more precise models. The result of this iterative process is that QSARs change over time.

As an example of the scope of the structure-activity based modelling, the following parameters are considered:

- physico-chemical properties
- the partitioning of pesticides among environmental compartments
- bioaccumulation potential

- aquatic toxicity.

One of the main limits of applicability of QSAR is that relationships can only be established, and consequently used as a prediction tool, for compounds with a common mode of toxic action (e.g. cholinesterase inhibitor or photosynthesis inhibitor). This is one of the major problems in the estimation of toxicity: What modes of action are recognised and how is a recognised mode of action assigned to a certain compound, either inferred from measured data such as toxicity dose (concentration)-response (effect) curves, or predicted from structural parameters.

2.2 QSAR modelling

A QSAR model is a mathematical expression that relates the variation of the biological activity in a series of structurally similar compounds to the variation in their chemical structure. Thus, a QSAR model is a mathematical equation describing the activity for a specific class of substances and derived from the quantified measured data belonging to these substances.

The strategy mainly rests on the concept that biological data measured for a few compounds selected may form the basis for a QSAR of a class. The developed QSAR models may permit the estimation of the corresponding missing data for all the non-tested compounds belonging to the class, regardless of their number.

In order to validate the QSAR models, measured and predicted values are compared. The experimental values used in this report are mostly obtained from letters of approval or denial for sale or import given according to the current statutory order from the Danish Ministry of the Environment where information from the applicants are evaluated by the Danish EPA's Pesticide Division. Other major sources of information are the Pesticide Manual (Tomlin 1994, 1997) and Linders ***et al.*** (1994). The experimental values are compared by linear regression analyses with QSAR estimates derived from QSAR models. The QSAR models used are the currently most preferred models.

The QSAR models or mathematical equations have been developed on the basis of experimental data on model substances. During the development of QSAR models, the calculations and testing were performed by using a great number of substances, e.g. high production volume substances or other industrial substances. These industrial substances had mostly simple structures.

QSAR was previously used in the chemical industry in the development of new substances and only within the last decade the models have been refined to the use in assessment of chemical substances effects, fate and behaviour in the environment.

The American Environmental Protection Agency (US-EPA) has developed a system of QSARs which are connected to a database (AQUIRE) and can therefore use the latest evaluated endpoint-values, whether physico-chemical, effect or fate data. This should improve the models as the reliability of model estimations relies on the precision of the input data. The model system is

called ASTER: Assessment Tools for the Evaluation of Risk (Russom 1991, Pedersen ***et al.*** 1995).

The US-EPA has also developed a computer programme for estimating the ecotoxicity of industrial chemicals based on structure activity relationships: ECOSAR. The programme uses specific QSARs for different chemical classes (US-EPA 1994). Because the programme was not complete at the time of this work, it was not used.

The value in using QSARs in the environmental assessment is that in the absence of experimental data employing QSAR may derive the missing variables. Besides, when several experimental studies on the same chemical substance are giving information on single endpoints or parameters which are not complementary or in the same range, the decision on which results to use may be supported by QSAR (TGD 1996).

When applying QSAR, it should be taken into account that a QSAR is an estimation method and therefore, there is a certain probability that the estimate is poor even for well-evaluated models. QSAR model estimates cannot be the only basis for preparing risk assessment. QSAR estimates should be seen as a complementary tool which, evaluated together with test results, can provide a more complete understanding of the physico-chemical and ecotoxicological characteristics of the substance. This means that QSARs are no better than the data on which they are based. Furthermore, it should be noted that QSAR models, generally, only exists for discrete organic substances and not for more complex substances or reaction mixtures.

Thus, QSARs can be used to assist data evaluation

- to contribute to the decision on whether further testing is necessary to clarify an endpoint of concern
- to establish input parameters which are necessary to conduct the exposure or effect assessment.

QSAR models should only be used in risk assessment if the models have been thoroughly evaluated and no experimental data or conflicting validated experimental data exist. As the work on QSAR model development and evaluation is being performed in national and international programmes, the various models change currently.

Environmental risk assessment is based on a comparison of two variables:

- the concentration of the chemical in the environment (exposure)
- the concentration of the chemical at which no adverse effects on the environment are expected or estimated to occur.

Concentration in the environment

Measurements of the actual concentration in the environment are to be preferred. However, in many cases the concentration that can be expected after the release of the chemical in the environment (exposure) is the most interesting issue. Fate modelling techniques may be applied to estimate these expected concentrations.

Fate models require an input of data for the various fate processes, e.g.:

- abiotic degradation (hydrolysis, photolysis, oxidation)

- biodegradation
- adsorption to soil, sediments, suspended particles
- volatilisation, evaporation
- leaching
- bioaccumulation

The rate or equilibrium constants of these fate processes can be measured in the laboratory and technical guidelines are developed to ensure comparable results (e.g. EU 1992, OECD 1993). To ensure a comparable result that can be used in the risk assessment, the laboratory results are used instead of field data where factors affecting the results may be less controllable.

The fate processes determine the extent to which the organisms are exposed to the substance, i.e. the extent to which the chemical is bioavailable.

Several models are developed to predict/estimate the environmental fate processes and based on the physico-chemical parameters. Physico-chemical properties are important data for the exposure analysis.

Especially, a few physico-chemical parameters and variables are observed to be important, i.e.:

- the size and structure of the chemical
- the water solubility
- vapour pressure
- octanol/water partition coefficient (lipophilicity)
- adsorption coefficient.

For a long time, the lipophilicity character has been shown to play a basic role in determining distribution phenomena as well as influencing the mechanisms of ecotoxicity of organic chemicals. The classic procedure for measuring lipophilicity of organic chemicals is based on the partition between octanol and water.

Effect concentration

The concentration, at which a chemical exerts an effect, depends on:

- its toxicokinetic behaviour
- uptake
- biotransformation
- distribution
- excretion/elimination
- its toxicodynamic behaviour
- interaction with receptor target

As in the environment, a number of processes in an organism such as uptake, distribution, biotransformation will determine the concentration of a compound at the target site. In addition, differences in the potency of chemicals to interact with the target will influence the effect concentration.

Conclusion

The development of QSAR is based on the assumption that chemical substances, which reach and interact with a target site by the same mechanism, perform likewise due to their similar chemical properties.

The analysis for QSAR is through regression method affording transparent relations and simple mathematical equations and leading to a quantitative correlation. However, for a meaningful regression analysis, precise and accurate input data are required which tend to limit the number of samples in the testing set. It also means that the data used should be carefully evaluated and not taken from any available handbook unless the data quality is known to be validated (Hart 1991).

3 Pesticides

Pesticides are chemicals that are especially chosen for their ability to affect "unwanted organisms" whether it may be animals, plants, fungi or micro-organisms without affecting non-target organisms. Thus, pesticides are biological active substances or preparations containing one or more substances with a broad range of biocidal activity and often with a specific mode of action.

3.1 Modes of action

It has been observed that chemicals of analogous structures have similar modes of action on the target organism. Dividing such chemicals into chemical classes therefore means that predictions of the mode of action are possible. Pesticides may act by contact or systemic mode of action. A contact action means that the pesticide by contact with the target organisms affects the surface or penetrates the surface to reach the target site. A systemic mode of action means that a pesticide is taken up by an organism and then acts after the uptake (e.g. insecticides taken up by eating or sucking insects from the plants the insecticide has entered).

Below some of the major chemical classes used in pesticides are presented.

Aryloxyalkanoic acids Aryloxyalkanoic acids (phenoxy acids) are selective systemic hormone type herbicides that are absorbed by the leaves and roots and translocated throughout the plant but concentrates in the meristematic regions where it inhibits growth.

Azoles Azoles are fungicides acting as steroid demethylation inhibitor.

Carbamates Carbamates may be herbicides or insecticides. As herbicides, carbamates are systemic herbicides, which are absorbed by the roots, leaves and stem, and translocated to active growth sites (meristems) where it inhibits elongation of roots and aerial parts. Some carbamates are insecticides with contact and stomach action and act as cholinesterase inhibitor.

Dinitroanilines Dinitroanilines are selective soil herbicides, which are absorbed by the roots. Dinitroanilines affect seed germination and prevent plant growth by inhibition of root and shoot development.

Organophosphorous Organophosphorous substances are usually insecticides with contact and stomach action and act as cholinesterase inhibitor affecting the nervous system. Organophosphorous herbicides do exist as selective herbicides, which are absorbed through the roots.

Pyrethroids Pyrethroids are usually non-systemic insecticides with contact action. They cause paralysis initially ("knock-down effect") and may lead to death later. Usually, they are non-phytotoxic.

Sulfonylureas Sulfonylureas are selective systemic herbicides, which are absorbed by the leaves and roots and translocated throughout the plant. Sulfonylureas inhibit the acetolactate synthesis. Plant growth is inhibited followed by the development of chlorotic patches, which spread acropetally and then basipetally.

Triazines Triazines are selective systemic herbicides, which are absorbed by the leaves and roots and then translocated acropetally in the xylem to accumulate in apical meristems. Triazines inhibit photosynthesis and interfere with other enzymatic processes.

Triazoles Triazoles are non-selective systemic herbicides, which are absorbed by the leaves and roots and then translocated in both the phloem and the xylem. Triazoles inhibit the chlorophyll formation and re-growth from buds.

Ureas Ureas are selective herbicides, which are absorbed by the roots and leaves. They inhibit photosynthesis.

3.2 QSAR and pesticides

Most QSARs are based on simple chemical structures and the use on more complex organic molecules which is often the case with pesticides, should be performed with this in mind. However, some studies have been using the QSAR models on pesticides. Generally, most aspects of pesticides are very well documented compared with other chemicals and this should improve the input data quality. However, data on metabolites and degradation products are usually missing and validated QSAR models may present estimates on whether a metabolite or degradation product should be considered for more study or not.

Evaluation of the validity of the latest accepted QSARs is performed by comparing experimental values and the QSAR model estimates using specified models.

The experimental values are based on information from the manufacturers (Tomlin 1994, 1997, Linders ***et al.*** (1994) or letters of approval of plant protection preparations from the Danish-EPA) and a Danish-EPA database (Clausen 1998). It means that data on ecotoxicological effects are based on evaluated and accepted studies.

The QSAR estimations on physico-chemical proportions are performed by programmes developed by Syracuse Research Corporation: MPBPVP, WSKOW, KOWWIN, HENRY, and PCKOCWIN. The programmes are stand-alone programmes but can be run together using the Estimation Programs Interface (EPIWIN) as an interface. The programmes require that the molecular structure be presented as a SMILES notation, cf. 3.2.1.

Fortunately, the programme includes a database where, by using CAS number, the programme itself presents the SMILES notation. If no SMILES notation exists it can relatively easy be performed.

The QSAR estimations on toxicity to aquatic organisms are performed by QSARs recommended in the EU technical guidance document (TGD 1996).

3.2.1 SMILES notation

Simplified Molecular Input Line Entry System (SMILES) is a simple chemical notation system to identify the molecule from its structure by a linear string of symbols. The system has been designed so that a computer can use it. The chemical structure is described from basal symbols and a few rules:

- The SMILES notation can begin at any atom in the molecular structure.
- Hydrogen atoms are not presented.
- Normal atoms are named by capital letters (C, O, N, S, P...) unless they are included in aromatic ring structures.
- Aromatic atoms are named by small letters (c, o, n, s).
- Single bonds are not shown, double bonds as "=" and triple bonds as "#".
- Branches are presented in brackets. A branch cannot begin a SMILES notation but must follow immediately after the atom to which it connects. If an atom has more than one branch, the branches are coded as consecutive pairs of parentheses.
- Ring structures are numbered to identify which atoms that are connected to present the ring structure, e.g. benzene: c1ccccc1, 1,3,5-triazin: c1ncncn1 (Lagersted 1987). More rings are introduced by increasing number.

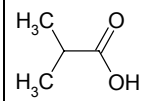
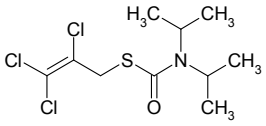
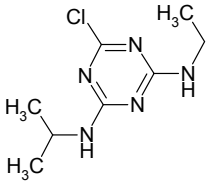
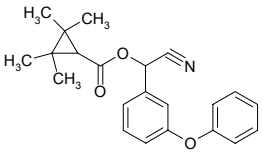
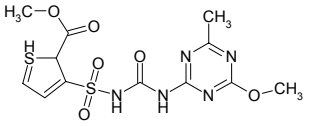
For a more comprehensive introduction to SMILES see to Weininger (1988).

Writing SMILES notation is relatively easy since a SMILES notation depicts a molecular structure as a two-dimensional picture. A single structure can be depicted correctly from different SMILES. This means that there may be more than one correct SMILES notation result if the rules are followed.

More complicated structures, such as some pesticides, may be difficult and time consuming to construct. A few examples have been presented for illustration (table 1).

Table 1
Examples of SMILES notation.

Eksempler på SMILES notation.

Substance	Structure	SMILES
Isobutyric acid		CC(C)C(=O)O or C(C)(C)C(=O)O or OC(=O)C(C)C or O=C(O)C(C)C
Benzene		c1ccccc1
Triallate		CC(C)N(C(C)C)C(=O)SCC(CL)=C(CL)CL
Atrazine		n(c(nc(n1)NC(C)C)NCC)c1CL
Fenpropathrin		C1(C)(C)C(C)(C)C1C(=O)OC (C(#N))c2cccc(Oc3ccccc3)c2
Thifensulfuron-methyl		n1c(C)nc(OC)nc1NC(=O)NS(=O) (=O)c2ccsc2C(=O)OC

3.3 Physico-chemical properties

3.3.1 Boiling point

The boiling point is defined as the temperature at which the vapour pressure of a liquid is equal to the pressure of the atmosphere on the liquid. For pure compounds, the normal boiling point is defined as the boiling point at one standard atmosphere of pressure on the liquid. Besides being an indicator for the physical state (liquid vs. gas) of a chemical, the boiling point also provides an indication of the volatility.

The boiling point is estimated by using the Stein and Brown (1994) method of group contributions that calculates boiling point (BP) of a compound by adding group increment values according to the relationship:

$$BP = 198.2 + \sum n_i g_i$$

Where g_i is a group increment value and n_i is the number of times the group occurs in the compound.

The resulting BP is then corrected by one of the following equations:

$BP(corr) = BP - 94.84 + 0.5577\ BP - 0.0007705\ (BP)^2$ [BP≤700°K]
$BP(corr) = BP + 282.7 - 0.5209\ BP$ [BP>700°K]

The Stein and Brown method was derived from a training set of 4426 organic compounds.

Other methods

Other methods are described in Lyman ***et al.*** (1982) but are either not validated or are using a reduced number of chemicals.

Pesticides

Boiling points for pesticides are usually not available. The available experimental values are either based on studies performed at non-comparable pressures or the substance decomposed before a boiling point was reached. Apparently, most pesticides are estimated to have boiling points in the vicinity of 400ºC according to the Stein and Brown method. The average estimated boiling point and standard deviation was 406 ±102ºC. Results of the estimations are presented in the appendix.

Conclusion

The validity of the estimations could not be evaluated due to the lack of experimental data on pesticide boiling points. Besides the Stein and Brown method, no other estimation method exists that has been validated so extensively or accurately for diverse structures.

3.3.2 Melting point

The melting point is defined as the temperature at which crystals are in equilibrium with the liquid phase at atmospheric pressure. The melting point is an important parameter since it affects the solubility. Solubility controls toxicity by affecting the bioavailability of the substance and the possibility of being transported to the active site within an organism. Primarily intermolecular forces and molecular symmetry holding the molecules in a crystal lattice control the melting point of a compound. The melting point is determined by the strength of the crystal lattice since melting point is a measure of the energy required to disrupt the crystal lattice. In the same way, the solubility can be regarded as a partitioning of the substance between its crystal lattice and the solvent. The melting point tends to increase with molecular size simply because the molecular surface area available for contact with other molecules increases (Dearden 1991).

Meylan and Howard (1994) estimated the melting point by two different methods. The first is an adaptation of the Joback group contribution method for melting point and the second is a simple Gold and Ogle method suggested by Lyman (1985).

The Joback adaptation is an extension of the original method to include the same groups as in the adapted Stein and Brown boiling point method. The Joback method overestimates MP for some structures.

The Gold and Ogle method simply relates melting point (MP) to boiling point (BP) as follows:

$$MP = 0.5839\ BP\ (°K)$$

The computer programme MPBPVP by Meylan and Howard (1994) performs minor evaluations. If the values are close to the model averages, the two estimates are averaged, if not, the programme performs and decides which estimate is more likely to be accurate and presents a "suggested" melting point. Although, the suggested MPBPVP estimates are usually adequate for screening purposes the overall accuracy is not outstanding. The accuracy of the "suggested" value was tested on a 666 compound data set containing a diverse mix of simple, moderately complex compounds and many pesticides and pharmaceutical compounds. MPBPVP estimates yielded a correlation coefficient (r^2) of 0.73. However, even if the estimated melting points can only be used for screening purposes, it seems to be the best method currently available (Meylan and Howard 1994).

Pesticides

Usually, the melting point of pesticides is known. Comparing the experimental melting points of the pesticides including salts and esters used in this study with the MPBPVP suggested melting points performed the correlation presented in figure 1.

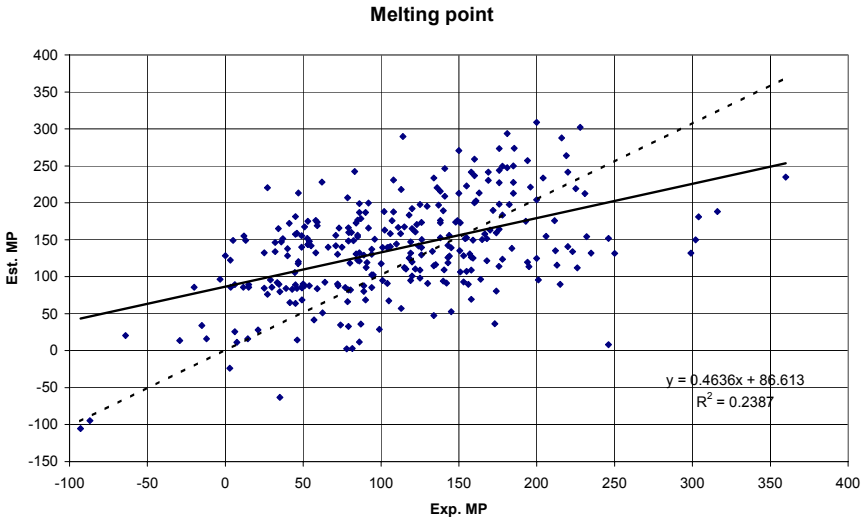


Figure 1
Experimental versus estimated melting points in ºC. The dotted line represents the ideal correlation; i.e. the intercept is set to 0 and the slope to 1. The dark line represents the linear correlation.

Eksperimentelle overfor estimerede smeltepunkter i ºC. Den stiplede linie repræsenterer ideal korrelation, dvs. skæringspunktet er sat til 0 og hældningen til 1. Den ubrudte linie repræsenterer lineær korrelation.

In figure 1, the dotted trend line is placed with the intercept 0 and the slope 1, which represents the ideal situation of a perfect match. The position of the dotted line relative to the marking demonstrates that most estimated values are apparently overestimated for the low experimental values and underestimated for the higher experimental values. The mean±SD value for experimental and estimated melting points was 112±69 and 140±69ºC, respectively.

The correlation between the experimental values from 297 melting points and estimated values indicates that the estimations are inaccurate, as can be seen from the correlation coefficient (r^2 =0.24) presented in the figure .

Conclusion

The correlation between experimental and estimated melting points was low. The method generally overestimated the melting point values for substances with an experimental melting point up to 100ºC. Furthermore it underestimated melting point values for substances with an experimental melting point above 250ºC. Thus, the currently best available method by Meylan and Howard (1994) cannot be used to estimate the melting point of pesticides with a sufficient accuracy in its present form.

3.3.3 Solubility in water

The water solubility reflects the maximum amount of a chemical that will dissolve in pure water at a given temperature. The water solubility is one of the most important physico-chemical properties in ecological hazard assessment and exposure assessment, including environmental fate. The spatial and temporal movement (mobility) of a substance within and between the environmental compartments of soil, water and air depends largely on its solubility in water. The knowledge of the solubility in water is essential when estimating biological degradation, bioaccumulation, hydrolysis, adsorption and the partition coefficient octanol/water. Highly water-soluble chemicals are potentially easier distributed by the hydrologic cycle, as they tend to have relatively low adsorption coefficients (i.e. low adsorption to soil and sediment).

As the term “insoluble” is sometimes seen in handbooks it must be emphasised that no organic chemical is completely insoluble in water. All organic chemicals are soluble to some extent. The range observed in pesticides is usually between µg/l to g/l. In a few instances, it may be even lower and some are infinitely soluble, i.e. total miscible with water.

Several approaches to estimate the water solubility have been developed (Lyman ***et al.*** 1982, Yalkowky and Banerjee 1992). Yalkowsky and Banerjee (1992) have reviewed most of the recent literature where a variety of estimation methods are available. The methods involve the application of group activity coefficients, partition coefficients, chromatographic parameters, boiling point, molecular volume, molecular surface area, molecular connectivity, parachor, solubility parameters, UNIFAC, linear solvation energy and multivariate statistical methods. After critical evaluation of the available methods in terms of range of applicability, accuracy, ease of use and strength of underlying theory, Yalkowsky and Banerjee (1992) concluded that only two methods could be considered for universal application:

- group activity coefficient techniques which include group contribution fragment methods
- correlations based upon log Kow.

Group activity coefficient method

The group activity coefficient method is demonstrated with the group contribution approach of Wakita ***et al.*** (1986) that derived the following equations for:

Liquids:	$\log S = -0.957 \sum f_i - 0.048$	(n=307, r=0.982, sd=0.245)
Solids:	$\log S = -0.963 \sum f_i - 0.208$	(n=112, r=0.986, sd=0.410)

Where $\sum f_i$ is the summation of all applicable fragment values. The fragment values are derived from experiments starting with small molecules and

increasing the molecular structure with known atoms or functional groups and calculate the contribution from each change in the molecular structure. The Wakita method was fairly accurate for its training set, which primarily consisted of hydrocarbons and simple monofunctional compounds. When applied to a test set of pesticides and drugs, the accuracy was reduced: standard deviation (S.D.) = 1.05 (Yalkowsky and Banerjee 1992).

Correlations using log Kow

At present, the most practical method to estimate water solubility involves regression derived correlations using log Kow. Most of the highly water-soluble substances show low log Kow values. Several correlations have been developed depending on the applied chemicals used in the calculations. Eighteen different regression equations that correlate water solubility to log Kow have been found in the literature (Lyman ***et al.*** 1982, Isnard & Lambert 1989). Only the two equations, which include pesticides, are shown below:

Lyman et al. 1982

log S (mg/l) =	-0.922 log Kow + 4.184	(n=90, r^2=0.740)
log S (µmol/l) =	-1.49 log Kow + 7.46	(n=34, r^2=0.970)

Some equations include the melting point (MP) for solids. For liquids, the MP is set to 25°C which zeroes out the melting point parameter.

Isnard and Lambert (1989) performed a correlation on 300 substances (166 liquids and 134 solids) including some pesticides and obtained following correlations where log S is the logarithm to the water solubility and MP is the melting point:

Isnard and Lambert 1989

log S (mg/l) = 6.05 - 1.29 logKow	(n=300, r=0.964, sd=0.631)
log S (mg/l) = 5.90 - 1.18 logKow - 0.0048(MP-25)	(n=300, sd=0.560)
or	
log S (mol/m^3) = 4.17 - 1.38 logKow	(n=300, r=0.965, sd=0.665)
log S (mol/m^3) = 4.00 - 1.26 logKow - 0.0054(MP-25)	(n=300, sd=0.582)

The two latter equations were recommended for liquids and solids in OECD (1993b). The equations can be changed to give the result in mol/l:

log S (mol/l) = 1.17 - 1.38 log Kow

log S (mol/l) = 1.0 - 1.26 log Kow - 0.0054 (MP -25)

Meylan and Howard (1994) have developed a QSAR model on water solubility where the water solubility in mol/l is estimated based on log Kow with and without a melting point. The first equation was developed based on a validation set of 85 substances with an experimental log Kow and water solubility values but with no available melting point. The second validation set included 817 compounds with measured water solubility and melting points.

The Meylan and Howard equations are shown below:

Meylan and Howard 1994

$$\log S \text{ (mol/l)} = 0.796 - 0.854 \log Kow - 0.00728MW + cf \quad (n=85, r^2=0.865, sd=0.961)$$

$$\log S \text{ (mol/l)} = 0.693 - 0.96 \log Kow - 0.0092(MP-25) - 0.00314MW + cf \quad (n=817, r^2=0.902, sd=0.615)$$

Where MW is the molecular weight, MP is the melting point and "cf" the correction factor. Knowledge of the melting point reduces the standard deviation and improves the correlation coefficient and this model should be used when a measured melting point is available. The melting point is only used for solids. The correction factor is applied to 15 structure types (e.g. alcohols, acids, selected phenols, amines, amino acids, etc). The calculations of the Meylan and Howard QSAR model can be performed on computer (WS-KOW, Syracuse, Meylan and Howard 1995).

Pesticides

Performing a correlation between the experimental water solubility from 377 pesticides and the result of Meylan and Howard computerised version (WSKOW) is presented in figure 2 using log values. The logarithmic values ($\log_{10}$) are used to reduce the range and to make the values comparable.

For a perfect match, the intercept should be 0 and the slope 1. If the estimated values were overestimated the values should be above the trend line with a slope of 1 and intercept 0. Such a trend line would be close to the linear regression line presented in figure 2 that had a slope of 0.8.

Performing regression between the experimental water solubility values and the values estimated using the computerised WSKOW model with melting point resulted in a correlation coefficient r^2 of 0.65. It is a poorer result than found by the training set used by Meylan and Howard (1994) but considering the wide diversity of the included pesticides the result cannot be considered unacceptable for a first estimate.

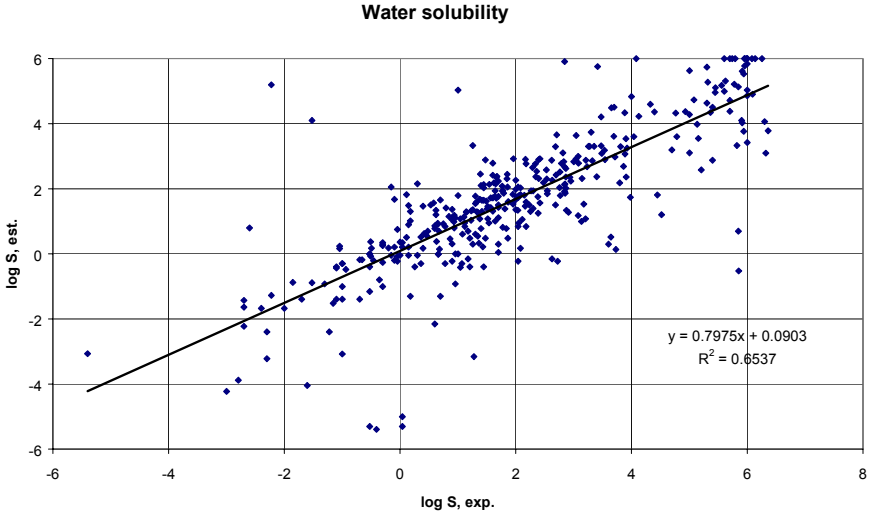


Figure 2
Correlation between the logarithm to the experimental water solubility and the logarithm to the estimated water solubility.

Korrelation mellem logaritmen til eksperimentel vandopløselighed og logaritmen til estimeret vandopløselighed.

Based on the measured water solubility and log Kow values from 322 pesticides, a linear regression analysis was performed. Figure 3 presents the result graphically.

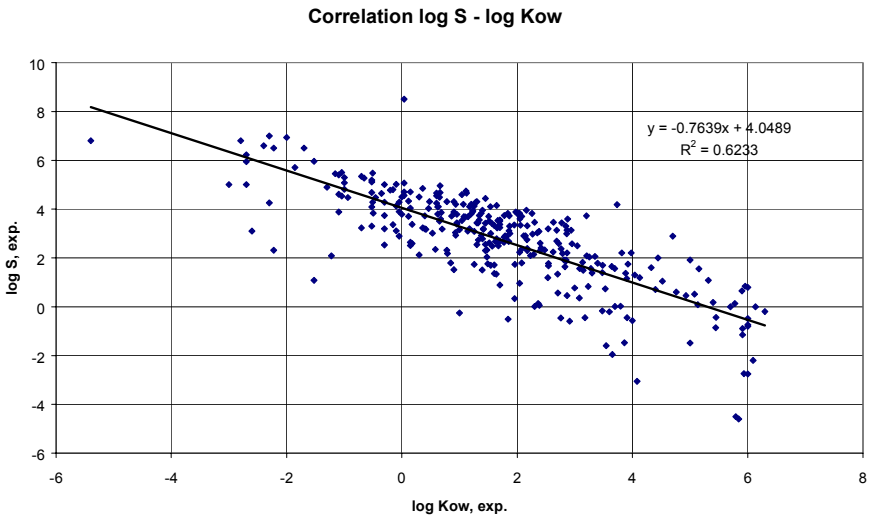


Figure 3
Correlation between the logarithm to the measured water solubility and log Kow.

Korrelation mellem logaritmen til målt vandopløselighed og log Kow.

The resulting correlations using mg/l (figure 3) or recalculating the solubility data to mmol/l were:

log S (mg/l) = -0.7639 log Kow + 4.0489 (n= 322, r^2=0.6233)
log S (mmol/l) = -0.844 log Kow + 1.5683 (n= 322, r^2=0.6245)

The result of the correlation seems relatively poor and no improvement was obtained by including the molecular weight. However, considering the variation in chemical classes etc. the result is not unacceptable. It should also be considered that the experimental data are based on temperatures varying from 20 to 25ºC whereas the estimated water solubility are estimated at 25ºC. Figure 3 also demonstrates the negative correlation between water solubility and octanol/water partition coefficient (lipophilicity).

Conclusion

The estimations of water solubility was reasonable acceptable using the selected computerised QSAR model although the correlation coefficient for pesticides was smaller than for the data used to develop the model. A linear regression analysis based on log water solubility and log Kow of the pesticides used in this report resulted in a QSAR model with an almost identical correlation coefficient. Thus, both methods may be used with the same degree of uncertainty.

3.3.4 Vapour pressure

The vapour pressure is defined as the pressure at which a solid is in equilibrium with its own vapour. The vapour pressure is a chemical specific property, which is important in evaluating the behaviour and fate of a pesticide in the environment. Especially, when evaluating the distribution into the environmental compartments soil, air and water and its persistence in the

compartments. Experimental or estimated vapour pressures given in mmHg or atm. are recalculated to Pa in this report.

Numerous equations and correlations for estimating vapour pressure are presented in the literature. They normally require information on:

- the critical temperature
- the critical pressure
- the heat of vaporisation
- the vapour pressure at some reference temperatures

The vapour pressure is estimated by three methods:

- the Antoine method (Lyman ***et al*** 1990)
- the modified Grain method (Lyman 1985)
- the Mackay method (Lyman 1985).

All three methods use the normal boiling point to estimate the vapour pressure.

The Antoine method

The Antoine method was developed for liquids and gases. The method is described in detail in Lyman ***et al.*** (1990). The general equation is:

$$\ln VP = [(\Delta H_{vb} (BP-C_2)^2) / (\Delta Z_b R BP^2)] * [1/(BP-C_2) - 1/(T-C_2)]$$

Where ΔH_{vb} is the heat of vaporisation at the boiling point (cal/mol)
BP is the temperature of the normal boiling point in ºK
C_2 is a constant estimated to be = -18 + 0.19BP
T is the temperature in ºK
ΔZ_b is assumed to have the value of 0.97.
R is the gas constant = 1.987 cal/mol × K

The modified Grain method

The modified Grain method is described in Lyman (1985). The method is a modification of the modified Watson method. It is applicable for solids, liquids and gasses. The method converts super-cooled liquid vapour pressure to a solid phase vapour pressure. It is probably the best all round VP estimation currently available (Meylan and Howard 1994) and is used by US-EPA in the PC-CHEM programme.

Mackay method

Mackay derived the following equation to estimate the vapour pressure:

$$\ln VP = - (4.4 + \ln BP)[1.803(BP/T-1) - 0.803 \ln (BP/T)] - 6.8 (MP/T-1)$$

The equation includes the boiling point (BP), the melting point (MP) and the temperature (T) in ºK. The melting point is ignored for liquids. Since the boiling point was usually unknown to pesticides, the method was not applicable.

MPBPVP

The computer estimations made by MPBPVP (Meylan and Howard 1994) report all three methods and a "suggested" value. For solids, the suggested vapour pressure is the modified Grain estimate. For liquids and gasses, the average of the Antoine and the modified Grain method is suggested. The Mackay method is not used, as it is limited to its derivation classes: hydrocarbons and halogenated compounds (both aliphatic and aromatic).

Using a data set of 805 compounds, a correlation coefficient (r^2) of 0.941 and a standard deviation, S.D., of 0.717 were observed.

Pesticides

For the pesticides, a linear regression analysis has been performed using log transformation due to the large variation in the experimental vapour pressure values. The result is presented graphically in figure 4.

The experimental vapour pressure values and values estimated by the model MPBPVP and presented as suggested values (Meylan and Howard 1994) were not well correlated for pesticides. The correlation coefficient r^2 was 0.46 for n = 308. The deviations seem to increase at decreasing vapour pressures. The reason for the low correlation coefficient may be the relatively few outliers. However, removing the outliers did not significantly improve the result.

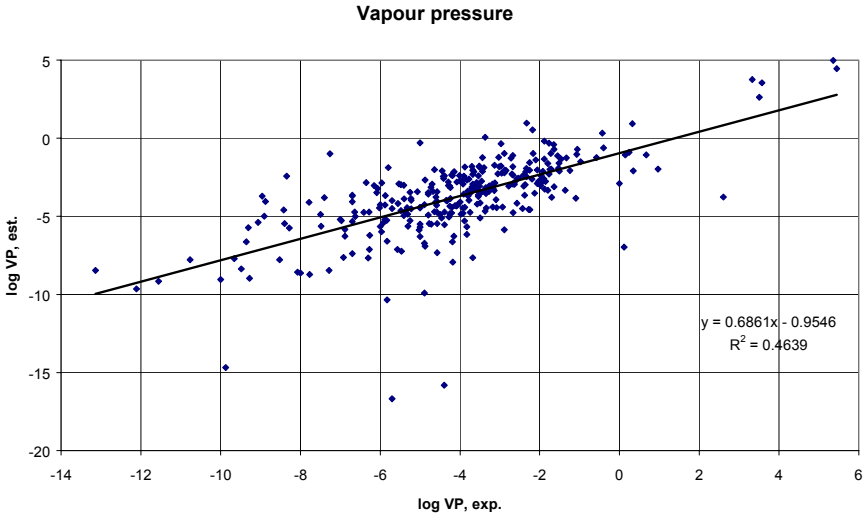


Figure 4
Correlation between the experimentally reported vapour pressure and the model-estimated vapour pressure (both logarithmic).

Korrelation mellem eksperimentelt rapporteret damptryk og model-estimeret damptryk (begge logaritmiske).

Conclusion

Generally, the presented QSAR model was not able to perform a sufficient close correlation of experimental and estimated vapour pressures from the included pesticide data set. However, the main part of the substances is relatively well correlated and the estimation method may be considered sufficient for a first estimate.

3.3.5 Henry's Law constant

Henry's constant is the ratio of chemical concentration in air to the concentration in water, when those two phases are in contact and are at equilibrium. The partitioning between water and air is a physical property that is described by the Henry's Law constant, H. The magnitude of H provides an indication of which of the two phases a chemical will tend to partition into at equilibrium. Henry's Law constant can be estimated from:

H = Vapour pressure x Molecular weight / Water solubility [Pa m^3/mol]

H can also be expressed as the ratio of the concentration in air and water, called the "dimensionless" H, H', where:

H' = concentration in air / concentration in water, i.e.
H' = $k_{air\text{-}water}$ = H / (gas constant (8.314) x temperature (ºK))

Where $k_{air\text{-}water}$ is the air-water partition coefficient.

QSAR models

QSAR estimations of H are based on a combination of connectivity indices and calculated polarisability (Nirmalakhandan and Speece 1988). A narrow range of chemical types was used to develop the method, which is not widely applicable.

QSARs based on group and bond contributions are developed from experimentally measured log $K_{air\text{-}water}$ values, when available. The methods of Hine and Mokerjee (1975) have been further developed and are now available in PC programme (HENRY in EPIWIN, Meylan and Howard 1992).

Compounds with large structures, which include many different types of bonds and groups, may have significant inaccuracies in their estimations.

Pesticides

For the pesticides in this project, no measured Henry's Law constants were available. It was decided to compare the computerised estimation with the calculated H values using:

H = VP (Pa) * MW (g/mol) / S (mg/l) [Pa m^3/mol]

This is the preferred estimation method when reliable measured data on vapour pressure and water solubility are available (Meylan and Howard 1991). In the PC-model, the group estimation methods were usually presenting the message "incomplete" in the estimation programme and therefore the bond contribution method was applied in the estimations (Meylan and Howard 1991).

The regression analysis between the calculated H and the H estimated by bond contribution method is shown graphically in Figure 6 and resulted in a correlation coefficient r^2 of 0.43 (n= 308). The results of the bond contribution method are relatively underestimated compared with the calculated values.

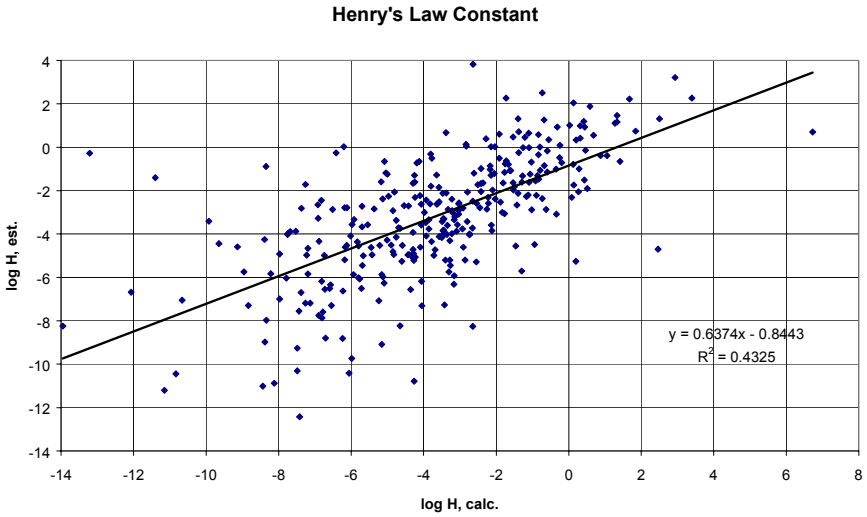


Figure 5
Correlations between Henry's Law constant calculated and estimated by structure analysis in HENRY PC-model (Meylan and Howard 1992).

Korrelation mellem Henrys Lov konstant beregnet og estimeret ud fra strukturanalysen i HENRY Pc-modellen (Meylan and Howard 1992).

No conclusion can be drawn from the used pesticide data set since values estimated by calculation and by computer model are not necessarily correct for the pesticide in question. It can be concluded that the two estimation methods are presenting comparable results with estimated H being slightly above calculated H below log H -2 and slightly above the calculated H above log H -2.

3.3.6 Octanol/water partition coefficient (Kow)

Hydrophobicity is one of the key parameters in QSARs for environmental endpoints. The property is usually modelled by the n-octanol/water partition coefficient (Kow) which is an established laboratory method to measure the hydrophobicity of a chemical. As such, Kow or log Kow is a key parameter in the assessment of environmental fate and the bioaccumulation potential. Kow has been found to be a good predictor for relatively non-specific processes. For instance, many distribution processes are found to be related to Kow, e.g. sorption to soil and sediment, partitioning into air and bioconcentration, and non-specific toxicity. This especially relates to non-polar organic chemicals. When more polar chemicals and more specific processes such as degradation, biodegradation and specific toxic interactions are the subject, other kinds of interactions (stereo-electronic) become more relevant (EEC report 1995).

The octanol/water partition coefficient is the ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of a two-phase system at equilibrium. Thus, the two-phase system consists of octanol as the non-polar solvent and water as the polar solvent. Since measured values range from below 10^{-4} to more than 10^{8}, the logarithm (log Kow) is normally used to characterise its value.

The literature contains several methods for estimating log Kow. The most common method for the estimation of Kow is based on fragment constants.

The fragmental approach is based on simple addition of the lipophilicity of the individual molecular fragments of a given molecule, i.e. atoms or larger functional groups. The most widely used fragment constant method was proposed by Hansch and Leo (1979) and initially computerised for use by Chou and Jurs in the CLOGP programme (Daylight Chemical Information Systems, New Orleans). The fragment constant method consists of determining the log Kow values of a set of small molecules very accurately and then calculating "fundamental" chemical fragments from these values. The method uses single atom "fundamental" fragments consisting of isolated carbons or a hydrogen or hetero-atom plus multiple atom fundamental fragments, e.g.-CN, and a large number of correction factors. Other methods have been developed but have, at present, not proven to be acceptable as a general estimation method (Meylan and Howard (1995). Meylan and Howard (1995) have evaluated 10 different methods and concluded that CLOGP and the AFC methods (cf. below) are the best comprehensive predictors currently available.

A major problem with most fragment constant approaches is their inability to estimate log Kow for a structure containing a fragment that has not been correlated.

Meylan and Howard (1995) have developed a new fragment constant approach, the atom/fragment contribution (AFC) method which was developed by multiple linear regressions of reliable experimental log Kow values. The regressions were performed in two stages: The first regression correlated atom/fragment values with log Kow and the second correlated correction factors. The log Kow is then estimated by summing up the values from a structure.

In general, each non-hydrogen atom, e.g. carbon, nitrogen, oxygen, sulphur, in a structure is a core for a fragment and the exact fragment is determined by what is connected to the atom. The result of the atom and/or fragment regression was:

$$\log Kow = \sum(f_i n_i) + 0.229 \qquad (n=1120,\ r^2=0.98,\ SD=0.22)$$

Where $\sum(f_i n_i)$ is the summation of f_i (the coefficient for each atom or fragment) times n_i (the number of times the atom/fragment occurs in the structure).

The general equation for estimating log Kow of any organic compound is

$$\log Kow = \sum(f_i n_i) + \sum(c_j n_j) + 0.229 \qquad (n=2351,\ r^2=0.982,\ SD=0.216)$$

Where $\sum(c_j n_j)$ is the summation of c_j (the coefficient for each correction factor) times n_j (the number of times the correction factor occurs or is applied in the structure).

Examples

Three calculation examples using pesticides are presented

Simazine

Simazine is a herbicide belonging to the triazines and has the molecular structure presented below:

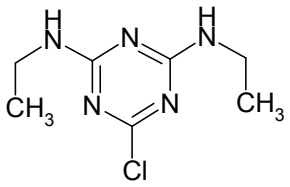


Table 2
Simazine, structure fragment analysis used to calculate log Kow.

Simazin, strukturfragmentanalyse anvendt til beregning af log Kow.

Fragment:	Coefficient	Frequency	Value
-CH_3	0.5473	2	1.0946
-CH_2	0.4911	2	0.9822
Aromatic carbon	0.2940	3	0.8820
Aromatic nitrogen	-0.7324	3	-2.1972
-N (one aromatic attachment)	-0.9170	2	-1.8340
-Cl (aromatic attachment	0.6445	1	0.6445
Correction factors:			
Symmetric triazine ring correction	0.8856	1	0.8856
Amino type triazine	0.8566	2	1.7132
Equation constant			0.2290
log Kow =			2.3999

Simazine has an experimental log Kow of 2.18. Based on structure fragment analysis the log Kow was estimated to be 2.40.

Thiodicarb

Thiodicarb is an insecticide belonging to the oxime carbamates and has the molecular structure:

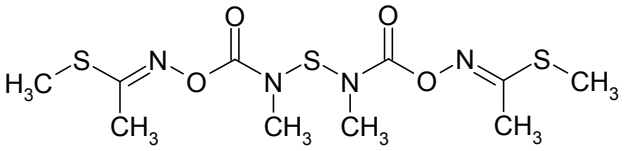


Table 3
Thiodicarb, structure fragment analysis used to calculate log Kow.

Thiodicarb, strukturfragmentanalyse anvendt til beregning af log Kow.

Fragment:	Coefficient	Frequency	Value
-CH_3	0.5473	6	3.2838
C (no hydrogens)	0.9723	2	1.9446
-N< (aliphatic attachment)	-1.8323	2	-3.6646
-ON (nitrogen attachment)	0.2352	2	0.4704
OC(=O)N (carbamate type carbonyl)	0.1283	2	0.2566
-N=C (aliphatic attachment)	-0.0010	2	-0.0020
-SC= (aliphatic C=)	-0.1000	2	-0.2000
-S- (two nitrogen attachments)	1.2000	1	1.2000
Correction factors:			
Di-N-aliphatic substituted carbamate	0.1984	2	0.3968
>C=NOC(=O)-	-1.0000	2	-2.0000
Equation constant			0.2290
log Kow =			1.9146

Thiodicarb has an experimental log Kow of 1.70. Based on structure fragment analysis the log Kow was estimated to be 1.91.

Thifensulfuron-methyl

Thifensulfuron-methyl is a herbicide belonging to the sulfonylureas. It has the molecular structure shown below.

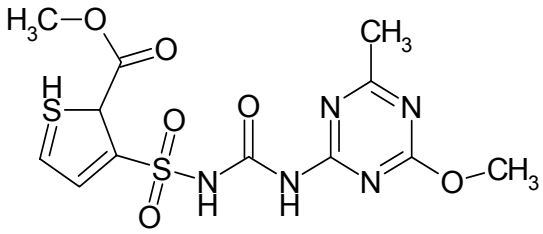


Table 4
Thifensulfuron-methyl, structure fragment analysis used to calculate log Kow.

Thifensulfuron-methyl, strukturfragmentanalyse anvendt til beregning af log Kow.

Fragment:	Coefficient	Frequency	Value
-CH_3	0.5473	3	1.6419
-NH (aliphatic attachment)	-1.4962	1	-1.4962
Aromatic carbon	0.2940	7	2.0580
Aromatic nitrogen	-0.7324	3	-2.1972
-N (one aromatic attachment)	-0.9170	1	-0.9170
-O- (one aromatic attachment)	-0.4664	1	-0.4664
Aromatic sulphur	0.4082	1	0.4082
-C(=O)O (ester, aromatic attachment)	-0.7121	1	-0.7121
-SO_2N (aromatic attachment)	-0.2079	1	-0.2079
-NC(=O)N- (urea type)	1.0453	1	1.0453
Correction factors:			
Symmetric triazine ring correction	0.8856	1	0.8856
Amino type triazine	0.8566	1	0.8566
Alkyloxy ortho to two nitrogens	0.8955	1	0.8955
-NC(=O)NS on triazine	-0.7500	1	-0.7500
Equation constant			0.2290
log Kow =			1.2733

Thifensulfuron-methyl has an experimental Kow of 1.6 at pH 5 and a Kow of 0.02 at pH 7.

The deviation demonstrates that the method results are “ion-corrected” for compounds that have log Kow values that vary with pH. The log Kow correction for ionisation is calculated as:

$$\log Kow_{corrected} = \log Kow_{pH} + \log(1+10^{pH-pKa}).$$

Thifensulfuron-methyl has a pKa value of 4.0. This would result in a corrected Kow at pH 7 = log (0.02) + log ($1+10^{7-4}$) = log 1.3.

Pesticides

Performing a correlation between 327 pesticides, an overestimation seems to be the case for pesticides of low experimental Kow values. In figure 6, the trend line with the intercept 0 and the slope 1 would be almost identical to the linear regression line that had the slope 0.87. Thus, the correlation is close to represent the ideal correlation.

A linear regression analysis between the experimental log Kow and the estimated log Kow gave a correlation coefficient r^2 of 0.72 (n = 327) (figure 6) which is sufficient close for predictive purposes.

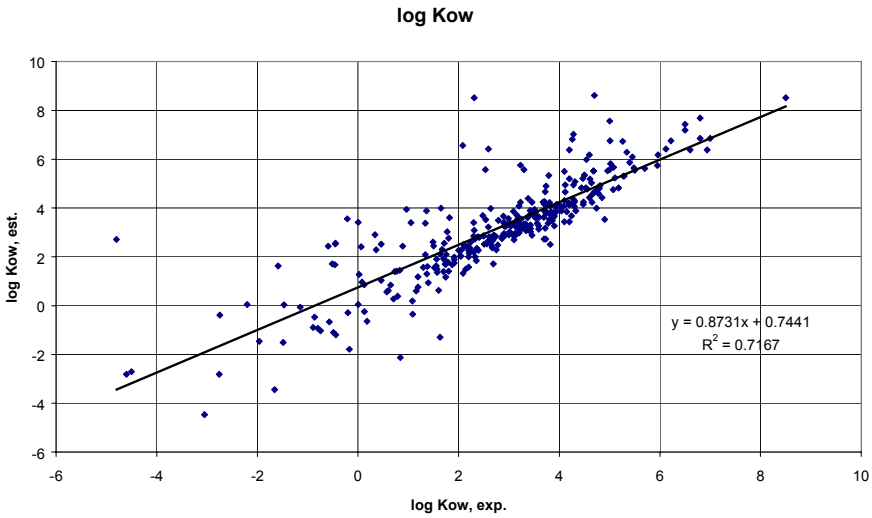


Figure 6
Correlation analysis between the experimental log Kow and the estimated log Kow.

Korrelationsanalyse mellem den eksperimentelle log Kow og den estimererede log Kow.

Some derivation may arise from imprecise or incorrect log Kow's or from "ionised" substances (cf. the thifensulfuron-methyl example above). However, the results are accurate enough to be used for the estimation on related chemical compounds, e.g. pesticide degradation and/or transformation products. Concerning the pesticide active substance itself, there should always be an evaluated measured value present and the value should consider different pH if the substance is depending on pH (Ribo 1988). This is especially important since the log Kow is an essential part of most predicting methods on adsorption, toxicity etc.

Very often several log Kow values may be found even as experimental data obtained from laboratory methods performed according to accepted guidelines (reverse phase HPLC, "shake-flask", "slow stirring method" etc). In such cases, QSAR models may be used in evaluating which value to decide on.

The method is, however, not recommendable for manual calculations since 130 fragments and 235 correction factors are included. The PC versions of the methods AFC or CLOGP are recommended instead.

Log Kow estimated from water solubility

Based on the selected pesticides in this report, a QSAR for manual calculation of an estimated log Kow based on water solubility can be suggested.

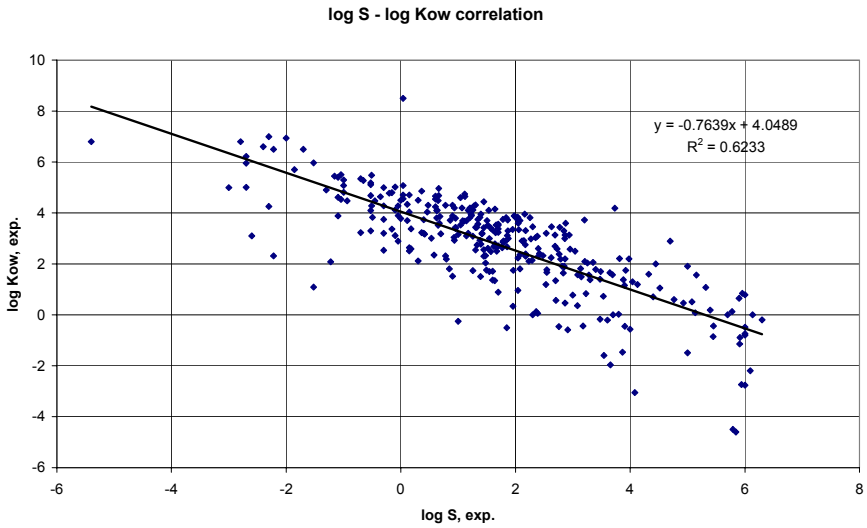


Figure 7
Correlation between experimental water solubility (mg/l) and log Kow.

Korrelation mellem eksperimentel vandopløselighed (mg/l) og log Kow.

Performing linear regression between the measured water solubility either as mg/l or mmol/l and log Kow resulted in the equations:

log Kow = - 0.7639 log S (mg/l) + 4.0489 (n=322, r^2 = 0.6233)
log Kow = - 0.7322 log S (mmol/l) + 2.2024 (n=322, r^2 = 0.6229)

The correlation coefficient was 0.62 which is reasonable acceptable for predictive purposes.

Conclusion

The octanol/water partition coefficient log Kow could be reasonably well estimated from the QSAR models based on structure fragment analysis. The method is complicated and recommended to be performed by available computer models. However, an alternative QSAR model may be used based on water solubility. For the pesticides used in this report, it resulted in a lower correlation coefficient but if the computerised model is not available the method should be sufficient in a screening procedure.

3.3.7 Sorption

The sorption (adsorption/desorption) to soil and sediments is a determining factor for the mobility of chemicals. This property also contributes to the distribution among soil, sediment and water phases, volatilisation from soil surfaces, and bioavailability. The extent of soil and sediment sorption is governed by a variety of physico-chemical properties of both the soil/sediment and the chemical, e.g. organic carbon content, clay content, humidity, pH value, cation exchange capacity, temperature, etc.

The sorption of non-polar substances may be regarded as a distribution process between the polar phase of the soil water and the organic phase of the soil component. The equilibrium constant of this partitioning between solid and solution phase constitutes the adsorption coefficient for soil and sediments. The sorption coefficient is defined, at steady state, as:

Kd = Concentration of chemical sorbed to soil / Mean concentration in aqueous solution.

As the organic fraction is the principal interaction site for hydrophobic compounds, a partition coefficient normalised for the content of organic carbon (OC) is used to reduce the variance of sorption coefficients:

Koc = (Kd/OC%) 100

The remaining variation may be due to other characteristics of soils (clay content, clay composition, surface area, cation exchange capacity, pH, etc.), the nature of the organic matter present and/or variation in the test methods. Numerous studies of the correlation of adsorption coefficient with these variables found that the organic carbon content usually gave the most significant correlations (Stevenson 1976).

Soil adsorption coefficients may be reported on a soil-organic matter basis (Kom). Since the organic carbon content of a soil can be measured more directly, reporting values as Koc are preferred. The ratio of organic matter to organic carbon varies from soil to soil but a value of 1.724 is often assumed when conversion is necessary, i.e. Koc =1.724 Kom (Lyman ***et al.*** 1990) based on an organic carbon content of 58% in organic matter.

Since Koc is accepted as essential in the evaluation of pesticides, many different procedures for estimating Koc have been developed. One general method correlates Koc with R_f-values obtained from soil thin-layer chromatography tests. Various authors have shown a reasonable good correlation between these properties but gave no regression equation (Briggs 1973, Hance 1967, Lambert 1968) or required an additional parameter (pore fraction of the soil (Hamaker 1975)). Briggs (1969) described a correlation between Koc and the Hammet and Taft energy constants for phenylureas but without presenting a regression equation.

Other factors affect the measured value of Koc under actual environmental conditions besides the differences in laboratory procedures (Lyman 1990):

- temperature
- pH of soil and water
- particle size distribution and surface area of solids
- concentration of dissolved organic matter in water
- non-equilibrium adsorption mechanisms or failure to reach equilibrium conditions
- solids to solution ratio
- loss of chemical due to volatilisation, degradation, adsorption to test flask walls etc.
- non-linear isotherm
- time factor

Temperature

Temperature may affect the measured values since adsorption is an exothermic process. Values of Koc usually decrease with increasing temperature.

pH of soil and water

Chemicals that tend to ionise are much affected by pH. Weak acids and weak bases show the greatest sensitivity to pH changes in the range normally met in soil and surface waters (pH 5 to pH 9).

Particle size distribution and surface area of solids The fine silt and clay fraction of soil and sediments may have a great tendency to absorb chemicals. The different clay fractions have different adsorptive capacities.

Non-equilibrium adsorption Non-equilibrium adsorption may occur when a chemical moves through an environmental compartment so rapidly that equilibrium conditions cannot be achieved.

Solids to solution ratio Changes in the water content of a soil or sediment will change the fraction of chemical that is adsorbed. As the water content is lowered, the fraction adsorbed will increase as the concentration in solution does.

Loss of chemical The chemical may be lost during the test due to volatilisation, degradation, adsorption to test flask walls etc. if this is not considered.

Non-linear isotherm If the adsorption isotherm is non-linear, the reported value of Koc will depend on the range of chemical concentrations used in the tests.

Time factor The time for the chemicals to adsorb/desorb varies depending on conditions, substance properties etc.

Models Several compilations of QSAR models for soil sorption are published in the literature. All of the available methods for estimating Koc involve empirical relationships with some other property of the chemical:

- water solubility
- octanol/water partition coefficient (Kow)
- bioconcentration factor etc.

Most models are based on Kow because hydrophobic interactions are the dominant type of interactions between non-polar substances and soil organic carbon. However, chemicals with more polar groups may interact by other types of interaction. It is therefore obvious that not one single model accurately predicts soil sorption coefficients and that different models should be used depending on which class of chemicals that the specific compound belongs to.

Some of the models/equations have been developed from training sets of insecticides, herbicides and fungicides or compounds of related structure. The relationships are regression equations usually expressed in the log-log form:

log Koc = a log (S, Kow, or BCF) + b

Where “a” and “b” are constants.

Examples of QSARs developed for estimating log Koc from experimental data on water solubility, log Kow and bioaccumulation factor BCF are given in Lyman ***et al.*** (1982) and presented in table 5 for different chemical classes.

The second equation in table 5 was derived from pesticides (Kenaga 1980). Individual results estimated for the pesticides selected for this report can be found in the appendix under the heading ”Koc, Lyman, est”.

Table 5
Estimation of Koc (Lyman et al. 1982).

Estimering af Koc (Lyman et al. 1982).

Chemical classes	Equation	n	r^2
Variable, mostly pesticides	log Koc = -0.55 log S + 3.64	106	0.71
Variable, mostly pesticides	log Koc = 0.544 log Kow + 1.377	45	0.74
Aromatics, polynuclear aromatics, triazines and dinitroanilin herbicides	log Koc = 0.937 log Kow - 0.0006	19	0.95
s-triazines and dinitroaniline herbicides	log Koc = 0.94 log Kow + 0.02	9	NA
Variety of insecticides, herbicides and fungicides	log Koc = 1.029 log Kow - 0.18	13	0.91
Substituted phenylureas and alkyl-N-phenylcarbamates	log Koc = 0.524 log Kow + 0.855	30	0.84
Variable, mostly pesticides	log Koc = 0.681 log BCF + 1.886	22	0.83

S: water solubility in mg/l. NA: not available. n: number. r^2: correlation coefficient.

The EU Technical Guidance Document (TGD 1996) for risk assessment presents 19 equations to estimate log Koc in soil and sediment for different chemical classes. The 19 QSAR models were developed by Sabljic ***et al.*** (1995). For values of log Kow, evaluated and recommended log Kow values (known as LOGPSTAR data) or reliable ClogP data were used. For log Koc, data from two literature compilations of soil sorption coefficients were used and median values when several measured Koc values were available (Sabljic ***et al***. 1995). The soil sorption data used in Sabljic ***et al.*** (1995) were determined for non-ionic species of respective chemicals and thus, the QSAR models presented in the table 6 will be applicable only for non-ionised chemicals:

Table 6
List of derived QSAR models for soil sorption with their chemical domains (Sabljic et al. 1995).

Liste over udledte QSAR modeller til estimering af adsorption med deres kemiske områder (Sabljic et al. 1995).

Chemical class	Regression equation	n	r^2	SE
Predominantly hydrophobics	log Koc = 0.81 log Kow + 0.10	81	0.89	0.45
Nonhydrophobics	log Koc = 0.52 log Kow + 1.02	390	0.63	0.56
Phenols, anilines, benzonitriles, and nitrobenzenes	log Koc = 0.63 log Kow + 0.90	54	0.75	0.40
Acetanilides, carbamates, esters, phenylureas, phosphates, triazines, triazoles, and uracils	log Koc = 0.47 log Kow + 1.09	216	0.68	0.43
Alcohols and organic acids	log Koc = 0.47 log Kow + 0.50	36	0.72	0.39
Acetanilides	log Koc = 0.40 log Kow + 1.12	21	0.51	0.34
Alcohols	log Koc = 0.39 log Kow + 0.50	13	0.77	0.40
Amides	log Koc = 0.33 log Kow + 1.25	28	0.46	0.49
Anilines	log Koc = 0.62 log Kow + 0.85	20	0.82	0.34
Carbamates	log Koc = 0.365 log Kow + 1.14	43	0.58	0.41
Dinitroanilines	log Koc = 0.38 log Kow + 1.92	20	0.83	0.24
Esters	log Koc = 0.49 log Kow + 1.05	25	0.76	0.46
Nitrobenzenes	log Koc = 0.77 log Kow + 0.55	10	0.70	0.58
Organic acids	log Koc = 0.60 log Kow + 0.32	23	0.75	0.34
Phenols and benzonitriles	log Koc = 0.57 log Kow + 1.08	24	0.75	0.37
Phenylureas	log Koc = 0.49 log Kow + 1.05	52	0.62	0.34
Phosphates	log Koc = 0.49 log Kow + 1.17	41	0.73	0.45
Triazines	log Koc = 0.30 log Kow + 1.50	16	0.32	0.38
Triazoles	log Koc = 0.47 log Kow + 1.405	15	0.66	0.48

n: Number of substances. r^2: Correlation coefficient. SE: Standard error.

In table 6, predominantly hydrophobics were in this context defined as compounds that contain only carbon, hydrogen and halogen atoms (i.e. C, H, F, Cl, Br, I). Nonhydrophobics were are all the chemicals not defined as predominantly hydrophobic. It means that the definition was based on molecular structure and does not imply anything about lipophilicity.

For agricultural chemicals (acetanilides, carbamates, esters, phenylurea, phosphates, triazines and uracils), the following equation was recommended (cf. table 6 above):

$\log Koc = 0.47 \log Kow + 1.09$ $(n=216, r^2=0.68, SE=0.43)$

Of other methods, the first order molecular connectivity index ($^1\chi$) has successfully been used to predict log Koc for hydrophobic organic compounds (Sabljic 1987, Bahnick and Douchette 1988). The calculation has been computerised and Meylan ***et al.*** (1992) describe the estimation methodology. Briefly, the equation used is:

$$\log Koc = 0.53\ ^1\chi + 0.62 + \sum P_f$$

Where $^1\chi$ is the first order molecular connectivity index and $\sum P_f$ is the summation product of all applicable correction factors (Meylan and Howard 1994). The calculations are performed by PCKOC part of the EPIWIN (Meylan and Howard 1994).

Pesticides

Because pesticides are the subjects of this report, correlations have been performed using both the model calculation programmes PCKOC (Epiwin, Syracuse) and the TGD recommended QSAR model by Sabljic ***et al.*** (1995).

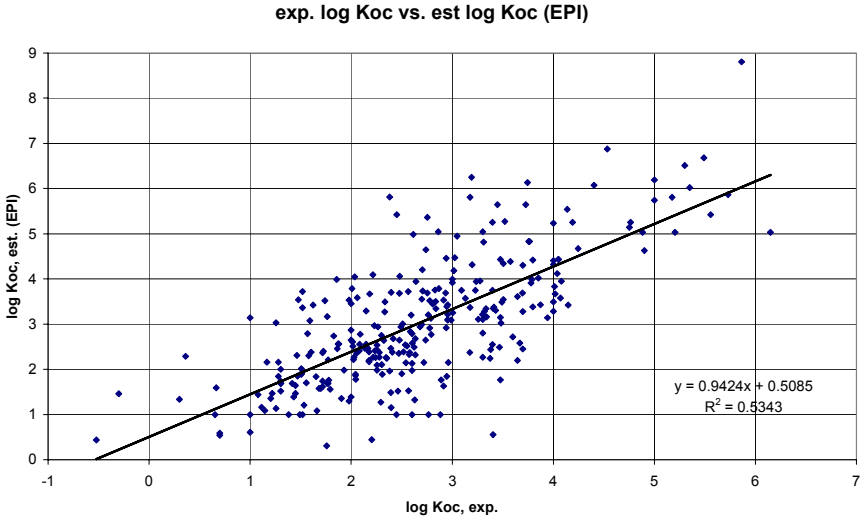


Figure 8
Correlation between experimental log Koc and log Koc estimated by PCKOC programme.

Korrelation mellem eksperimentel log Koc og log Koc vurderet efter PCKOC-program.

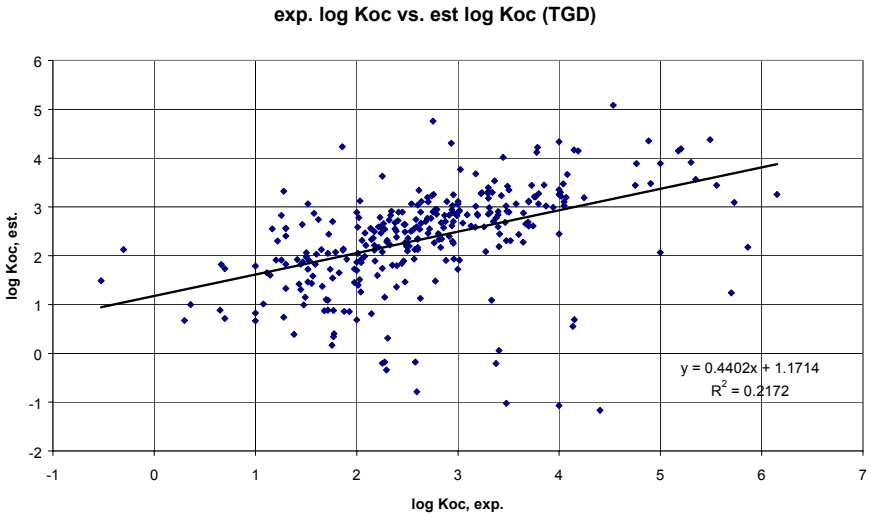


Figure 9
Correlation between experimental log Koc and log Koc estimated by TGD's QSAR model for pesticides (Table 6, 4th equation).

Korrelation mellem eksperimentel log Koc og log Koc vurderet efter TGDs QSAR-model for pesticider (Tabel 6, 4. ligning).

Performing a linear regression between the experimental Koc and the Koc estimated by the computer model EPIWIN (Meylan and Howard, Syracuse) resulted in a correlation coefficient r^2 of 0.53 (n= 306) (cf. figure 8). Performing the same regression using the QSAR model recommended in TGD for agricultural chemicals (cf. above) resulted in a correlation coefficient r^2 of 0.22 (n= 306) (cf. figure 9). It would normally result in the EPIWIN model to be recommended. However, the poor result of the TGD model seem to be related to outliers whereas the main points are closer to the regression line than in the EPIWIN estimates and the TGD QSAR models for Koc estimation developed by Sabljic ***et al***. may be used with care.

Generally, all the correlation coefficients of the QSARs examined in this study were poor. The slope of the correlation equation for the EPI and the TGD recommended QSAR for hydrophobic substances were the closer to 1 (n = 305. y = log Koc. x = log Kow. Individual values can be found in the appendix):

QSAR equation used:	Correlation equation:	r^2:
EPI structure analysis (figure 8)	y=0.9424 x + 0.5085	0.5343
Lyman ***et al***. 1982 (2nd eq. table 5)	y=0.5006 x + 1.4658	0.2236
TGD, hydrophobics (1st eq., table 6)	y=0.7454 x + 0.2322	0.2236
TGD, non-hydrophobics (2nd eq., table 6)	y=0.4785 x + 1.1049	0.2236
TGD, pesticides (4th eq., table 6)	y=0.4402 x + 1.3714	0.2172

Performing a linear regression analysis between the experimental log Kow and experimental log Koc demonstrates problems in estimating Koc from low log Kow values, cf. figure 10.

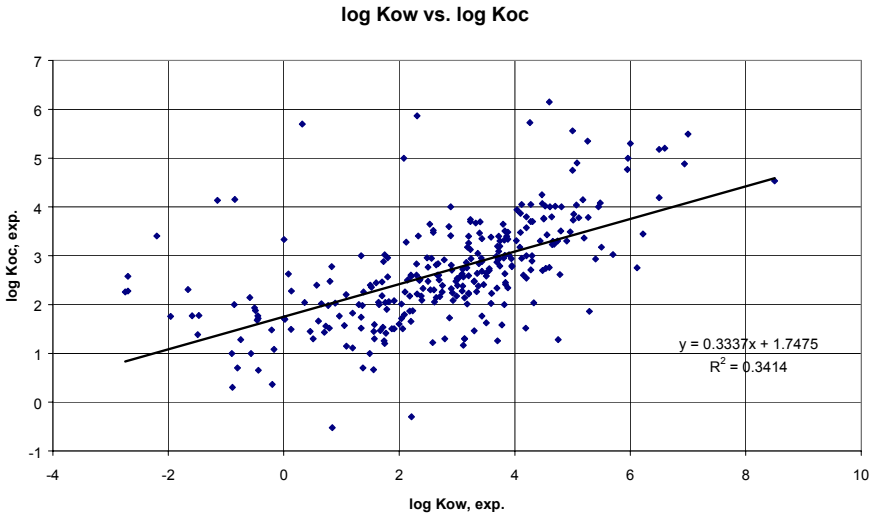


Figure 10
Correlation between experimental log Kow and experimental log Koc.

Korrelation mellem eksperimentel log Kow og eksperimentel log Koc.

Based on 300 pesticides, the correlation coefficient r^2 was 0.34 and unacceptably low but an improvement compared to the Lyman and TGD correlations. Apparently, the data are not linear. A polynomial regression of the 2nd order was tried (figure 11) and resulted in the equation:

$$\log Koc = 0.055 \log Kow^2 + 0.0764 \log Kow + 1.8476$$

The correlation coefficient r^2 was 0.41 using data from 300 pesticides. The graph demonstrated that a linear correlation might be most valid between log -1 to 5. The individual results are presented in the appendix under the heading log Koc, OCH estimate.

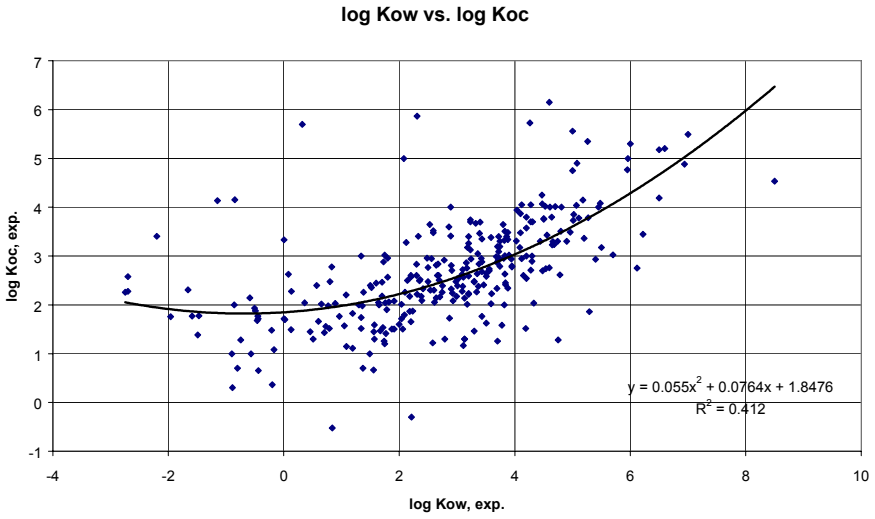


Figure 11
Correlation between experimental log Kow and experimental log Koc. Trend line adapted by polynomial regression (n=300).

Korrelation mellem eksperimentel log Kow og eksperimentel log Koc. Kurven er fastlagt ud fra en polynomial regression (n=300).

A new linear regression analysis was tried after leaving out the pesticides with the lowest log Kow values. The result is presented in figure 12.

Reducing the number of outliers by narrowing the log Kow range from 0 to 8.5 increased the correlation coefficient to 0.39. The resulting regression equation or derived QSAR model was:

log Koc = 0.4389 log Kow + 1.3752 (n= 273, r^2=0.3851)

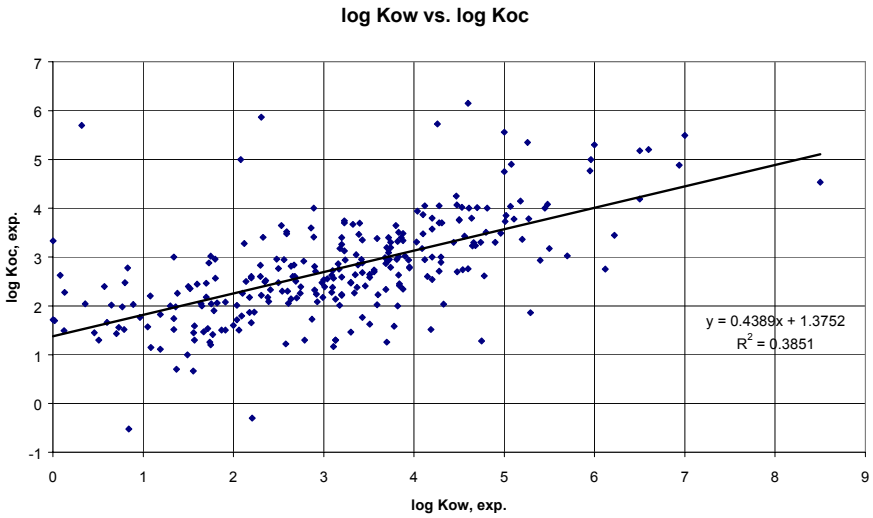


Figure 12
Correlation between experimental log Kow and experimental log Koc. Outliers below log Kow 0 was removed.

Korrelation mellem eksperiment log Kow og eksperimentel log Koc. Data med log Kow mindre end 0 er udeladt.

Using the water solubility to estimate the adsorption coefficient did improve the result (figure 13).

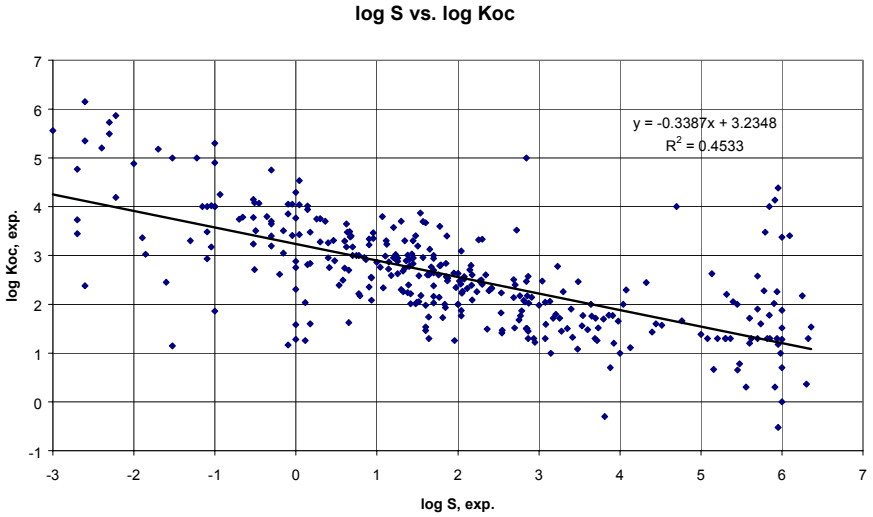


Figure 13
Correlation between experimental water solubility (log S) and experimental log Koc.

Korrelation mellem eksperimentel vandopløselighed (log S) og eksperimentel log Koc.

The resulting correlation was:

log Koc = -0.3387 log S + 3.2348 (n= 338, r^2=0.45)

The result is close to the QSAR observed for pesticides by Kanazawa (1989), although for a fewer number:

LOG KOC = -0-356 LOG S + 3.01 (N=15, R=-0.887, P<0-001)

Conclusion

The soil adsorption coefficient factor is very important in the evaluation of the mobility of pesticides and since the known methods for estimation are approximate at best, measured values should be recommended.

If however, measured data for some reason are not present; the QSAR model to estimate Koc developed by Sabljic ***et al***. (1995) and recommended in TGD (1996) or the calculation programme PCKOC may be used. However, based on 338 pesticides in this project, QSAR models, based on log Kow or the water solubility, were derived which had correlation coefficients which were better than the model by Sabljic ***et al*** (1995). These QSARs derived for pesticides could be considered when evaluating experimental results are either not present or conflicting.

3.4 Bioaccumulation

3.4.1 Bioaccumulation factor for aquatic organisms

The uptake of chemical substances into living organisms occurs mostly by direct adsorption but also along trophic web. The internal concentration, e.g. in fish, may increase by accumulation to a level causing toxic effects, even if the internal concentration remains below the critical limit (OECD 1993b). The accumulated substance may then be passed on to other organisms higher up in the food web which were not directly exposed themselves.

The bioaccumulation or bioconcentration factor (BCF) in aquatic organisms is defined as the ratio between the concentration of the chemical in biota and the concentration in water at equilibrium.

Procedures for estimating the bioconcentration potential have been reviewed by e.g. Lyman ***et al.*** (1982), Connell (1988), Nendza (1991b), and OECD (1993b). Comparison of non-ionic organic chemicals exhibiting substantial bioconcentration revealed several common characteristics. The bioconcentration potential of a chemical was directly related to its lipophilicity and inversely related to its water solubility, molecular charge and degree of ionisation (Lyman ***et al***. 1982, Connell 1988). In fish, the lipid tissue is the principal site for bioaccumulation and since n-octanol is often a satisfactory surrogate for lipids, linear correlations are usually observed between log BCF and log Kow. Most QSAR models on bioconcentration are based on log Kow. The simplest form of the relationships is based on the partition process of the lipid phase of fish and water:

BCF = a × Kow (where a is the lipid fraction actually ranging 0.02 - 0.2)

It is generally agreed that a linear relationship exists for chemicals, which are not biotransformed with a log Kow < 6. Veith ***et al.*** (1979) developed a linear

model based on fathead minnows (***Pimephales promelas***) valid for log Kow < 6:

log BCF = 0.85 log Kow - 0.70 (n = 55, r^2 = 0.90)

In the log Kow range above 6, the measured log BCF data tend to decrease with increasing log Kow.

Performing a regression analysis, using the Veith ***et al.*** (1979) developed QSAR on the pesticides used in this report, would result in the following correlation (figure 14):

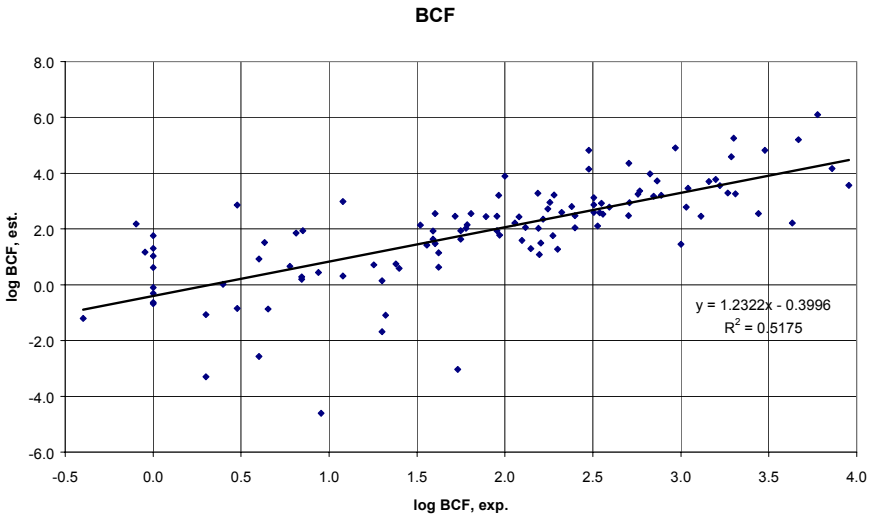


Figure 14
Correlation between the experimental log BCF and the estimated log BCF (Veith et al. 1979).

Korrelation mellem den eksperimentelle log BCF og den estimerede log BCF (Veith et al. 1979).

The correlation between the experimental values and the estimated values seems to be acceptable with a correlation coefficient, r^2, of 0.52 (figure 14). The result is less accurate than Veith ***et al.*** (1979) but it is to be expected considering the diverse group of chemical compounds, different fish species and different laboratories although the amount of data (n=112) included was higher.

Developing a new QSAR, based on regression analysis between measured log Kow and experimental log BCF for 112 pesticides, would result in a similar correlation coefficient (figure 15):

log BCF = 0.3324 log Kow + 0.7545 (n = 112, r^2 = 0.502).

The QSAR is still inaccurate but being at the same level as Veith ***et al***. (1979) and may be used for screening purposes.

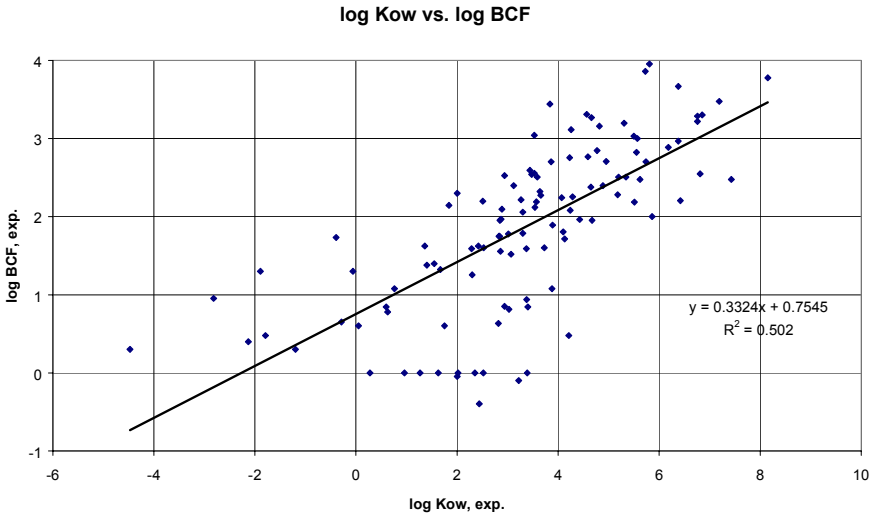


Figure 15
Correlation between experimental log Kow and experimental log BCF based on 112 pesticides.

Korrelation mellem eksperimentel log Kow og eksperimentel log BCF baseret på 112 pesticider.

3.4.2 Bioaccumulation factor for terrestrial organisms

In water, the bioconcentration factor are based on the concentration in the aquatic organism or part of the aquatic organism (e.g. whole fish or part of fish) divided by the concentration in water presumably under equilibrium conditions.

The maximum amount of a chemical in water is governed by the water solubility of the chemical, which can be very low. In soil, the situation is different since no saturation limit is imposed by solubility. The biology of the soil living organism determines whether the bioavailability is a question of the water solubility of the substance or not.

Distribution of pesticides in soil from use application is rarely uniform. If applied to soil surfaces, the upper few centimetres usually contain the majority of the substance and the measured concentration depends on the depth of the soil sampled for analysis. For instance, if the application is 1 kg/ha and assumed uniformly distributed in soil 2.5 cm, 5 cm, 10 cm or 25 cm deep with the density 1500 kg/m^3, the estimated concentration in soil would be 2.67, 1.33, 0.66 or 0.26 mg/kg soil, respectively.

Thus, bioconcentration factors for terrestrial animals on treated soil do not have the same basis for a denominator as for aquatic animals in treated water (Kenaga 1980). Because of the difficulty in determining and deciding on a uniform soil residue denominator for BCF, very little data comparable to aquatic organisms are available for terrestrial organisms.

Earthworms

For the assessment of secondary poisoning in the terrestrial food chain, the bioconcentration factor in worms is necessary. The bioconcentration factor is defined as:

$$BCF_{earthworm} = C_{earthworm} / C_{pore\ water}$$

As the concentration in soil and the concentration in pore water are related through the Koc where Koc = $C_{soil(oc)}$ / $C_{pore\ water}$, the calculation could be performed using the concentration in soil and the soil/water partition coefficient assuming steady state:

$$BCF_{earthworm} = (C_{earthworm} \cdot Koc) / C_{soil(oc)}$$

QSAR

Finally, the QSAR models may be used. Van Gestel and Ma (1988) determined the BCF for two species of earthworms for five chlorophenols and found a relationship with log Kow. Connel and Markwell (1990) increased the data amount from literature and developed a model based on log Kow. The model was generated on data on pesticides with a log Kow range of 1-6. The BCF-log Kow relationship applies generally to neutral organic substances, which are not easily biotransformed. The relationship is not valid for ionised substances and organometals. The model needs further validation.

The QSAR for BCF in earthworms developed by Connel and Markwell (1990) is presented below:

log BCF = 1.0 log Kow - 0.6 (n=100, r^2=0.91)

Pesticides

Only a very few data exist on BCF in earthworms for pesticides that are precise enough to be used in a comparison. Therefore, the accuracy of the estimation from the QSAR by Connel and Markwell (1990) could not be compared.

3.5 Aquatic toxicity

3.5.1 QSAR models on aquatic ecotoxicity

Within the aquatic ecotoxicology, QSAR models have been used to estimate biological effects of various chemical substances. For instance, frequently the octanol-water coefficient (log Kow) of a substance has been used to estimate the ecotoxicity potential of the substance to organisms.

Most literature on developing QSARs for toxicity estimations has assumed that compounds from the same chemical class should behave in a toxicologically similar manner (cf. section 3.1). Recent literature indicates that similarity in mode of toxic action is not necessarily related to typical chemical classification but to molecular structures. As a consequence, QSAR development and application have been evolving from a chemical class perspective to one that is more consistent with assumptions regarding modes of toxic action (TGD 1996, Russom ***et al.*** 1997).

For instance, Russom ***et al.*** (1997) have performed a classification of chemicals into 8 modes of toxic action based on fathead minnow (***Pimephales promelas***) exposed in 96 hours flow-through studies to 617 chemicals.

The Russom ***et al.***(1997) classification on modes of toxic action included:

- base-line narcosis or narcosis I
- polar narcosis or narcosis II

- ester narcosis or narcosis III
- oxidative phosphorylation uncoupling
- respiratory inhibition
- electrophile/proelectrophile reactivity
- acetylcholinesterase inhibition
- several mechanisms of CNS seizure responses

A few comments are given below on the most essential action mechanisms relating to pesticides.

Base-line narcosis or non-polar narcosis

Base-line toxicity or the "minimum toxicity" is related to the hydrophobicity of the substance and is also referred to as non-polar narcosis. In absence of specific toxic mechanisms, the internal effect concentration is almost constant and a substance will then be as toxic as predicted by its hydrophobicity due to the relation with bioconcentration (McCarthy and MacKay 1993). Indications of non-polar narcosis are the change of EC_{50} over time. The ratio $EC_{50\ (24\ hours)}/EC_{50\ (96\ hours)}$ approximately 1.0 is considered indicative of non-polar narcosis. Excess toxicity values, calculated by dividing predicted "narcosis I" EC_{50} values by the observed values, greater than 10 indicate that the substance does not act by non-polar narcosis (Russom ***et al.*** 1997). Examples of pesticides classified as having the toxic mode of action of non-polar narcosis are alachlor, bromacil and diuron.

Polar narcosis

The polar narcosis class consists of more polar chemicals such as phenols, esters and anilines. The mode of action of these substances is not very specific but they are significantly more toxic than predicted by non-polar narcosis.

Acetylcholinesterase inhibition

Several insecticides are acting by acetylcholinesterase inhibition, e.g. carbamates and organophosphorous pesticides. Examples of pesticides are azinphos-methyl, carbaryl, carbofuran, chlorpyriphos, diazinon, malathion and methomyl.

CNS seizure responses

Central Nervous System (CNS) seizure/stimulant responses. In literature and handbooks, the mode of action is often called contact action or contact and stomach action. Examples of pesticides are organochlorines and pyrethroids such as dicofol, fenvalerate and permethrin (Russom 1997).

QSARs for the acute and long term effects on fish, daphnia and algae are present for chemicals that act by non-specific mode of action (non-polar narcosis as well as polar narcosis).

The latest evaluation of current models in ecotoxicity resulted in the QSAR models mentioned in the tables 7 and 8 (Verhaar ***et al.*** 1992, 1995).

Table 7
QSARs for non-polar narcosis (Verhaar et al. 1995, TGD 1996).

QSAR for ikke-polær narkotisk virkende stoffer (Verhaar et al. 1995, TGD 1996).

Species	Regression equation (mol/l)	Statistics		
		n	r^2	SE
Fish *Pimephales promelas*	log LC_{50} (96h) = -0.85 log Kow - 1.39	58	0.94	0.36
Daphnia: *Daphnia magna*	log EC_{50} (48h) = -0.95 log Kow - 1.32	49	0.95	0.34
Daphnia magna (repro.)	log NOEC (16d) = -1.05 log Kow - 1.85	10	0.97	0.39
Algae: *Selenastrum capricornutum*	log EC_{50} (72-96h) = -1.0 log Kow - 1.23	10	0.93	0.17

The models are generated by linear regression analysis. The experimental data were generated according to OECD test guidelines or comparable methods.

QSAR models for chemicals, which act by polar narcosis (esters, phenols and anilines), are also available. The mode of action of these compounds is also not very specific but they are significantly more toxic than predicted by non-polar narcosis.

Table 8
QSARs for polar narcosis (Verhaar et al 1995, TGD 1996).

QSAR for polær narkotisk virkende stoffer (Verhaar et al. 1995, TGD 1996).

Species	Regression equation (mol/l)	Statistics		
		n	r^2	SE
Fish *Pimephales promelas*	log LC_{50} (96h) = -0.73 log Kow - 2.16	86	0.90	0.33
Daphnia: *Daphnia magna*	log EC_{50} (48h) = -0.56 log Kow - 2.79	37	0.73	0.37

The models were generated by linear regression analysis. The experimental data were generated according to OECD test guidelines or comparable methods.

Classification

For classification purposes, the Danish EPA has developed a programme to estimate the minimum acute aquatic toxicity: QTOXMIN. The programme QTOXMIN is available in Pedersen ***et al.*** (1995) and in Pedersen and Falck (1997).

However, the use of QSAR data for classification is currently under discussion. At this stage it is proposed that the use of QSAR estimations for base-line acute aquatic toxicity should be limited and only used if the prerequisites below are fulfilled (Pedersen ***et al.*** 1995):

- No measured data on acute aquatic toxicity are available even after the data collection procedure outlined in Pedersen ***et al.*** (1995) has been followed.

- Estimated QSAR-based effect concentrations on the three species fish, daphnia and/or algae are not above either the measured or estimated water solubility value.

- The estimated QSAR-based effect concentration on fish, daphnia or algae is below 1 mg/l.

The QSAR equations recommended are (results in mol/l):

Fish:	log LC_{50} (96h) = - 0.85 log Kow - 1.41	n=68, r^2= 0.94, SE=0.35
Daphnia:	log EC_{50} (48h) = - 0.95 log Kow - 1.19	n=17, r^2=0.99, SE=0.21
Algae:	log EC_{50} (72h) = - 1.0 log Kow - 1.23	n=10, r^2=0.93, SE=0.17

The equations are applicable for neutral, organic, non-reactive and non-ionisable compounds such as alcohols, ketones, ethers, alkyl and aryl halides, and can also be used for aromatic hydrocarbons, halogenated aromatic and aliphatic hydrocarbons as well as sulphides and disulphides (Pedersen ***et al.*** 1995).

Generally, the differences in acute toxicity between non-polar and polar narcotic acting substances are only significant for substances with a log Kow value less than 2.7. Thus, for polar acting narcotic substances with a log Kow value above 2.7, the presented QSAR equations can also be used as a reliable predictor of their acute aquatic toxicity. For polar narcotic acting substances with a log Kow value less than 2.7, and especially for reactive substances and for substances with a specific mode of action, the presented QSAR equations will significantly underestimate the acute toxicity (Pedersen ***et al.*** 1995, Pedersen and Falck 1997).

The QSAR equations recommended for classification are the same or almost the same as the equations recommended in TGD (1996), which are used in the estimations of aquatic toxicity of pesticides in this report.

Pesticides

It is important to realise that most of the QSARs developed and the QSARs presented above are based on chemicals that are biased toward industrial organic chemicals, which are not overtly designed to have biological activity. Pesticides are mostly reacting in a specific mode of action and no QSARs have been recommended for substances that act by more specific modes of action (TGD 1996).

3.5.2 Correlations between experimental and estimated ecotoxicity

Base-line toxicity correlations

In figure 16, the correlations on estimated acute toxicity in the aquatic organisms where estimated values are based on the QSARs for non-polar narcosis substances are presented. It is primarily performed to illustrate the concept of "minimum" toxicity than estimated EC_{50} values as only few pesticides have been identified as non-polar narcosis and then on a level D confidence, e.g. diuron, bromacil and alachlor (Rossum ***et al.*** 1997). For comparison, EC_{50}-values have been analysed using both QSAR for polar as well as for non-polar substances. The estimated values in mol/l are recalculated to mg/l by multiplying with molecular weight and a factor 1000.

Fish

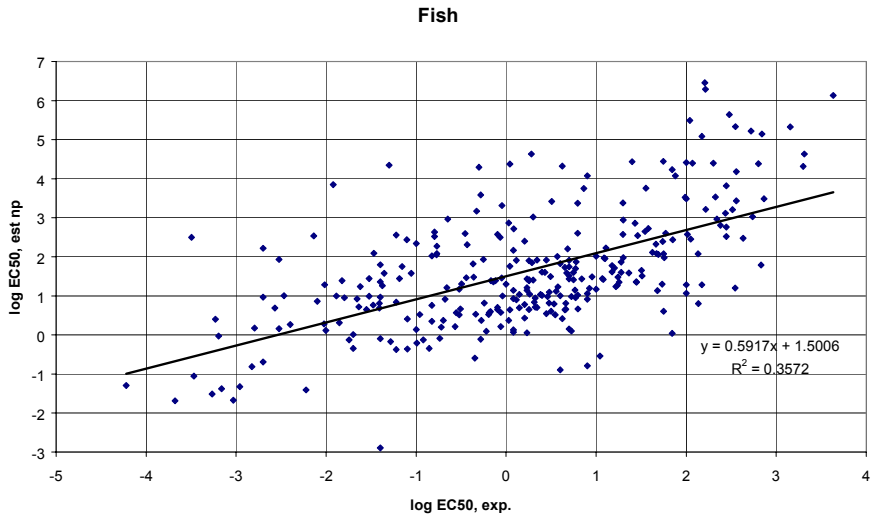


Figure 16
Correlation between experimental and estimated EC_{50}-values (log) with non-polar narcosis type QSAR.

Korrelation mellem eksperimentelle og estimerede EC_{50}-værdier (log) med ikke-polær narkosetype QSAR).

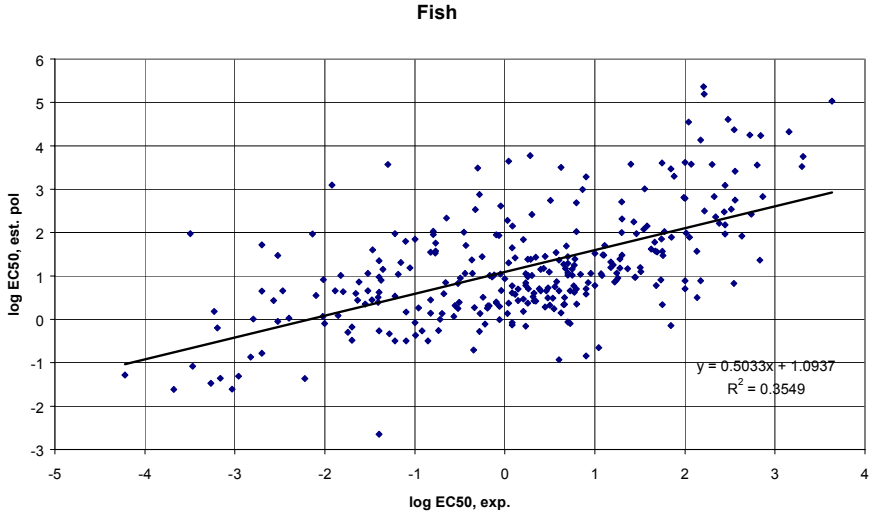


Figure 17
Fish: Correlation between experimental EC_{50} and estimated EC_{50} based on polar narcosis type QSAR.

Fisk: Korrelation mellem eksperimentel EC_{50} - og estimerede EC_{50} værdier baseret på QSAR for polært narkotisk virkende stoffer.

As expected, the estimated values on acute fish toxicity are overestimated i.e. above the trend line with intercept 0 and the slope 1. Thus, the true EC_{50}-value is below the estimated value. For chemicals with a specific mode of action, the effect concentration is generally between 10 and 10000 times lower than predicted by baseline toxicity QSAR equations (Verhaar ***et al.*** 1992). The same applies to daphnia and algae (cf. below).

The linear regression analysis of the relationship between the experimental log EC_{50} and the estimated log EC_{50} for fish resulted in a correlation coefficient r^2 of 0.35 based on n = 297. The result was approximately the same irrespective of whether the non-polar or the polar QSAR was used. It is far from satisfactory but the QSAR model may be used for screening purposes.

Daphnia

For comparison, linear regression analyses of the relationship between the experimental log EC_{50} and the estimated log EC_{50} for daphnia are performed for both non-polar and polar narcosis type QSARs (figures 18 and 19). The correlation coefficient r^2 for non-polar narcosis type QSAR was 0.28 and the correlation coefficient r^2 for polar narcosis type QSAR was 0.27. The number of data sets was 255. The result indicates that the available QSAR models for estimating acute toxicity to daphnia are not acceptable for pesticides in general at present.

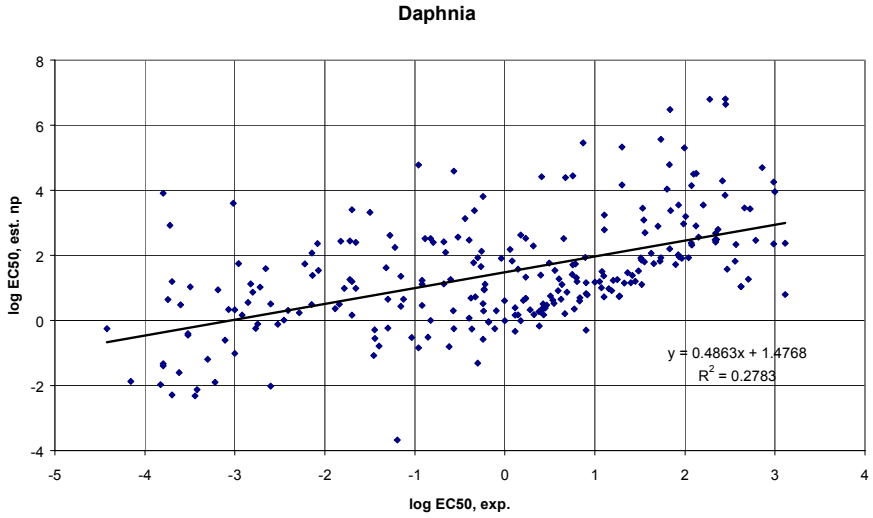


Figure 18
Daphnia: Correlation between experimental EC_{50} and estimated EC_{50} values based on non-polar narcosis type QSAR.

Dafnier: Korrelation mellem eksperimentelle EC_{50} og estimerede EC_{50} -værdier baseret på QSAR for ikke-polære narkotisk virkende stoffer.

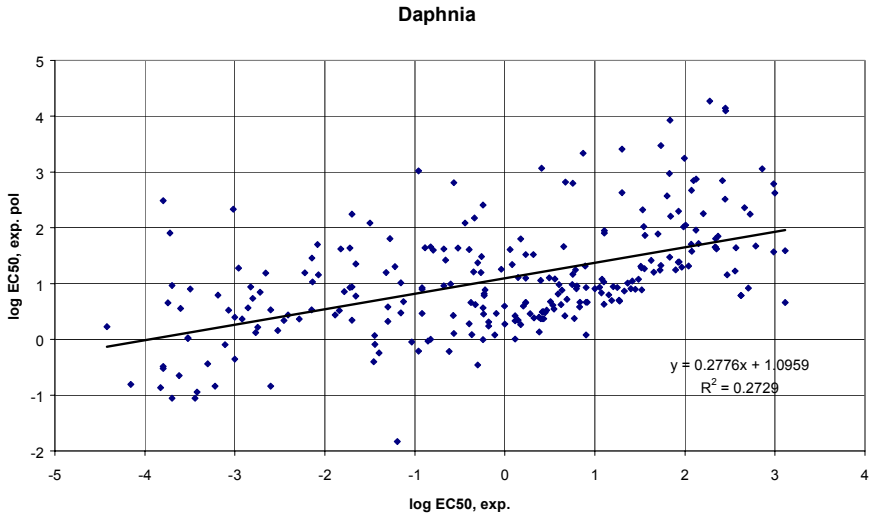


Figure 19
Daphnia: Correlation between experimental EC_{50} and estimated EC_{50} values based on polar narcosis type QSAR.

Dafnier: Korrelation mellem eksperimentelle EC_{50} og estimerede EC_{50} -værdier baseret på QSAR for polære narkotisk virkende stoffer.

Daphnia, chronic

Long-term effect studies (16 days) on ***Daphnia*** have also been used to develop a QSARs on daphnia reproduction.

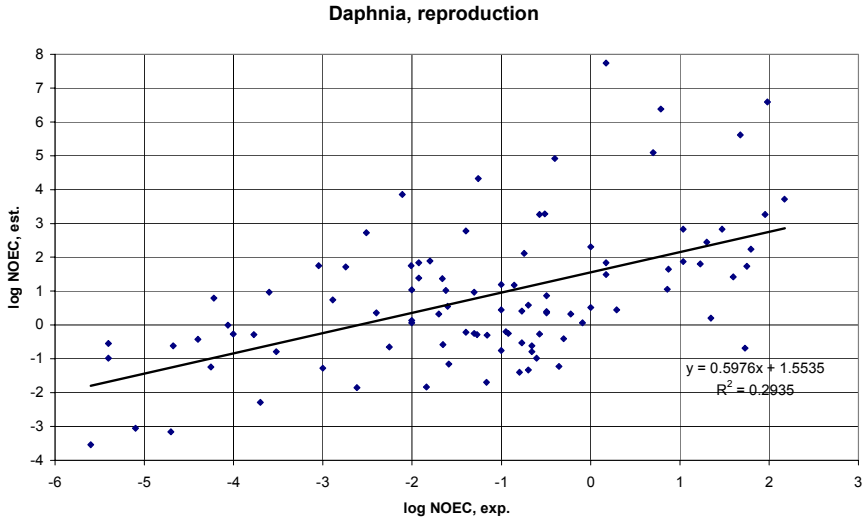


Figure 20
Correlation between experimental Daphnia NOEC (16-21 days) and NOEC values based on non-polar narcosis type QSAR.

Korrelation mellem eksperimentel dafnie NOEC (16-21 dage) og NOEC værdier baseret på QSAR for ikke-polære narkotisk virkende stoffer.

A linear regression analysis of the relationship between the log NOEC from experimental Daphnia reproduction tests and the currently recommended QSAR (table 7) resulted in a correlation coefficient r^2 of 0.29 based on n = 96 (figure 20). The correlation was lower than the recommended QSAR which was based on n=10. It should also be noted that the QSAR for estimating daphnia reproduction NOEC was based on 16-day tests and the experimental results in this report are mainly from 21-day tests. This could reduce the

comparability. The result indicates that the used QSAR model for estimating chronic ***Daphnia*** NOEC values is not recommendable for pesticides in general.

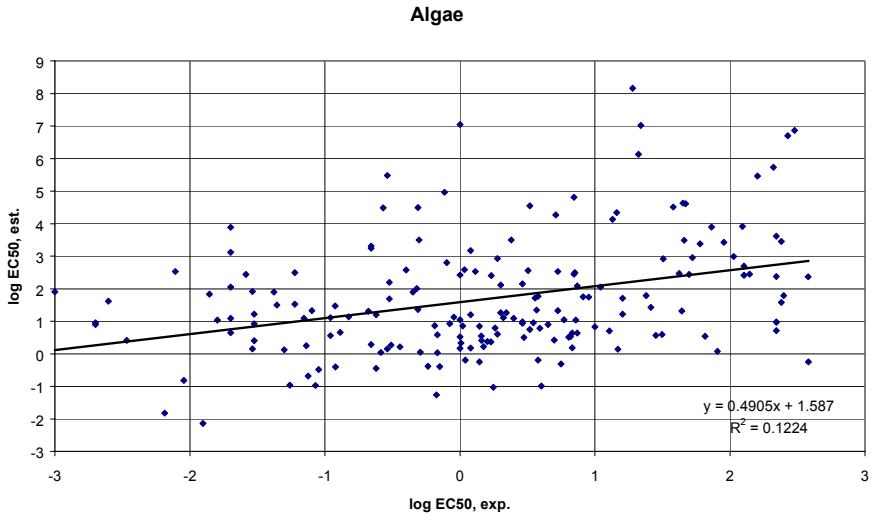


Figure 21
Correlations between the experimental log EC_{50} and estimated log EC_{50} for algae (non-polar narcosis).

Korrelation mellem eksperimentel EC_{50} og estimeret EC_{50} -værdier for alger (ikke-polær narkotisk virkende stoffer).

Algae

Linear regression analyses of the relationship between the experimental log EC_{50} and the estimated log EC_{50} for algae for non-polar type QSARs (figure 21) resulted in the correlation coefficient r^2 0.12. The number of data sets was 193. For algae, the correlation was so low that it must be concluded that the resulting estimations are unacceptably poor.

Discussion

The situation with the present data set is that it has been chosen as a mixture of different pesticides to evaluate whether the evolved QSARs could be used in general. The general conclusion is that the results demonstrate that the available QSAR models should be used with great precaution, as they are not developed specifically for pesticides.

Individual results of the estimation can be found in the appendix. Generally, the results support the concept of minimum toxicity, i.e. if the substance is estimated to be toxic the experimental results may be expected to confirm that the substance is more toxic than estimated.

If the pesticides were selected according to function, mode of action or chemical class another result might have appeared. The following two sections presents examples of QSARs developed for specific pesticides (3.5.3) and the QSARs derived from the pesticides used in the report (3.5.4).

3.5.3 QSARs developed for specific pesticides

Two examples of developed QSAR models for pesticides from the same chemical class and assumed same mode of action are presented below.

Phenylureas

Phenylurea herbicides have been selected as model compounds representing a well-defined class of chemical structure mostly acting by a uniform mode of action by Nendza (1991) and Nendza ***et al.*** (1991). Satisfactory estimates on the phenylureas fish toxicity were obtained from a log Kow dependent QSAR. The toxicity to algae and plants which were the most sensitive species corresponding to the mode of action (interacts with the electron transport chain in the photolysis reactions) could be estimated by including the Hill reaction inhibition in the QSAR. Nendza ***et al.*** (1991) used the following equations with satisfactory results:

Fish: $\log 1/LC_{50}$ (mmol/l) = 0.62 log Kow - 0.56 (n=118, r=0.91, s=30)

QSARs derived for non-reactive chemicals underestimate the effects of phenylureas on algae significantly. Regarding their mode of action, the inhibition of algae photosystem should be included. Nendza ***et al.*** (1991) presents a QSAR modelling the interaction with the electron transport chain (pI_{50} Hill reaction) giving acceptable estimates of the phenylureas' algae toxicity by including the ionisation potential (IP) besides log Kow as descriptors:

Algae: pI_{50} = 0.93 log Kow + 0.69 IP - 3.03 (n=12, r= 0.97, s= 0.37)

In Nendza (1991), the equation on algae toxicity is changed and instead tabulated electronic properties (σ) is employed:

Algae (log 1/[mmol/l]):
$\log 1/C = 1.89 \log Kow - 0.17 \log Kow^2 - 0.65 \sigma - 0.66$

The results from Nendza ***et al.*** (1991) are presented in table 9.

For algae, it was observed that the estimated EC_{50} values were always below the experimental values (cf. table 9).

Table 9
Phenylurea herbicides log Kow and experimental (exp.) and estimated (calculated.) toxicity (log 1/(mmol/l) (Nendza et al. 1991).

Phenylurea herbiciders log Kow, eksperimentel (exp.) og estimeret (calc.) toksicitet (log 1/(mmol/l) (Nendza et al. 1991).

Compound	Log Kow	Fish log LC_{50}		Algae log EC_{50}	
		Exp.	Calc.	Exp.	Calc.
Buturon	1.6	2.57	0.43	3.13	1.94
Chlorbromuron	3.05	2.82	1.33	5.17	3.50
Chloroxuron	4.00	0.80	1.92	5.08	4.03
Chlorotoluron	2.53	-0.06	1.01		2.86
Defenuron	1.10	1.55	0.12		1.36
Diuron	2.75	-0.57	1.15	5.33	3.23
Fenuron	0.87	0.82	-0.02		1.17
Isoproturon	2.44	1.36	0.95		2.60
Fluometuron	2.28	1.19	0.85	3.82	2.91
Linuron	3.18	0.85	1.41		3.69
Metobromuron	2.46	1.06	1.06	3.51	2.81
Metoxuron	1.68	0.46	0.48		2.02
Monolinuron	2.31	0.42	0.87	3.24	2.71
Monuron	1.88		0.61	3.94	2.27
Neburon	4.09	0.22	1.98	5.06	4.51
Siduron	3.65		1.70		3.74

Organophosphorous

QSARs have also been developed for the toxicity of organophosphorous pesticides to ***Daphnia*** (Vighi ***et al.*** 1991). The 22 tested chemicals were belonging to the subclasses: phosphates, phosphorothionates, phosphorodithionates, and phosphonates. They all had a specific mode of action: cholinesterase inhibition. The QSARs were obtained by multilinear correlations with independent variables: log Kow, first order valence molecular connectivity ($^1\chi^v$) and complementary information content (CIC) as independent variables for a number of chemical substances.

For ***Daphnia,*** the best equation obtained was:

$$\log 1/EC_{50} = 0.55 \log Kow - 0.085 (\log Kow)^2 - 3.93IC - 0.016 (^1\chi^v_{ox})^2 + 0.13\alpha_3 - 0.0006(\alpha_3)^2 + 4.58$$

$$(n=22, r^2=0.895, s=0.67)$$

where the molecular connectivity indices developed by Hall and Kier (1981) and information index of neighbourhood symmetry, IC (information content), were used as descriptor of topological information. Valence molecular connectivity indices encode information on volumetric and electronic characteristics of the bonds in the molecule and are also calculated for the oxygen metabolites, $^1\chi^v_{ox}$. The variable α_3 describes the electronegativity of the leaving group in the acetylenesterase inhibition reaction (Vighi ***et al.*** 1991). The approach was considered satisfactory in describing the toxicity of a relatively heterogeneous set of organophosphorous compounds after introduction of variables able to describe the particular reactivity of these compounds characterised by a highly specific biological activity.

3.5.4 QSARs derived from pesticides in the report

Based on the approximately 400 pesticides including some salts and esters selected for this study (cf. appendix), it was decided to study whether dividing the pesticides into minor groups would improve the predictability. Furthermore, it was decided to use the mode of action as basis. At first the pesticides were divided into five main groups and then further subdivided if sufficient data were present:

Fungicides	
Herbicides	Growth inhibitors
	Photosynthesis inhibitors
Insecticides	Cholinesterase inhibitors
	Contact and stomach action (CSA)
Plant growth regulators (PGR)	
Rodenticides	

Linear regression analyses were performed between the experimental EC_{50} values and the experimental log Kow. The analyses were performed using both mg/l and mmol/l on account of the general idea that the molecular weight influenced the effect level. Graphic presentations of the correlations between experimental EC_{50}-values and log Kow are presented below for fish, daphnia and algae.

Fish

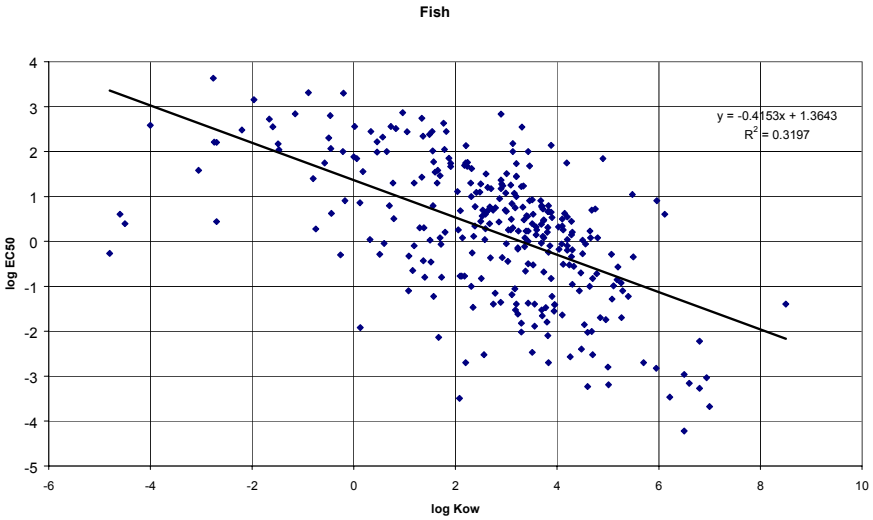


Figure 22
Correlation between experimental log Kow and experimental EC_{50} for fish (n=300) for all pesticides in the appendix.

Korrelation mellem eksperimentel log Kow og eksperimentel EC_{50} for fisk (n=300) for alle pesticider i appendiks.

Using all the selected pesticides and performing a linear regression analysis of the correlation between experimental log Kow and the acute toxicity (cf. figure 22), the resulting equation for fish was:

$\log EC_{50}$ (mg/l) = -0.4153 log Kow + 1.3643 (n=300, r^2 = 0.3197)

The reduced correlation compared with the previous section may be the result of data from several fish species and a broader variety of pesticides included in the calculation. However, a trend is obvious and the result may be sufficient for a screening procedure.

Removing the data with the lowest log Kow values (log Kow values ≤4) improved the correlation coefficient slightly (Figure 23). The resulting equation for acute fish toxicity was then:

$\log EC_{50}$ (mg/l) = -0.5076 log Kow + 1.6739 (n=296, r^2 = 0.3786)

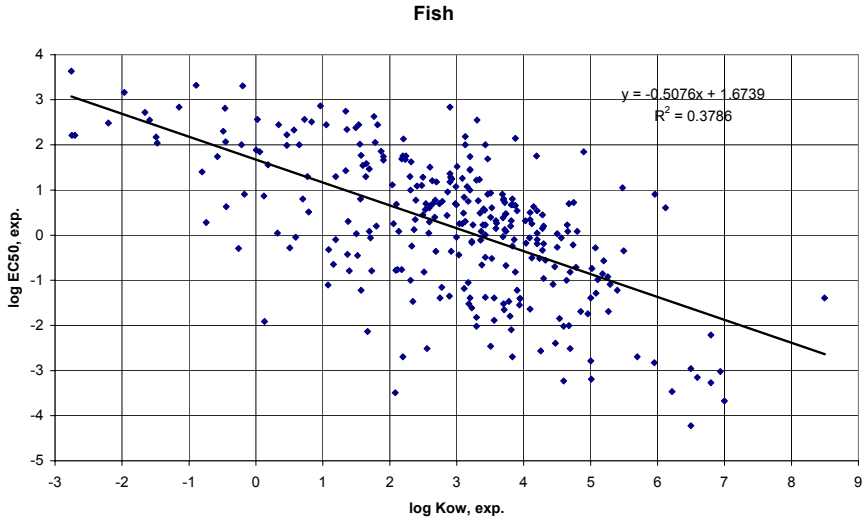


Figure 23
Correlation between experimental log Kow and experimental EC_{50} for fish (n=296).

Korrelation mellem eksperimentel log Kow og eksperimentel EC_{50} for fisk (n=296).

Many of the literature QSARs are presented using the mol/l instead of mg/l in the models estimating toxicity. It indicates that the molecular size or properties related to the molecular weight is important to the estimated toxicity. As the argument seems reasonable a recalculation of the measured data to mmol/l was performed. The result is presented in figure 24.

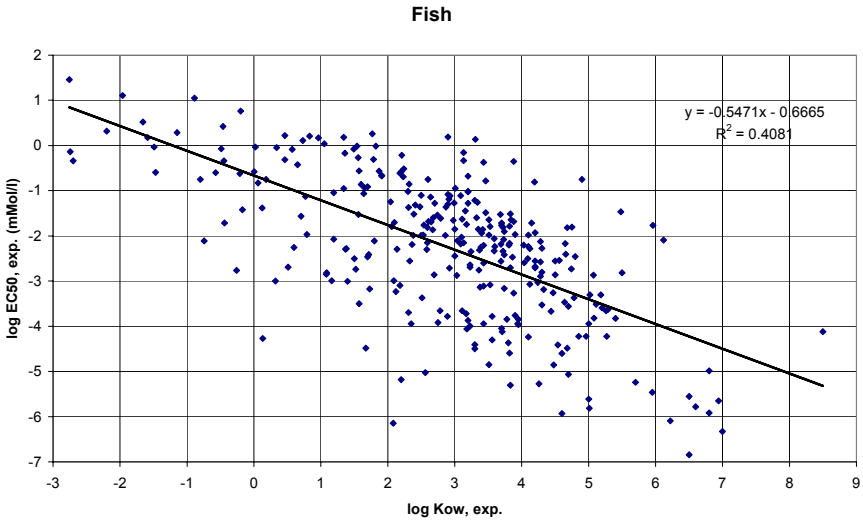


Figure 24
Correlation between log Kow and experimental EC_{50} for fish (n=296) in mmol/l.

Korrelation mellem log Kow og eksperimentel EC_{50} for fisk (n=296) mmol/l.

The resulting equation for acute fish toxicity was:

log EC_{50} (mmol/l) = 0.5471 log Kow - 0.6666 (n=296, r^2 = 0.4081)

The correlation coefficient was slightly higher. The reason was probably that the variation of molecular weights for the used pesticides was relatively narrow (299±103 g/mol, n=409). Using mmol/l instead of mg/l had minor effect on the correlation coefficient. Mainly results from mmol/l are shown in the figures and both equations are presented in the text.

Mode of action

The data on fish acute toxicity were divided into:

pH of soil and water

- fungicides
- herbicides
- herbicides with a growth inhibition mode of action
- herbicides with a photosynthesis mode of action
- insecticides
- insecticides with a cholinesterase inhibition mode of action
- insecticides with a contact and systemic action
- plant growth regulators
- rodenticides.

The axes in the following charts are kept constant for comparison.

For fungicides, 59 corresponding experimental log Kow and EC_{50} values were found. In figure 25, a trend is indicated but the dispersion is high. This could be expected since fungicides do not have a specific action mode towards fish.

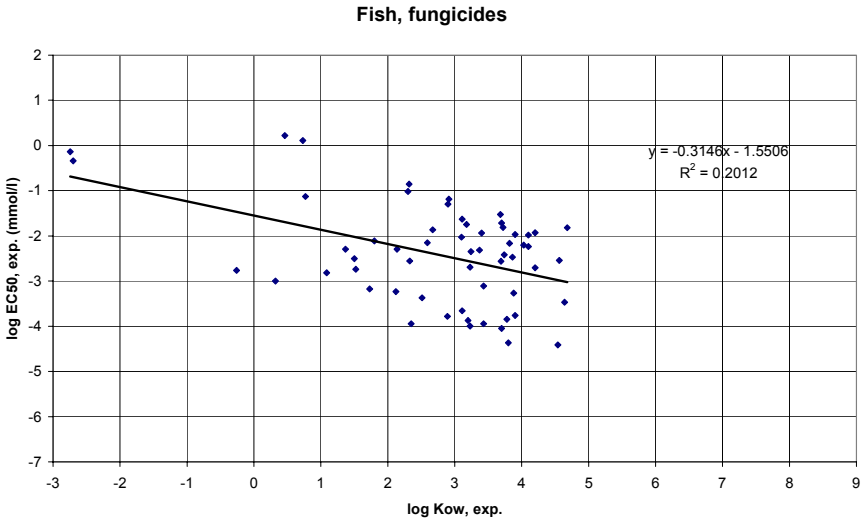


Figure 25
Correlation between log Kow and experimental EC_{50} for fish using data on fungicides (n=59).

Korrelation mellem log Kow og eksperimentel EC_{50} for fisk med data for fungicider (n=59).

The resulting equations for acute fish toxicity using fungicide data were:

$\log EC_{50}$ (mg/l) = -0.2963 log Kow + 0.8584 (n=59, r^2 = 0.1890)
$\log EC_{50}$ (mmol/l) = -0.3146 log Kow - 1.5506 (n=59, r^2 = 0.2012)

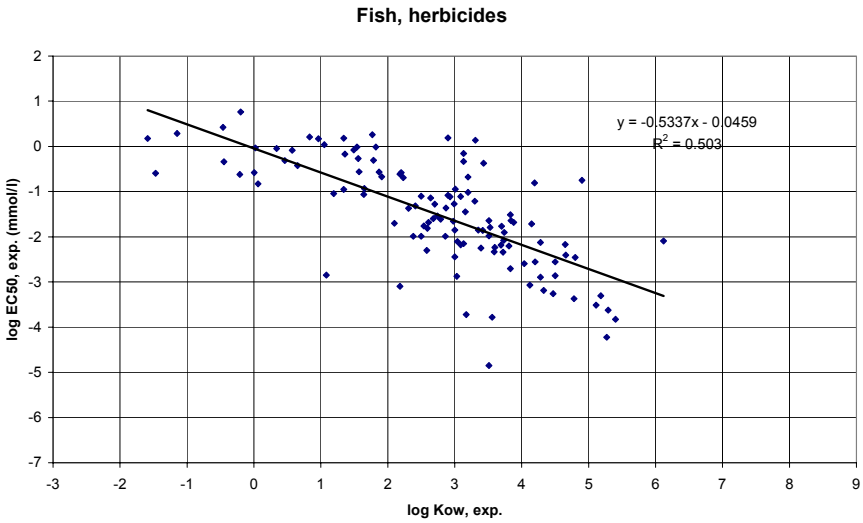


Figure 26
Correlation between log Kow and experimental EC_{50} for fish using data on herbicides (n=118).

Korrelation mellem log Kow og eksperimentel EC_{50} for fisk ved anvendelse af herbicid data (n=118).

For herbicides, all available data on experimental log Kow and fish EC_{50} were used and presented in figure 26. The resulting equations for acute fish toxicity using herbicide data were:

log EC_{50} (mg/l) = -0.5193 log Kow + 2.3548 (n=118, r^2 = 0.4814)
log EC_{50} (mmol/l) = -0.5337 log Kow - 0.0459 (n=118, r^2 = 0.5030)

The data on herbicides was divided into herbicides with a growth inhibition mode of action and herbicides with a photosynthesis inhibition mode of action.

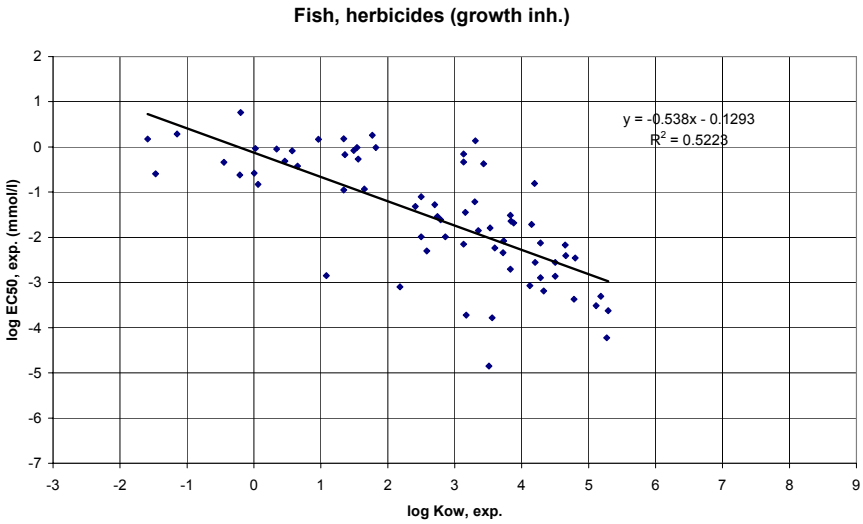


Figure 27
Correlation between log Kow and experimental EC_{50} for fish using data on herbicides with growth inhibition mode of action (n=69).

Korrelation mellem log Kow og eksperimentel EC_{50} for fisk ved anvendelse af herbicid data med vækshæmmende virkningsmekanisme (n=69).

The resulting equations for acute fish toxicity using data on herbicides with a growth inhibition mode of action (cf. figure 27) were:

log EC_{50} (mg/l) = -0.6344 log Kow + 2.3145 (n=69, r^2 = 0.5122)
log EC_{50} (mmol/l) = -0.538 log Kow - 0.1293 (n=69, r^2 = 0.5223)

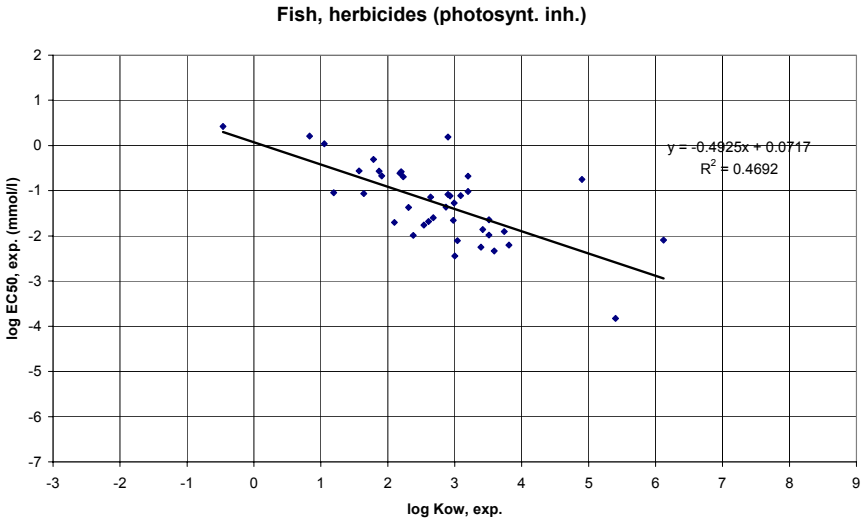


Figure 28
Correlation between log Kow and experimental EC_{50} for fish using data on herbicides with photosynthesis inhibition mode of action (n=40).

Korrelation mellem log Kow og eksperimentel EC_{50} for fisk ved anvendelse af data for herbicider med fotosyntesehæmmende (n=40). virkningsmekanisme.

The resulting equations for acute fish toxicity using data on herbicides with a photosynthesis inhibition mode of action (cf. figure 28) were:

$\log EC_{50}$ (mg/l) = -0.4394 log Kow + 2.3336 (n=40, r^2 = 0.3913)
$\log EC_{50}$ (mmol/l) = -0.4925 log Kow + 0.0717 (n=40, r^2 = 0.4692)

Compared to the result using fungicides, the estimations on fish acute toxicity using herbicide data were improved. The correlation coefficients for herbicides with a growth inhibition mode of action were slightly higher than for herbicides characterised with a photosynthesis inhibition mode of action.

The two modes of action is based on action modes taking place in plants and would be expected to be meaningless to fish. However, some herbicides are toxic to fish and the reason may be a general toxic action or a specific toxic action to enzymatic systems in fish. Whatever the reason, log Kow data on herbicides seems to an acceptable variable to estimate the general acute toxicity to fish.

For insecticides, all the data on experimental log Kow and acute toxicity are used and presented in figure 29. The data are then divided into insecticides with a cholinesterase inhibition mode of action and insecticides with a contact and systemic mode of action.

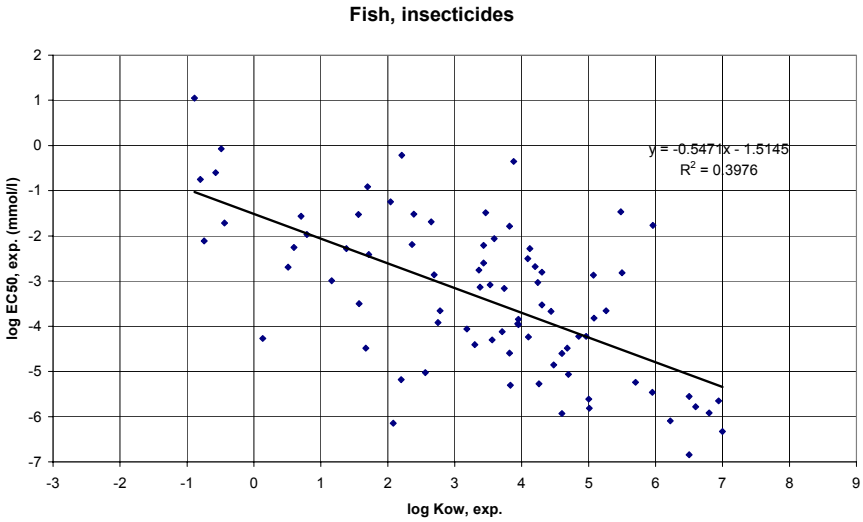


Figure 29
Correlation between log Kow and experimental EC_{50} for fish using data on insecticides (n=81).

Korrelation mellem log Kow og eksperimentel EC_{50} for fisk ved anvendelse af insekticiddata (n=81).

The equations for acute fish toxicity using insecticide data were:

$\log EC_{50}$ (mg/l) = -0.4998 log Kow + 0.8155 (n=81, r^2 = 0.3652)
$\log EC_{50}$ (mmol/l) = -0.5471 log Kow - 1.5145 (n=81, r^2 = 0.3976)

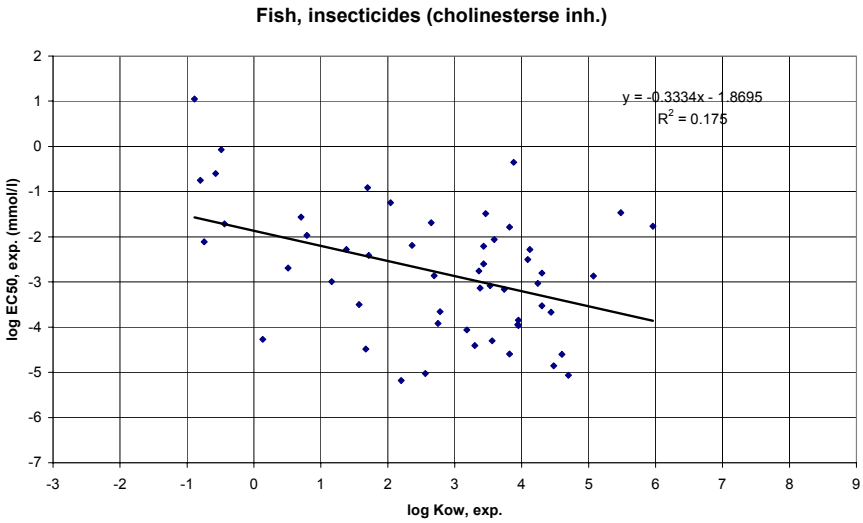


Figure 30
Correlation between log Kow and experimental EC_{50} for fish using data on insecticides with cholinesterase inhibition mode of action (n=53).

Korrelation mellem log Kow og eksperimentel EC_{50} for fisk ved anvendelse af insekticiddata for insekticider med cholinesterasehæmmende virkningsmekanisme (n=53).

The equations for acute fish toxicity using data on insecticides with a cholinesterase inhibition mode of action were:

log EC_{50} (mg/l) = -0.2903 log Kow + 0.4699 (n=53, r^2 = 0.1403)
log EC_{50} (mmol/l) = -0.3334 log Kow - 1.8695 (n=53, r^2 = 0.1750)

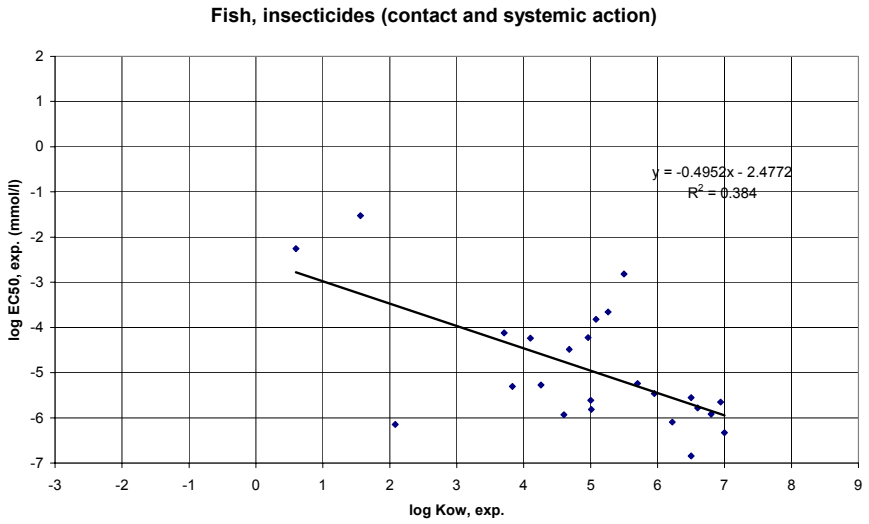


Figure 31
Correlation between log Kow and experimental EC_{50} for fish using data on insecticides with contact and systemic mode of action (n=24).

Korrelation mellem log Kow og eksperimentel EC_{50} for fisk ved anvendelse af data for insekticider med kontakt og systemisk virkningsmekanisme (n=24).

The equations for acute fish toxicity using data on insecticides with a contact and systemic mode of action were:

log EC_{50} (mg/l) = -0.4515 log Kow - 0.111 (n=24, r^2 = 0.3690)
log EC_{50} (mmol/l) = -0.4952 log Kow - 2.4772 (n=24, r^2 = 0.3840)

Comparing the figures on fungicides, herbicides and insecticides, it can be observed that the data points occupy a lower position in the charts that indicate a higher toxicity of insecticides to fish. This is not surprising since for instance a cholinesterase inhibition mode of action should also affect fish.

The data points are widely scattered which result in a low correlation coefficient. However, it should be remembered that several fish species, laboratories etc. are included and that it is the lowest experimental values found on acute toxicity that are used as effect data. These factors may result in the observed scattering of data points.

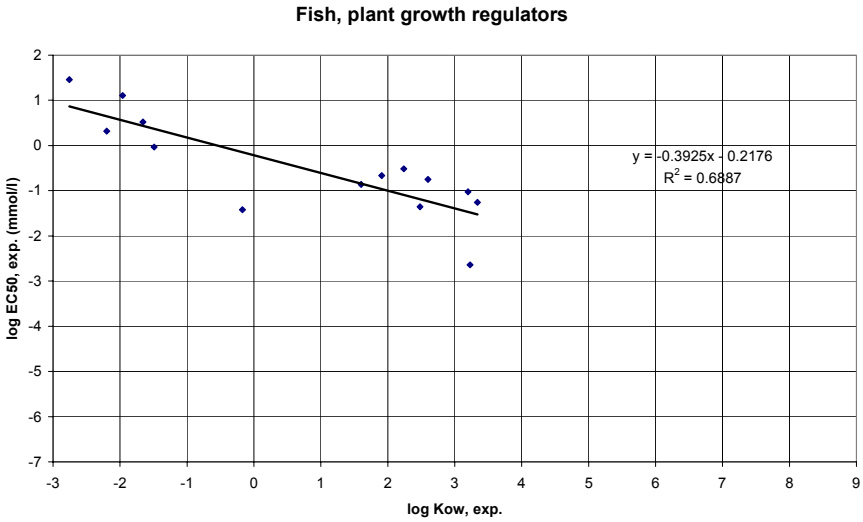


Figure 32
Correlation between log Kow and experimental EC_{50} for fish using data on plant growth regulators (n=14).

Korrelation mellem log Kow og eksperimentel EC_{50} for fisk ved anvendelse af data fra plantevækst regulatorer (n=14).

For plant growth regulators, only few data sets were available (cf. figure 32). The equations for acute fish toxicity using plant growth regulator data were:

$\log EC_{50}$ (mg/l) = -0.3391 log Kow + 2.054 (n=14, r^2 = 0.6495)
$\log EC_{50}$ (mmol/l) = -0.3925 log Kow - 0.2176 (n=14, r^2 = 0.6887)

The correlation coefficient was high and the estimations on toxicity based on log Kow were acceptable for plant regulators.

The data points are located in the upper end of the chart indicating lower toxicity than insecticides. It is not surprising since plant growth regulators usually affects meristematic tissues. The result could be compared with the results on rodenticides (cf. figure 33) where a high correlation coefficient was also observed.

The equations for acute fish toxicity using rodenticide data were:

$\log EC_{50}$ (mg/l) = -0.5838 log Kow + 2.7154 (n=5, r^2 = 0.6390)
$\log EC_{50}$ (mmol/l) = -0.617 log Kow + 0.2194 (n=5, r^2 = 0.6228)

It should be noted that the regression equations on both plant regulators and rodenticides are based on few data sets and should be used with this in mind.

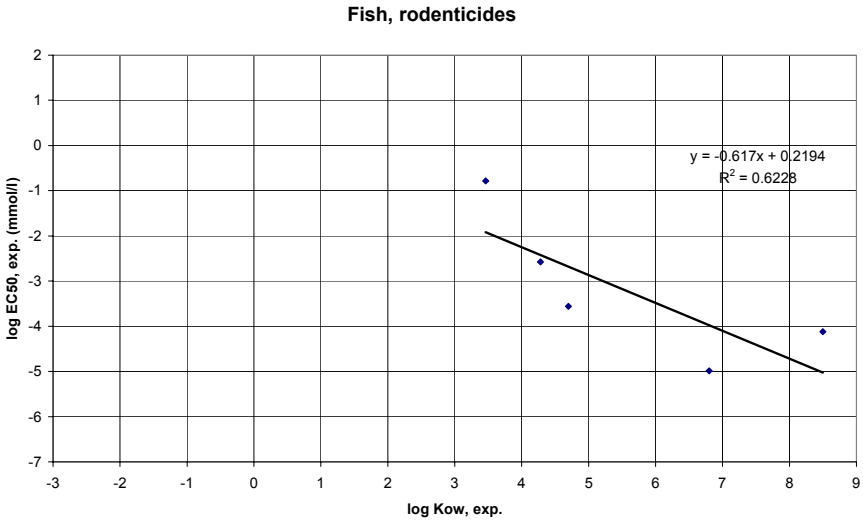


Figure 33
Correlation between log Kow and experimental EC_{50} for fish using rodenticides (n=5).

Korrelation mellem log Kow og eksperimentel EC_{50} for fisk med rottemidler (n=5).

Daphnia

For daphnia the same procedure as in fish was repeated using the same subdivision of pesticides.

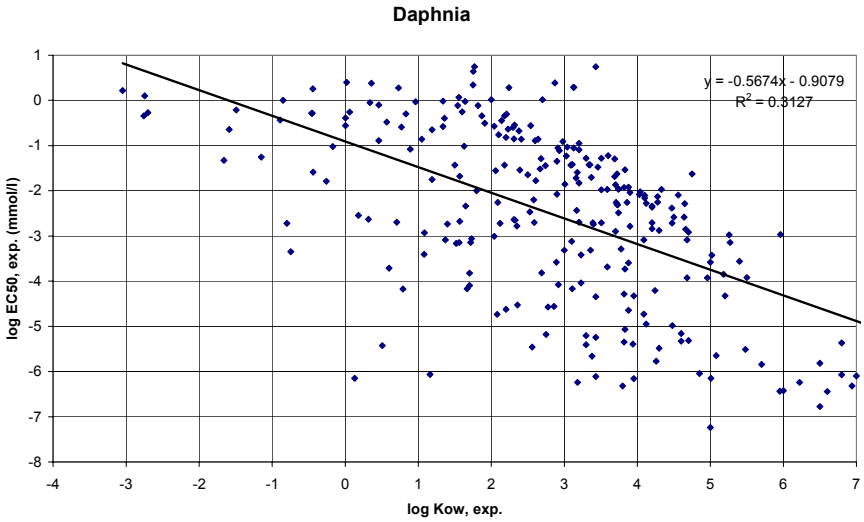


Figure 34
Correlation between log Kow and experimental EC_{50} values for Daphnia (n=255).

Korrelation mellem log Kow og eksperimentelle EC_{50}-værdier for dafnier (n=255).

Using all the selected pesticides and performing a regression analysis of the correlation between the experimental log Kow and the acute toxicity, the resulting equations for estimating acute daphnia toxicity were:

$\log EC_{50}$ (mg/l) = - 0.5166 log Kow + 1.39 (n=255, r^2 = 0.2743)
$\log EC_{50}$ (mmol/l) = - 0.5674 log Kow - 0.9079 (n=255, r^2 = 0.3127)

The reduced correlation compared with the Verhaar ***et al.*** QSARs may be the result of data from a broader variety of pesticides, data sources and/or study

methodologies included in the applied values. The low correlation coefficient of 0.31 does not indicate a predictive value to be sufficient even for a screening procedure.

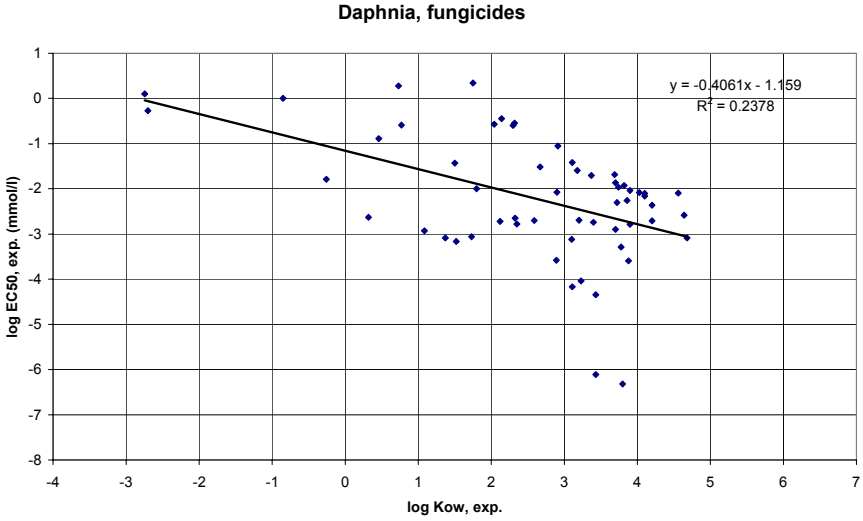


Figure 35
Correlation between log Kow and experimental EC_{50} for daphnia using data on fungicides (n=57).

Korrelation mellem log Kow og eksperimentel EC_{50} for dafnier med data for fungicider (n=57).

The resulting equations for acute daphnia toxicity using fungicide data were:

log EC_{50} (mg/l) = -0.3149 log Kow + 1.0021 (n=57, r^2 = 0.1518)
log EC_{50} (mmol/l) = -0.4061 log Kow - 1.159 (n=57, r^2 = 0.2378)

As with the fish data, the data points were widely dispersed and the correlation coefficient was low.

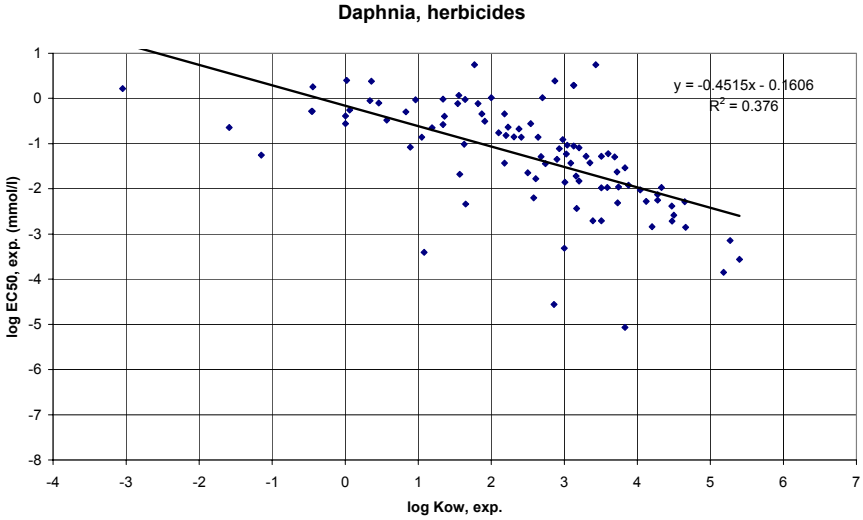


Figure 36
Correlation between log Kow and experimental EC_{50} for daphnia using data on herbicides (n=97).

Korrelation mellem log Kow og eksperimentel EC_{50} for dafnier ved anvendelse af herbicid data (n=97).

The resulting equations for acute daphnia toxicity using all available herbicide data (cf. figure 36) were:

$\log EC_{50}$ (mg/l) = -0.4388 log Kow + 2.2407 (n=97, r^2 = 0.3578)
$\log EC_{50}$ (mmol/l) = -0.4515 log Kow - 0.1606 (n=97, r^2 = 0.3760)

The correlation coefficients were low and with a low toxicity as indicated by the position on the chart (figure 36). The same comments on expected toxicity presented for fish above also applies to daphnia.

The herbicide data were divided into herbicides with a growth inhibition mode of action (cf. figure 37) and herbicides with a photosynthesis inhibition mode of action (cf. figure 38).

The resulting equations for acute daphnia toxicity using data on herbicides with a growth inhibition mode of action were:

$\log EC_{50}$ (mg/l) = -0.4263 log Kow + 2.1565 (n=58, r^2 = 0.3344)
$\log EC_{50}$ (mmol/l) = -0.4344 log Kow - 0.2771 (n=58, r^2 = 0.3547)

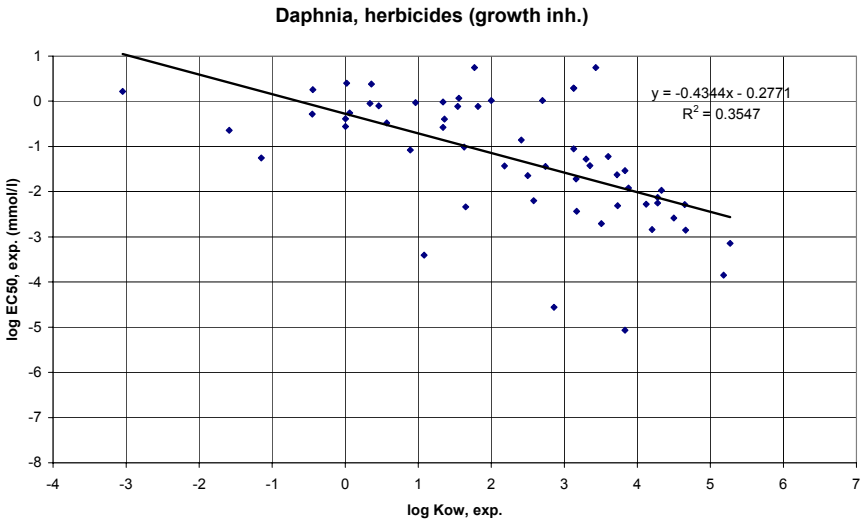


Figure 37
Correlation between log Kow and experimental EC_{50} for daphnia using data on herbicides with growth inhibition mode of action (n=58).

Korrelation mellem log Kow og eksperimentel EC_{50} for dafnier ved anvendelse af data fra herbicider med vækshæmmende virkningsmekanisme.

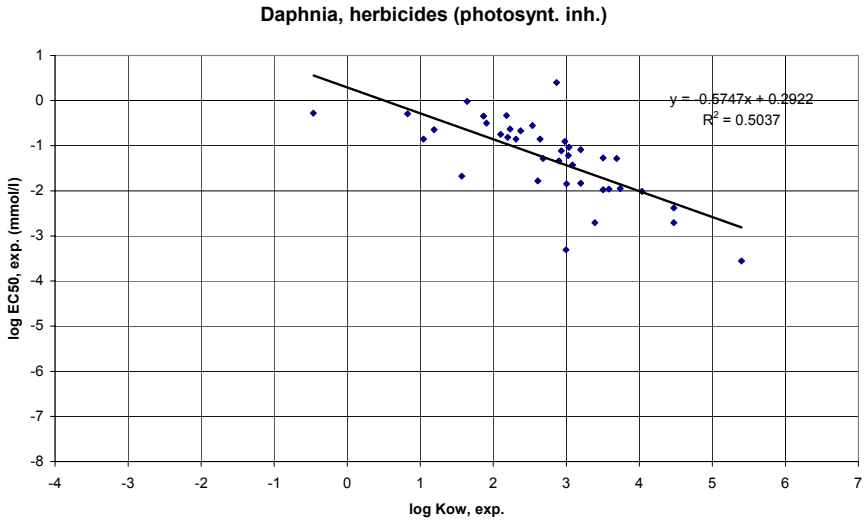


Figure 38
Correlation between log Kow and experimental EC_{50} for daphnia using data on herbicides with photosynthesis inhibition mode of action (n=39).

Korrelation mellem log Kow og eksperimentel EC_{50} for dafnier ved anvendelse af data fra herbicider med fotosyntesehæmmende virkningsmekanisme (n=39).

The resulting equations for acute daphnia toxicity using data on herbicides with a photosynthesis inhibition mode of action were:

$\log EC_{50}$ (mg/l) = -0.5284 log Kow + 2.569 (n=39, r^2 = 0.4788)
$\log EC_{50}$ (mg/l) = -0.5747 log Kow + 2.922 (n=39, r^2 = 0.5037)

The correlation coefficient for data on herbicides with a photosynthesis inhibition mode of action was considerably higher than for the other data sets on herbicides. No explanation can be given. The position of the data points indicates relatively low toxicity of herbicides to daphnia that was not unexpected.

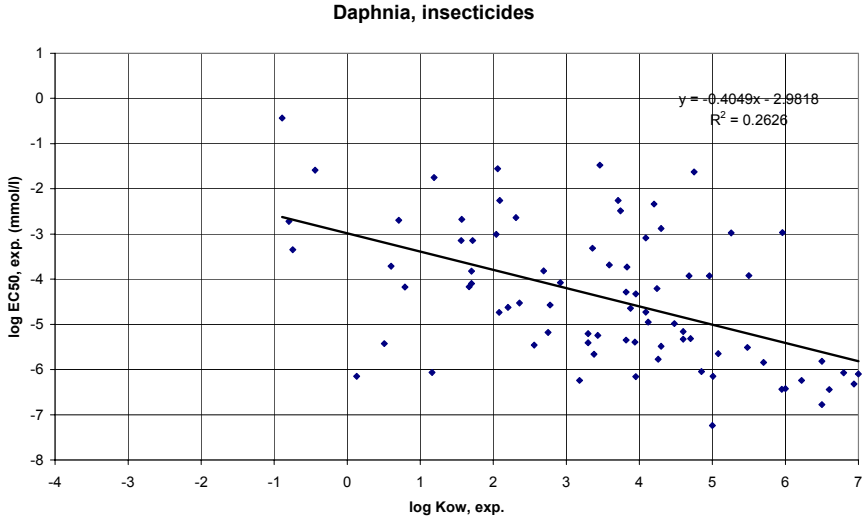


Figure 39
Correlation between log Kow and experimental EC_{50} for daphnia using data on insecticides (n=79).

Korrelation mellem log Kow og eksperimentel EC_{50} for dafnier ved anvendelse af insekticiddata (n=79).

The equations for acute daphnia toxicity using insecticide data were:

log EC_{50} (mg/l) = -0.3521 log Kow - 0.6848 (n=79, r^2 = 0.2203)
log EC_{50} (mmol/l) = -0.4049521 log Kow - 2.9818 (n=79, r^2 = 0.2626)

For insecticides, using all available data sets it could be observed by the position in the chart (figure 39) that insecticides were more toxic to daphnia than herbicides and fungicides as expected.

The equations for acute daphnia toxicity using data on insecticides with a cholinesterase inhibition mode of action (cf. figure 40) were:

log EC_{50} (mg/l) = -0.2711 log Kow - 1.1177 (n=43, r^2 = 0.1243)
log EC_{50} (mmol/l) = -0.3156 log Kow - 3.4422 (n=43, r^2 = 0.1582)

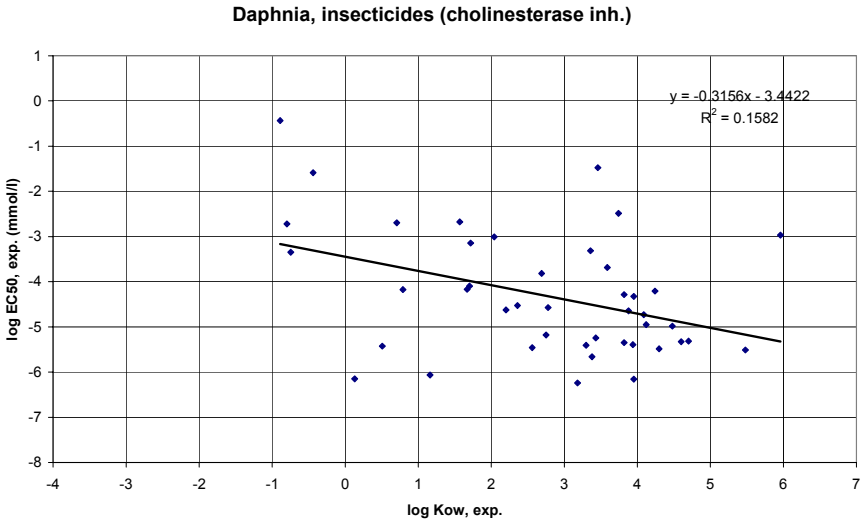


Figure 40
Correlation between log Kow and experimental EC_{50} for daphnia using data on insecticides with cholinesterase inhibition mode of action (n=43).

Korrelation mellem log Kow og eksperimentel EC_{50} for dafnier ved anvendelse af data for insekticider med cholinesterasehæmmende virkningsmekanisme (n=43).

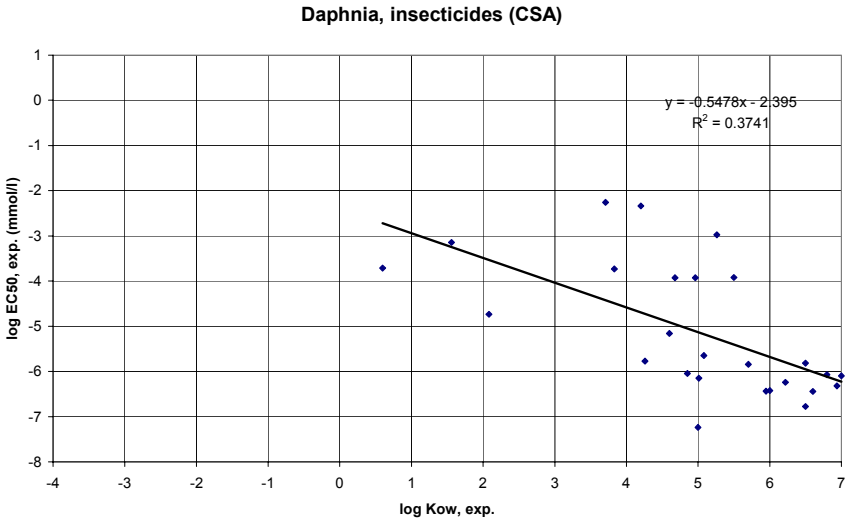


Figure 41
Correlation between log Kow and experimental EC_{50} for daphnia using data on insecticides with contact and systemic mode of action (n=26).

Korrelation mellem log Kow og eksperimentel EC_{50} for dafnier ved anvendelse af data for insekticider med kontakt og systemisk virkningsmekanisme (n=26).

The equations for acute fish toxicity using data on insecticides with a contact and systemic mode of action were:

$\log EC_{50}$ (mg/l) = -0.5026 log Kow - 0.043 (n=26, r^2 = 0.3465)
$\log EC_{50}$ (mmol/l) = -0.5478 log Kow - 2.395 (n=26, r^2 = 0.3741)

The data points from all insecticides were widely scattered. Dividing the data on insecticides into modes of action did not improve the correlation coefficients. Primarily data on ***Daphnia magna*** and a few data on ***Daphnia pulex*** were included. No other crustacean species were used. Data were based on OECD standard 48-hour tests. However, test conditions, media etc. may differ and may be part of an explanation.

For plant growth regulators, only a few data sets were available. As indicated by figure 42 they were less toxic than the insecticides which was not unexpected due to their specific mode of action on plant meristematic tissues.

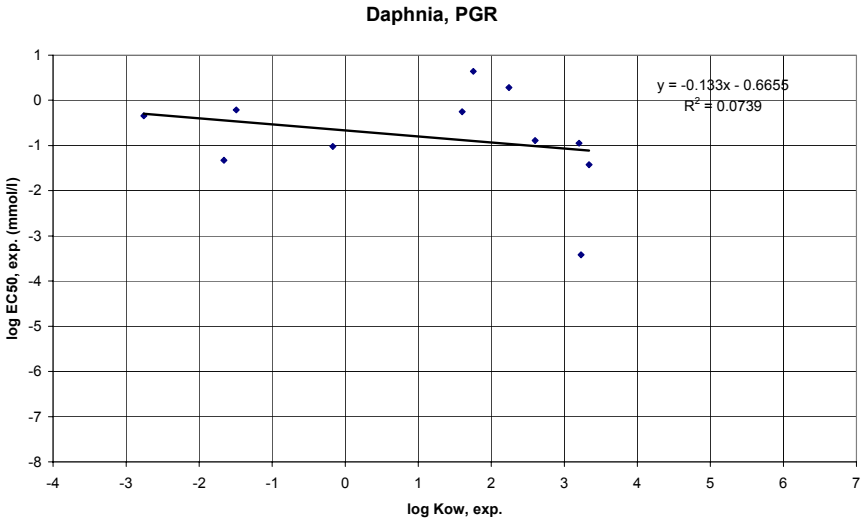


Figure 42
Correlation between log Kow and experimental EC_{50} for daphnia using data on plant growth regulators (n=11).

Korrelation mellem log Kow og eksperimentel EC_{50} for dafnier ved anvendelse af data fra plantevækst regulatorer (n=11).

The equations for acute daphnia toxicity using plant growth regulator data were:

$\log EC_{50}$ (mg/l) = -0.0887 log Kow + 1.6166 (n=11, r^2 = 0.0364)
$\log EC_{50}$ (mmol/l) = -0.133 log Kow - 0.6655 (n=11, r^2 = 0.0739)

The correlation was very low and the data points few. The data indicate a low toxicity of plant growth regulators to daphnia. Another parameter than Kow should be searched for as descriptor.

Daphnia reproduction

For chronic toxicity, experimental 21-day NOEC data on Daphnia magna reproduction were used. However, sufficient data were not available to perform a division further than to the main groups of fungicides, herbicides and insecticides.

Using all available pesticide data sets on daphnia reproduction resulted in figure 43.

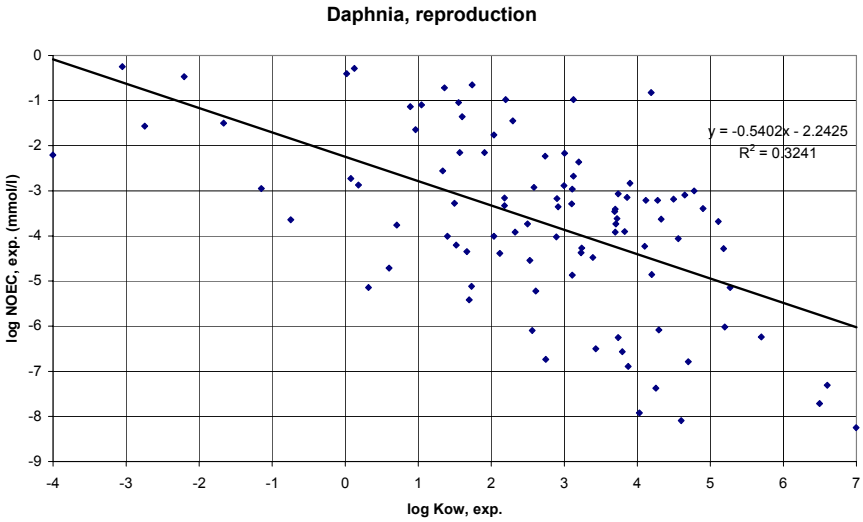


Figure 43
Correlation between experimental log Kow and experimental daphnia NOEC (21 days) values.

Korrelation mellem eksperimentel log Kow og eksperimentelle værdier for dafniers NOEC (21 dage).

Performing linear regression analyses between experimental log Kow and experimental NOEC values from daphnia reproduction tests resulted in the regression equations:

log NOEC (21d, mg/l) = -0.5052 log Kow + 0.1325(n=96, r^2=0.3002)
log NOEC (21d, mmol/l) = -0.5402 log Kow - 2.2425(n=96, r^2=0.3241)

The correlation coefficients were close to the correlation observed when the QSAR from Verhaar ***et al.*** (1995) was used (cf. figure 20). In other words, the above-derived QSAR model may also be used for estimating the daphnia reproduction NOEC with the same precision as the recommended QSAR. The correlation coefficient was low. However, seeking for QSAR models to be used in general, low correlation coefficients may be accepted and the results used with precaution for indicative purposes only.

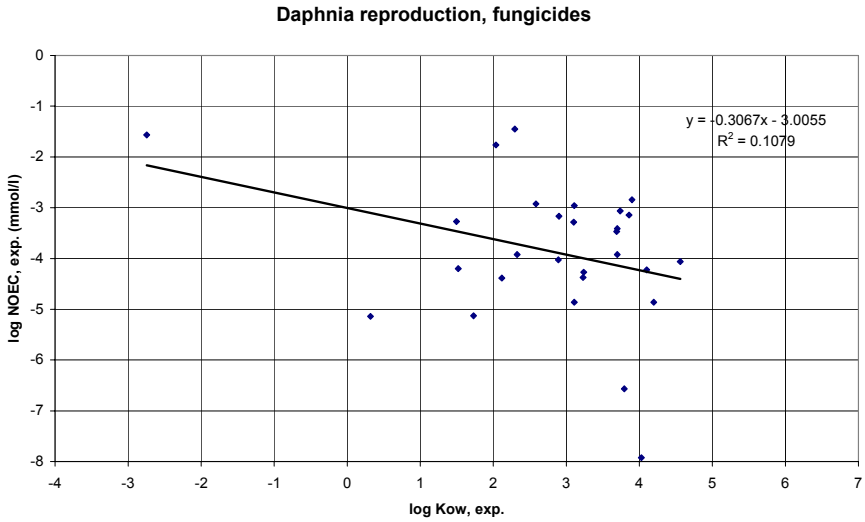


Figure 44
Correlation between experimental log Kow and experimental Daphnia NOEC (21 days) using data on fungicides.

Korrelation mellem data for eksperimentel log Kow og eksperimentel dafnie NOEC (21 dage) fra svampemidler.

The resulting equations for chronic daphnia toxicity using fungicide data were:

log NOEC (mg/l) = -0.3035 log Kow - 0.5229 (n=28, r^2 = 0.1106)
log NOEC (mmol/l) = -0.3067 log Kow - 3.0055 (n=28, r^2 = 0.1079)

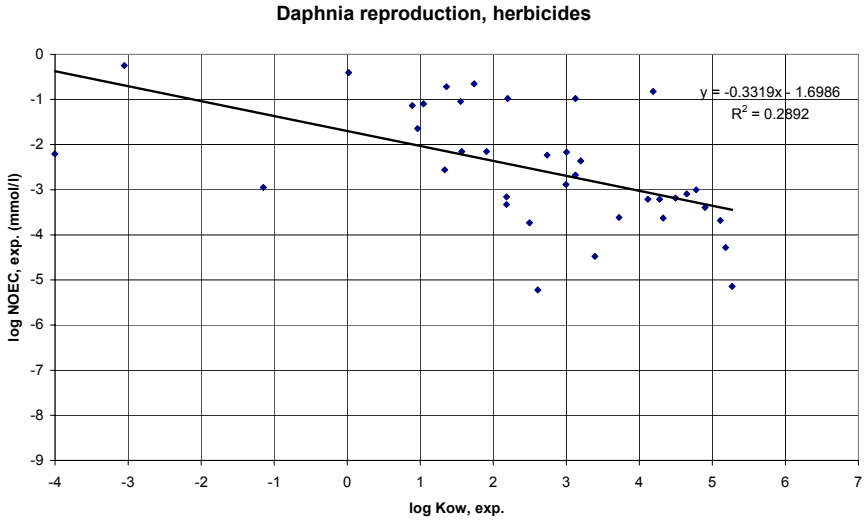


Figure 45
Correlation between experimental log Kow and experimental Daphnia NOEC (21 days) using data on herbicides.

Korrelation mellem data for eksperimentel log Kow og eksperimentel dafnie NOEC (21 dage) for herbicider.

The resulting equations for chronic daphnia toxicity using herbicide data were:

log NOEC (mg/l) = -0.3163 log Kow + 0.7216 (n=37, r^2 = 0.2647)
log NOEC (mmol/l) = -0.3319 log Kow - 1.6986 (n=37, r^2 = 0.2892)

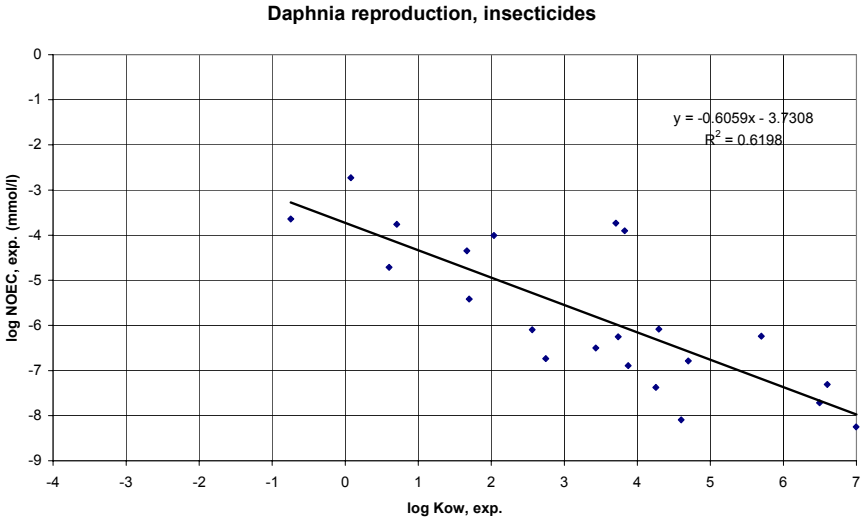


Figure 46
Correlation between experimental log Kow and experimental Daphnia NOEC (21 days) using data on insecticides.

Korrelation mellem data for eksperimentel log Kow og eksperimentel dafnie NOEC (21 dage) for insekticider.

The resulting equations for chronic daphnia toxicity using insecticide data were:

log NOEC (mg/l) = -0.5516 log Kow - 1.425 (n=22, r^2 = 0.5682)
log NOEC (mmol/l) = -0.6059 log Kow - 3.7308 (n=22, r^2 = 0.6198)

Data on rodenticides were insufficient for analysis to be performed.

For estimating the chronic toxicity to daphnia using daphnia reproduction NOEC as end point and log Kow as descriptor, the resulting equations on fungicides and herbicides were meaningless. This may be the result of the designated substances' mode of action in contrast to insecticides where a toxic action is expected. The only derived equations with high correlation coefficients were data on insecticides. Although the data points were few a clear tendency was observed. However, more data should be included before a general use of the equation is recommendable.

Algae

The same procedure as for fish and daphnia is performed on acute algae tests. The data are from tests performed according to OECD test guidelines and the end point was inhibition EC_{50} values after 72 to 96 hours.

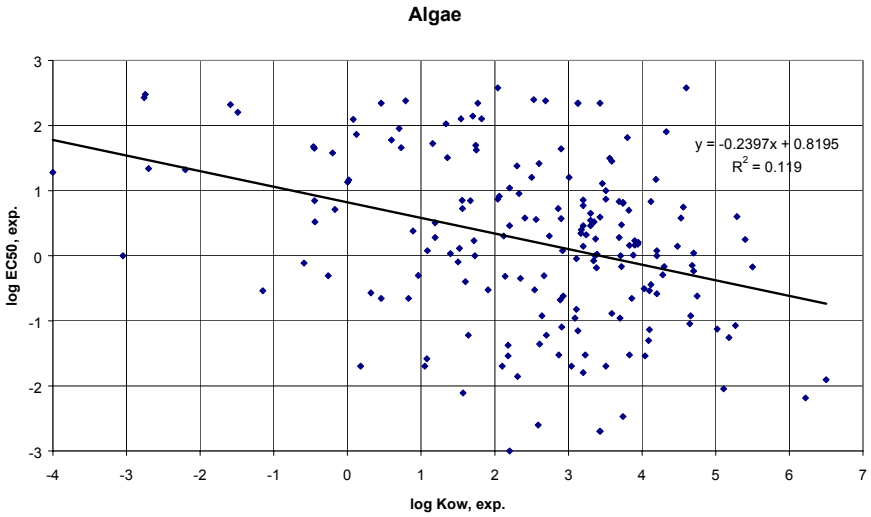


Figure 47
Correlation between log Kow and experimental EC_{50} values for algae.

Korrelation mellem log Kow og eksperimentelle EC_{50} værdier for alger.

Using all the selected pesticides and performing a regression analysis on the experimental log Kow and the acute toxicity data, the resulting equation for algae was:

$\log EC_{50}$ (mg/l) = - 0.2397 log Kow + 0.8195 (n=183, r^2 = 0.1190)

The reduced correlation compared with the Van Leeuwen ***et al.*** QSARs may be the result of data from a broader variety of pesticides (Verhaar ***et al.*** n=10) and/or study methodologies included in the applied values. The low correlation coefficient of 0.12 does not indicate a predictive value to be sufficient even for a screening procedure.

For algae, the QSAR from Verhaar ***et al.*** (1995) was expressed in mol/l where the results above were analysed using mg/l. Using mmol/l is presented in the figure below (figure 48).

Transforming the toxicity data to mmol/l, the resulting equation for algae was:

$\log EC_{50}$ (mmol/l) = - 0.2679 log Kow - 1.5452 (n=183, r^2 = 0.1451)

Thus, only a minor improvement in the correlation coefficient is observed The data points are still widely dispersed and only a weak tendency evolved from the change.

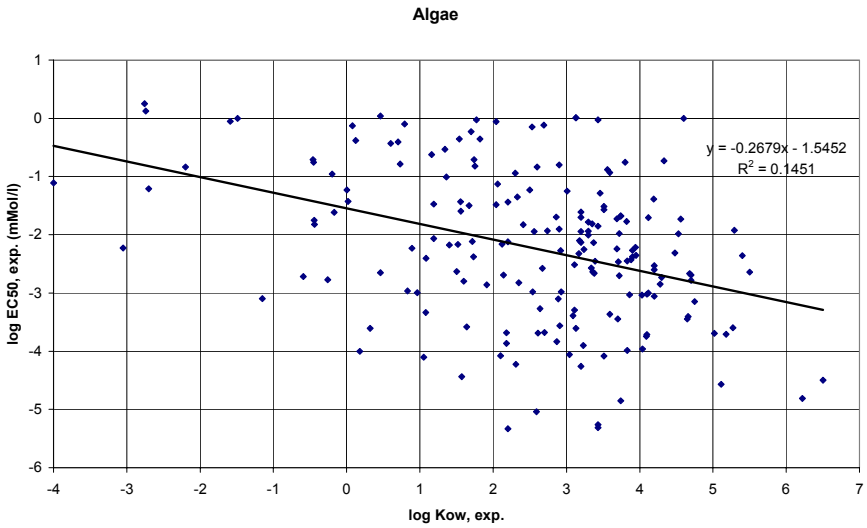


Figure 48
Correlation between log Kow and log experimental EC_{50} (mmol/l).

Korrelation mellem log Kow og log eksperimentel EC_{50} (mmol/l).

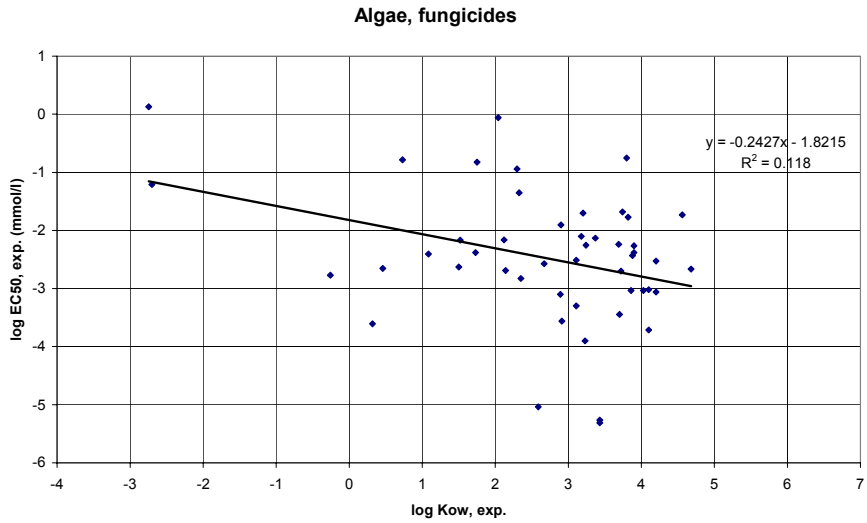


Figure 49
Correlation between log Kow and experimental EC_{50} for algae using data on fungicides (n=48).

Korrelation mellem log Kow og eksperimentel EC_{50} for alger med data for fungicider (n=48).

The resulting equations for acute algae toxicity using fungicide data were:

$\log EC_{50}$ (mg/l) = -0.2325 log Kow + 0.623 (n=48, r^2 = 0.1112)
$\log EC_{50}$ (mmol/l) = -0.2427 log Kow - 1.8215 (n=48, r^2 = 0.1180)

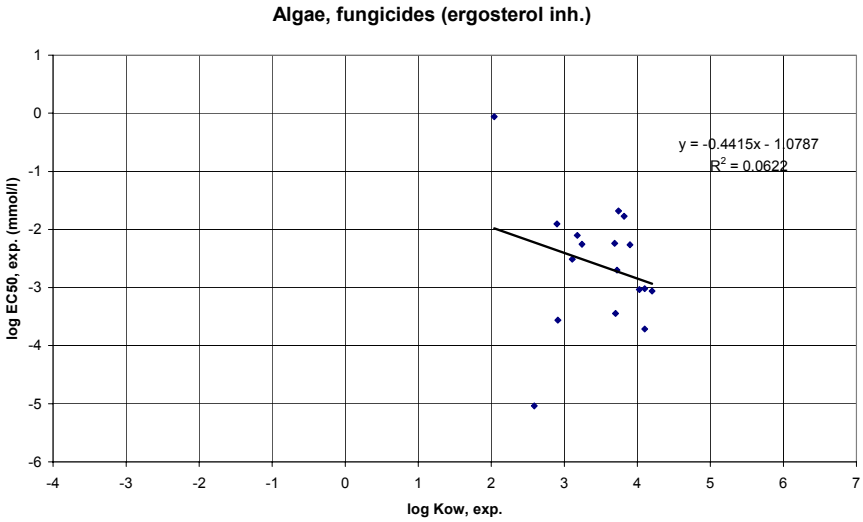


Figure 50
Correlation between log Kow and experimental EC_{50} for algae using data on fungicides with ergosterol inhibition mode of action (n=17).

Korrelation mellem log Kow og eksperimentel EC_{50} for alger med data for fungicider med ergosterolhæmmende virkningsmekanisme (n=17).

The resulting equations for acute algae toxicity using fungicide data on fungicides with ergosterol inhibition mode of action were:

$\log EC_{50}$ (mg/l) = -0.4549 log Kow + 1.4752 (n=17, r^2 = 0.0629)
$\log EC_{50}$ (mmol/l) = -0.4415 log Kow - 1.0787 (n=17, r^2 = 0.0622)

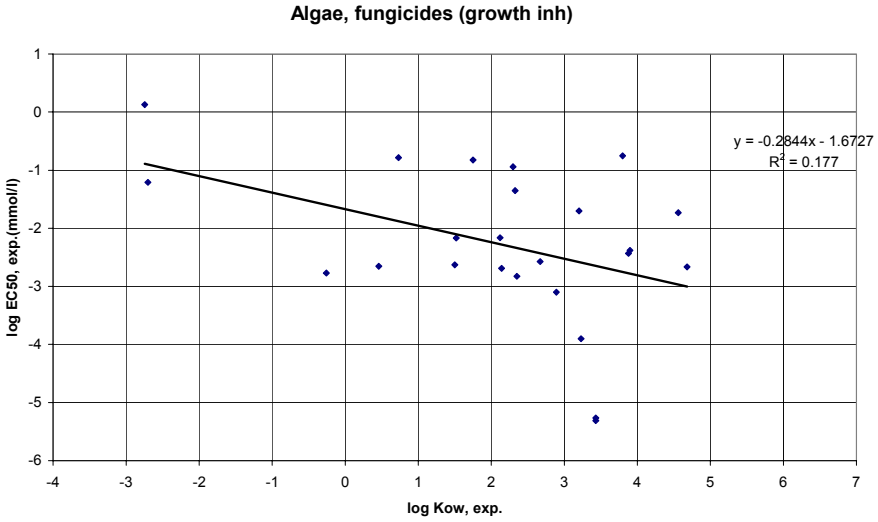


Figure 51
Correlation between log Kow and experimental EC_{50} for algae using data on fungicides with growth inhibition mode of action (n=24).

Korrelation mellem log Kow og eksperimentel EC_{50} for alger med data for fungicider med vækshæmmende virkningsmekanisme (n=24).

The resulting equations for acute algae toxicity using fungicide data on fungicides with a growth inhibition mode of action were:

$\log EC_{50}$ (mg/l) = -0.2669 log Kow + 0.7178 (n=24, r^2 = 0.1605)
$\log EC_{50}$ (mmol/l) = -0.2844 log Kow - 1.6727 (n=24, r^2 = 0.1770)

Based on fungicides, neither all available data nor a selection of data on fungicides with ergosterol inhibition mode of action resulted in any usable regression equations. The data points were scattered and no tendency could be observed.

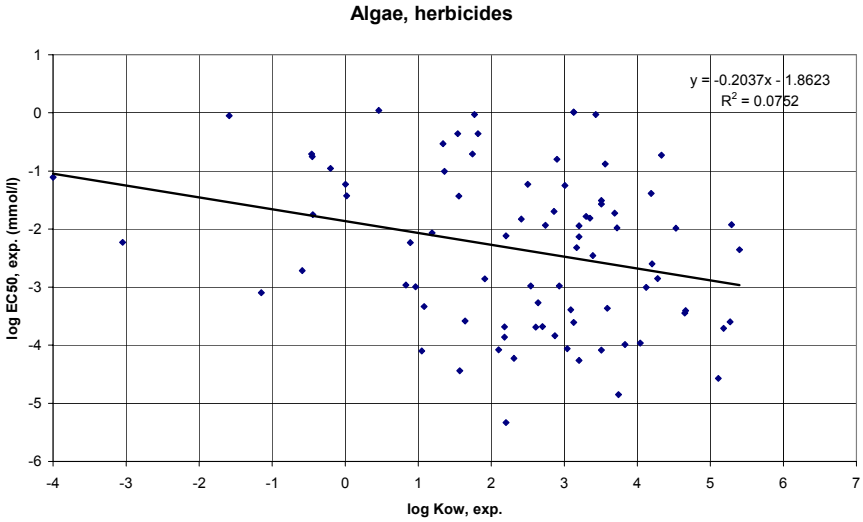


Figure 52
Correlation between log Kow and experimental EC_{50} for algae using data on herbicides (n=82).

Korrelation mellem log Kow og eksperimentel EC_{50} for alger ved anvendelse af herbiciddata (n=82).

The resulting equations for acute algae toxicity using all available herbicide data were:

$\log EC_{50}$ (mg/l) = -0.1898 log Kow +025345 (n=82, r^2 = 0.0636)
$\log EC_{50}$ (mmol/l) = -0.2037 log Kow - 1.8623 (n=82, r^2 = 0.0752)

It was surprising that using herbicide data sets did not show any tendency. Results from different algae species are included. Algae species are known to differ considerably in sensitivity to chemicals. Another explanation could be that the general mode of action in herbicides does not apply to algae which normally is considered as aquatic micro-plants.

A subdivision of data on herbicides with growth inhibition (cf. figure 53) and photosynthesis inhibition mode of action (cf. figure 54) was performed.

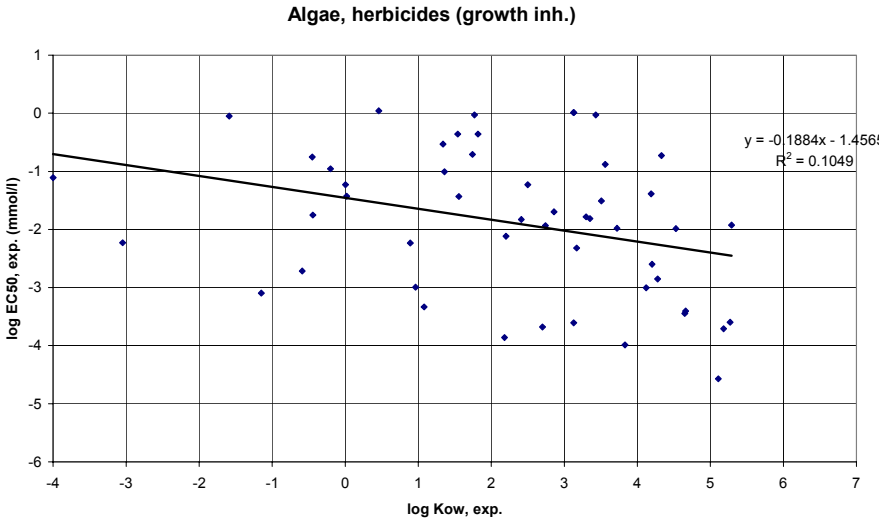


Figure 53
Correlation between log Kow and EC_{50} for algae using data on herbicides with growth inhibition mode of action (n=51).

Korrelation mellem log Kow og EC_{50} for alger ved anvendelse af data fra herbicider med vækshæmmende virkningsmekanisme (n=51).

The resulting equations for acute algae toxicity using data on herbicides with a growth inhibition mode of action were:

$\log EC_{50}$ (mg/l) = -0.1768 log Kow + 0.9666 (n=51, r^2 = 0.0934)
$\log EC_{50}$ (mmol/l) = -0.1884 log Kow - 1.456 (n=51, r^2 = 0.1049)

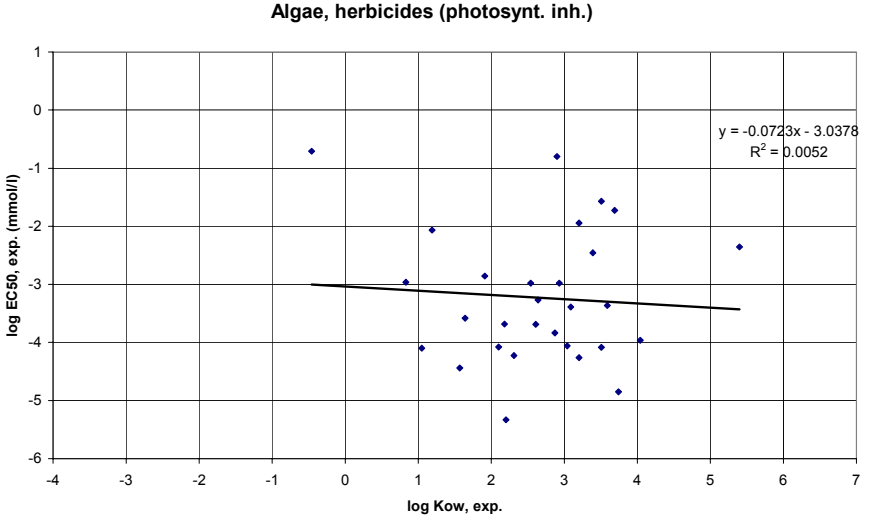


Figure 54
Correlation between log Kow and EC_{50} for algae using data on herbicides with photosynthesis inhibition mode of action (n=29).

Korrelation mellem log Kow og EC_{50} for alger ved anvendelse af data for herbicider med fotosyntesehæmmende virkningsmekanisme (n=29).

The resulting equations for acute algae toxicity using data on herbicides with a photosynthesis inhibition mode of action were:

$\log EC_{50}$ (mg/l) = -0.0294 log Kow - 0.7492 (n=29, r^2 = 0.0008)
$\log EC_{50}$ (mmol/l) = -0.0723 log Kow - 3.0378 (n=29, r^2 = 0.0052)

The subdivision of herbicide data sets did not improve the correlation coefficients. No acceptable regression equations could be deducted.

Regression analyses on experimental log Kow and insecticides (cf. figure 55) and selected insecticides with cholinesterase inhibition mode of action (cf. figure 56) were performed.

Figure 55
Correlation between log Kow and experimental EC_{50} for algae using data on insecticides (n=34).

Korrelation mellem log Kow og eksperimentel EC_{50} for alger ved anvendelse af insekticiddata (n=34).

The equations for acute algae toxicity using insecticide data were:

$\log EC_{50}$ (mg/l) = -0.4461 log Kow + 1.9898 (n=34, r^2 = 0.4395)
$\log EC_{50}$ (mmol/l) = -0.494 log Kow - 0.3145 (n=34, r^2 = 0.4908)

A tendency was observed and although the correlation coefficient was low the resulting regression equations may be used for indicative purposes. However, the number of data sets is small and more data should be included before further recommendation can be considered.

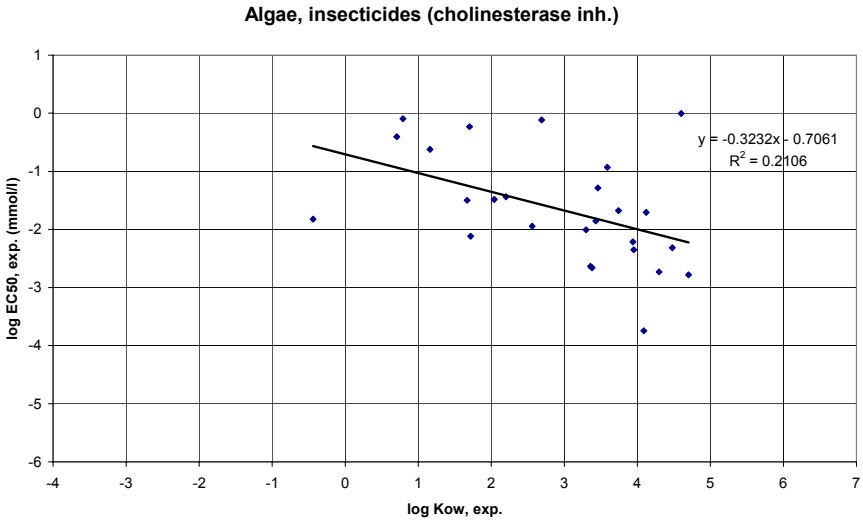


Figure 56
Correlation between log Kow and experimental EC_{50} for algae using data on insecticides with cholinesterase inhibition mode of action (n=26).

Korrelation mellem log Kow og eksperimentel EC_{50} for alger ved anvendelse af data for insekticider med cholinesterasehæmmende virkningsmekanisme (n=26).

The equations for acute algae toxicity using data on insecticides with a cholinesterase inhibition mode of action were:

$\log EC_{50}$ (mg/l) = -0.2843 log Kow + 1.6348 (n=26, r^2 = 0.1692)
$\log EC_{50}$ (mmol/l) = -0.3232 log Kow - 0.7061 (n=26, r^2 = 0.2106)

No result was gained by selecting data sets on insecticides with a cholinesterase inhibiting mode of action. It is not unexpected since the mode of action is irrelevant for algae.

Using data on plant growth regulators, a positive result would be expected. The equations for acute algae toxicity using plant growth regulator data were:

$\log EC_{50}$ (mg/l) = -0.2735 log Kow + 1.1986 (n=8, r^2 = 0.4655)
$\log EC_{50}$ (mmol/l) = -0.3192 log Kow - 1.0879 (n=8, r^2 = 0.5149)

A tendency was observed but the data too few to be conclusive. More data is needed before any recommendations can be made.

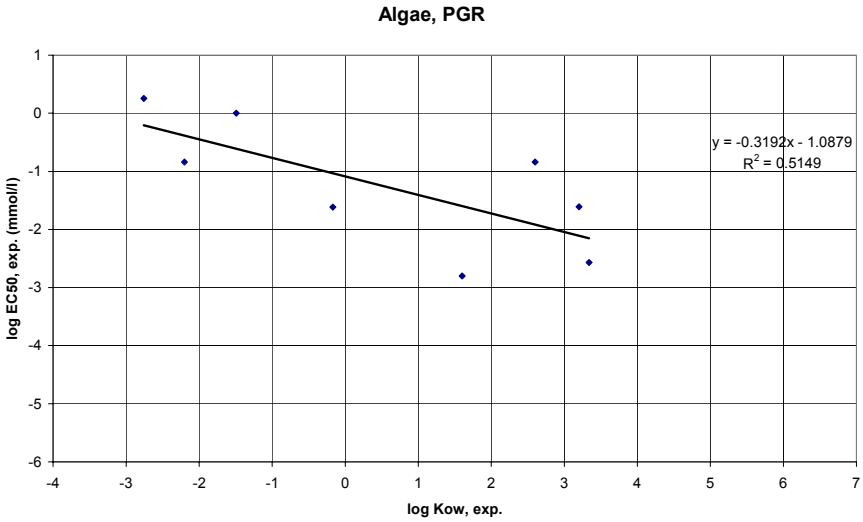


Figure 57
Correlation between log Kow and experimental EC_{50} for algae using data on plant growth regulators (n=8).

Korrelation mellem log Kow og eksperimentel EC_{50} for alger ved anvendelse af data for plantevækst regulatorer (n=8).

3.5.5 Discussion on estimated ecotoxicity

Based on the results using the available recommended QSARs it could be observed that the estimated acute toxicity was generally underestimated. Using the experimental results from pesticides, improved results could be obtained for some organisms whereas for others (e.g. algae) no correlation could be observed using log Kow as descriptor. Dividing the data sets into primary functional areas (fungicides, herbicides, insecticides, plant growth regulators and rodenticides) according to the assumption that the manufacturers recommended the substance for the use areas where the largest effects would be expected, generally low correlations were observed. A further subdivision into the pesticides' mode of action resulted in improvements for some of the correlations and the opposite for others (cf. table 10).

It is generally agreed that when measuring the effect of a chemical it is at the molecular level that the chemical has an impact. Therefore the QSARs should be developed based on effect concentrations expressed on a molar basis. Including the molecular weight in the calculations improved the correlations slightly (cf. table 10). However, for the pesticides where the variation in the molecular weight was relatively small (mean molecular weight of the studied pesticides and standard deviation was 299 and 103, respectively) the improvements by using mmol/l instead of mg/l were low.

Table 10
Correlations between log Kow and experimental effect concentrations in mg/l or mmol/l

Korrelationer mellem log Kow og effektkoncentrationer i mg/l eller mmol/l

Test	Group	Mode of action	Equation	No. and correlation
Fish acute	Pesticides		log EC_{50} (mg/l) = -0.4153 log Kow + 1.3643	(n=300, r^2 = 0.3197)
			log EC_{50} (mg/l) = -0.5076 log Kow + 1.6739	(n=296, r^2 = 0.3786)
			log EC_{50} (mmol/l) = 0.5471 log Kow - 0.6666	(n=296, r^2 = 0.4081)
	Fungicides		log EC_{50} (mg/l) = -0.2963 log Kow + 0.8584	(n=59, r^2 = 0.1890)
			log EC_{50} (mmol/l) = -0.3146 log Kow - 1.5506	(n=59, r^2 = 0.2012)
	Herbicides	All	log EC_{50} (mg/l) = -0.5193 log Kow + 2.3548	(n=118, r^2 = 0.4814)
			log EC_{50} (mmol/l) = -0.5337 log Kow - 0.0459	(n=118, r^2 = 0.5030)
		Growth. inh	log EC_{50} (mg/l) = -0.6344 log Kow + 2.3145	(n=69, r^2 = 0.5122)
			log EC_{50} (mmol/l) = -0.538 log Kow - 0.1293	(n=69, r^2 = 0.5223)
		Photosyn. inh.	log EC_{50} (mg/l) = -0.4394 log Kow + 2.3336	(n=40, r^2 = 0.3913)
			log EC_{50} (mmol/l) = -0.4925 log Kow + 0.0717	(n=40, r^2 = 0.4692)
	Insecticides	All	log EC_{50} (mg/l) = -0.4998 log Kow + 0.8155	(n=81, r^2 = 0.3652)
			log EC_{50} (mmol/l) = -0.5471 log Kow - 1.5145	(n=81, r^2 = 0.3976)
		Cholinest. inh.	log EC_{50} (mg/l) = -0.2903 log Kow + 0.4699	(n=53, r^2 = 0.1403)
			log EC_{50} (mmol/l) = -0.3334 log Kow - 1.8695	(n=53, r^2 = 0.1750)
		CSA	log EC_{50} (mg/l) = -0.4515 log Kow - 0.111	(n=24, r^2 = 0.3690)
			log EC_{50} (mmol/l) = -0.4952 log Kow - 2.4772	(n=24, r^2 = 0.3840)
	PGR		log EC_{50} (mg/l) = -0.3391 log Kow + 2.054	(n=14, r^2 = 0.6495)
			log EC_{50} (mmol/l) = -0.3925 log Kow - 0.2176	(n=14, r^2 = 0.6887)
	Rodenticides		log EC_{50} (mg/l) = -0.5838 log Kow + 2.7154	(n=5, r^2 = 0.6390)
			log EC_{50} (mmol/l) = -0.617 log Kow + 0.2194	(n=5, r^2 = 0.6228)
Daphnia Acute	Pesticides		log EC_{50} (mg/l) = - 0.5166 log Kow + 1.39	(n=255, r^2 = 0.2743)
			log EC_{50} (mmol/l) = - 0.5674 log Kow - 0.9079	(n=255, r^2 = 0.3127)
	Fungicides		log EC_{50} (mg/l) = -0.3149 log Kow + 1.0021	(n=57, r^2 = 0.1518)
			log EC_{50} (mmol/l) = -0.4061 log Kow - 1.159	(n=57, r^2 = 0.2378)
	Herbicides		log EC_{50} (mg/l) = -0.4388 log Kow + 2.2407	(n=97, r^2 = 0.3578)
			log EC_{50} (mmol/l) = -0.4515 log Kow - 0.1606	(n=97, r^2 = 0.3760)
		Growth inh.	log EC_{50} (mg/l) = -0.4263 log Kow + 2.1565	(n=58, r^2 = 0.3344)
			log EC_{50} (mmol/l) = -0.4344 log Kow - 0.2771	(n=58, r^2 = 0.3547)
		Photosynt. inh.	log EC_{50} (mg/l) = -0.5284 log Kow + 2.569	(n=39, r^2 = 0.4788)
			log EC_{50} (mg/l) = -0.5747 log Kow + 2.922	(n=39, r^2 = 0.5037)
	Insecticides		log EC_{50} (mg/l) = -0.3521 log Kow - 0.6848	(n=79, r^2 = 0.2203)
			log EC_{50} (mmol/l) = -0.4049521 log Kow - 2.9818	(n=79, r^2 = 0.2626)
		Cholinest. inh.	log EC_{50} (mg/l) = -0.2711 log Kow - 1.1177	(n=43, r^2 = 0.1243)
			log EC_{50} (mmol/l) = -0.3156 log Kow - 3.4422	(n=43, r^2 = 0.1582)
		CSA	log EC_{50} (mg/l) = -0.5026 log Kow - 0.043	(n=26, r^2 = 0.3465)
			log EC_{50} (mmol/l) = -0.5478 log Kow - 2.395	(n=26, r^2 = 0.3741)
	PGR		log EC_{50} (mg/l) = -0.0887 log Kow + 1.6166	(n=11, r^2 = 0.0364)
			log EC_{50} (mmol/l) = -0.133 log Kow - 0.6655	(n=11, r^2 = 0.0739)
Daphnia Reprod.	Pesticides		log NOEC (mg/l) = -0.5052 log Kow + 0.1325	(n=96, r^2= 0.3002)
			log NOEC (mmol/l) = -0.5402 log Kow - 2.2425	(n=96, r^2= 0.3241)
	Fungicides		log NOEC (mg/l) = -0.3035 log Kow - 0.5229	(n=28, r^2 = 0.1106)
			log NOEC (mmol/l) = -0.3067 log Kow - 3.0055	(n=28, r^2 = 0.1079)
	Herbicides		log NOEC (mg/l) = -0.3163 log Kow + 0.7216	(n=37, r^2 = 0.2647)
			log NOEC (mmol/l) = -0.3319 log Kow - 1.6986	(n=37, r^2 = 0.2892)
	Insecticides		log EC_{50} (mg/l) = -0.5516 log Kow - 1.425	(n=22, r^2 = 0.5682)
			log EC_{50} (mmol/l) = -0.6059 log Kow - 3.7308	(n=22, r^2 = 0.6198)
Algae acute	Pesticides		log EC_{50} (mg/l) = - 0.2397 log Kow + 0.8195	(n=183, r^2 = 0.1190)
			log EC_{50} (mmol/l) = - 0.2679 log Kow - 1.5452	(n=183, r^2 = 0.1451)
	Fungicides	All	log EC_{50} (mg/l) = -0.2325 log Kow + 0.623	(n=48, r^2 = 0.1112)
			log EC_{50} (mmol/l) = -0.2427 log Kow - 1.8215	(n=48, r^2 = 0.1180)
		Ergosterol inh.	log EC_{50} (mg/l) = -0.4549 log Kow + 1.4752	(n=17, r^2 = 0.0629)
			log EC_{50} (mmol/l) = -0.4415 log Kow - 1.0787	(n=17, r^2 = 0.0622)
		Growth inh.	log EC_{50} (mg/l) = -0.2669 log Kow + 0.7178	(n=24, r^2 = 0.1605)
			log EC_{50} (mmol/l) = -0.2844 log Kow - 1.6727	(n=24, r^2 = 0.1770)
	Herbicides	All	log EC_{50} (mg/l) = -0.1898 log Kow +025345	(n=82, r^2 = 0.0636)
			log EC_{50} (mmol/l) = -0.2037 log Kow - 1.8623	(n=82, r^2 = 0.0752)
		Growth inh.	log EC_{50} (mg/l) = -0.1768 log Kow + 0.9666	(n=51, r^2 = 0.0934)
			log EC_{50} (mmol/l) = -0.1884 log Kow - 1.456	(n=51, r^2 = 0.1049)
		Photosyn. inh.	log EC_{50} (mg/l) = -0.0294 log Kow - 0.7492	(n=29, r^2 = 0.0008)
			log EC_{50} (mmol/l) = -0.0723 log Kow - 3.0378	(n=29, r^2 = 0.0052)

Test	Group	Mode of action	Equation	No. and correlation
	Insecticides	All	log EC_{50} (mg/l) = -0.4461 log Kow + 1.9898	(n=34, r^2 = 0.4395)
			log EC_{50} (mmol/l) = -0.494 log Kow - 0.3145	(n=34, r^2 = 0.4908)
		Cholinest. inh.	log EC_{50} (mg/l) = -0.2843 log Kow + 1.6348	(n=26, r^2 = 0.1692)
			log EC_{50} (mmol/l) = -0.3232 log Kow - 0.7061	(n=26, r^2 = 0.2106)
	PGR		log EC_{50} (mg/l) = -0.2735 log Kow + 1.1986	(n=8, r^2 = 0.4655)
			log EC_{50} (mmol/l) = -0.3192 log Kow - 1.0879	(n=8, r^2 = 0.5149)

PGR: Plant growth regulators. CSA: Contact and stomach action. Inh: Inhibitor

The problems in reaching an acceptable correlation may be multiple. The toxicity values are from several species of fish, but primarily the lowest value has been used unless ***Pimephales promelas*** or ***Oncorhynchus my-kiss*** was present. Then they were preferred. The experimental Kow value may be incorrect if they are temperature or pH dependent. Generally, there is a large agreement with the experimental and estimated log Kow. However, discrepancies did occur and especially for ionisable substances the deviation could be large. The result may be to perform several QSARs according to more specific organism types, or according to chemical group e.g. from traditional chemical classification according to functional group. There is a high correlation between chemical functional groups and toxic mode of action. Another explanation could be that there is no direct relationship between log Kow and toxicity for specific acting substances. The exposure time is also determining for the effect of substances with a high log Kow.

Data reliability

To evaluate the predictive potential of QSARs, reliable biological and ecotoxicological databases must be assembled and computerised. These databases should be validated or reviewed as to data quality. Currently, such works are performed e.g. by the US-EPA in the database AQUIRE and the chemical industry ECETOC (ECETOC 1993).

A procedure for data collection and interpretation for substances to be evaluated for classification as dangerous to the environment has been presented in Pedersen ***et al.*** (1995).

Biological results may be numerically imprecise and are generally not generated for use in QSAR prediction. For instance, results from limit tests or results above water solubility or just designated “more than” cannot be used in QSARs. However, such data may be useful for demonstrating trends. But it must be kept in mind that individual results may not be quantitatively exact (Rispin 1981).

Isomers

Pesticides with one or more centres of asymmetry in the molecule represent a special problem in estimation of toxicity. For geometric isomers, the physico-chemical properties usually differ but optical isomers have identical physico-chemical properties, at least in solution. Such isomers may nevertheless differ greatly in their biological activity (Ariëns 1984).

This makes ecotoxicity results based on racemic mixtures without know-ledge of the isomer ratio disputable, taking into account the fact that the individual isomers may differ essentially in their action.

4 Summary of conclusions

Traditional QSAR models are based on a few key physico-chemical data (typically melting point, octanol/water partition coefficient) which are then used to calculate other physico-chemical parameters if they are missing. The calculation equations should be based on experimental laboratory studies performed by accepted guidelines and the results based on regression analyses.

The conclusions of this project comparing experimental values with QSAR model estimations are summarised below. The main object was to study whether the currently recommended general QSARs could be used to perform acceptable estimates on pesticides physico-chemical properties and aquatic toxicity. The study was expanded by examining whether general or specific regression equations could be derived for log Kow and pesticides after subdivision into fungicides, herbicides, insecticides, plant growth regulators and rodenticides. No attempt has been made to improve on regression equations by removing outliers.

Melting point

The correlation between experimental and estimated melting points was low. The used method generally overestimated the melting point values. Thus, the currently best available method by Meylan and Howard (1994) is not recommendable for pesticides in its present form.

Water solubility

The estimations of water solubility were acceptable using the selected computerised QSAR model although the correlation coefficient for pesticides was smaller than for the data used to develop the model. A linear regression analysis based on log water solubility and log Kow of the pesticides used in this report resulted in a QSAR model with a slightly reduced correlation coefficient.

Vapour pressure

The presented QSAR model on vapour pressure was not able to perform a sufficient close correlation of experimental and estimated vapour pressures from the included pesticide data set. However, it should be noted that the experimental values were based on test results varying between 20ºC and 25ºC whereas the vapour pressures were estimated at 25ºC.

Henry's Law constant

For Henry's Law constant, no conclusion can be drawn from the used pesticide data set since values estimated by calculation and by computer model may not be correct for the pesticide in question. However, it can be concluded that the two estimation methods are presenting comparable results.

Log Kow

The octanol/water partition coefficient log Kow could be reasonably well estimated from the QSAR models based on structure fragment analysis. The method is complicated and recommended to be performed by available computer models. However, an alternative QSAR model may be used based on water solubility. For the pesticides used in this report, it resulted in a lower correlation coefficient but both methods should be sufficient in a screening procedure.

Adsorption

The soil adsorption coefficient factor Koc is very important in the evaluation of the mobility of pesticides. Since the known methods for estimation are approximate at best, measured values should be used if they are available. If however, measured data on Koc for some reason are not present, the PCKOC programme (Meylan and Howard 1994) or the QSAR model to estimate Koc developed by Sabljic ***et al.*** (1995) and recommended in TGD (1996) can be used. Based on 338 pesticides in this project, a QSAR model was derived which had a correlation coefficient close to the model by Sabljic ***et al.*** (1995). For comparison of the outcome of each QSAR estimation on individual pesticides the results are presented in the appendix.

Ecotoxicity

It is important to realise that most of the QSARs developed and the QSARs presented above are based on chemicals that are biased toward industrial organic chemicals that are not overtly designed to have biological activity. Pesticides are mostly reacting in a specific mode of action and no QSARs have been recommended for substances that act by more specific modes of action (TGD 1996).

The situation with the present data set is that it has been chosen as a mixture of different pesticides to evaluate whether the evolved QSARs could be used in general. If another choice had been made, e.g. the used pesticides were selected according to function, mode of action or chemical class, another result may have appeared. However, the chosen pesticides included in this report represent too many chemical classes to collect a sufficient number in each class for analysis. On the other hand, the results demonstrate that the available QSAR models should be used with great precaution, as they are not developed specifically for pesticides.

QSARs have been developed with acceptable results for most industrial chemicals. The recommended QSARs on ecotoxicity were not recommendable for pesticides in general. However, the results cannot be used without further development for chemicals like pesticides with specific biological mode of action.

The study demonstrates that, by dividing the pesticides according to their mode of action, improved correlations could be found for some organisms and some modes of action. The problems in reaching an acceptable QSAR for estimating ecotoxicity may be multiple (cf. discussion in section 3.5.5). Another explanation for the result could be that there is no direct relationship between log Kow and toxicity for specific acting substances.

The conclusion is that no QSARs of a sufficient and reliable quality are currently available for estimating ecotoxicity of pesticides. The values can only be acquired from regular studies.

The general idea is not that QSARs shall replace experimentally derived data for pesticides. It must be kept in the mind that the purpose of using QSAR models is to give a qualified estimate of an endpoint in replacement of a missing experimental data.

However, using the QSAR models with precaution and keeping in mind their background presents reasonable good estimates to perform preliminary assessments on physico-chemical properties and in very precautions way of degradation products and /or metabolites. As demonstrated by the studies by e.g. Nendza ***et al.*** (1991) and Vighi ***et al.*** (1991), positive results can be

obtained but they must await a thorough evaluation before they can be recommended for pesticides in general or for specified groups.

Relating to degradation products and transformation products QSARs may be useful in the priority of toxicity studies and which endpoint should be studied.

QSARs have been found to have great predictive values for chemicals of less complicated structures or other modes of reaction than pesticides and the use is recommended in the TGD (1996) as a useful part of the risk assessment procedure. The area of developing QSAR models for more complicated structures and chemicals with specific modes of action is therefore currently an area of high priority.

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Appendix A

A list of the abbreviations used in the appendix is located after the tables.

Table 1
Pestcide ISO name, chemical class, use, mode of action, CAS No., molecular formula and molecular weight (MW).

Pesticid ISO navn, kemisk klasse, anvendelse, virkningsmekanisme, CAS nr., molekylformel og molekylvægt (MW).

Name (ISO)	Chemical class	Use	Mode of action	CAS No.	Molecular formula	MW g/mol
Acephate	Organophosphorous	I	Cholinesterase inh.	30560-19-1	C4 H10 N O3 P S	183.16
Acetochlor	Chloroacetanilide	H	prot.synt.inh.	34256-82-1	C14 H20 Cl N O2	269.77
Acifluorfen	Diphenyl ether	H	prophyrinoxidase inh.	50594-66-6	C14 H7 Cl F3 N O5	361.66
Acifluorfen sodium	Diphenyl ether	H	prophyrinoxidase inh.	62476-59-9	C14 H6 Cl F3 N O5 Na	383.65
Aclonifen	Diphenyl ether	H	prophyrinoxidase inh.	74070-46-5	C12 H9 Cl N2 O3	264.67
Acrinathrin	Pyrethroid	A, I	CSA	101007-06-1	C26 H21 F6 N O5	541.45
Acrolein	Propenal	H	Enzyme reaction	107-02-8	C3 H4 O	56.06
Alachlor	Chloroacetanilide	H	prot.synt.inh.	15972-60-8	C14 H20 Cl N O2	269.77
Alanycarb	Oxime carbamate	I	Cholinesterase inh.	83130-01-2	C17 H25 N3 O4 S2	399.53
Aldicarb	Oxime carbamate	I	Cholinesterase inh.	116-06-3	C7 H14 N2 O2 S	190.27
Aldoxycarb	Oxime carbamate	I	Cholinesterase inh.	1646-88-4	C7 H14 N2 O4 S	222.26
Allethrin	Pyrethroid	I	CSRA	584-79-2	C19 H26 O3	302.42
Alloxydim sodium	Cyclohexanedione oxime	H	Mitosis inh.	66003-55-2	C17 H24 N O5 Na	345.37
Ametryn	Triazine	H	Photo+enzym inh.	834-12-8	C9 H17 N5 S	227.33
Amidosulfuron	Sulfonylurea	H	Acetolactat synt.inh	120923-37-7	C9 H15 N5 O7 S2	369.37
Amitraz	Amidine	A, I	CSA	33089-61-1	C19 H23 N3	293.42
Amitrole	Triazole	H	Chloroph.form.inh.	61-82-5	C2 H4 N4	84.08
Ancymidol	Pyrimidinyl carbinol	PGR	Gibbereli.synt.inh.	12771-68-5	C15 H16 N2 O2	256.31
Anilazine	Triazine aniline	F	Contact action	101-05-3	C9 H5 Cl3 N4	275.53
Asulam	Sulfanilylcarbamate	H	Cell div. inh.	3337-71-1	C8 H10 N2 O4 S	230.24
Asulam sodium	Sulfanilylcarbamate	H	Cell div. inh.	2302-17-2	C7 H7 N2 O4 S Na	238.19
Atrazine	Triazine	H	Photo+enzym inh.	1912-24-9	C8 H14 Cl N5	215.69
Azaconazole	Azole	F	Steroid demeth.inh.	60207-31-0	C12 H11 Cl2 N3 O2	300.15
Azamethiphos	Organophosphorous	I	Cholinesterase inh.	35575-96-3	C9 H10 Cl N2 O5 P S	324.68
Azinphos-ethyl	Organophosphorous	I	Cholinesterase inh.	2642-71-9	C12 H16 N3 O3 P S2	345.37
Azinphos-methyl	Organophosphorous	I	Cholinesterase inh..	86-50-0	C10 H12 N3 O3 P S2	317.33
Benalaxyl	Acylalanine	F	Growth inh.	71626-11-4	C20 H23 N O3	325.41
Benazolin	Benzothiazolin	H	Growth inh.	3813-05-6	C9 H6 Cl N O3 S	243.67
Benazolin ethyl	Benzothiazolin	H	Growth inh.	25059-80-7	C11 H10 Cl N O3 S	271.72
Bendiocarb	Carbamate	I	Cholinesterase inh..	22781-23-3	C11 H13 N O4	223.23
Benfluralin	Dinitroaniline	H	Growth inh.	1861-40-1	C13 H16 F3 N3 O4	335.29
Benfuracarb	Carbamate	I	Cholinesterase inh.	82560-54-1	C20 H30 N2 O5 S	410.53
Benfuresate	Benzofuranyl alkanesulfonate	H	Growth inh.	68505-69-1	C12 H16 O4 S	256.32
Benomyl	Benzimidazole	F	Growth inh.	17804-35-2	C14 H18 N4 O3	290.32
Bensulfuron methyl	Sulfonylurea	H	Aminoacid synt.inh.	83055-99-6	C16 H18 N4 O7 S	410.40
Bensulide	Organophosphorous	H	Germination inh.	741-58-2	C14 H24 N O4 P S3	397.51
Bensultap	Dimethylaminopropanedithiol	I	Cholinesterase inh.	17606-31-4	C17 H21 N O4 S4	431.60

Name (ISO)	Chemical class	Use	Mode of action	CAS No.	Molecular formula	MW g/mol
Bentazone	Benzothiadiazinone	H	Photosynt.inh.	25057-89-0	C10 H12 N2 O3 S	240.28
Bentazone sodium	Benzothiadiazinone	H	Photosynt.inh.	50723-80-3	C10 H11 N2 O3 S Na	262.26
Bifenox	Diphenyl ether	H	Photosynt.inh.	42576-02-3	C14 H9 Cl2 N O5	342.14
Bifenthrin	Pyrethroid	I	CSA	82657-04-3	C23 H22 Cl F3 O2	422.88
Bioallethrin	Pyrethroid	I	CSRA	584-79-2	C19 H26 O3	302.42
Bioresmethrin	Pyrethroid	I	CSA	28434-01-7	C22 H26 O3	338.45
Bitertanol	Azole	F	Ergosterol synt.inh.	70585-36-3	C20 H23 N3 O2	337.42
Brodifacoum	Coumarin anticoagulant	R	Vit. K inh.	56073-10-0	C31 H23 Br O3	523.43
Bromacil	Uracil	H	Photosynt.inh.	314-40-9	C9 H13 Br N2 O2	261.12
Bromacil lithium	Uracil	H	Photosynt.inh.		C9 H12 Br N2 O2 Li	267.05
Bromadiolone	Coumarin anticoagulant	R	Vit. K inh.	28772-56-7	C30 H23 Br O4	527.42
Bromethalin	Diphenylamin	R	Oxidat. phospho. inh	63333-35-7	C14 H7 Br3 F3 N3 O4	577.94
Bromofenoxim	Hydroxybenzonitril	H	Contact action	13181-17-4	C13 H7 Br2 N3 O6	461.02
Bromoxynil	Hydroxybenzonitril	H	Photosynt.inh.	1689-84-5	C7 H3 Br2 N O	276.92
Bromoxynil octanoate	Hydroxybenzonitril	H	Photosynt.inh.	1689-99-2	C15 H17 Br2 N O2	403.12
Bromoxynil butyrate	Hydroxybenzonitril	H	Photosynt.inh.	3861-41-4	C11 H9 Br2 N O2	347.01
Bromoxynil potassium	Hydroxybenzonitril	H	Photosynt.inh.	2961-68-4	C7 H2 Br2 N O K	315.01
Bromuconazole	Azole	F	Ergosterol synt. inh.	116255-48-2	C13 H12 Br Cl2 N3 O	377.07
Bronopol	Alkyl halide	B	Dehydrogenase inh.	52-51-7	C3 H6 Br N O4	199.99
Butylate	Thiocarbamate	H	Growth inh.	2008-41-5	C11 H23 N O S	217.40
Captafol	N-trihalomethylthio	F	Spore germ. inh.	2425-06-1	C10 H9 Cl4 N O2 S	349.06
Captan	N-trihalomethylthio	F	Spore germ. inh.	133-06-2	C9 H8 Cl3 N O2 S	300.59
Carbaryl	Carbamate	I	Cholinesterase inh.	63-25-2	C12 H11 N O2	201.23
Carbendazim	Benzimidazole	F	Growth inh.	10605-21-7	C9 H9 N3 O2	191.19
Carbetamide	Carbamate	H	Cell div. inh.	16118-49-3	C12 H16 N2 O3	236.27
Carbofuran	Carbamate	I	Cholinesterase inh.	1563-66-2	C12 H15 N O3	221.25
Carbosulfan	Carbamate	I	Cholinesterase inh.	55285-14-8	C20 H32 N2 O3 S	380.55
Carboxin	Phenylamide	F	syst fung	5234-68-4	C12 H13 N O2 S	235.31
Chinomethionate	Quinoxaline	F	Cont. fung.	2439-01-2	C10 H6 N2 O S2	234.29
Chloramben	Benzoic acid	H	Growth inh.	133-90-4	C7 H5 Cl2 N O2	206.03
Chloramben sodium	Benzoic acid	H	Growth inh.		C7 H4 Cl2 N O2 Na	228.01
Chlordimeform hydrochloride		A		19750-95-9	C10 H14 Cl2 N2	233.20
Chlorfenac sodium (Fenac)	trichlorofenyl	H		2439-00-1	C8 H4 Cl3 Na O2	261.47
Chlorfenvinphos	Organophosphorous	I	Cholinesterase inh.	470-90-6	C12 H14 Cl3 O4 P	359.58
Chloridazon (Pyridazon)	Pyridazinone	H	Photosynt.inh.	1698-60-8	C10 H8 Cl N3 O	221.65
Chlorimuron ethyl	Sulfonylurea	H	Amino acid synt.inh	90982-32-4	C15 H15 Cl N4 O6 S	414.82
Chlormequat chloride	Quarternary ammonium	PGR	Cell elong inh.	999-81-5	C5 H13 Cl2 N	158.07
Chlorobenzilate	Benzilate	A	CA	510-15-6	C16 H14 Cl2 O3	325.19
Chloroneb	arom hydrocarb deriv	F	syst fung	2675-77-6	C8 H8 Cl2 O2	207.06
Chloropicrin	trichloronitromethane	I	fumigant	76-06-2	C Cl3 N O2	164.39
Chlorothalonil	tetrachlorobenzene	F	syst fung	1897-45-6	C8 Cl4 N2	265.92
Chloroxuron	Urea	H	Photosynt.inh.	1982-47-4	C15 H15 Cl N2 O2	290.75
Chlorpropham	Carbamate	H	Growth inh.	101-21-3	C10 H12 Cl N O2	213.67
Chlorpyrifos	Organophosphorous	I	Cholinesterase inh.	2921-88-2	C9 H11 Cl3 N O3 P S	350.59
Chlorpyrifos methyl	Organophosphorous	I	Cholinesterase inh.	5598-13-0	C7 H7 Cl3 N O3 P S	322.53
Chlorsulfuron	Sulfonylurea	H	Amino acid synt.inh	64902-72-3	C12 H12 Cl N5 O4 S	357.77
Chlorthal dimethyl (DCPA)	Benzoic acid	H	Growth inh.	1861-32-1	C10 H6 Cl4 O4	331.97
Clethodim	Cyclohexanedione oxime	H	Mitosis inh.	99129-21-2	C17 H26 Cl N O3 S	359.92
Clofentezine	bischlorophenyl-tetrazine	A	Embryo-dev. inh	74115-24-5	C14 H8 Cl2 N4	303.15
Clomazone	Oxazalodinone	H	Growth inh.	81777-89-1	C12 H14 Cl N O2	239.70
Cloprop (3-CPA)	Aryloxyalkanoic acid	PGR	Growth reg.	101-10-0	C9 H9 Cl O3	200.62
Cloprop ammonium	Aryloxyalkanoic acid	PGR	Growth reg.	5825-87-6	C9 H10 Cl N O2	199.64
Cloprop sodium	Aryloxyalkanoic acid	PGR	Growth reg.		C9 H8 Cl O3 Na	222.60
Clopyralide	Pyridinecarboxylic acid	H	auxin type reaction	1702-17-6	C6 H3 Cl2 N O2	192.00
Clopyralid-olamine	Pyridinecarboxylic acid	H	auxin type reaction	57754-85-5	C8 H10 Cl2 N2 O3	253.10
Coumatetralyl	Coumarin anticoagulant	R	Prothrombin	5836-29-3	C19 H16 O3	292.34

Name (ISO)	Chemical class	Use	Mode of action	CAS No.	Molecular formula	MW g/mol
			blocking			
Cyanazine	1,3,5-Triazine	H	Photosynt.inh.	21725-46-2	C9 H13 Cl N6	240.70
Cyanophos	Organophosphorous	I	Cholinesterase inh.	2636-26-2	C9 H10 N O3 P S	243.22
Cycloate	Thiocarbamate	H	Growth inh.	1134-23-2	C11 H21 N O S	215.37
Cycloxidim	Cyclohexanedione oxime	H	Mitosis inh.	101205-02-1	C17 H27 N O3 S	325.47
Cyfluthrin	Pyrethroid	I	CSA	68359-37-5	C22 H18 Cl2 F N O3	434.30
Cyhalothrin	Pyrethroid	I	CSA	68085-85-8	C23 H19 Cl F3 N O3	449.85
Cypermethrin	Pyrethroid	I	CSA	52315-07-8	C22 H19 Cl2 N O3	416.31
alpha-Cypermethrin	Pyrethroid	I	CSA	67375-30-8	C22 H19 Cl2 N O3	416.31
Cyproconazole	Azole	F	Ergosterol synt.inh.	94361-06-5	C15 H18 Cl N3 O	291.78
Cyromazine	Triazine-triamine	I	Growth regulator	66215-27-8	C6 H10 N6	166.19
2,4-D	Aryloxyalkanoic acid	H	Growth inh.	94-75-7	C8 H6 Cl2 O3	221.04
2,4-D-dimethylammonium	Aryloxyalkanoic acid	H	Growth inh.	2008-39-1	C10 H13 Cl2 N O3	266.13
2,4-D methylester	Aryloxyalkanoic acid	H	Growth inh.	1928-38-7	C9 H8 Cl2 O3	235.07
Dalapon sodium	Dichloropropionic acid	H	totalherbicide	127-20-8	C3 H3 Cl2 O2 Na	164.95
Daminozide	Hydrazide	PGR	Plant growth reg.	1596-84-5	C6 H12 N2 O3	160.17
Dazomet	Methyl isothiocyanate	F, H, I	Soil sterilant	533-74-4	C5 H10 N2 S2	162.27
2,4-DB	Aryloxyalkanoic acid	H	Growth inh.	94-82-6	C10 H10 Cl2 O3	249.10
2,4-DB butoxyethyl	Aryloxyalkanoic acid	H	Growth inh.	32357-46-3	C16 H22 Cl2 O4	294.20
Deltamethrin	Pyrethroid	I	CSA	52918-63-5	C22 H19 Br2 N O3	505.21
Desmedipham	Bis-carbamate	H	Photosynt. inh	13684-56-5	C16 H16 N2 O4	300.32
Desmetryn	1,3,5-Triazine	H	Photosynt. inh	1014-69-3	C8 H15 N5 S	213.30
Diazinon	Organophosphorous	I	Cholinesterase inh.	333-41-5	C12 H21 N2 O3 P S	304.35
Dicamba	Benzoic acid	H	auxinlike growth reg.	1918-00-9	C8 H6 Cl2 O3	221.04
Dicamba sodium	Benzoic acid	H	auxinlike growth reg.	1982-69-0	C8 H5 Cl2 O3 Na	243.02
Dichlobenil	Dichlorobenzonitrile	H	Growth inh.	1194-65-6	C7 H3 Cl2 N	172.01
Dichlofluanid	N-trihalomethylthio	F	contact fung.	1085-98-9	C9 H11 Cl2 F N2 O2 S2	333.22
1,3-Dichloropropene	Halogenated hydrocarbon	N	Soil fumigant	542-75-6	C3 H4 Cl2	111.00
Dichlorprop (2,4-DP)	Aryloxyalkanoic acid	H	Auxintype growth reg.	7547-66-2	C9 H8 Cl2 O3	235.10
Dichlorprop butoxyethyl	Aryloxyalkanoic acid	H	Auxintype growth reg.		C15 H20 Cl2 O4	335.23
Dichlorprop-P	Aryloxyalkanoic acid	H	Hormonetype	15165-67-0	C9 H8 Cl2 O3	235.07
Dichlorvos	Organophosphorous	I	Cholinesterase inh.	62-73-7	C4 H7 Cl2 O4 P	220.98
Dicloran (DCNA)	dichloronitroaniline	F	Growth effects	99-30-9	C6 H4 Cl2 N2 O2	207.02
Dicofol	Organochlorine	A	Contact action	115-32-2	C14 H9 Cl5 O	370.49
Dicrotophos	Organophosphorous	I	Cholinesterase inh.	141-66-2	C8 H16 N O5 P	237.19
Dienochlor	Organochlorine	A	Contact action	2227-17-0	C10 Cl10	474.64
Diethatyl-ethyl	Chloroacetanilide	H	Cell div. inh.	38727-55-8	C16 H22 Cl N O3	311.81
Difenacoum	Coumarin anticoagulant	R	Vit. K inh.	56073-07-5	C31 H24 O3	444.53
Difenoconazole	Azole	F	demethylation inh.	119446-68-3	C19 H17 Cl2 N3 O3	406.27
Difenoxuron	Urea	H	Photosynt. inh	14214-32-5	C16 H18 N2 O3	286.33
Difenzoquat methylsulfate	diphenyl-pyrazolium	H	Meristem inh.	43222-48-6	C18 H20 N2 O4 S	360.44
Difethialone	Benzothiine	R	anticoagulant rod.	104653-34-1	C31 H23 Br O2 S	539.49
Diflubenzuron	Benzoylurea	I	Chitin synt.inh.	35367-38-5	C14 H9 Cl F2 N2 O2	310.69
Diflufenican	Anilide	H	Photosynt. inh.	83164-33-4	C19 H11 F5 N2 O2	394.30
Dimethachlor	Chloroacetanilide	H	Cell div. inh.	50563-36-5	C13 H18 Cl N O2	255.75
Dimethipin	dimethyldithiine	PGR	Protein synt. inh.	55290-64-7	C6 H10 O4 S2	210.26
Dimethoate	Organophosphorous	I	Cholinesterase inh.	60-51-5	C5 H12 N O3 P S2	229.25
Dinocap	dinitrophenol der.	F	131-72-6	39300-45-3	C18 H24 N2 O6	364.41
Dinoseb	Dinitrophenol	H	electron transp. inh	88-85-7	C10 H12 N2 O5	240.22
Dinoseb-olamin	Dinitrophenol	H	electron transp. inh		C12 H19 N3 O6	301.30
Dinoseb acetic acid	Dinitrophenol	H	electron transp. inh	2813-95-8	C12 H14 N2 O6	282.20
Dinoterb	Dinitrophenol	H	Contact action	1420-07-1	C10 H12 N2 O5	240.22
Diphenamid	Diphenyl-amide	H	Root elong. inh.	957-51-7	C16 H17 N O	239.32
Dipropetryn	1,3,5-triazine	H	Photosynt. inh.	4147-51-7	C11 H21 N5 S	255.38
Diquat dibromide	Bipyridyl	H	Photosynt.elect.divert.	85-00-7	C12 H12 Br2 N2	344.06

Name (ISO)	Chemical class	Use	Mode of action	CAS No.	Molecular formula	MW g/mol
Disulfoton	Organophosphorous	I	Cholinesterase inh.	298-04-4	C8 H19 O2 P S3	274.39
Dithianon	dioxonaphthol-dithiin	F	Spore germ. inh.	3347-22-6	C14 H4 N2 O2 S2	296.32
Diuron	Urea	H	Photosynt. inh.	330-54-1	C9 H10 Cl2 N2 O	233.10
DNOC	Dinitrophenol	H, I	CSA	534-52-1	C7 H6 N2 O5	198.14
Dodine	Guanidine	F	Cont., syst., fung	2439-10-3	C15 H33 N3 O2	287.44
Endosulfan	Organochlorine	I	CSA	115-29-7	C9 H6 Cl6 O3 S	406.91
Endothal	cyclohexanedicarboxylacid	H	Growth inh.	145-73-3	C8 H10 O5	186.17
Endothal sodium	cyclohexanedicarboxylacid	H	Growth inh.	129-67-9	C8 H8 O5 Na2	230.13
EPTC	Thiocarbamate	H	Systemic action	759-94-4	C9 H19 N O S	189.32
Esfenvalerate	Pyrethroid	I	CSA	66230-04-4	C25 H22 Cl N O3	419.91
Ethalfluralin	Dinitroaniline	H	Growth inh.	55283-68-6	C13 H14 F3 N3 O4	333.27
Ethametsulfuron-methyl	Sulfonylurea	H	Amino acid synt.inh	97780-06-8	C15 H18 N6 O6 S	410.41
Ethephon	Chloroethylphosphonic acid	PGR	Ethylene generator	16672-87-0	C2 H6 Cl O3 P	144.50
Ethiofencarb	Carbamate	I	Cholinesterase inh.	29973-13-5	C11 H15 N O2 S	225.31
Ethion	Organophosphorous	I	Cholinesterase inh.	563-12-2	C9 H22 O4 P2 S4	384.46
Ethirimol	Pyrimidine	F	Spore germ. inh.	23947-60-6	C11 H19 N3 O	209.29
Ethofumesate	Benzofuranyl alkanesulfonate	H	Growth inh.	26225-79-6	C13 H18 O5 S	286.35
Ethoprophos	Organophosphorous	I	Cholinesterase inh.	13194-48-4	C8 H19 O2 P S2	242.33
Etridiazole	1,2,4-thiadiazole	F	Cont.fung	2593-15-9	C5 H5 Cl3 N2 O S	247.53
Etrimfos	Organophosphorous	I	Cholinesterase inh.	38260-54-7	C10 H17 N2 O4 P	292.29
Fenamiphos	Organophosphorous	N	cont. nematicide	22224-92-6	C13 H22 N O3 P S	303.36
Fenarimol	Pyrimidinyl carbinol	F	Ergosterol synt.inh.	60168-88-9	C17 H12 Cl2 N2 O	331.20
Fenbuconazole	Azole	F	syst fung	114369-43-6	C19 H17 Cl N4	336.83
Fenbutatin oxide	Organotin	A	CSA	13356-08-6	C60 H78 O Sn2	1052.70
Fenitrothion	Organophosphorous	I	Cholinesterase inh.	122-14-5	C9 H12 N O5 P S	277.23
Fenoxaprop	Aryloxyphenoxypropionic acid	H	Fatty acid synt.inh.	73519-55-8	C16 H12 Cl N O5	333.73
Fenoxaprop-ethyl	Aryloxyphenoxypropionic acid	H	Fatty acid synt.inh.	66441-23-4	C18 H16 Cl N O5	361.78
Fenoxaprop-P-ethyl	Aryloxyphenoxypropionic acid	H	Fatty acid synt.inh.	71283-80-2	C18 H16 Cl N O5	361.78
Fenoxycarb	Carbamate	I	Metamorph. inh	79127-80-3	C17 H19 N O4	301.35
Fenpiclonil	Cyanopyrrole	F	Cont. act. fung	74738-17-3	C11 H6 Cl2 N2	237.09
Fenpropathrin	Pyrethroid	I	CSA	64257-84-7	C22 H23 N O3	349.43
Fenpropidin	Morpholine analogue	F	Ergosterol synt.inh.	67306-00-7	C19 H31 N	273.47
Fenpropimorph	Morpholine	F	Ergosterol synt.inh.	67564-91-4	C20 H33 N O	303.49
Fenthion	Organophosphorous	I	Cholinesterase inh.	55-38-9	C10 H15 O3 P S2	278.32
Fentin acetate	Organotin	F	Multi-site inh.	900-95-8	C20 H18 O2 Sn	409.60
Fentin hydroxide	Organotin	F	Multi-site inh.	76-87-9	C18 H16 O Sn	367.02
Fenvalerate	Pyrethroid	I	CSA	51630-58-1	C25 H22 Cl N O3	419.91
Ferbam	Dimethyldithiocarbamate	F	Fung.	14484-64-1	C9 H18 Fe N3 S6	416.50
Flamprop methyl	Arylalanine	H	Plant growth inh.	52756-25-9	C17 H15 Cl F N O3	335.77
Flamprop-M isopropyl	Arylalanine	H	Plant growth inh.	63782-90-1	C19 H19 Cl F N O3	363.82
Flocoumafen	Coumarin anticoagulant	R	Vit. K inh.	90035-08-8	C33 H25 F3 O4	542.56
Fluazifob	Aryloxyphenoxypropionic acid	H	Growth inh.	69335-91-7	C15 H12 F3 N O4	327.26
Fluazifop-butyl	Aryloxyphenoxypropionic acid	H	Growth inh.	69806-50-4	C19 H20 F3 N O4	383.37
Fluazifop-P-butyl	Aryloxyphenoxypropionic acid	H	Growth inh.	79241-46-6	C19 H20 F3 N O4	383.37
Flucythrinate	Pyrethroid	I	CSA	70124-77-5	C26 H23 F2 N O4	451.47
Flumetralin	Dinitroaniline	PGR	Plant growth reg.	62924-70-3	C16 H21 Cl F4 N3 O4	421.74
Fluometuron	Urea	H	Photosynt. inh.	2164-17-2	C10 H11 F3 N2 O	232.21
Flurenol-butyl	fluorenecarboxylic acid	PGR	Plant growth inh.	2314-09-2	C18 H18 O3	282.34
Fluridone	Pyridone	H	Carotenoid synt.inh.	59756-60-4	C19 H14 F3 N O	329.32
Fluroxypyr	Aryloxyalkanoic acid	H	auxin type reaction	69377-81-7	C7 H5 Cl2 F N2 O3	255.03
Fluroxypyr-meptyl	Aryloxyalkanoic acid	H	auxin type reaction	81406-37-3	C15 H21 Cl2 F N2 O3	367.25

Name (ISO)	Chemical class	Use	Mode of action	CAS No.	Molecular formula	MW g/mol
Flurprimidol	Pyrimidinyl carbinol	PGR	Gibbereli.synt.inh.	56425-91-3	C15 H15 F3 N2 O2	312.29
Flusilazole	Azole	F	Ergosterol synt.inh.	85509-19-9	C16 H15 F2 N3 Si	315.40
tau-Fluvalinate	Pyrethroid	I	CSA	102851-06-9	C26 H22 Cl F3 N2 O3	502.93
Folpet	Trihalomethylthio	F	Cont. fung.	133-07-3	C9 H4 Cl3 N O2 S	296.56
Fomesafen	Diphenyl ether	H	Photosynt. inh.	72178-02-0	C15 H10 Cl F3 N2 O6 S	438.76
Fomesafen sodium	Diphenyl ether	H	Photosynt. inh.		C15 H9 Cl F3 N2 O6 S Na	460.75
Fonofos	Organophosphorous	I	Cholinesterase inh.	944-22-9	C10 H15 O P S2	246.32
Formetanate hydrochloride	Carbamate	I	Cholinesterase inh.	23422-53-9	C11 H16 Cl N3 O2	257.71
Formothion	Organophosphorous	I	Cholinesterase inh.	2540-82-1	C6 H12 N O4 P S2	257.26
Fosamine ammonium	Organophosphorous	H	Bud dev. inh.	25954-13-6	C3 H11 N2 O4 P	170.10
Fosetyl-aluminium	Organophosphorous	F	Growth inh.	39148-24-8	C6 H18 Al O9 P3	354.10
Fuberidazole	Benzimidazole	F	Mitosis inh.	3878-19-1	C11 H8 N2 O	184.20
Furathiocarb	Carbamate	I	Cholinesterase inh.	65907-30-4	C18 H26 N2 O5 S	382.48
Glufosinate ammonium	Phosphinic acid	H	Photosynt. inh.	77182-82-2	C5 H15 N2 O4 P	198.16
Glyphosate	Phosphinic acid	H	Amino acid synt.inh	1071-83-6	C3 H8 N O5 P	169.07
Glyphosate isopropylammonium	Phosphinic acid	H	Amino acid synt.inh	38641-94-0	C6 H17 N2 O5 P	228.19
Glyphosate trimesium	Phosphinic acid	H	Amino acid synt.inh	81591-81-3	C6 H16 N O5 P S	245.20
Guazatine	Guanidine	F	Contact action	13516-27-3	C18 H41 N7	355.57
Guazatine acetates	Guanidine	F	Contact action	115044-19-4	Mixture	
Haloxyfop	Aryloxyphenoxypropionic acid	H	Growth inh.	69806-34-4	C15 H11 Cl F3 N O4	361.71
Haloxyfop ethoxyethyl	Aryloxyphenoxypropionic acid	H	Growth inh.	87237-48-7	C19 H19 Cl F3 N O5	433.81
Hexaconazole	Azole	F	Ergosterol synt. inh.	79983-71-4	C14 H17 Cl2 N3 O	314.22
Hexazinone	1,3,5-triazine-dione	H	Photosynt. inh	51235-04-2	C12 H20 N4 O2	252.32
Hexythiazox	Thiazolidinone	A	CSA	78587-05-0	C17 H21 Cl N2 O2 S	352.88
Hydramethylnon	Pyrimidinone hydrazone	I	SA	67485-29-4	C25 H24 F6 N4	494.49
Hymexazol	Isoxazole	F	Syst.fung.inh	10004-44-1	C4 H5 N O2	99.10
Imazalil	Azole	F	Ergosterol synt.inh.	35554-44-0	C14 H14 Cl2 N2 O	297.19
Imazamethabenz-methyl (m)	Imidazolinone	H	Amino acid synt. inh.	81405-85-8	C16 H20 N2 O3	288.35
Imazamethabenz-methyl (p)	Imidazolinone	H	Amino acid synt. inh.	81405-85-8	C16 H20 N2 O3	288.35
Imazapyr	Imidazolinone	H	Amino acid synt. inh.	81334-34-1	C13 H15 N3 O3	261.28
Imazaquin	Imidazolinone	H	Amino acid synt. inh.	81335-37-7	C17 H17 N3 O3	311.34
Imazaquin ammonium	Imidazolinone	H	Amino acid synt. inh.	81335-47-9	C17 H20 N4 O3	328.37
Imazethapyr	Imidazolinone	H	Amino acid synt. inh.	81335-77-5	C15 H19 N3 O3	289.34
Imidacloprid	Nitroimidazolidinylideneamine	H	Acetylcholin rec. inh.	138261-41-3	C9 H10 Cl N5 O2	255.67
4-Indol-3-ylbutyric acid	indolylbutyric acid	PGR	Cell div.and elong. inh.	133-32-4	C12 H13 N O2	203.24
Ioxynil	Hydroxybenzonitril	H	Photosynt. inh.	1689-83-4	C7 H3 I2 N O	370.92
Ioxynil octanoate	Hydroxybenzonitril	H	Photosynt. inh.	3861-47-0	C15 H17 I2 N O2	497.12
Iprodione	Dichloroanilide	F	Germ. and growth inh.	36734-19-7	C13 H13 Cl2 N3 O3	330.17
Isazofos	Organophosphorous	I	Cholinesterase inh.	42509-80-8	C9 H17 Cl N3 O3 P S	313.75
Isofenphos	Organophosphorous	I	Cholinesterase inh.	25311-71-1	C15 H24 N O4 P S	345.40
Isopropalin	Dinitroaniline	H	Cell div. inh.	33820-53-0	C15 H23 N3 O4	309.30
Isoproturon	Urea	H	Photosynt. inh.	34123-59-6	C12 H18 N2 O	206.30
Isoxaben	Amide	H	Amino acid synt. inh.	82558-50-7	C18 H24 N2 O4	332.40
Lactofen	Diphenyl ether	H		77501-63-4	C19 H15 Cl F3 N O7	461.78
Lambda-Cyhalothrin	Pyrethroid	I	CSA	91465-08-6	C23 H19 Cl F3 N O3	449.86
Lenacil	Uracil	H	Photosynt. inh.	2164-08-1	C13 H18 N2 O2	234.30
Lindane (Gamma HCH)	Organochlorine	I	CSA	58-89-9	C6 H6 Cl6	290.85

Name (ISO)	Chemical class	Use	Mode of action	CAS No.	Molecular formula	MW g/mol
Linuron	Urea	H	Photosynt. inh	330-55-2	C9 H10 Cl2 N2 O2	249.11
Malathion	Organophosphorous	I	Cholinesterase inh.	121-75-5	C10 H19 O6 P S2	330.35
Maleic hydrazide	Pyridazinone	PGR	Cell div. inh.	123-33-1	C4 H4 N2 O2	112.09
Maleic hydrazide potassium	Pyridazinone	PGR	Cell div. inh.	51542-52-0	C4 H3 K N2 O2	150.18
Mancozeb	Alkylenebis(dithiocarbamate)	F	Contact action	8018-01-7	(C4 H6 Mn N2 S4)x (Zn)y	271.0_m
Maneb	Alkylenebis(dithiocarbamate)	F	Contact action	12427-38-2	(C4 H6 Mn N2 S4)x	265.3_x
MCPA	Arylalkanoic acid	H	Growth inh. (hormone)	94-74-6	C9 H9 Cl O3	200.62
MCPA octyl ester	Arylalkanoic acid	H	Growth inh. (hormone)		C17 H25 Cl O3	312.84
MCPA dimethylammonium	Arylalkanoic acid	H	Growth inh. (hormone)		C11 H16 Cl N O3	245.71
MCPB	Arylalkanoic acid	H	Growth inh. (hormone)	94-81-5	C11 H13 Cl O3	228.70
MCPB sodium	Arylalkanoic acid	H	Growth inh. (hormone)	6062-26-6	C11 H12 Cl Na O3	250.66
Mecoprop (MCPP)	Arylalkanoic acid	H	Growth inh. (hormone)	7085-19-0	C10 H11 Cl O3	214.65
Mecoprop dimethylamine	Arylalkanoic acid	H	Growth inh. (hormone)		C12 H18 Cl N O3	259.74
Mecoprop-P	Arylalkanoic acid	H	Growth inh. (hormone)	16484-77-8	C10 H11 Cl O3	214.65
Mecoprop-P dimethylammonium	Arylalkanoic acid	H	Growth inh. (hormone)	66423-09-4	C12 H18 Cl N O3	259.74
Mepiquat chloride	Quarternary ammonium	PGR	Gibbereli.synt.inh.	24307-26-4	C7 H16 Cl N	149.67
Mepronil	Anilide	F	Syst. act.fung	55814-41-0	C17 H19 N O2	269.35
Metalaxyl	Acylalanine	F	Protein synt. inh.	57837-19-1	C15 H21 N O4	279.34
Metaldehyde	Oxacyclo-octane	M	CSA	108-62-3	C8 H16 O4	176.21
Metam (metham) sodium	Mehtyl isothiocyanate pre.	I, F, N	Soil sterilant	137-42-8	C2 H4 N Na S2	129.18
Metamitron	Triazinone	H	Photosynt. inh.	41394-05-2	C10 H10 N4 O	202.22
Methabenzthiazuron	Urea	H	Photosynt. inh.	18691-97-9	C10 H11 N3 O S	221.30
Methamidophos	Organophosphorous	I	Cholinesterase inh.	10265-92-6	C2 H8 N O2 P S	141.13
Methazole	Phenylurea pre.	H		20354-26-1	C9 H6 Cl2 N2 O3	261.07
Methidathion	Organophosphorous	I	Cholinesterase inh.	950-37-8	C6 H11 N2 O4 P S3	302.32
Methiocarb (Mercaptodimethur)	Carbamate	M	CSA	2032-65-7	C11 H15 N O2 S	225.31
Methomyl	Oxime carbamate	I	CSA	16752-77-5	C5 H10 N2 O2 S	162.21
Methoxychlor	Diphenyl ethane	I	CSA	72-43-5	C16 H15 Cl3 O2	345.65
Methylarsonate, sodium hydrogen	Organoarsenic	H	Cont. herb.	2163-80-6	C H4 As Na O3	161.90
Methyl Bromide	Alkyl halide	I, N	Soil sterilant	74-83-9	C H3 Br	94.94
Methyl isothiocyanate	Isothiocyanate	F	Soil sterilant	556-61-6	C2 H3 N S	73.11
Metiram	Alkylenebis(dithiocarbamate)	F	Cont. fung.	9006-42-2	C16 H33 N11 S16 Zn3	1088.70
Metolachlor	Chloroacetanilide	H	Germ. and growth inh.	51218-45-2	C15 H22 Cl N O2	283.80
Metoxuron	Urea	H	Photosynt. inh.	19937-59-8	C10 H13 Cl N2 O2	228.68
Metribuzin	Triazinone	H	Photosynt. inh.	21087-64-9	C8 H14 N4 O S	214.30
Metsulfuron-methyl	Sulfonylurea	H	Amino acid synt.inh.	74223-64-6	C14 H15 N5 O6 S	381.37
Mevinphos	Organophosphorous	I	Cholinesterase inh.	26718-65-0	C7 H13 O6 P	224.15
Monocrotophos	Organophosphorous	I	Cholinesterase inh.	6923-22-4	C7 H14 N O5 P	223.20
Monolinuron	Urea	H	Photosynt. inh.	1746-81-2	C9 H11 Cl N2 O2	214.65
Muscalure	Pheromone	I	Sex pheromone	27519-02-4	C23 H46	322.60
Naled	Organophosphorous	I	Cholinesterase inh.	300-76-5	C4 H7 Br2 Cl2 O4 P	380.79
2-(1-Naphthyl)acetamide	Aryl acetic acid	PGR	Synthetic auxin	86-86-2	C12 H11 N O	185.23
2-(1-Naphthyl)acetic acid	Aryl acetic acid	PGR	Synthetic auxin	86-87-3	C12 H10 O2	186.21
2-(1-Naphthyl)acetate, ethylester	Aryl acetic acid	PGR	Synthetic auxin	2122-70-5	C14 H14 O2	214.27
2-(1-Naphthyl)acetate sodium	Aryl acetic acid	PGR	Synthetic auxin		C12 H9 O2 Na	208.19

Name (ISO)	Chemical class	Use	Mode of action	CAS No.	Molecular formula	MW g/mol
Napropamide	Arylalkanamide	H	Cell div. inh.	15299-99-7	C17 H21 N O2	271.36
Naptalam	N-arylphthalamic acid	H	IAA transp. inh.	132-66-1	C18 H13 N O3	291.31
Naptalam sodium	N-arylphthalamic acid	H	IAA transp. inh.	132-67-2	C18 H12 N O3 Na	313.29
Nitrapyrin	Pyridine	B	Nitrification inh.	1929-82-4	C6 H3 Cl4 N	230.91
Norflurazon	Pyridazinone	H	Photosynt. inh.	27314-13-2	C12 H9 Cl F3 N3 O	303.67
Nuarimol	Pyrimidinyl carbinol	F	Ergosterol synt. inh.	63284-71-9	C17 H12 Cl F N2 O	314.75
1,4,4a,5a,6,9,9a,9b-Octahydro-dibenzofuran-4a-carbaldehyde	Dibenzofuran	I rep.	insect repellent	126-15-8	C13 H16 O2	204.27
Oryzalin	Dinitroaniline	H	Growth inh.	19044-88-3	C12 H8 N4 O6 S	346.36
Oxadiazon	Oxadiazolone	H	CA	19666-30-9	C15 H18 Cl2 N2 O3	345.23
Oxadixyl	Xylidide	F	Syst. act.fung	77732-09-3	C14 H18 N2 O4	278.31
Oxamyl	Oxime carbamate	I	Cholinesterase inh.	23135-22-0	C7 H13 N3 O3 S	219.26
Oxycarboxin	Phenylamide	F	Syst.fung.inh	5259-88-1	C12 H13 N O4 S	267.30
Oxydemeton-methyl	Organophosphorous	I	Cholinesterase inh.	301-12-2	C6 H15 O4 P S2	246.28
Oxyfluorfen	Diphenyl ether	H	prophyrinoxidase inh.	42874-03-3	C15 H11 Cl F3 N O4	361.71
Paclobutrazol	Azole	PGR	Gibberelli.synt. inh	76738-62-0	C15 H20 Cl N3 O	293.80
Paraquat dichloride	Bipyridyl	H	Cell and cytopl. destr.	1910-42-5	C12 H14 Cl2 N2	257.16
Parathion ethyl	Organophosphorous	H	Cholinesterase inh.	56-38-2	C10 H14 N O5 P S	291.27
Parathion methyl	Organophosphorous	H	Cholinesterase inh.	298-00-0	C8 H10 N O5 P S	263.21
Pebulate	Thiocarbamate	H	Germination inh.	1114-71-2	C10 H21 N O S	203.36
Penconazole	Azole	H	Ergosterol synt. inh.	66246-88-6	C13 H15 Cl2 N3	284.19
Pencycuron	Phenylurea	F	non-systemic fung	66063-05-6	C19 H21 Cl N2 O	328.84
Pendimethalin	Dinitroaniline	H	Growth inh.	40487-42-1	C13 H19 N3 O4	281.31
Permethrin	Pyethroid	I	CSA	52645-53-1	C21 H20 Cl2 O3	391.30
Phenmedipham	Biscarbamate	H	Photosynt. inh.	13684-63-4	C16 H16 N2 O4	300.32
Phorate	Organophosphorous	I	Cholinesterase inh.	298-02-2	C7 H17 O2 P S3	260.38
Phosalone	Organophosphorous	I	Cholinesterase inh.	2310-17-0	C12 H15 Cl N O4 P S2	367.80
Phosmet	Organophosphorous	I	Cholinesterase inh.	732-11-6	C11 H12 N O4 P S2	317.33
Phosphamidon	Organophosphorous	I	Cholinesterase inh.	13171-21-6	C10 H19 Cl N O5 P	299.69
Phoxim	Organophosphorous	I	Cholinesterase inh.	14816-18-6	C12 H15 N2 O3 P S	298.30
Picloram	Pyridinecarboxylic acid	H	Growth inh.	1918-02-1	C6 H3 Cl3 N2 O2	241.46
Picloram potassium	Pyridinecarboxylic acid	H	Growth inh.	2545-60-0	C6 H2 Cl3 N2 O2 K	279.55
Piperalin	Dichlorobenzoate	F		3478-94-2	C16 H21 Cl2 N O2	330.25
Piperonyl butoxide	Methylenedioxyphenyl	I	I synergist	51-03-6	C19 H30 O5	338.45
Pirimicarb	Carbamate	I	Cholinesterase inh.	23103-98-2	C11 H18 N4 O2	238.29
Pirimiphos-ethyl	Organophosphorous	I	Contact and resp.act.	23505-41-1	C13 H24 N3 O3 P S	333.39
Pirimiphos-methyl	Organophosphorous	I	Contact and resp.act.	29232-93-7	C11 H20 N3 O3 P S	305.34
Primisulfuron-methyl	Sulfonylurea	H	Amino acid synt. inh.	86209-51-0	C15 H12 F4 N4 O7 S	468.34
Prochloraz	Azole	F	Ergosterol.synt. inh.	67747-09-5	C15 H16 Cl3 N3 O2	376.67
Profenofos	Organophosphorous	I	Cholinesterase inh.	41198-08-7	C11 H15 Br Cl O3 P S	373.60
Prometon	Triazine	H	Photosynt. inh.	1610-18-0	C10 H19 N5 O	225.30
Prometryn	Triazine	H	Photosynt. inh.	7287-19-6	C10 H19 N5 S	241.36
Propachlor	Chloroacetanilide	H	Growth inh.	1918-16-7	C11 H14 Cl N O	211.69
Propamocarb hydrochloride	Carbamate	F	Multi-site inh.	25606-41-1	C9 H21 Cl N2 O2	224.73
Propaquizafop	Aryloxyphenoxypropionic acid	H	fatty acid synt. inh.	111479-05-1	C22 H22 Cl N3 O5	443.89
Propargite	Sulfite	A	CA	2312-35-8	C19 H26 O4 S	350.48
Propazine	Triazine	H	Photosynt. inh.	139-40-2	C9 H16 Cl N5	229.71
Propetamphos	Organophosphorous	I	Cholinesterase inh.	31218-83-4	C10 H20 N O4 P S	281.30
Propham (IPC)	Carbamate	PGR	Growth inh.	122-42-9	C10 H13 N O2	179.22
Propiconazole	Azole	F	Ergosterol synt. inh.	60207-90-1	C15 H17 Cl2 N3 O2	342.20
Propineb	Alkylenebis(dithiocarbamate)	F	Fung.inh.	12071-83-9	(C5 H8 N2 S4 Zn)x	289.80

Name (ISO)	Chemical class	Use	Mode of action	CAS No.	Molecular formula	MW g/mol
Propoxur	Carbamate	I	CSA	114-26-1	C11 H15 N O3	209.25
Propyzamide	Amide	H	Photosynt. inh.	23950-58-5	C12 H11 Cl2 N O	256.13
Prosulfocarb	Thiocarbamate	H	Growth inh.	52888-80-9	C14 H21 N O S	251.39
Prosulfuron	Sulfonylurea	H	Enz.synt.inh.	94125-34-5	C15 H16 F3 N5 O4 S	419.40
Pyrazophos	Organophosphate ester	F	Syst fung.	13457-18-6	C14 H20 N3 O5 P S	373.37
Pyrethrins (extract)	Pyrethrins	I	Contact action	8003-34-7	C21 H28 O3	328.46
Pyrethrins I (chrysanthemates)	Pyrethrins	I	Contact action	121-21-1	C21 H28 O3	328.46
Pyrethrins II (pyrethrates)	Pyrethrins	I	Contact action	121-29-9	C22 H28 O5	372.47
Pyridate	Pyridazine	H	Photosynt. inh	55512-33-9	C19 H23 Cl N2 O2 S	378.92
Pyriproxyfen	Phenyl ether	I		95737-68-1	C20 H19 N O3	321.38
Quintozene (PCNB)	Hydrocarbon der.	F	Soil fung.	82-68-8	C6 Cl5 N O2	295.34
Quizalofop-ethyl	Aryloxyphenoxypropionic acid	H	Growth inh.	76578-14-8	C19 H17 Cl N2 O4	372.80
Rimsulfuron	Sulfonylurea	H	Enz.synt.inh.	122931-48-0	C14 H17 N5 O7 S2	431.40
Rotenone	CA	I	CSA	83-79-4	C23 H22 O6	394.43
Sethoxydim	Cyclohexanedione oxime	H	Mitosis inh.	74051-80-2	C17 H29 N O3 S	327.50
Siduron	Urea	H	Photosynt. inh.	1982-49-6	C14 H20 N2 O	232.33
Simazine	Triazine	H	Photosynt. inh.	122-34-9	C7 H12 Cl N5	201.66
Sulfometuron methyl	Sulfonylurea	H	Amino acid synt. inh.	74222-97-2	C15 H16 N4 O5 S	364.38
Sulprofos	Organophosphorous	I	Cholinesterase inh.	35400-43-2	C12 H19 O2 P S3	322.44
2,4,5-T	Aryloxyalkanoic acid	H	auxin type reaction	93-76-5	C8 H5 Cl3 O3	255.46
2,4,5-T trihydroxyethyl-ammonium	Aryloxyalkanoic acid	H	auxin type reaction	3813-14-7	C14 H19 Cl3 N O6	403.67
2,3,6-TBA	Benzoic acid	H	Oxidat. phospho. inh	50-31-7	C7 H3 Cl3 O2	225.46
TCA-sodium	Alkanoic acid	H	Growth inh.	650-51-1	C2 Cl3 Na O2	185.37
Tebuconazole	Azole	F	Ergosterolsynt. inh.	107534-96-3	C16 H22 Cl N3 O	307.83
Tebuthiuron	Urea	H	Photosynt. inh.	34014-18-1	C9 H16 N4 O S	228.32
Tefluthrin	Pyrethroid	I	CSA	79538-32-2	C17 H14 Cl F7 O2	418.74
Temephos	Organophosphorous	I	Cholinesterase inh.	3383-96-8	C16 H20 O6 P2 S3	466.46
Terbacil	Uracil	H	Photosynt.inh.	5902-51-2	C9 H13 Cl N2 O2	216.67
Terbufos	Organophosphorous	I	Cholinesterase inh.	13071-79-9	C9 H21 O2 P S3	288.43
Terbutryn	Triazine	H	Photosynt. inh.	886-50-0	C10 H19 N5 S	241.36
Terbutylazine	Triazine	H	Photosynt. inh.	5915-41-3	C9 H16 Cl N5	229.71
Tetrachlorvinphos	Organophosphorous	I	Cholinesterase inh.	22248-79-9	C10 H9 Cl4 O4 P	365.97
Tetradifon	Diphenyl	A	Sterilisation	116-29-0	C12 H6 Cl4 O2 S	356.05
Thiabendazole	Benzimidazole	F	Growth inh.	148-79-8	C10 H7 N3 S	201.25
Thidiazuron	Phenylurea	PGR	Stim abscission layer	51707-55-2	C9 H8 N4 O S	220.25
Thifensulfuron methyl	Sulfonylurea	H	Amino acid synt. inh.	79277-27-3	C12 H13 N5 O6 S2	387.39
Thiobencarb	Thiocarbamate	H	Photosynt. inh.	28249-77-6	C12 H16 Cl N O S	257.78
2-(Thiocyanomethylthio)-benzothiazol (TCMTB)	Benzothiazol	F	Growth inh., syst act.	21564-17-0	C9 H6 N2 S3	238.35
Thiodicarb	Oxime carbamate	I, M	Cholinesterase inh.	59669-26-0	C10 H18 N4 O4 S3	354.46
Thiofanox	Oxime carbamate	I, M	Cholinesterase inh.	39196-18-4	C9 H18 N2 O2 S	218.32
Thiometon	Organophosphorous	I	Cholinesterase inh.	640-15-3	C6 H15 O2 P S3	246.34
Thiophanate-methyl	Benzimidazole	F	Syst.fung.inh	23564-05-8	C12 H14 N4 O4 S2	342.39
Thiram	Dimethyldithiocarbamate	F	CA	137-26-8	C6 H12 N2 S4	240.42
Tolclofos-methyl	Organophosphorous	F	Phospholipid synt.inh.	57018-04-9	C9 H11 Cl2 O3 P S	301.13
Tolylfluanid	N-trihalomethylthio	F	Multi-site act.fung.	731-27-1	C10 H13 Cl2 F N2 O2 S2	347.25
Camphechlor (Toxaphene)	Camphene mixt.	I	CSA	8001-35-2	C10 H10 Cl8	413.80
Tralomethrin	Pyrethroid	I	CSA	66841-25-6	C22 H19 Br4 N O3	655.02
Triadimefon	Azole	F	Ergosterol synt. inh.	43121-43-3	C14 H16 Cl N3 O2	293.76
Triadimenol	Azole	F	Ergosterol synt. inh.	55219-65-3	C14 H18 Cl N3 O2	295.77

Name (ISO)	Chemical class	Use	Mode of action	CAS No.	Molecular formula	MW g/mol
Triallate	Thiocarbamate	H	Growth inh.	2303-17-5	C10 H16 Cl3 N O S	304.66
Triasulfuron	Sulfonylurea	H	Amino acid synt. inh.	82097-50-5	C14 H16 Cl N5 O5 S	401.83
Triazamate		I	Cholinesterase inh.	112143-82-5	C13 H22 N4 O3 S	314.41
Tribenuron methyl	Sulfonylurea	H	Amino acid synt. inh.	101200-48-0	C15 H17 N5 O6 S	395.39
S,S,S-tributyl phosphorotrithioate (Tribufos)	Organophosphorous	PGR	Stim abscission layer	78-48-8	C12 H27 O P S3	314.50
Trichlorfon	Organophosphorous	I	Cholinesterase inh.	52-68-6	C4 H8 Cl3 O4 P	257.44
Triclopyr	Aryloxyalkanoic acid	H	auxin type reaction	55335-06-3	C7 H4 Cl3 N O3	256.47
Triclopyr-butotyl	Aryloxyalkanoic acid	H	auxin type reaction	64470-88-8	C13 H16 Cl3 N O4	356.64
Triclopyr-triethylammonium	Aryloxyalkanoic acid	H	auxin type reaction		C13 H19 Cl3 N2 O3	357.66
Tridemorph	Morpholine	F	Ergosterol synt. inh.	24602-86-6	C09 H39 N O	297.53
Tridiphane		H		58138-08-2	C10 H7 Cl5 O	320.43
Trifluralin	Dinitroaniline	H	Cell div. inh.	1582-09-8	C13 H16 F3 N3 O4	335.29
Triflusulfuron methyl	Sulfonylurea	H	Amino acid synt. inh	126535-15-7	C17 H19 F3 N6 O6 S	492.43
Triforine	Trichloromethylformamide	F	Ergosterol synt. inh.	26644-46-2	C10 H14 Cl6 N4 O2	434.97
Trimethacarb	Carbamate	I	CSA	12407-86-2	C11 H15 N O2	193.24
Trinexapac ethyl	dioxocyclohexanecarboxylate	PGR	Gibberelli. synt.inh.	95266-40-3	C13 H16 O5	252.27
Vernolate	Thiocarbamate	H	Growth inh.	1929-77-7	C10 H21 N O S	203.35
Vinclozolin	Dicarboximide	H	Spore germin. inh.	50471-44-8	C12 H9 Cl2 N O3	286.12
Zineb	Alkylenebis(dithiocarbamate)	F	Cont. fung.	12122-67-7	C4 H6 N2 S4 Zn	275.80
Ziram	Dimethyldithiocarbamate	F	Cont.fung.	137-30-4	C6 H12 N2 S4 Zn	305.80
Total number (of 409)	398	409	396	399	409	408

Table 2
Melting point (MP), boiling point (BP), water solubility (S), vapour pressure (VP) and Henry's Law constant.

Smeltepunkt (MP), kogepunkt (BP), vandopløselighed (S), damptryk (VP) og Henrys Lov Konstant.

Name (ISO)	MP		BP		S		VP		Henry's Law Constant	
	ºC	ºC	ºC	ºC	mg/l	EPI	Pa	Pa	Pa m^3/mol	Pa m^3/mol
	exp.	est.	exp.	est.	exp.	est.	exp.	est.	est. (bond)	calculated
Acephate	89.00	80.07		340.48	818000	405400	2.26E-04	7.16E-03	2.85E-07	5.06E-08
Acetochlor	0.00	128.45		378.17	223	233	4.53E-06	3.73E-03	2.26E-03	5.48E-06
Acifluorfen	151.00	185.94		442.92	120	1.5	1.00E-05	2.04E-06	6.11E-06	3.01E-05
Acifluorfen sodium	276.00	277.47		638.89	250000	756	<1.00E-05	1.53E-12		
Aclonifen	81.00	160.01		399.65	1.4	7.8	1.60E-05	3.31E-04	2.70E-04	3.02E-03
Acrinathrin	81.50	2.91		451.29	<0.02	0.0025	3.90E-07	1.77E-05	2.53E-02	
Acrolein	-87.00	-94.61	52.50	57.87	208000	188500	2.93E+04	2.87E+04	3.85E+00	7.90E+00
Alachlor	40.00	128.45	>100	378.17	241	57.5	2.90E-03	2.73E-03	2.26E-03	3.25E-03
Alanycarb	46.80	117.51		452.42	20	35.2	4.70E-06	3.61E-05	1.74E-08	9.39E-05
Aldicarb	99.00	28.81		251.95	4930	4068	1.30E-02	6.44E-01	3.62E-04	5.02E-04
Aldoxycarb	140.00	94.21		316.50	10000	67790	1.20E-02	7.45E-03	2.87E-06	2.67E-04
Allethrin	liq.	126.18	>140	374.02	4.6	0.98	1.60E-02	4.60E-04	6.20E-07	1.05E+00
Alloxydim sodium	185.50	273.89		631.21	2000000	11680	<0.000133	2.71E-12		
Ametryn	84.00	130.58		341.98	185	85.6	3.65E-04	7.42E-03	6.94E-04	4.49E-04
Amidosulfuron	160.00	236.61		551.41		125700	2.20E-05	7.37E-09	1.42E-07	
Amitraz	86.00	132.34		396.72	0.09	1.72	3.40E-04	3.47E-04	1.50E-03	1.11E+00
Amitrole	158.00	69.52		258.30	280000	90300	5.50E-08	1.01E-01	5.47E-05	1.65E-11
Ancymidol	110.00	144.33		376.26	650	1275	2.67E-05	1.77E-05	5.88E-08	1.05E-05
Anilazine	159.00	149.42		364.74	8	2.04	8.20E-07	3.32E-04	3.45E-02	2.82E-05
Asulam	143.00	142.46		382.35	5000	32050	<1.33E-03	1.89E-04	1.72E-07	
Asulam sodium		264.62		611.37	550000	1000000		1.17E-11		
Atrazine	175.80	113.91		313.03	33	28.5	3.90E-05	3.52E-03	4.53E-04	2.55E-04
Azaconazole	112.60	158.17		383.48	300	155.3	8.60E-06	3.77E-04	5.89E-05	8.60E-06
Azamethiphos	89.00	87.59		452.52	1100	4340	4.90E-06	1.37E-05	6.41E-08	1.45E-06
Azinphos-ethyl	50.00	90.06		477.85	5	44.96	3.20E-04	7.80E-06	5.11E-05	2.21E-02
Azinphos-methyl	72.40	87.80		454.64	28	133.6	1.80E-04	1.81E-05	2.90E-05	2.04E-03
Benalaxyl	79.00	166.16		438.37	37	26.5	6.70E-04	3.89E-05	7.94E-05	5.89E-03
Benazolin	193.00	175.09		419.70	500	264.8	1.00E-07	6.31E-06	8.85E-05	4.87E-08
Benazolin ethyl	79.20	159.76		398.25	47	238.9	3.70E-04	3.75E-04	3.76E-02	2.14E-03
Bendiocarb	125.00	98.27		315.15	40	614.9	4.60E-03	1.17E-02	6.67E-06	2.57E-02
Benfluralin	66.00	139.97	>121	382.17	0.1	0.5	8.70E-03	1.24E-03	2.15E+01	2.92E+01
Benfuracarb	liq.	163.99		443.93	8	0.6	2.66E-05	3.45E-06	3.06E-07	1.37E-03
Benfuresate	32.00	133.81		360.96	261	829.7	1.43E-03	8.36E-03	5.50E-03	1.40E-03
Benomyl	140.00	189.25	dec	450.02	2	141.6	<4.9E-06	4.52E-06	1.90E-10	
Bensulfuron methyl	185.00	249.90		579.86	120	65.7	2.80E-12	7.01E-10	3.64E-09	9.58E-12
Bensulide	34.40	89.63		473.44	5.6	8.4	1.07E-04	1.40E-05	3.32E-04	7.60E-03
Bensultap	83.00	242.44		563.88	0.7	112.6	2.10E-04	2.27E-08	4.46E-09	1.29E-01
Bentazone	138.00	173.04		415.31	570	108	4.60E-04	3.41E-05	2.02E-05	1.94E-04
Bentazone sodium		285.44		655.93	2300000	6048		4.32E-13		
Bifenox	85.00	176.73		425.15	0.35	0.62	3.20E-04	7.16E-05	1.66E-04	3.13E-01
Bifenthrin	51.00	167.36		437.29	0.1	0.00084	2.40E-05	7.80E-05	1.94E+00	1.01E-01
Bioallethrin	liq.	126.18		374.02	4.6	0.98	4.39E-02	4.60E-04	6.20E-02	2.89E+00
Bioresmethrin	32.00	146.28		405.44	<0.3	0.019	1.86E-05	7.08E-04	5.63E-01	
Bitertanol	137.00	196.84		466.26	2.9	3.6	2.20E-10	1.96E-08	1.65E-07	2.56E-08
Brodifacoum	228.00	302.03		691.46	1.1	0.000005	4.00E-05	1.56E-16	5.47E-08	1.90E-02
Bromacil	149.00	175.78		421.19	700	133	4.10E-05	1.85E-05	1.41E-05	1.53E-05
Bromacil lithium		272.93		629.16	700	469		3.16E-12		
Bromadiolone	200.00	308.78		705.90	19	0.0007	2.00E-06	2.07E-17	4.11E-09	5.55E-05
Bromethalin	150.00	212.79		500.41	0.0016	0.00013	1.30E-05	1.91E-07	4.08E-04	4.70E+00
Bromofenoxim	196.00	221.33		518.70	2.6	4.2	1.00E-08	2.31E-09	1.10E-09	1.77E-06
Bromoxynil	194.00	119.50		327.67	130	11.36	<1.00E-03	2.76E-04	8.71E-05	

Name (ISO)	MP		BP		S		VP		Henry's Law Constant	
	°C	°C	°C	°C	mg/l	EPI	Pa	Pa	Pa m^3/mol	Pa m^3/mol
	exp.	est.	exp.	est.	exp.	est.	exp.	est.	est. (bond)	calculated
Bromoxynil octanoate	45.00	157.62		413.69	0.08	0.04	1.90E-04	3.37E-04	5.51E-02	9.57E-01
Bromoxynil butyrate		133.46		367.27	27	1.64	1.33E-02	5.56E-04	1.77E-02	1.71E-01
Bromoxynil potassium	360.00	234.70		547.36	61000	4026		1.25E-09		
Bromuconazole	84.00	172.71		414.60	50	27.05	4.00E-06	1.33E-04	2.56E-05	3.02E-05
Bronopol	130.00	90.85		300.57	250000	32370	1.68E-03	8.38E-04	1.16E-06	1.34E-06
Butylate		60.29	>138	299.57	44	10.15	1.73	1.25E-01	2.75E+00	8.55E+00
Captafol	160.00	200.12		473.28	1.4	30.78		7.10E-07	2.18E-04	
Captan	178.00	183.46		437.61	3.8	36.6	1.70E-05	3.41E-06	4.65E-04	1.34E-03
Carbaryl	142.00	91.20		327.50	120	105.4	4.10E-05	3.92E-03	3.18E-04	6.88E-05
Carbendazim	302.00	149.71		404.73	8	23.3	1.50E-04	6.84E-07	1.51E-07	3.58E-03
Carbetamide	119.00	147.15		393.23	3500	782.3		1.89E-04	1.46E-05	
Carbofuran	153.00	92.80		311.41	351	86.8	7.20E-05	7.01E-03	1.65E-04	4.54E-05
Carbosulfan	liq.	176.02	126.00	441.52	0.3	0.07	4.10E-05	2.88E-06	2.27E-04	5.20E-02
Carboxin	92.00	165.94		407.15	195	451.8	2.50E-05	1.68E-04	7.56E-07	3.02E-05
Chinomethionate	170.00	162.86		393.52	1	2.3	2.60E-05	5.05E-05	1.28E-01	6.09E-03
Chloramben	200.00	124.67		348.90	700	83.61	<0.93	2.67E-04	2.13E-06	
Chloramben sodium		233.55		544.86	900000	597800		1.49E-09		
Chlordimeform hydrochloride		40.94		265.33	50000	1577	4.27E-04	1.15E+00	5.01E-02	1.99E-06
Chlorfenac sodium (Fenac)		227.82		532.58	500000	24030		3.61E-09		
Chlorfenvinphos	-20.00	85.90		397.78	145	29	1	1.25E-03	5.24E-03	2.48E+00
Chloridazon (Pyridazon)	206.00	154.76		381.24	340	383	1.00E-05	3.81E-05	6.63E-07	6.52E-06
Chlorimuron ethyl	181.00	247.58		574.90	1200	14.9	5.33E-10	1.05E-09	1.03E-06	1.84E-10
Chlormequat chloride	235.00	132.06		368.52	>1000000	1000000	1.00E-05	3.47E-05	1.98E-07	
Chlorobenzilate	37.00	151.43	157.00	403.32	13	9	1.20E-04	1.57E-05	1.32E-02	3.00E-03
Chloroneb	134.00	47.69	268.00	252.91	8	11.2	0.4	2.45E-01	1.05E+00	1.04E+01
Chloropicrin	-64.00	20.30	112.40	155.18	1620	761	3200	4.20E+02	1.86E-01	3.25E+02
Chlorothalonil	250.00	131.51	350.00	354.86	0.9	0.84	7.60E-05	4.83E-05	1.54E-02	2.25E-02
Chloroxuron	151.00	173.18		431.37	2.5	1.5	2.39E-07	9.86E-06	1.59E-06	2.78E-05
Chlorpropham	41.40	64.92		283.19	89	67	1.07E-03	4.43E-01	2.89E-03	2.57E-03
Chlorpyrifos	43.00	82.93		377.43	1.4	1.6	2.70E-03	2.67E-03	2.55E-01	6.76E-01
Chlorpyrifos methyl	46.00	84.08		354.22	4	7.2	5.60E-03	8.98E-03	1.45E-01	4.52E-01
Chlorsulfuron	176.00	227.06		530.95	27900	65.16	3.00E-09	1.63E-08	8.76E-07	3.85E-11
Chlorthal dimethyl (DCPA)	156.00	89.69		343.19	0.5	0.55	2.10E-04	1.17E-03	6.83E-03	1.39E-01
Clethodim	liq.	177.50		461.94	5400	1.36	<10E-6	9.25E-09	1.18E-06	
Clofentezine	182.30	197.87		468.46	0.0025	6.3	1.30E-07	5.21E-07	1.58E-04	1.58E-02
Clomazone	25.00	132.37	275.00	359.07	1100	832	1.92E-02	1.07E-02	7.42E-06	4.18E-03
Cloprop (3-CPA)		90.51		313.01	1200	981		3.04E-02	1.67E-03	
Cloprop ammonium		123.07		344.85		1786		2.47E-03	3.41E-05	
Cloprop sodium		218.14		511.86	200000	544800		1.59E-08		
Clopyralide	151.00	106.56		308.01	143000	3508	1.33E-03	8.85E-03	4.99E-04	1.79E-06
Clopyralid-olamine		211.04		496.66	560000	1000000		3.32E-10	2.11E-16	
Coumatetralyl	172.00	189.63		481.73	425	0.7	8.50E-09	2.71E-09	2.22E-05	5.85E-09
Cyanazine	168.00	151.63		369.47	171	32	2.00E-07	2.03E-04	1.88E-07	2.82E-07
Cyanophos	14.50	15.98	119.00	339.33	46	225	1.05E-01	3.15E-02	4.17E-02	5.55E-01
Cycloate	11.50	85.71	145.00	322.62	95	42.2	2.13E-03	7.76E-02	1.22E+00	4.83E-03
Cycloxidim	41.00	172.34		451.86	40	20.5	1.00E-05	5.11E-07	9.65E-07	8.14E-05
Cyfluthrin	64.00	92.74		447.81	0.002	0.037	9.60E-07	3.51E-05	9.33E-02	2.08E-01
Cyhalothrin	liq.	68.66	187.00	436.49	0.000004	0.000853	1.00E-06	5.49E-05	1.36E+00	1.12E+02
Cypermethrin	80.50	82.07		450.48	0.004	0.021	2.30E-07	1.88E-05	7.99E-02	2.39E-02
alpha-Cypermethrin	79.00	82.07		450.48	0.01	0.021	2.30E-05	1.95E-05	7.99E-02	9.58E-01

Name (ISO)	MP		BP		S		VP		Henry's Law Constant	
	°C	°C	°C	°C	mg/l	EPI	Pa	Pa	Pa m^3/mol	Pa m^3/mol
	exp.	est.	exp.	est.	exp.	est.	exp.	est.	est. (bond)	calculated
Cyproconazole	106.00	158.36	>250	389.82	140	63.29	3.46E-05	7.89E-06	1.74E-05	7.21E-05
Cyromazine	220.00	140.86		346.43	136000	9669	4.48E-07	1.44E-03	3.27E-08	5.47E-10
2,4-D	140.50	109.13		329.17	890	171.1	1.10E-02	3.72E-03	9.33E-04	2.73E-03
2,4-D-dimethylammonium	86.00	198.75		470.35	796000	12510	1.07E-07	5.31E-06	1.47E-11	3.58E-11
2,4-D methylester		74.53		289.14	100	95		1.57E-01	2.99E-01	
Dalapon sodium	>191	173.84		429.22	900000	1000000	<1.00E-05	6.13E-06		
Daminozide	157.00	130.91		350.31	100000	421900	2.27E-02	7.72E-04	2.25E-10	3.64E-05
Dazomet	104.00	90.98		294.76	3000	2103	3.70E-04	5.80E-02	2.88E+02	2.00E-05
2,4-DB	118.00	125.28		353.19	46	51.6		1.77E-03	2.32E-04	
2,4-DB butoxyethyl		134.39		390.20	709000	0.3		1.52E-04	2.71E-03	
Deltamethrin	101.00	139.52		490.92	<0.0002	0.0063	<1.33E-05	1.13E-06	6.14E-03	
Desmedipham	120.00	119.92		396.03	9	12.6	4.00E-08	1.59E-04	6.97E-06	1.33E-06
Desmetryn	85.00	122.60		329.71	580	328	1.33E-04	1.41E-02	5.23E-04	4.89E-05
Diazinon	liq.	87.58	>125	366.20	60	6.5	1.20E-02	1.81E-03	8.85E-03	6.09E-02
Dicamba	115.00	112.26	>200	329.17	6500	1958	4.50E-03	7.05E-03	3.57E-04	1.53E-04
Dicamba sodium		224.71		525.94	360000	151500		5.81E-09		
Dichlobenil	145.00	52.67	270.00	252.19	21.2	19.6	8.80E-02	1.93E-01	2.90E+00	7.14E-01
Dichlofluanid	106.00	140.58		385.73	1.3	65.3	2.10E-05	3.96E-04	6.83E-02	5.38E-03
1,3-Dichloropropene	<-50	-72.77	108.00	107.80	2250	1994	3700	3.56E+03	2.48E+03	1.83E+02
Dichlorprop (2,4-DP)	116.00	110.38		334.17	350	70.16	<1E-05	5.25E-03	1.24E-03	
Dichlorprop butoxyethyl		125.13		371.61	50	1.1	4.00E-04	5.40E-04	1.44E-02	2.68E-03
Dichlorprop-P	122.00	110.38		334.17	590	62	6.20E-05	4.52E-03	1.24E-03	2.47E-05
Dichlorvos	liq.	18.07	234.10	251.76	8000	3475	2.10E+00	8.41E+00	8.69E-02	5.80E-02
Dicofol	79.00	148.32	>193	397.63	0.8	1.6	5.30E-05	8.86E-06	5.66E-05	2.45E-02
Dicloran (DCNA)	195.00	113.77		320.34	7	14	2.60E-04	1.43E-03	4.17E-04	7.69E-03
Dicrotophos	liq.	79.21	400.00	337.53	1000000	72910	9.3	1.06E-02	1.22E-07	2.21E-03
Dienochlor	122.00	160.53		388.53	0.025	0.00009	2.90E-04	2.28E-04	6.93E+01	5.51E+00
Diethatyl-ethyl	49.00	155.46		415.50	112	9	4.27E-04	2.16E-05	6.11E-04	1.19E-03
Difenacoum	216.00	287.69		660.75	2.5	0.000075	<0.00016	2.17E-15	1.38E-07	
Difenoconazole	78.60	206.96		487.93	16	0.4	3.30E-08	2.28E-06	1.71E-06	8.38E-07
Difenoxuron	138.00	176.21		436.33	20	59	1.24E-09	1.04E-05	1.28E-07	1.78E-08
Difenzoquat methylsulfate	150.00	270.74		624.46	817000	10590	1.30E-05	1.20E-10	1.12E-14	5.74E-09
Difethialone	233.00	300.08		687.27	0.39	0.000004	7.40E-05	2.75E-17		1.02E-01
Diflubenzuron	231.00	212.45		499.68	0.08	0.4	1.20E-07	2.33E-08	1.21E-06	4.66E-04
Diflufenican	161.00	202.41		478.02	0.05	0.12	7.00E-05	5.21E-07	3.82E-07	5.52E-01
Dimethachlor	47.00	120.55		366.57	2100	727	2.10E-03	4.47E-03	8.54E-05	2.56E-04
Dimethipin	168.00	121.79		342.22	3000	16310	5.10E-05	9.24E-04	5.45E-04	3.57E-06
Dimethoate	49.00	86.01		360.80	25000	23110	1.10E-03	5.87E-03	2.14E-06	1.01E-05
Dinocap	liq.	190.91	139.00	466.85	4	0.007	5.30E-09	1.77E-06	6.78E-04	4.83E-07
Dinoseb	40.00	138.02	320.00	372.11	50	58	1.07E-02	9.20E-04	7.22E-03	5.14E-02
Dinoseb-olamin		249.45		578.88	2200	2730		3.28E-15	1.71E-18	
Dinoseb acetic acid		144.40		386.65	1600	12	8.00E-02	1.44E-04	2.64E-04	1.41E-02
Dinoterb	126.00	139.35		367.51	4.5	8	2.00E-02	1.63E-04	7.22E-03	1.07E+00
Diphenamid	135.00	116.32		365.79	260	37	4.00E-06	5.80E-04	3.56E-05	3.68E-06
Dipropetryn	105.00	139.71		358.29	16	3	9.87E-05	1.84E-03	1.23E-03	1.58E-03
Diquat dibromide		138.15		380.21	700000	134500	<1.3E-05	2.41E-04	1.44E-08	
Disulfoton	<-25	6.90	>128	332.07	25	6	1.30E-02	4.67E-02	2.13E-01	1.43E-01
Dithianon	225.00	219.02		513.75	0.5	2	6.60E-05	1.18E-08	3.94E-12	3.91E-02
Diuron	158.00	126.39		353.86	42	151	1.10E-06	1.39E-03	5.40E-05	6.11E-06
DNOC	86.00	121.23	312.00	344.23	150	591	1.40E-02	1.72E-03	3.09E-03	1.85E-02
Dodine	136.00	220.33		516.55	700	810800	1.3	1.07E-07	6.10E-14	5.34E-01

Name (ISO)	MP		BP		S		VP		Henry's Law Constant	
	ºC	ºC	ºC	ºC	mg/l	EPI	Pa	Pa	Pa m^3/mol	Pa m^3/mol
	exp.	est.	exp.	est.	exp.	est.	exp.	est.	est. (bond)	calculated
Endosulfan	>80	166.48		401.28	0.32	1.49	8.30E-04	3.60E-05	9.15E-03	1.06E+00
Endothal	144.00	128.18		349.86	100000	1259		1.11E-03	3.67E-10	
Endothal sodium		194.76		485.47	100000	19250		1.40E-07		
EPTC	<-30	60.53	>127	287.60	344	197	1.00E-05	5.01E-01	1.56E+00	5.50E-06
Esfenvalerate	59.00	83.72	151.00	480.19	0.002	0.023	2.00E-07	5.59E-06	1.21E-02	4.20E-02
Ethalfluralin	55.00	141.89	256.00	378.14	0.3	0.97	1.17E-02	1.97E-03	1.88E+01	1.30E+01
Ethametsulfuron-methyl	194.00	256.94		594.93	50	13	7.73E-13	2.24E-10	7.11E-12	6.34E-12
Ethephon	74.00	34.64	265.00	306.96	1239000	79940	<1E-5	2.12E-03	5.78E-07	
Ethiofencarb	33.40	92.31		324.33	1800	2013	9.40E-04	5.96E-02	5.09E-05	1.18E-04
Ethion	-12.00	15.89	164.00	415.18	1.1	1.6	2.00E-04	4.72E-04	1.71E-02	6.99E-02
Ethirimol	159.00	125.33		334.73	150	7	2.67E-04	4.89E-04	3.20E-04	3.73E-04
Ethofumesate	71.00	141.80		381.25	50	172	6.50E-04	1.16E-03	1.19E-04	3.72E-03
Ethoprophos	liq.	42.23	86.00	322.52	750	22	4.65E-02	5.44E-02	3.14E-02	1.50E-02
Etridiazole	liq.	101.86	>95	284.78	50	32	1.90E-02	1.04E-01	6.80E-03	9.41E-02
Etrimfos	-3.40	96.37		362.04	40	260	8.60E-03	9.10E-03	2.45E-03	6.28E-02
Fenamiphos	49.20	84.78		390.08	700	79	1.20E-04	1.16E-03	9.79E-06	5.20E-05
Fenarimol	118.00	183.34		437.36	14	19	6.50E-05	2.32E-07	4.27E-08	1.54E-03
Fenbuconazole	125.00	197.68		468.06	0.2	0.66	5.00E-06	2.35E-06	1.55E-05	8.42E-03
Fenbutatin oxide	138.00				0.0127		8.50E-08			7.05E-03
Fenitrothion	3.40	85.77	140.00	359.98	21	39	1.80E-02	1.02E-02	1.88E-02	2.38E-01
Fenoxaprop		197.78		468.28		5		3.48E-07	4.66E-09	
Fenoxaprop-ethyl	86.00	186.82		446.83	0.8	0.63	4.20E-06	2.04E-05	1.99E-06	1.90E-03
Fenoxaprop-P-ethyl	90.00	186.82		446.83	0.9	0.6	5.30E-07	1.85E-05	1.99E-06	2.13E-04
Fenoxycarb	53.00	143.45		400.64	6	7	8.67E-07	5.91E-04	1.47E-06	4.35E-05
Fenpiclonil	145.00	139.14		380.80	4.8	1.4	1.10E-09	1.96E-04	3.75E-04	5.43E-08
Fenpropathrin	45.00	63.96		409.15	0.014	0.132	7.30E-04	4.36E-04	2.08E-01	1.82E+01
Fenpropidin	liq.	103.81		340.72	530	0.6	1.70E-02	4.96E-03	1.86E+00	8.77E-03
Fenpropimorph	liq.	121.28	>250	360.46	4.3	2.4	2.30E-03	1.10E-03	2.18E-02	1.62E-01
Fenthion	7.50	11.27		349.16	4.2	21.7	7.40E-04	1.84E-02	1.39E-01	4.90E-02
Fentin acetate	122.00		>350		9		<1.90E-03			
Fentin hydroxide	119.00		>350		1		<4.71E-05			
Fenvalerate	liq.	83.72		480.19	0.002	0.006	1.92E-05	3.17E-06	1.21E-02	4.03E+00
Ferbam	180d				120		1.33E-03			4.62E-03
Flamprop methyl	85.00	153.72		419.59	35	26	4.70E-05	9.81E-05	1.39E-04	4.51E-04
Flamprop-M isopropyl	73.00	165.81		435.80	12	4	8.50E-05	5.17E-05	2.44E-04	2.58E-03
Flocoumafen	181.00	293.76		673.73	1.1	0.00001	1.33E-10	2.09E-15	7.43E-08	6.56E-08
Fluazifob		162.84		402.25		18.6		3.75E-05	5.12E-06	
Fluazifop-butyl	13.00	149.02		404.01	1	0.9	5.50E-05	8.85E-04	3.84E-03	2.11E-02
Fluazifop-P-butyl	5.00	149.02		404.01	2	0.9	5.40E-04	8.85E-04	3.84E-03	1.04E-01
Flucythrinate	liq.	75.21		480.43	0.06	0.004	1.20E-06	3.81E-06	3.80E-03	9.03E-03
Flumetralin	102.00	188.09		447.53	0.07	0.03	3.20E-05	1.33E-05	6.40E-01	1.93E-01
Fluometuron	164.00	96.34		317.72	110	53	1.25E-04	3.76E-03	8.55E-04	2.64E-04
Flurenol-butyl	71.00	156.00		408.53	37	52	1.30E-04	5.11E-06	1.47E-02	9.92E-04
Fluridone	154.00	151.48		399.56	10	62	1.30E-05	5.48E-05	1.75E-05	4.28E-04
Fluroxypyr	232.00	154.36		375.32	91	840	3.78E-09	2.59E-05	4.60E-09	1.06E-08
Fluroxypyr-meptyl	59.00	169.01		416.49	0.09	1.47	1.35E-06	2.12E-04	1.07E-05	5.50E-03
Flurprimidol	94.00	130.56	264.00	359.10	114	62	1.00E-04	8.20E-05	1.05E-06	2.74E-04
Flusilazole	53.00	143.59		373.97	0.5	1.8	3.90E-05	2.60E-03	5.13E-02	2.46E-02
tau-Fluvalinate	liq.	156.17	>164	505.30	0.005	0.0006	<1.30E-05	1.23E-07	1.47E-03	
Folpet	177d	188.69		448.81	0.8	47.35	1.30E-03	1.36E-06	1.56E-04	4.82E-01
Fomesafen	220.00	241.62		562.13	>600	0.7	<1.00E-04	7.80E-10	7.63E-08	
Fomesafen sodium		349.84		802.76	700000	5	0	7.14E-18		
Fonofos	liq.	0.66	>130	323.68	16.9	10.7	2.80E-02	7.33E-02	1.13E+01	4.08E-01

Name (ISO)	MP		BP		S		VP		Henry's Law Constant	
	ºC	ºC	ºC	ºC	mg/l	EPI	Pa	Pa	Pa m^3/mol	Pa m^3/mol
	exp.	est.	exp.	est.	exp.	est.	exp.	est.	est. (bond)	calculated
Formetanate hydrochloride	201.00	95.53		326.35	500000	52110	1.60E-06	1.32E-02	7.01E-06	8.25E-10
Formothion	25.00	84.73		389.76	2600	574500	1.13E-04	1.96E-03	1.50E-05	1.12E-05
Fosamine ammonium	174.00	80.54		342.09	1790000	1000000	5.30E-04	7.74E-04	1.45E-09	5.04E-08
Fosetyl-aluminium	200.00				120000		<1.30E-05			
Fuberidazole	292d	148.61		411.74	71	275.5	2.00E-06	3.17E-05	2.85E-03	5.19E-06
Furathiocarb	liq.	155.16	>250	427.71	11	0.38	3.90E-06	1.09E-05	8.02E-04	1.36E-04
Glufosinate ammonium	215.00	89.93		476.56	1370000	1000000	<1.00E-04	1.22E-09	2.56E-19	
Glyphosate	200.00	204.23		417.49	12000	1000000		4.32E-08	4.13E-14	
Glyphosate isopropylammonium		90.27		480.00	900000	1000000		8.08E-09	6.35E-22	4.56E-10
Glyphosate trimesium		86.99		405.22	1000000	1000000	4.00E-05	1.83E-06	2.50E-13	9.81E-09
Guazatine		216.12		507.55		28		2.16E-08	4.33E-17	
Guazatine acetates	>60				3000000		8.00E-07			
Haloxyfop	107.00	175.67		420.95	43.4	58	1.33E-06	5.36E-05	3.76E-06	1.11E-05
Haloxyfop ethoxyethyl	58.00	176.31		434.76	1.3	3.2	1.64E-08	7.72E-05	2.50E-05	5.47E-06
Hexaconazole	111.00	166.79		401.93	17	21	1.00E-05	3.09E-06	2.21E-05	1.85E-04
Hexazinone	115.00	167.52		408.34	33000	16	2.67E-05	8.97E-05	4.16E-08	2.04E-07
Hexythiazox	108.00	230.58		538.50	0.5	0.1	3.40E-06	5.88E-08	2.32E-04	2.40E-03
Hydramethylnon	185.00	212.75		500.33	0.006	155200	2.70E-06	7.66E-08	8.23E-06	2.23E-01
Hymexazol	86.00	11.88		164.31	85000	23720	<1.33E-01	3.87E+01	6.60E-04	
Imazalil	52.70	151.76	>340	407.11	180	20	1.58E-04	4.13E-04	7.35E-03	2.61E-04
Imazamethabenz-methyl (m)	113.00	217.95		511.46	1370	10	1.50E-06	2.55E-07	1.94E-06	3.16E-07
Imazamethabenz-methyl (p)	113.00	217.95		511.46	857	10	1.50E-06	2.55E-07	1.94E-06	5.05E-07
Imazapyr	169.00	230.52		538.36	11000	4034	<1.30E-05	1.23E-08	7.17E-12	
Imazaquin	219.00	263.64		609.26	90	34	<1.30E-05	4.79E-11	7.00E-13	
Imazaquin ammonium		319.37		728.56	160000	380		1.84E-15	3.36E-21	
Imazethapyr	169.00	241.36		561.56	1400	209	<1.30E-05	3.19E-09	1.05E-11	
Imidacloprid	143.80	156.00		378.84	510	4547	2.00E-07	2.25E-04	1.05E-08	1.00E-07
4-Indol-3-ylbutyric acid	124.00	141.38		386.53	250	784	<1.00E-05	2.43E-04	1.30E-06	
Ioxynil	212.00	134.99		366.01	50	2	<1.00E-03	1.87E-05	2.95E-05	
Ioxynil octanoate	59.00	173.97		450.18	insol	0.01	3.70E-03	3.13E-05	1.86E-02	
Iprodione	134.00	233.57		544.90	13.9	19.6	5.00E-07	2.11E-08	1.05E-08	1.19E-05
Isazofos	liq.	86.12	>120	399.28	69	6	7.45E-03	2.99E-04	1.48E-01	3.39E-02
Isofenphos	oil	59.29		395.75	18	2	4.40E-04	6.74E-04	1.60E-03	8.44E-03
Isopropalin	liq.	152.04		406.57	0.1	0.1	1.17E-03	3.89E-05	4.80E+00	3.62E+00
Isoproturon	158.00	108.78		344.22	65	24	3.30E-06	1.05E-03	1.92E-04	1.05E-05
Isoxaben	176.00	198.17		469.11	1.4	0.9	5.50E-07	5.93E-07	2.08E-08	1.31E-04
Lactofen		177.99		458.69	0.1	0.04	1.07E-06	1.03E-06	5.81E-05	4.94E-03
Lambda-Cyhalothrin	49.20	68.66		436.49	0.005	0.004	2.00E-07	8.52E-05	1.37E+00	1.80E-02
Lenacil	316.00	188.07		447.48	6	0.5	2.00E-07	4.04E-08	5.04E-05	7.81E-06
Lindane (Gamma HCH)	113.00	56.98		304.35	7.3	2.9	5.60E-03	2.80E-02	2.59E+01	2.23E-01
Linuron	94.00	137.23		365.91	75	40	5.10E-05	1.59E-03	1.17E-03	1.69E-04
Malathion	2.85	-23.58	>156	351.17	148	811	1.07E-03	1.65E-02	8.50E-05	2.38E-03
Maleic hydrazide	299.00	131.88		367.60	4507	30770	<1.00E-05	1.91E-07	3.04E-08	
Maleic hydrazide potassium		244.50		568.30	400000	1000000		2.73E-10		
Mancozeb					6		<1.33E-05			
Maneb					6		6.37E-05			
MCPA	120.00	100.97		321.20	734	105	2.30E-05	9.57E-03	1.39E-03	6.29E-06
MCPA octyl ester		120.04		371.04	5	0.05	2.00E-04	6.32E-04	3.23E+00	1.25E-02
MCPA dimethylammonium		195.43		463.25	866000	5844		4.95E-07	2.19E-11	
MCPB	100.00	117.51	>280	346.09	44	86	9.83E-05	4.05E-03	3.47E-04	5.11E-04
MCPB sodium		232.24		542.05	200000	43050		1.83E-09		
Mecoprop (MCPP)	94.00	102.33		326.42	734	230	3.10E-04	1.36E-02	1.84E-03	9.07E-05

Name (ISO)	MP		BP		S		VP		Henry's Law Constant	
	°C	°C	°C	°C	mg/l	EPI	Pa	Pa	Pa m^3/mol	Pa m^3/mol
	exp.	est.	exp.	est.	exp.	est.	exp.	est.	est. (bond)	calculated
Mecoprop dimethylamine		197.59		467.86	660000	2148		3.59E-07	2.91E-11	
Mecoprop-P	95.00	102.33		326.42	860	225	4.00E-04	1.33E-02	1.84E-03	9.98E-05
Mecoprop-P dimethylammonium		197.59		467.86		2148		3.59E-07	2.91E-11	
Mepiquat chloride	223.00	133.82		368.11	1000000	1000000	<1.00E-05	4.95E-05	4.37E-07	
Mepronil	92.00	171.32		429.96	12.7	13.5	5.60E-05	4.41E-05	1.43E-05	1.19E-03
Metalaxyl	72.00	130.49		377.88	8400	1760	7.50E-04	1.37E-03	8.16E-05	2.49E-05
Metaldehyde	246.00	8.00		221.88	230	343		8.98E-02	7.24E-04	
Metam (metham) sodium	dec.	194.10		460.40	963000	1000000	2.67E+03	6.04E-07		3.58E-01
Metamitron	166.60	157.88		382.87	1700	474	2.00E-06	1.00E-04	5.93E-07	2.38E-07
Methabenzthiazuron	120.00	165.20		398.53	59	85	5.90E-06	1.37E-04	6.37E-08	2.21E-05
Methamidophos	46.10	14.56		222.87	1000000	690200	4.70E-03	9.04E+00	8.80E-05	6.63E-07
Methazole	123.00	170.42		420.17	1.5	20	1.33E-04	3.79E-05	2.95E-02	2.31E-02
Methidathion	39.00	84.31		418.78	220	592	4.49E-04	2.88E-04	7.19E-04	6.17E-04
Methiocarb (Mercaptodimethur)	119.00	95.12		324.32	24	47	3.60E-05	8.29E-03	1.16E-04	3.38E-04
Methomyl	78.00	2.65		228.00	57900	21390	6.64E-03	3.41E+00	2.05E-04	1.86E-05
Methoxychlor	89.00	129.34		377.87	0.1	0.5		9.20E-04	9.88E-03	
Methylarsonate, sodium hydrogen	113.00				1400000		1.00E-05			1.16E-09
Methyl Bromide	-93.00	-105.39	4.50	26.06	13400	16980	2.27E+05	9.76E+04		1.61E+03
Methyl isothiocyanate	35.00	-63.26	118.00	90.58	7600	21530	2.13E+03	5.81E+03	3.15E+02	2.05E+01
Metiram	d 140.00				0.1		<1.00E-05			
Metolachlor		136.10		382.78	488	32	4.20E-03	2.20E-04	1.51E-04	2.44E-03
Metoxuron	126.00	129.46		358.82	678	677	4.30E-03	1.07E-03	4.31E-06	1.45E-03
Metribuzin	126.20	150.38		366.80	1220	617	5.80E-05	6.89E-04	1.83E-07	1.02E-05
Metsulfuron-methyl	158.00	241.37		561.64	9500	55	3.30E-10	4.24E-09	7.62E-09	1.32E-11
Mevinphos	21.00	28.06		288.73	600000	164000	1.70E-02	4.72E-01	3.94E-04	6.35E-06
Monocrotophos	54.00	87.72		366.68	1000000	1000000	2.90E-04	3.81E-03	5.52E-08	6.47E-08
Monolinuron	80.00	118.43		347.22	735	424	1.30E-03	5.99E-03	1.58E-03	3.80E-04
Muscalure	liq.	79.05	378.00	372.80	0.3	0.000005	4.70E-03	3.40E-03	5.30E+06	5.05E+00
Naled	27.00	76.37		327.79	2000	5430	2.66E-01	5.64E-02	5.52E-05	5.06E-02
2-(1-Naphthyl)acetamide	184.00	138.50		380.45	100	183.4	<1.00E-05	7.21E-05	8.93E-06	
2-(1-Naphthyl)acetic acid (NAA)	134.00	114.68		351.44	420	750	<1.00E-05	1.31E-03	4.38E-04	
2-(1-Naphthyl)acetate, ethylester	liq.	83.45	175.00	329.17	105	57	2.13E-03	1.51E-02	1.85E-01	4.35E-03
2-(1-Naphthyl)acetate sodium		234.74		547.4	419000	207300		1.24E-09		
Napropamide	75.00	140.02		399.40	74	39	5.30E-04	3.85E-04	3.82E-05	1.94E-03
Naptalam	185.00	227.46		531.82	200	25	<133	1.21E-08	2.43E-10	
Naptalam sodium		319.00		727.78	231000	21930		1.95E-15		
Nitrapyrin	62.50	51.22		244.94	40	52	3.70E-01	2.08E+00	1.61E+00	2.14E+00
Norflurazon	174.00	159.26		387.18	28	44	2.80E-06	6.48E-05	1.27E-05	3.04E-05
Nuarimol	126.00	173.25		173.25	26	44	<2.7E-06	8.20E-07	6.73E-08	
1,4,4a,5a,6,9,9a,9b-Octahydro-dibenzofuran-4a-carbaldehyde	liq.	75.47		294.58		2126		1.15E-01	8.09E-02	
Oryzalin	141.00	208.73	265dec	491.73	2.5	29	<1.33E-06	3.99E-07	1.94E-04	
Oxadiazon	87.00	178.65		431.28	0.7	0.9	<1.00E-04	4.29E-06	3.26E-03	
Oxadixyl	104.00	173.03		437.03	3400	1548	3.33E-06	2.32E-05	4.33E-05	2.73E-07
Oxamyl	101.00	94.99		333.58	282000	128000	3.10E-02	7.81E-03	3.58E-06	2.41E-05
Oxycarboxin	120.00	192.18		456.29	1000	678	5.60E-06	5.23E-06	6.01E-09	1.50E-06
Oxydemeton-methyl	<-20	83.92		353.65	1000000	108400	3.80E-03	3.93E-03	1.64E-08	9.36E-07

Name (ISO)	MP		BP		S		VP		Henry's Law Constant	
	ºC	ºC	ºC	ºC	mg/l	EPI	Pa	Pa	Pa m^3/mol	Pa m^3/mol
	exp.	est.	exp.	est.	exp.	est.	exp.	est.	est. (bond)	calculated
Oxyfluorfen	85.00	156.08	358.00	395.75	0.116	0.33	2.67E-05	3.75E-04	2.38E-02	8.33E-02
Paclobutrazol	165.00	150.11		386.27	26	20	1.00E-06	2.25E-06	3.95E-05	1.13E-05
Paraquat dichloride	300d	108.59		351.92	620000	1000000	<1.00E-04	1.35E-05	3.26E-08	
Parathion ethyl	6.10	89.16		371.59	24	12	8.90E-04	5.37E-03	3.00E-02	1.08E-02
Parathion methyl	35.00	79.69		348.38	60	88	2.00E-04	1.56E-02	1.70E-02	8.77E-04
Pebulate	liq.	70.54		302.57	100	23	4.7	8.45E-02	2.07E+00	9.56E+00
Penconazole	58.00	132.47		360.64	73	3	2.10E-04	4.85E-03	4.55E-01	8.18E-04
Pencycuron	129.50	195.39		469.84	0.3	0.4	5.00E-10	1.89E-06	8.06E-06	5.48E-07
Pendimethalin	54.00	148.09		393.77	0.3	1	4.00E-03	8.48E-04	1.47E-01	3.75E+00
Permethrin	34.00	164.97	>290	437.64	0.006	0.053	4.50E-05	1.08E-04	2.92E-02	2.93E+00
Phenmedipham	143.00	126.18		396.02	4.7	5	1.33E-09	8.85E-05	5.80E-06	8.50E-08
Phorate	<-15	-2.49	>119	319.06	22	19	8.50E-02	9.40E-02	1.60E-01	1.01E+00
Phosalone	45.00	88.99		466.82	3	5	6.13E-05	1.64E-05	3.99E-02	7.52E-03
Phosmet	72.00	90.27		480.00	25	125	6.50E-05	4.02E-03	9.14E-04	8.25E-04
Phosphamidon	liq.	82.61	>162	375.21	1000000	2608	2.20E-03	1.24E-03	1.54E-07	6.59E-07
Phoxim	6.10	25.81		399.30	1.5	10.4	2.10E-03	1.15E-03	7.49E+00	4.18E-01
Picloram	215 dec	153.29		373.03	430	184	8.20E-05	4.71E-05	1.31E-07	4.60E-05
Picloram potassium		244.83		568.99	400000	100000		2.60E-10		
Piperalin	liq.	140.80		384.82	20	4	399	1.75E-04	2.31E-03	6.59E+03
Piperonyl butoxide	liq.	152.74	>180	408.30	insol.	0.6	1.17E-04	3.47E-05	9.01E-06	
Pirimicarb	90.5	112.43		326.21	3060	1223	9.70E-04	1.49E-02	2.65E-04	7.55E-05
Pirimiphos-ethyl	15.00	85.65	>194	396.07	2.3	3.3	6.80E-04	5.95E-04	4.52E-01	9.86E-02
Pirimiphos-methyl	15.00	89.53		372.87	8.6	15.4	2.00E-03	5.01E-03	2.56E-01	7.10E-02
Primisulfuron-methyl	170dec	240.07		558.80	243	17.7	<5.00E-06	3.67E-09	1.41E-07	
Prochloraz	47.00	213.06		501.00	34.4	8.9	1.50E-04	2.17E-06	7.68E-07	1.64E-03
Profenofos	liq.	86.45		401.58	28	0.4	1.24E-04	2.61E-04	3.54E-03	1.65E-03
Prometon	91.00	119.07		324.15	720	73	3.06E-04	1.65E-02	4.38E-04	9.58E-05
Prometryn	119.00	132.03		346.68	33	12	1.69E-04	2.47E-03	9.21E-04	1.24E-03
Propachlor	77.00	85.56		322.84	613	606	3.06E-02	2.47E-02	7.95E-03	1.06E-02
Propamocarb hydrochloride	45.00	181.20		432.79	867000	339400	8.00E-04	1.15E-04	8.55E-13	2.07E-07
Propaquizafop	62.00	227.97		532.91	0.63	1.52	4.40E-10	2.36E-07	2.54E-07	3.10E-07
Propargite	liq.	173.22		441.80	0.5	2.2	6.00E-06	1.05E-04	9.29E-03	4.21E-03
Propazine	213.00	115.70		318.46	8.6	6.2	3.90E-06	9.72E-04	6.02E-04	1.04E-04
Propetamphos	liq.	13.64		329.86	110	114	1.90E-03	5.25E-02	5.95E-03	4.86E-03
Propham (IPC)	87.00	35.98		256.75	250	208	consid.	6.36E-01	3.90E-03	
Propiconazole	liq.	172.86		414.93	110	7	5.60E-05	1.41E-05	1.38E-04	1.74E-04
Propineb	150dec				10		<1.00E-03			
Propoxur	90.00	68.65		289.92	1900	1993	1.30E-03	1.05E-01	3.39E-04	1.43E-04
Propyzamide	155.00	152.87		382.22	15	5	5.80E-05	1.40E-04	1.04E-04	9.90E-04
Prosulfocarb	<-10	117.45	129.00	368.31	13.2	6.9	6.90E-05	6.44E-03	9.48E-02	1.31E-03
Prosulfuron	155dec	230.76		538.88	4000	2	<3.50E-06	1.76E-08	1.81E-05	
Pyrazophos	51.00	87.73		453.92	4.2	16	6.01E-06	3.03E-05	1.23E-07	5.34E-04
Pyrethrins (extract)	liq.	143.07		398.43		0.05	2.93E+02	7.73E-05	6.64E-02	/0!
Pyrethrins I (chrysanthemates)	liq.	142.27		400.80	0.2	0.04	2.67E-03	6.90E-05	7.83E-02	4.38E+00
Pyrethrins II (pyrethrates)	liq.	132.12		421.81	9	0.12	5.33E-03	2.75E-05	7.49E-05	2.21E-01
Pyridate	27.00	220.30		516.49	1.5	0.05	1.30E-07	1.47E-06	1.14E-01	3.28E-05
Pyriproxyfen	46.00	158.63		424.22		0.5	2.90E-04	1.83E-04	6.42E-05	
Quintozene (PCNB)	143.00	118.99	328.00	335.30	0.44	0.16	1.27E-02	2.51E-03	4.81E-01	8.52E+00
Quizalofop-ethyl	92.00	199.71		472.42	0.31	2.34	8.66E-10	4.08E-06	7.50E-06	1.04E-06
Rimsulfuron	176.00	273.19		629.72	7300	491	1.50E-06	4.44E-11	2.19E-11	8.86E-08
Rotenone	163.00	213.16		501.20	15	0.7	<1.00E-03	1.30E-07	1.13E-08	

Name (ISO)	MP		BP		S		VP		Henry's Law Constant	
	°C	°C	°C	°C	mg/l	EPI	Pa	Pa	Pa m^3/mol	Pa m^3/mol
	exp.	est.	exp.	est.	exp.	est.	exp.	est.	est. (bond)	calculated
Sethoxydim	liq.	161.06		440.96	4390	3.3	<1.33E-05	6.07E-08	2.19E-06	
Siduron	133.00	134.43		37.36	18	23	<0.1	3.23E-04	1.08E-04	
Simazine	226.00	112.05		307.45	6.2	26	2.94E-06	1.22E-03	3.41E-04	9.56E-05
Sulfometuron methyl	204.00	233.33		544.14	70	205	7.30E-14	3.51E-09	3.77E-08	3.80E-13
Sulprofos	-15.00	34.08		393.58	0.31	0.85	8.40E-05	1.59E-03	1.62E-01	8.74E-02
2,4,5-T	153.00	128.28		348.68	150	39	7.00E-07	9.36E-04	6.92E-04	1.19E-06
2,4,5-T trihydroxyethyl-ammonium	114	289.56		664.75	500000	1000000		9.25E-16	3.59E-17	
2,3,6-TBA	125.00	108.94		323.63	7700	1165	<3.2E+00	1.87E-02	4.47E-03	
TCA-sodium	165dec	180.76		436.04	1200000	1000000	<1.00E-04	3.47E-06		
Tebuconazole	102.40	162.86		394.85	32	24	1.30E-06	6.15E-06	5.25E-05	1.25E-05
Tebuthiuron	162dec	163.19		394.23	2500	233	2.70E-04	6.00E-05	6.86E-07	2.47E-05
Tefluthrin	44.60	105.70		327.38	0.02	0.04	8.00E-03	3.99E-02	4.69E+01	1.67E+02
Temephos	30.00	85.97		480.00	0.03	0.13		1.05E-05	1.99E-04	
Terbacil	176.00	164.19		396.37	710	140	6.25E-05	3.68E-05	5.09E-05	1.91E-05
Terbufos	-29.20	13.79		332.08	4.5	8.8	3.46E-02	4.67E-02	2.82E-01	2.22E+00
Terbutryn	104.00	139.64		349.08	22	3.5	2.25E-04	8.92E-04	9.21E-04	2.47E-03
Terbutylazine	178.00	123.48		321.23	8.5	9.7	1.50E-04	2.15E-03	6.02E-04	4.05E-03
Tetrachlorvinphos	94.00	85.24		393.27	11	12	5.60E-06	3.47E-04	2.20E-03	1.86E-04
Tetradifon	148.00	173.71		427.63	0.08	0.37	3.20E-08	1.32E-05	7.62E-03	1.42E-04
Thiabendazole	304.00	181.09		443.05	30	3	5.33E-07	7.38E-08	2.03E-06	3.58E-06
Thidiazuron	211.50	175.90		421.44	31	42	4.00E-09	3.51E-06	3.64E-08	2.84E-08
Thifensulfuron methyl	176.00	244.06		567.36	6270	151	1.70E-08	1.88E-09	4.13E-09	1.05E-09
Thiobencarb	3.30	122.33		363.80	28	107	2.2	8.26E-03	3.98E-02	2.03E+01
2-(Thiocyanomethylthio)-benzothiazol (TCMTB)	12.00	155.22		404.85	45	143	3.12E-04	8.45E-04	6.58E-07	1.65E-03
Thiodicarb	173.00	36.24		403.54	35	137	5.70E-03	2.67E-05	9.91E-06	5.77E-02
Thiofanox	57.00	41.51		279.73	5200	955	2.26E-02	3.83E-01	6.36E-04	9.49E-04
Thiometon	liq.	-12.19		305.14	200	87	2.30E-02	1.97E-01	1.21E-01	2.83E-02
Thiophanate-methyl	172d			185.26	24.6	286	9.50E-06	1.32E-06	2.98E-08	1.32E-04
Thiram	155.00	107.25		339.43	18	2118	2.30E-03	1.47E-03	2.72E+00	3.07E-02
Tolclofos-methyl	79.00	32.77		341.59	1.1	2.2	5.70E-02	8.52E-03	2.61E+00	1.56E+01
Tolylfluanid	96.00	150.76		397.33	0.9	5.6	1.60E-05	2.64E-04	7.54E-02	6.17E-03
Camphechlor (Toxaphene)	65.00	14.48		382.58	3	0.013	5.33E-04	1.24E-03	4.41E+00	7.35E-02
Tralomethrin	138.00	215.54		547.16	0.001	0.00006	1.70E-11	1.67E-08	3.66E-05	1.11E-05
Triadimefon	82.30	148.64		376.67	72	113	2.00E-05	1.15E-03	1.18E-04	8.16E-05
Triadimenol	138.00	152.51		386.72	62	73	2.00E-07	4.73E-06	1.60E-06	9.54E-07
Triallate	29.00	95.64		342.74	4	6	1.60E-02	2.41E-02	5.73E-01	1.22E+00
Triasulfuron	178.00	249.31		578.60	815	19	1.00E-10	9.12E-10	3.27E-08	4.93E-11
Triazamate	53.00	174.89		419.27	488	1984	1.60E-04	2.03E-04	1.80E-08	1.03E-04
Tribenuron methyl	141.00	246.31		572.17	1500	34	5.20E-08	3.51E-09	1.56E-07	1.37E-08
S,S.S-tributyl phosphorotrithioate (Tribufos)	<-25	85.01		391.67	2.3	0.5	3.50E-04	1.76E-03	5.35E-02	4.79E-02
Trichlorfon	78.50	66.10		292.62	120000	54640	2.10E-04	8.93E-03	2.69E-07	4.51E-07
Triclopyr	150.50	135.20		354.11	8100	232	2.00E-04	7.41E-04	5.21E-04	6.33E-06
Triclopyr-butotyl		146.81		391.13	23	2.1	1.68E-04	1.06E-04	6.06E-03	2.61E-03
Triclopyr-triethylammonium		231.20		539.82	2100000	1248		2.13E-09	5.52E-10	
Tridemorph	liq.	105.80		352.92	11.7	0.5	6.40E-03	2.43E-03	1.34E+00	1.63E-01
Tridiphane		106.56		323.14	1.8	0.4	2.93E-02	1.20E-02	4.15E-02	5.22E+00
Trifluralin	49.00	139.97		382.17	0.221	0.658	9.50E-03	1.80E-03	2.15E+01	1.44E+01
Triflusulfuron methyl	160.00	259.09		599.53	110	0.6	<1.00E-05	4.17E-10	1.27E-09	
Triforine	155.00	222.90		522.06	30	776	2.70E-05	4.73E-08	1.20E-10	3.91E-04
Trimethacarb	105.00	67.59		283.05	58	121	6.80E-03	1.05E-01	4.38E-03	2.27E-02
Trinexapac ethyl	36.00	147.05	>270	402.34	21100	39420	2.16E-03	1.68E-05	7.33E-10	2.58E-05
Vernolate	liq.	70.54	>150	302.57	108	22	1.39	8.45E-02	2.07E+00	2.62E+00

Name (ISO)	MP		BP		S		VP		Henry's Law Constant	
	ºC	ºC	ºC	ºC	mg/l	EPI	Pa	Pa	Pa m^3/mol	Pa m^3/mol
	exp.	est.	exp.	est.	exp.	est.	exp.	est.	est. (bond)	calculated
Vinclozolin	108.00	187.73		446.77	3.4	32	1.60E-05	1.21E-05	2.39E-01	1.35E-03
Zineb	157dec	209.21		492.75	10	107700	<1.00E-05	2.49E-07		
Ziram	246.00	151.88		401.87	0.03	12550	<1.00E-06	4.00E-06		
Total number	368	396	61	397	400	396	369	400	373	316

Table 3
Kow, log Kow, adsorption coefficient (Kd and Koc ranges and the log Koc used in the report) and Koc estimated by Lyman, TGD (non-hydrophobis and hydrophobics) and this study (OCH).

Kow, log Kow, adsorption koefficienter (kd og Koc variationsbredder samt log Koc anvendt i rapporten) samt log Koc estimeret efter QSARs opstillet af Lyman, TGD og denne rapport (OCH).

Name (ISO)	Kow			Adsorption Coefficient								
		log Kow	log Kow	Kd	Koc	Koc used	log Koc	EPI	Lyman	TGD, nhf	TGD, hf	OCH
	exp.	exp.	est.	exp.	exp. range	exp.	exp.	est	est.	est.	est	est.
Acephate	0.13	-0.89	-0.90			2	0.30	1.34	0.89	-0.62	0.34	1.82
Acetochlor	1082	3.03	3.37					2.25	3.03	2.55	2.81	2.58
Acifluorfen	5012	3.70	4.17					3.46	3.39	3.10	3.23	2.88
Acifluorfen sodium	15	1.19	0.37		44-684	113	2.05	3.50	2.02	1.06	1.65	2.02
Aclonifen	11000	4.04	3.88		5318-12164	8741	3.94	3.14	3.57	3.37	3.45	3.05
Acrinathrin	180000	5.26	6.73	2460-2780	127500-319610	223555	5.35	6.02	4.24	4.36	4.21	3.77
Acrolein	12.1	1.08	0.19	0.003-0.28	51-270	160	2.20	0.44	1.96	0.97	1.58	1.99
Alachlor	1230	3.09	3.37	5.1-8.6	68-190	190	2.28	2.27	3.06	2.60	2.85	2.61
Alanycarb	2700	3.43	3.16					3.65	3.24	2.88	3.06	2.76
Aldicarb	37	1.57	1.36		1.3-4.2, 8-30	20	1.30	1.52	2.23	1.37	1.89	2.10
Aldoxycarb	0.27	-0.57	-0.67			10	1.00	1.00	1.07	-0.36	0.54	1.82
Allethrin	91200	4.96	5.52			3100	3.49	3.49	4.08	4.12	4.02	3.58
Alloxydim sodium	0.63	-0.20	-0.29		0-4.6	2.3	0.36	2.29	1.27	-0.06	0.77	1.83
Ametryn	955	2.98	3.32		300	300	2.48	2.65	3.00	2.51	2.78	2.56
Amidosulfuron	43	1.63	-1.29					1.00	2.26	1.42	1.93	2.12
Amitraz	310000	5.50	5.55		1000-2000	1500	3.18	5.81	4.37	4.56	4.37	3.93
Amitrole	0.14	-0.86	-0.47			100	2.00	1.39	0.91	-0.60	0.36	1.82
Ancymidol	80.6	1.91	1.99			120	2.08	2.41	2.42	1.65	2.10	2.19
Anilazine	1050	3.88	3.64	9.2-37.9	1600-3000	2187	3.34	3.16	3.49	3.24	3.34	2.97
Asulam	1.01	0.004	0.05		18.3-115.3	52	1.72	1.62	1.38	0.10	0.90	1.85
Asulam sodium			-4.05			40	1.60	1.00	-0.83	-3.18	-1.65	2.44
Atrazine	384	2.61	2.82	0.4-2.3	55-135	113	2.05	2.36	2.80	2.21	2.54	2.42
Azaconazole	209	2.32	2.73					2.98	2.64	1.98	2.36	2.32
Azamethiphos	11	1.05	1					1.00	1.95	0.95	1.56	1.99
Azinphos-ethyl	1514	3.18	3.51		467-3155	1486	3.17	2.38	3.11	2.68	2.90	2.65
Azinphos-methyl	360	2.56	2.53	4.0-12.6	500-2000	882	2.95	1.84	2.77	2.17	2.51	2.40
Benalaxyl	2500	3.40	3.69		2728-7173	4951	3.69	3.69	3.23	2.85	3.04	2.74
Benazolin	22	1.34	2.08	0.4, 1.0	29, 36	33	1.52	1.00	2.11	1.19	1.74	2.05
Benazolin ethyl	315.3	2.50	2.86	8, 15	438, 726	582	2.76	1.00	2.74	2.13	2.48	2.38
Bendiocarb	52	1.72	2.55		28-40	34	1.53	1.21	2.31	1.49	1.98	2.14
Benfluralin	195000	5.29	5.31	27-117		9000	3.95	3.99	4.25	4.38	4.23	3.79
Benfuracarb	20000	4.30	4.06					3.28	3.72	3.58	3.61	3.19
Benfuresate	257	2.41	2.8		140-259	214	2.33	3.27	2.69	2.05	2.42	2.35
Benomyl	131	2.12	2.44	6.1-90	950-3620	1883	3.27	3.96	2.53	1.82	2.24	2.26
Bensulfuron methyl	63	1.80	1.41			370	2.57	1.52	2.36	1.56	2.03	2.16
Bensulide	15849	4.20	4.12			1000	3.00	4.00	3.66	3.50	3.55	3.14
Bensultap	2300	3.36	3.21		510-1700	1120	3.05	4.95	3.20	2.82	3.02	2.73
Bentazone	0.35	-0.46	1.67	0.4-3.1	13.3-175	48	1.68	1.57	1.13	-0.27	0.61	1.82
Bentazone sodium			0.61			34	1.53	1.57	1.71	0.59	1.28	1.91
Bifenox	30000	4.48	4.15	50-300	500-23000	11750	4.07	3.58	3.81	3.73	3.72	3.29
Bifenthrin	>1.0E+6	>6	8.15	990-5400	1.3-3.0E+5	200000	5.30	6.51	5.81	6.70	6.03	6.12
Bioallethrin	48000	4.68	5.52					3.49	3.92	3.89	3.85	3.41
Bioresmethrin	>50000	>4.7	7.11					5.63	5.24	5.86	5.38	5.17
Bitertanol	10641	4.03	4.07	19.6-40	1782-2238	2040	3.31	4.81	3.57	3.36	3.44	3.05
Brodifacoum	3.2E+08	8.50	8.51	358-1265	18000-51000	34300	4.54	6.88	6.00	6.99	6.26	6.47

Name (ISO)	Kow			Adsorption Coefficient								
		log Kow	log Kow	Kd	Koc	Koc used	log Koc	EPI	Lyman	TGD, nhf	TGD, hf	OCH
	exp.	exp.	est.	exp.	exp. range	exp.	exp.	est	est.	est.	est	est.
Bromacil	74.5	1.87	1.68			32	1.51	2.02	2.39	1.61	2.08	2.18
Bromacil lithium			0.35			32	1.51	2.09	1.57	0.38	1.12	1.88
Bromadiolone	19000	4.28	7.02					5.32	3.71	3.57	3.60	3.18
Bromethalin	6.3E+06	6.80	7.68					5.02	5.08	5.61	5.18	4.91
Bromofenoxim	1494	3.17	3.55		1100	568	2.75	5.36	3.10	2.67	2.90	2.64
Bromoxynil	794	2.90	3.39	1.4-12.5	108-328	210	2.32	2.64	2.95	2.45	2.73	2.53
Bromoxynil octanoate	2.5E+05	5.40	5.86	7	630, 1093	862	2.94	3.69	4.31	4.47	4.30	3.86
Bromoxynil butyrate			3.90			1079	3.03	2.62	3.50	3.26	3.36	2.98
Bromoxynil potassium			0.15					2.64	1.46	0.22	0.99	1.86
Bromuconazole	1738	3.24	3.54	4.5-38	474-1539	871	2.94	4.46	3.14	2.72	2.94	2.67
Bronopol	1.5	0.18	-0.64					0.00	1.47	0.25	1.01	1.86
Butylate	14125	4.15	3.85			400	2.60	2.79	3.63	3.46	3.51	3.11
Captafol	324	2.51	2.52					3.44	2.74	2.13	2.48	2.39
Captan	610	2.35	1.84	3.0-8.0	100-567	310	2.49	2.94	2.66	2.00	2.38	2.33
Carbaryl	229	2.36	2.35		230-390	330	2.52	2.38	2.66	2.01	2.39	2.33
Carbendazim	33	1.52	1.55	1.6-6.3	200-250	225	2.35	2.25	2.20	1.33	1.86	2.09
Carbetamide	0.026	-1.59	1.63		60-120	59	1.77	2.21	0.51	-1.19	-0.10	1.87
Carbofuran	47	1.67	2.30		14-160	29.4	1.47	1.85	2.29	1.45	1.95	2.13
Carbosulfan	1995	3.30	5.57					4.18	3.17	2.77	2.98	2.70
Carboxin	138	2.14	1.49		260, 373	317	2.50	1.90	2.54	1.83	2.25	2.26
Chinomethionate	6020	3.78	3.37		45-90	38	1.58	2.30	3.43	3.16	3.28	2.92
Chloramben			1.90					1.03	2.41	1.46	2.10	2.19
Chloramben sodium			-1.50			15	1.18	1.03	0.56	-1.12	-0.05	1.86
Chlordimeform hydrochloride	776	2.89	2.89			10000	4.00	3.49	2.95	2.44	2.72	2.53
Chlorfenac sodium (Fenac)			-0.08			20	1.30	2.07	1.33	0.04	0.85	1.84
Chlorfenvinphos	9001	3.95	4.15		313, 930	620	2.79	2.77	3.53	3.30	3.39	3.01
Chloridazon (Pyridazon)	15.6	1.19	0.76	0.3-2.5	52-94, 89-340	67	1.83	2.74	2.02	1.06	1.65	2.02
Chlorimuron ethyl	2.3	0.36	2.29			110	2.04	1.89	1.57	0.39	1.13	1.88
Chlormequat chloride	0.022	-1.66	-3.44	2.4	203	203	2.31	1.89	0.47	-1.24	-0.15	1.87
Chlorobenzilate	54954	4.74	3.99			2000	3.30	3.10	3.96	3.94	3.89	3.45
Chloroneb			3.44			1650	3.22	2.36	3.25	2.89	3.07	2.76
Chloropicrin	123	2.09	1.32			62	1.79	1.56	2.51	1.79	2.22	2.25
Chlorothalonil	776	2.89	3.66	0.3-29	1600-14000	2578	3.41	3.38	2.95	2.44	2.72	2.53
Chloroxuron	1585	3.20	4.08		1015-2600	1806	3.26	3.11	3.12	2.69	2.92	2.66
Chlorpropham	2250	3.35	3.30		203-662	432	2.64	2.32	3.20	2.81	3.01	2.72
Chlorpyrifos	50000	4.70	4.66	50-260	3680-14400	10323	4.01	3.83	3.93	3.91	3.86	3.42
Chlorpyrifos methyl	17300	4.24	3.68					3.30	3.68	3.53	3.57	3.16
Chlorsulfuron	1.26	2.00	2.26		40	40	1.60	2.38	2.47	1.72	2.16	2.22
Chlorthal dimethyl (DCPA)	19000	4.28	4.24			5000	3.70	2.45	3.71	3.57	3.60	3.18
Clethodim	1.5E+04	4.19	4.21	0.05-0.23	33	33	1.52	3.72	3.66	3.49	3.54	3.13
Clofentezine	1259	3.10	2.70		100-2070	240	2.38	5.81	3.06	2.61	2.85	2.61
Clomazone	316	2.50	2.86			300	2.48	3.68	2.74	2.13	2.48	2.38
Cloprop (3-CPA)			2.39			20	1.30	1.47	2.68	2.04	2.41	2.34
Cloprop ammonium			1.63					2.41	2.26	1.42	1.93	2.13
Cloprop sodium			-1.42			20	1.30	1.47	0.60	-1.05	0.01	1.85
Clopyralide	36	1.56	1.63	0.01-0.38	0.4-12.9	4.6	0.66	1.59	2.22	1.36	1.88	2.10
Clopyralid-olamine			-1.98			6	0.78	1.58	0.30	-1.50	-0.35	1.91
Coumatetralyl	2884	3.46	4.23					3.51	3.26	2.90	3.08	2.77
Cyanazine	126	2.10	2.51	0.5-6.8	32-418	180	2.26	2.09	2.52	1.80	2.22	2.25
Cyanophos	447	2.65	2.48					2.43	2.82	2.25	2.57	2.44
Cycloate	7586	3.88	3.81		11, 430	221	2.34	2.26	3.49	3.24	3.34	2.97
Cycloxidim	23	1.36	3.88		<10-183	95	1.98	3.53	2.12	1.20	1.76	2.05

Name (ISO)	Kow			Adsorption Coefficient								
		log Kow	log Kow	Kd	Koc	Koc used	log Koc	EPI	Lyman	TGD, nhf	TGD, hf	OCH
	exp.	exp.	est.	exp.	exp. range	exp.	exp.	est	est.	est.	est	est.
Cyfluthrin	891251	5.95	5.74			58185	4.76	5.25	4.61	4.92	4.65	4.25
Cyhalothrin	6309573	6.80	6.85					5.68	5.08	5.61	5.18	4.91
Cypermethrin	3891000	6.60	6.38	2000	160000	160000	5.20	5.03	4.97	5.45	5.06	4.75
alpha-Cypermethrin	8700000	6.94	6.38			76344	4.88	5.03	5.15	5.72	5.27	5.03
Cyproconazole	819	2.91	3.25	4.1, 16	307, 707	507	2.71	4.21	2.96	2.46	2.73	2.54
Cyromazine	0.86	0.08	0.96	0.5-50.4	40-1784	425	2.63	1.32	1.42	0.16	0.95	1.85
2,4-D	646	2.58	2.62		3.1-63	16.5	1.22	1.47	2.78	2.19	2.53	2.41
2,4-D-dimethylammonium	4	0.65	0.84	0.13-0.3	72-136	104	2.02	2.51	1.73	0.63	1.31	1.92
2,4-D methylester			2.9			100	2.00	2.20	2.95	2.45	2.73	2.53
Dalapon sodium	6.92	0.84	-2.13			0.3	-0.52	0.44	1.83	0.78	1.43	1.95
Daminozide	0.032	-1.49	-1.51	0.1-0.6	18-46	24.1	1.38	1.00	0.57	-1.11	-0.04	1.86
Dazomet	25	1.40	0.94					1.14	2.14	1.23	1.78	2.06
2,4-DB	3388	3.53	3.6					2.00	3.30	2.96	3.12	2.80
2,4-DB butoxyethyl			5.08			20	1.30	3.06	4.14	4.21	4.10	3.66
Deltamethrin	39811	4.60	6.18	1800-6000	0.71-3.14E+06	1413000	6.15	5.03	3.88	3.83	3.80	3.36
Desmedipham	2459	3.39	3.22	100-160	1500-10000	2934	3.47	2.49	3.22	2.85	3.04	2.74
Desmetryn	240	2.38	2.82		150	150	2.18	2.38	2.67	2.03	2.40	2.34
Diazinon	5454	3.74	3.86	3.7-114	440-850	616	2.79	3.13	3.41	3.13	3.26	2.90
Dicamba	0.16	2.21	2.14	0-0.11	0-1	0.5	-0.30	1.46	2.58	1.89	2.29	2.29
Dicamba sodium			-0.9			2	0.30	1.46	0.89	-0.63	0.33	1.82
Dichlobenil	550	2.74	2.83	0.6-60	95-680	180	2.26	2.43	2.87	2.32	2.63	2.47
Dichlofluanid	5000	3.70	2.72		7-30	18	1.26	3.03	3.39	3.10	3.23	2.88
1,3-Dichloropropene	115	2.06	2.29		32	32	1.51	1.91	2.50	1.77	2.20	2.24
Dichlorprop (2,4-DP)	59.1	1.77	3.03		12.0-40	26	1.41	1.69	2.34	1.53	2.02	2.16
Dichlorprop butoxyethyl			4.52		1000	1000	3.00	2.75	3.84	3.76	3.75	3.32
Dichlorprop-P	2700	3.43	3.03			58	1.76	1.69	3.24	2.88	3.06	2.76
Dichlorvos	35.5	1.16	0.6					1.60	2.01	1.04	1.63	2.01
Dicloran (DCNA)	63	1.80	2.76		760-1062	911	2.96	2.15	2.36	1.56	2.03	2.16
Dicofol	105000	5.02	5.81	8.4-82.8	5900-8380	7100	3.85	4.02	4.11	4.17	4.06	3.62
Dicrotophos	0.32	-0.49	-1.10			75	1.88	2.56	1.11	-0.30	0.59	1.82
Dienochlor	>7000	>3.84	8.39		196-384	283	2.45	5.42	5.94	6.90	6.19	6.36
Diethatyl-ethyl	3970	3.60	3.62		100-240	170	2.23	2.96	3.34	3.02	3.17	2.84
Difenacoum			7.62					6.67	5.52	6.27	5.70	5.62
Difenoconazole	15849	4.20	5.2	2.1-97.7	400-7734	3760	3.58	4.38	3.66	3.50	3.55	3.14
Difenoxuron	348	2.54	3.52		165-233	199	2.30	2.75	2.76	2.16	2.50	2.40
Difenzoquat methylsulfate	0.07	-1.15	-0.06	1.2-685	1350-23600	13700	4.14	5.54	0.75	-0.83	0.18	1.83
Difethialone	148000	5.17	9.82			2.7 E+09	9.43	6.99	4.19	4.29	4.16	3.71
Diflubenzuron	7586	3.88	3.59	38-3400	2800-18908	3043	3.48	3.03	3.49	3.24	3.34	2.97
Diflufenican	80000	4.90	3.53	10.0-50	1600-2400	2000	3.30	5.04	4.04	4.07	3.99	3.54
Dimethachlor	148	2.17	2.33					1.96	2.56	1.86	2.27	2.27
Dimethipin	0.67	-0.17	-1.79	0.04-13.6	3.3-26.6	12	1.08	1.44	1.28	-0.04	0.79	1.84
Dimethoate	5.06	0.70	0.28		16.2-51.9	27	1.43	1.39	1.76	0.67	1.34	1.93
Dinocap	34400	4.54	5.98			550	2.74	4.65	3.85	3.78	3.76	3.33
Dinoseb	3631	3.56	3.67			500	2.70	3.55	3.31	2.98	3.14	2.82
Dinoseb-olamin			0.30			63	1.80	2.99	1.54	0.34	1.09	1.88
Dinoseb acetic acid	5248	3.72	3.17					2.98	3.40	3.11	3.24	2.89
Dinoterb	3236	3.51	3.64		30-53	42	1.62	3.42	3.29	2.94	3.11	2.79
Diphenamid			2.86			210	2.32	4.19	2.93	2.42	2.70	2.52
Dipropetryn	6460	3.81	4.22			900	2.95	3.10	3.45	3.19	3.30	2.94
Diquat dibromide	2.5E-05	-4.60	-2.82	3387	3241-17800	10000	4.00	3.29	-1.13	-3.63	-2.00	2.66
Disulfoton	8913	3.95	3.86			600	2.78	2.91	3.53	3.30	3.39	3.01

Name (ISO)	Kow			Adsorption Coefficient								
		log Kow	log Kow	Kd	Koc	Koc used	log Koc	EPI	Lyman	TGD, nhf	TGD, hf	OCH
	exp.	exp.	est.	exp.	exp. range	exp.	exp.	est	est.	est.	est	est.
Dithianon	1585	3.20	2.98	18-56	1000-4000	2500	3.40	2.55	3.12	2.69	2.92	2.66
Diuron	480	2.68	2.67	2.4-14.3	400	400	2.60	2.13	2.83	2.27	2.59	2.45
DNOC	245	2.39	2.27		53-193	123	2.09	2.78	2.68	2.04	2.41	2.34
Dodine			-0.88			100000	5.00	4.19	0.90	-0.61	0.35	1.82
Endosulfan	55000	3.83	3.84	29-72	2800-3600	3200	3.51	4.34	3.46	3.20	3.31	2.95
Endothal	82	1.91	1.89					1.00	2.42	1.65	2.10	2.19
Endothal sodium			0.23					1.00	1.50	0.29	1.04	1.87
EPTC	1893	3.20	3.02	0.8-3	140-260	172	2.24	2.41	3.12	2.69	2.92	2.66
Esfenvalerate	1659587	6.22	6.76	4.4-71	600-	2792	3.45	5.65	4.76	5.14	4.82	4.45
Ethalfluralin	130000	5.11	5.23	12.0-97	4000-8000	6000	3.78	3.91	4.16	4.24	4.12	3.67
Ethametsulfuron-methyl	7.8	0.89	2.43	0.4-4.1	66-150	107	2.03	2.27	1.86	0.82	1.46	1.96
Ethephon	0.603	-2.20	0.05	2.4-57	608-3220	2540	3.40	0.55	0.18	-1.68	-0.49	1.95
Ethiofencarb	110	2.04	2.04	0.4-1.6	41-64	52	1.72	2.37	2.49	1.75	2.19	2.23
Ethion	120000	5.07	4.75		6451-15435	10958	4.04	4.12	4.14	4.21	4.09	3.65
Ethirimol	200	2.30	3.40	1.5-72	97-950	402	2.60	2.58	2.63	1.96	2.35	2.31
Ethofumesate	501	2.70	2.89	1.0-9.8	97-209	146	2.16	2.46	2.85	2.29	2.60	2.45
Ethoprophos	3890	3.59	3.14	1.08-3.78	60-150	105	2.02	2.21	3.33	3.01	3.16	2.83
Etridiazole	2340	3.37	3.60	5.31, 1.41		240	2.38	1.96	3.21	2.83	3.02	2.73
Etrimfos	2000	3.30	2.94	0.6-13	7-127	29	1.46	2.31	3.17	2.77	2.98	2.70
Fenamiphos	2000	3.30	3.29		70-550	295	2.47	2.35	3.17	2.77	2.98	2.70
Fenarimol	4900	3.69	3.62	1.5-11.9	500-1030	739	2.87	3.79	3.38	3.09	3.22	2.88
Fenbuconazole	1700	3.23	4.23		2100-9000	5550	3.74	6.13	3.13	2.72	2.93	2.67
Fenbutatin oxide	158489	5.20				2300	3.36		4.21	4.31	4.18	3.73
Fenitrothion	2692	3.43	3.3	5.0-18	252-593	479	2.68	2.94	3.24	2.88	3.06	2.76
Fenoxaprop			4.17	1.0-4.3	109-188	143	2.16	3.44	3.65	3.48	3.53	3.12
Fenoxaprop-ethyl	13200	4.12	4.95	57-149	5600-16800	11200	4.05	4.43	3.62	3.44	3.50	3.10
Fenoxaprop-P-ethyl	19000	4.28	4.95	57-149	5600-16800	11200	4.05	4.43	3.71	3.57	3.60	3.18
Fenoxycarb	20000	4.30	4.24			1000	3.00	3.92	3.72	3.58	3.61	3.19
Fenpiclonil	7200	3.86	3.48	18-94	1750-3300	2496	3.40	3.75	3.48	3.23	3.33	2.96
Fenpropathrin	500000	5.70	5.62		764-4700	1062	3.03	4.47	4.48	4.72	4.49	4.07
Fenpropidin	388	2.59	6.42	20-120	2100-5300	3302	3.52	5.28	2.79	2.20	2.53	2.41
Fenpropimorph	12589	4.10	5.50		862-4500	2988	3.48	4.43	3.61	3.42	3.48	3.09
Fenthion	12300	4.09	4.08			1500	3.18	3.37	3.60	3.41	3.48	3.08
Fentin acetate	2700	3.43			1700-4000	2240	3.35		3.24	2.88	3.06	2.76
Fentin hydroxide	2700	3.43			580-1334	754	2.88		3.24	2.88	3.06	2.76
Fenvalerate	103000	5.01	6.76	4.4-105	1040-12040	5350	3.73	5.65	4.10	4.16	4.06	3.61
Ferbam	6.3	0.80				300	2.48		1.81	0.75	1.40	1.94
Flamprop methyl	1000	3.00	3.33					3.04	3.01	2.53	2.79	2.57
Flamprop-M isopropyl	4893	3.69	4.24			216	2.33	3.49	3.38	3.09	3.22	2.88
Flocoumafen	50119	4.70	8.61					7.40	3.93	3.91	3.86	3.42
Fluazifob	1500	3.18	3.58	0.14-0.26	8.3-51.1	20.4	1.31	3.30	3.11	2.68	2.90	2.65
Fluazifop-butyl	31623	4.50	5.34	71.2	5836	5836	3.77	4.83	3.83	3.75	3.74	3.31
Fluazifop-P-butyl	31623	4.50	5.34			5700	3.76	4.83	3.83	3.75	3.74	3.31
Flucythrinate	120	2.08	6.56			100000	5.00	5.74	2.51	1.78	2.21	2.24
Flumetralin	281838	5.45	6.09			10000	4.00	5.23	4.34	4.51	4.33	3.90
Fluometuron	171	2.23	2.35		31-117	74	1.87	2.56	2.59	1.91	2.30	2.29
Flurenol-butyl	302	2.48	3.69	1.6-5	106-1700	903	2.96	3.21	2.73	2.11	2.46	2.38
Fluridone	1450	3.16	3.7	3.0-16	350-1100	725	2.86	5.04	3.10	2.66	2.89	2.64
Fluroxypyr	55	1.74	1.17		<43	18	1.26	1.14	2.32	1.51	2.00	2.15
Fluroxypyr-meptyl	6140	4.53	4.82	175-288	4310-16550	10430	4.02	3.67	3.84	3.77	3.75	3.32
Flurprimidol	933	3.34	3.07	1.7-8.7	140-238	184	2.26	2.94	3.19	2.81	3.00	2.72
Flusilazole	5550	3.74	4.89	12.0-76	990-2044	1555	3.19	6.25	3.41	3.13	3.26	2.90
tau-Fluvalinate	18197	4.26	6.81	2246-4607	1.3e5-1.6e6	537000	5.73	5.86	3.69	3.55	3.58	3.17
Folpet	1279	3.11	2.84	0.1-0.2	7.4-21.9	14.65	1.17	2.16	3.07	2.62	2.86	2.62
Fomesafen	800	2.90	3.41					4.04	2.95	2.45	2.73	2.53

Name (ISO)	Kow			Adsorption Coefficient								
		log Kow	log Kow	Kd	Koc	Koc used	log Koc	EPI	Lyman	TGD, nhf	TGD, hf	OCH
	exp.	exp.	est.	exp.	exp. range	exp.	exp.	est	est.	est.	est	est.
Fomesafen sodium			2.35			60	1.78	4.04	2.66	2.00	2.38	2.33
Fonofos	8700	3.94	4.02	15.3	870	870	2.94	2.92	3.52	3.29	3.38	3.00
Formetanate hydrochloride	<0.002	<-2.70	0.74	1.49-3.0	140-620	380	2.58	2.37	1.78	0.70	1.37	1.93
Formothion	0.28	-0.56	-0.48		4->21	21	1.32	1.00	1.07	-0.36	0.54	1.82
Fosamine ammonium			-4.54			150	2.18	1.35	-1.09	-3.58	-1.96	2.63
Fosetyl-aluminium	0.002	-2.70		1-6.5	81-311	190	2.28		-0.09	-2.09	-0.80	2.04
Fuberidazole	468	2.67	2.37	6.2-16.9	574-745	688	2.84	3.35	2.83	2.26	2.58	2.44
Furathiocarb	39800	4.60	4.43	3.0-110	450-708	577	2.76	3.21	3.88	3.83	3.80	3.36
Glufosinate ammonium	<1.25	<0.1	-4.81					1.78	-1.24	-3.80	-2.13	2.75
Glyphosate	0.0009	-3.05	-4.47	18-377		197	2.29	1.27	-0.28	-2.37	-1.02	2.13
Glyphosate isopropylammonium			-3.87			240	2.38	2.28	-0.73	-3.03	-1.54	2.38
Glyphosate trimesium	0.0001	-4.00		9.0-21.2	820-1090	394	2.60		-0.80	-3.14	-1.62	2.42
Guazatine	1.6E-05	-4.80	2.71			25283	4.40	6.08	-1.23	-3.79	-2.12	2.75
Guazatine acetates	0.14	-0.85		85-2405	3646-46250	14150	4.15		0.91	-0.59	0.36	1.82
Haloxyfop	22	1.34	3.38		32-77			3.52	2.11	1.19	1.74	2.05
Haloxyfop ethoxyethyl	21400	4.33	3.88		87-128	108	2.03	4.05	3.73	3.61	3.63	3.21
Hexaconazole	7943	3.90	3.66		420-1660	1040	3.02	4.18	3.50	3.26	3.36	2.98
Hexazinone	11.3	1.05	3.40	0.2-10.8	24.7-2327	37	1.57	2.79	1.95	0.95	1.56	1.99
Hexythiazox	340	2.53	5.57	33, 93	3300, 6200	4407	3.64	3.61	2.75	2.15	2.49	2.39
Hydramethylnon	206	2.31	8.51			730000	5.86	8.80	2.63	1.97	2.36	2.32
Hymexazol	2.9	0.46	1.03					2.37	1.63	0.47	1.19	1.89
Imazalil	6607	3.82	4.10	38-209	2080-8170	2080	3.32	3.29	3.46	3.19	3.31	2.94
Imazamethabenz-methyl (m)	66	1.82	3.6	0.32-10.5	86-145	115.5	2.06	3.59	2.37	1.57	2.05	2.17
Imazamethabenz-methyl (p)	35	1.54	3.6	0.18-8.5		100	2.00	3.59	2.21	1.35	1.87	2.10
Imazapyr	20	1.30	1.57			100	2.00	2.65	2.08	1.15	1.72	2.04
Imazaquin	2.2	0.34	2.9					3.69	1.56	0.38	1.11	1.88
Imazaquin ammonium			0.04			20	1.30	4.53	1.40	0.13	0.93	1.85
Imazethapyr	31	1.49	2.6			10	1.00	3.14	2.19	1.31	1.84	2.08
Imidacloprid	3.7	0.57	0.56		180-317	248	2.39	3.70	1.69	0.56	1.26	1.91
4-Indol-3-ylbutyric acid	200	2.30	2.84					2.74	2.63	1.96	2.35	2.31
Ioxynil	3236	3.51	3.94	3.5-182	250-1046	438	2.64	3.94	3.29	2.94	3.11	2.79
Ioxynil octanoate	1320000	6.12	6.42		235-1420	568	2.75	3.69	4.71	5.06	4.76	4.38
Iprodione	1259	3.10	2.85	1.5-11.7	373-1551	525	2.72	2.15	3.06	2.61	2.85	2.61
Isazofos	6600	3.82	4.08		100	100	2.00	2.87	3.46	3.19	3.31	2.94
Isofenphos	13200	4.12	4.65	5.8-10.1	600-1345	882	2.95	3.39	3.62	3.44	3.50	3.10
Isopropalin			5.8		10000	10000	4.00	3.83	4.53	4.80	4.55	4.14
Isoproturon	740	2.87	2.84	0.8-4.2	46-108	53	1.72	2.40	2.94	2.42	2.71	2.52
Isoxaben	436	2.64	3.98	6.4-13	700-1300	648	2.81	3.47	2.81	2.24	2.56	2.43
Lactofen	64560	4.81	4.92			10000	4.00	4.41	3.99	4.00	3.93	3.49
Lambda-Cyhalothrin	1.0E+7	7.00	6.85		1.3e+6-0.6e+6	310000	5.49	6.68	5.19	5.77	5.31	5.08
Lenacil	203	2.31	3.09	0.35-2.8	75-254	165	2.22	2.27	2.63	1.97	2.36	2.32
Lindane (Gamma HCH)	5107	3.71	4.26		870-1670	819	2.91	3.53	3.40	3.11	3.24	2.89
Linuron	1010	3.00	2.91		500-600	343	2.54	2.54	3.01	2.53	2.79	2.57
Malathion	560	2.75	2.29	0.8-2.5	151-308	247	2.39	1.48	2.87	2.33	2.63	2.47
Maleic hydrazide	0.011	-1.96	-1.46		35-79	57	1.76	0.31	0.31	-1.49	-0.33	1.91
Maleic hydrazide potassium			-4.01	0.1-2.6	21-83	52	1.72	0.31	-0.80	-3.15	-1.63	2.43
Mancozeb	22	1.34		7.2-10.1	618-2334	998	3.00		2.11	1.19	1.74	2.05
Maneb	56	1.75		2.0-8.4	720-1715	1040	3.02		2.33	1.52	2.00	2.15
MCPA	7.43	0.87	2.52	0.7-1.0	29.2-50	28	1.45	1.47	1.85	0.80	1.45	1.96
MCPA octyl ester			6.24			1000	3.00	4.06	4.77	5.15	4.83	4.47
MCPA dimethylammonium			0.74			20	1.30	2.51	1.78	0.70	1.37	1.93
MCPB	617	2.79	3.5			20	1.30	2.00	2.89	2.36	2.66	2.49

Name (ISO)	Kow			Adsorption Coefficient								
		log Kow	log Kow	Kd	Koc	Koc used	log Koc	EPI	Lyman	TGD, nhf	TGD, hf	OCH
	exp.	exp.	est.	exp.	exp. range	exp.	exp.	est	est.	est.	est	est.
MCPB sodium			-0.31			20	1.30	2.00	1.21	-0.15	0.70	1.83
Mecoprop (MCPP)		3.13	2.94		12.0-25.0	20	1.30	1.69	3.08	2.64	2.87	2.63
Mecoprop dimethylamine			1.16			20	1.30	2.73	2.01	1.04	1.63	2.01
Mecoprop-P		3.13	2.94			20	1.30	1.69	3.08	2.64	2.87	2.63
Mecoprop-P dimethylammonium			1.16			20	1.30	2.73	2.01	1.04	1.63	2.01
Mepiquat chloride	0.0017	-2.76	-2.82	4.0-17	67-4685	2376	3.38	2.24	-0.12	-2.14	-0.84	2.06
Mepronil	4786	3.68	4.24	11.3-69.2	689-1375	974	2.99	3.09	3.38	3.08	3.22	2.87
Metalaxyl	56	1.75	1.7		12-21.0	16	1.20	1.35	2.33	1.52	2.00	2.15
Metaldehyde	1.33	0.12	0.85	0.1-0.4	12.6-35.5	31	1.49	1.00	1.44	0.20	0.98	1.86
Metam (metham) sodium	<10	<1	-0.92			10	1.00	0.61	0.88	-0.65	0.32	1.82
Metamitron	6.76	0.83	1.44	11.0-40	400-1100	600	2.78	3.52	1.83	0.77	1.42	1.95
Methabenzthiazuron	437	2.64	2.65	5.6-8.9	103-176	140	2.15	3.29	2.81	2.24	2.56	2.43
Methamidophos	0.16	-0.80	-0.93		2-34	5	0.70	0.59	0.94	-0.55	0.40	1.82
Methazole	386	2.59	3.22			3000	3.48	1.77	2.79	2.20	2.53	2.41
Methidathion	158	2.20	1.58			400	2.60	1.00	2.57	1.88	2.29	2.28
Methiocarb (Mercaptodimethur)	832	2.92	2.87	12.6	517	174	2.24	2.26	2.97	2.47	2.74	2.54
Methomyl	1.24	0.60	0.61	0.2-1.4	32.2-59.1	45.65	1.66	1.08	1.70	0.59	1.28	1.91
Methoxychlor	120200	5.08	5.67			80000	4.90	4.63	4.14	4.21	4.10	3.66
Methylarsonate, sodium hydrogen	1	0	-3.89	0.5-39.4	250-2850	1550	3.19		1.38	0.10	0.90	1.85
Methyl Bromide	15	1.19	1.18		4, 22	13	1.11	1.16	2.02	1.06	1.65	2.02
Methyl isothiocyanate	23.5	1.37	1.30		3-7	5	0.70	0.54	2.12	1.21	1.76	2.06
Metiram	2.1	0.32				500000	5.70		1.55	0.36	1.10	1.88
Metolachlor	1350	3.13	3.24	0.1-10	21-309	137	2.14	2.47	3.08	2.64	2.87	2.63
Metoxuron	44	1.64	2.11		51-170	111	2.05	1.78	2.27	1.43	1.93	2.12
Metribuzin	37	1.57	1.49	0.1-1.9	7.3-160	39	1.59	3.08	2.23	1.37	1.89	2.10
Metsulfuron-methyl	158	2.20	2	0.4-1.4	35-54	45	1.65	1.84	2.57	1.88	2.29	2.28
Mevinphos	1.34	0.13	-0.24		9.9, 190	190	2.28	2.37	1.45	0.21	0.98	1.86
Monocrotophos			-1.31			1	0.00	2.37	0.66	-0.96	0.07	1.84
Monolinuron	160	2.20	2.26		250-500	375	2.57	2.33	2.57	1.88	2.29	2.28
Muscalure	12300	4.09	11.42					6.69	3.60	3.41	3.48	3.08
Naled	24	1.38	1.6			180	2.26	1.98	2.13	1.22	1.77	2.06
2-(1-Naphthyl)acetamide			1.72			100	2.00	3.41	2.31	1.49	1.98	2.14
2-(1-Naphthyl)acetic acid (NAA)	174	2.24	2.6					2.47	2.60	1.91	2.31	2.29
2-(1-Naphthyl)acetate, ethylester			3.75			300	2.48	3.47	3.42	3.14	3.26	2.91
2-(1-Naphthyl)acetate sodium			-0.84			20	1.30	2.47	0.92	-0.58	0.37	1.82
Napropamide	1995	3.30	3.33	3.3-14.8		301	2.48	4.06	3.17	2.77	2.98	2.70
Naptalam	1.01	0.004	3.41	14.98	2152	2152	3.33	3.34	1.38	0.10	0.90	1.85
Naptalam sodium			-0.39			20	1.30	2.57	1.16	-0.22	0.65	1.83
Nitrapyrin	2090	3.32	3.35	0.4-133	250-9100	4675	3.67	2.58	3.19	2.79	2.99	2.71
Norflurazon	200	2.30	2.19		298-1055	677	2.83	3.75	2.63	1.96	2.35	2.31
Nuarimol	1500	3.18	3.17		2.0-6.0	102	2.01	3.79	3.10	2.67	2.90	2.65
1,4,4a,5a,6,9,9a,9b-Octahydro-dibenzofuran-4a-carbaldehyde			1.51					2.07	2.20	1.32	1.85	2.09
Oryzalin	5420	3.73	2.73	2.1-12.9	700-1100	900	2.95	3.09	3.41	3.12	3.25	2.90
Oxadiazon	63100	4.80	4.81		3200	3200	3.51	3.54	3.99	3.99	3.92	3.48
Oxadixyl	5.4	0.73	1.4	0.2-13	24-50	36	1.56	1.70	1.77	0.69	1.36	1.93
Oxamyl	0.36	-0.44	-1.2	0.02-6.2	2.6-8.7	4.5	0.65	1.00	1.14	-0.26	0.62	1.82
Oxycarboxin	5.92	0.77	1.41			95	1.98	1.30	1.80	0.72	1.39	1.94

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	exp.	exp.	est.	exp.	exp. range	exp.	exp.	est	est.	est.	est	est.
Oxydemeton-methyl	0.18	-0.74	-1.03	0.1-0.5	5.0-34	19	1.28	2.16	0.97	-0.50	0.43	1.82
Oxyfluorfen	29400	4.47	5.21		2891-32381	17636	4.25	4.67	3.81	3.72	3.72	3.29
Paclobutrazol	1585	3.20	3.36	1.3-10.9	-361	164	2.21	4.09	3.12	2.69	2.92	2.66
Paraquat dichloride	3.2E-05	-4.50	-2.71			3000	3.48	3.15	-1.07	-3.55	-1.94	2.62
Parathion ethyl	6609	3.83	3.73		580-1643	1013	3.01	3.25	3.46	3.20	3.31	2.95
Parathion methyl	725	2.86	2.75			3980	3.60	2.72	2.93	2.42	2.70	2.52
Pebulate	6760	3.83	3.51			430	2.63	2.68	3.46	3.20	3.31	2.95
Penconazole	5248	3.72	4.67	10-69.8	802-3500	2500	3.40	5.25	3.40	3.11	3.24	2.89
Pencycuron	66069	4.68	5.51	43-397	1309-2276	1730	3.24	3.94	3.92	3.89	3.85	3.41
Pendimethalin	152000	5.18	4.82	30-380	13000-15000	14033	4.15	3.42	4.19	4.30	4.16	3.72
Permethrin	1621000	6.50	7.43	439	15460	15460	4.19	5.25	4.91	5.37	5.00	4.67
Phenmedipham	3857	3.59	3.27			2400	3.38	2.44	3.33	3.01	3.16	2.83
Phorate	3630	3.56	3.37		543	543	2.73	2.65	3.31	2.98	3.14	2.82
Phosalone	20000	4.30	4.29		519-1042	780	2.89	1.77	3.72	3.58	3.61	3.19
Phosmet	600	2.78	2.48			820	2.91	1.63	2.89	2.35	2.65	2.49
Phosphamidon	6.2	0.79	0.38	0.03-3.3	4.2-116	32.9	1.52	3.36	1.81	0.74	1.40	1.94
Phoxim	2400	3.38	4.39	7.2	686	686	2.84	3.50	3.22	2.84	3.03	2.73
Picloram			1.36					1.26	2.12	1.20	1.76	2.05
Picloram potassium			-2.36			16	1.20	1.26	0.09	-1.81	-0.59	1.97
Piperalin	20417	4.31	5.08			5000	3.70	4.30	3.72	3.59	3.62	3.20
Piperonyl butoxide	56200	4.75	47.29		7.8-38	19	1.28	1.84	3.96	3.95	3.89	3.45
Pirimicarb	50	1.70	1.4	0.2-52	45-730	290	2.46	1.52	2.30	1.48	1.97	2.14
Pirimiphos-ethyl	70795	4.85	4.42					2.67	4.02	4.03	3.96	3.51
Pirimiphos-methyl	15849	4.20	3.44		224-470	348	2.54	2.14	3.66	3.50	3.55	3.14
Primisulfuron-methyl	1.15	0.06	2.41		weak ads			2.18	1.41	0.15	0.94	1.85
Prochloraz	12600	4.10	3.44	152-256	4850-10000	7440	3.87	3.43	3.61	3.42	3.48	3.09
Profenofos	27542	4.44	4.82			2000	3.30	2.27	3.79	3.70	3.70	3.27
Prometon	975	2.99	3.57		150	150	2.18	2.20	3.00	2.52	2.78	2.57
Prometryn	3230	3.51	3.73		186-576	384	2.58	2.84	3.29	2.94	3.11	2.79
Propachlor	150	2.18	2.42	0.3-1.8	33-91	73	1.86	2.45	2.56	1.87	2.27	2.28
Propamocarb hydrochloride	0.0018	-2.74	-0.39	0.7-5.2	41-360	180	2.26	2.53	-0.12	-2.12	-0.83	2.05
Propaquizafop	34410	4.78	4.59	2.4-9.3	347-472	411	2.61	4.99	3.98	3.97	3.91	3.47
Propargite	100000	5.00	5.57		23000-90000	56500	4.75	5.14	4.10	4.15	4.05	3.60
Propazine	850	2.93	3.24	2.3-4.7	110-144	121	2.08	2.55	2.97	2.47	2.75	2.54
Propetamphos	6600	3.82	2.51					2.09	3.46	3.19	3.31	2.94
Propham (IPC)	400	2.60	2.66			200	2.30	2.11	2.79	2.21	2.54	2.42
Propiconazole	5248	3.72	4.13		734-1740	1236	3.09	3.75	3.40	3.11	3.24	2.89
Propineb	0.55	-0.26							1.24	-0.11	0.74	1.83
Propoxur	36	1.56	1.9		3-52	28	1.45	1.65	2.23	1.36	1.88	2.10
Propyzamide	1570	3.20	3.57	0.4-30.4	100-1340	391	2.59	3.20	3.12	2.69	2.92	2.66
Prosulfocarb	44668	4.65	4.23	11.7-32.8	1367-2340	1693	3.23	3.75	3.91	3.87	3.83	3.39
Prosulfuron	0.62	-0.21	3.56		18-41	30	1.48	3.54	1.26	-0.07	0.77	1.83
Pyrazophos	6300	3.80	3.53	12-34.1	3900-4600	4433	3.65	2.19	3.44	3.18	3.29	2.93
Pyrethrins (extract)	>1000	>3	6.15		7.6-38	14	1.15	4.02	4.72	5.08	4.77	4.40
Pyrethrins I (chrysanthemates)	218776	5.34	6.28					4.02	4.28	4.43	4.26	3.82
Pyrethrins II (pyrethrates)	6166	3.79	5.33					3.48	3.44	3.17	3.29	2.93
Pyridate	>1000	>3	5.73	~1				4.95	4.49	4.74	4.51	4.09
Pyriproxyfen			5.55		4980-34200	19600	4.29	5.61	4.40	4.60	4.40	3.97
Quintozene (PCNB)	44000	4.64	5.03		2966-9584	6275	3.80	3.38	3.90	3.86	3.82	3.39
Quizalofop-ethyl	19000	4.28	4.35			510	2.71	3.73	3.71	3.57	3.60	3.18
Rimsulfuron	0.034	-1.47	0.03		55-64	60	1.78	1.76	0.58	-1.09	-0.03	1.85
Rotenone	12600	4.10	4.31					5.54	3.61	3.42	3.48	3.09
Sethoxydim	44.7	1.65	3.99			100	2.00	3.45	2.27	1.44	1.94	2.12

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	exp.	exp.	est.	exp.	exp. range	exp.	exp.	est	est.	est.	est	est.
Siduron	1230	3.09	3.86			420	2.62	2.49	3.06	2.60	2.85	2.61
Simazine	151	2.18	2.4	0.37-4.66	103-377	150	2.18	2.17	2.56	1.87	2.27	2.28
Sulfometuron methyl	0.31	-0.51	1.71	1.78	85	85	1.93	1.98	1.10	-0.31	0.58	1.82
Sulprofos	302000	5.48	5.65			12000	4.08	3.95	4.36	4.54	4.35	3.92
2,4,5-T	2040	3.31	3.26					1.69	3.18	2.78	2.99	2.70
2,4,5-T trihydroxyethyl-ammonium			-2.49			80	1.90	1.41	0.02	-1.92	-0.67	2.00
2,3,6-TBA			2.71					1.82	2.85	2.30	2.61	2.46
TCA-sodium			-2.37					0.44	0.09	-1.82	-0.59	1.98
Tebuconazole	5000	3.70	3.89	8.4-16.8	958-2100	1570	3.20	4.32	3.39	3.10	3.23	2.88
Tebuthiuron	61	1.79	1.78	0.1-1.8	38-156	80	1.90	1.36	2.35	1.55	2.02	2.16
Tefluthrin	3200000	6.50	7.19	760-1800	100000-280000	150000	5.18	5.81	4.91	5.37	5.00	4.67
Temephos	910000	5.96	6.17	73-541		100000	5.00	6.19	4.62	4.93	4.65	4.26
Terbacil	82	1.91	1.75	0.05-2.6	3-123	32	1.51	1.89	2.42	1.65	2.10	2.19
Terbufos	30200	4.48	4.24			500	2.70	2.99	3.81	3.73	3.72	3.29
Terbutryn	5500	3.74	3.77		2000	2000	3.30	2.80	3.41	3.13	3.26	2.90
Terbutylazine	1096	3.04	3.27	2.2-9.36	162-443	356	2.55	2.52	3.03	2.56	2.82	2.59
Tetrachlorvinphos	3390	3.53	3.81					2.46	3.30	2.96	3.12	2.80
Tetradifon	40740	4.61	5.18		imm			4.32	3.88	3.83	3.80	3.37
Thiabendazole	213	2.33	2.00	2.8-22	1104-3993	2549	3.41	3.35	2.64	1.99	2.37	2.32
Thidiazuron	57	1.76	2.10			110	2.04	1.86	2.33	1.52	2.01	2.15
Thifensulfuron methyl	1.05	0.02	1.27	0.1-8.6	32-67	50	1.70	1.57	1.39	0.12	0.91	1.85
Thiobencarb	2630	3.42	3.90			900	2.95	3.43	3.24	2.87	3.05	2.75
2-(Thiocyanomethylthio)-benzothiazol (TCMTB)	1698	3.23	3.12	1.9-38.4	1152-1614	1345	3.13	3.57	3.13	2.72	2.93	2.67
Thiodicarb	50	1.70	1.91		126-178	152	2.18	3.67	2.30	1.48	1.97	2.14
Thiofanox			2.16		2.9-28	18	1.26	1.99	2.55	1.85	2.26	2.27
Thiometon	2884	3.46	2.88		11-402	256	2.41	2.38	3.26	2.90	3.08	2.77
Thiophanate-methyl	32	1.50	2.45	0.3-5.7	26-580	249	2.40	1.16	2.19	1.32	1.85	2.09
Thiram	53.7	1.73	1.70	3.7-78.3	260-4300	762	2.88	1.00	2.32	1.50	1.99	2.14
Tolclofos-methyl	36300	4.56	4.77		946-5384	2685	3.43	3.30	3.86	3.79	3.77	3.34
Tolylfluanid	8900	3.90	3.27					3.24	3.50	3.26	3.36	2.98
Camphechlor (Toxaphene)	316000	5.50	6.79			100000	5.00		4.37	4.56	4.37	3.93
Tralomethrin	100000	5.00	7.56	197-8784	43800-675700	359750	5.56	5.42	4.10	4.15	4.05	3.60
Triadimefon	1510	3.11	2.94	3.5-9.3	275-535	367	2.56	3.72	3.07	2.62	2.86	2.62
Triadimenol	800	2.90	2.95	1.9-5.7	189-1023	640	2.81	3.45	2.95	2.45	2.73	2.53
Triallate	45709	4.66	4.57	5.3-35	575-1583	1986	3.30	3.22	3.91	3.87	3.84	3.40
Triasulfuron	0.26	-0.59	2.44	0.05-2.7	7.4-47	140	2.15	2.55	1.06	-0.38	0.53	1.82
Triazamate	490	2.69	1.71	0.5-5.5	171-418	322	2.51	3.00	2.84	2.28	2.59	2.45
Tribenuron methyl	0.36	-0.44	2.55	0.2-2.0	30-80	52	1.72	1.74	1.14	-0.26	0.62	1.82
S,S,S-tributyl phosphorotrithioate (Tribufos)	1700	3.23	5.75			5000	3.70	3.28	3.13	2.72	2.93	2.67
Trichlorfon	3.2	0.51			10, 20	20	1.30	1.73	1.65	0.51	1.22	1.90
Triclopyr	0.35	-0.45	2.53	87-225	59	59	1.77	1.69	1.13	-0.26	0.62	1.82
Triclopyr-butotyl			4.01			780	2.89	2.75	3.56	3.35	3.43	3.04
Triclopyr-triethylammonium			0.77			20	1.30	3.66	1.80	0.72	1.39	1.94
Tridemorph	15800	4.20	6.38		2500-10000	6250	3.80	4.42	3.66	3.50	3.55	3.14
Tridiphane			5.18			5600	3.75	3.24	4.19	4.30	4.16	3.72
Trifluralin	118000	5.27	5.31	18.6-155.6	4300-8700	6125	3.79	3.99	4.24	4.37	4.22	3.78
Triflusulfuron methyl	9.2	0.96	3.94	0.4-1.3	35-132	58	1.76	3.17	1.90	0.88	1.51	1.97
Triforine	110	2.04	2.02	2.8-6.3	88-117	103	2.01	2.60	2.49	1.75	2.19	2.23

Name (ISO)	Kow			Adsorption Coefficient								
		log Kow	log Kow	Kd	Koc	Koc used	log Koc	EPI	Lyman	TGD, nhf	TGD, hf	OCH
	exp.	exp.	est.	exp.	exp. range	exp.	exp.	est	est.	est.	est	est.
Trimethacarb	457	2.66	2.81			400	2.60	1.98	2.82	2.25	2.58	2.44
Trinexapac ethyl	275	1.60	0.63	1.5-18	140-600	280	2.45	1.00	2.25	1.40	1.91	2.11
Vernolate	6918	3.84	3.51			260	2.41	2.68	3.47	3.21	3.32	2.95
Vinclozolin	1027	3.01	3.03	0.6-9.7	100-327	246	2.39	2.46	3.01	2.54	2.80	2.58
Zineb	<20	<1.3	-1.89					1.00	0.35	-1.43	-0.29	1.90
Ziram	12	1.09	-0.35		7-21	14	1.15	1.09	1.97	0.98	1.58	2.00
Total number	359	359	397	160	249	353	353	397	409	409	409	409

Table 4
Bioaccumulation factor (BCF) and acute effect concentrations for fish, daphnia and algae. The experimental acute effect levels are the lowest observed in the accepted literature.

Bioakkumuleringsfaktor (BCF) og akutte effektkoncentrationer for fisk, dafnier og alger. Den eksperimentelle effektkoncentration angivet er den laveste, der blev fundet i den anvendte litteratur.

Name (ISO)	BCF	fish	Fish mg/l	LC50,96h		Daphnia mg/l	EC50, 48h		Algae mg/l	IC50,72h
	exp.	est.	exp.	est., np	est., pol.	exp.	est., np	est., pol.	exp.	est., np.
Acephate	3	0.03	2050	4.26E+04	5.66E+03	67.2	6.14E+04	9.36E+02	>1000	8.37E+04
Acetochlor		75	0.36	2.92E+01	1.15E+01	16	1.71E+01	8.79E+00		1.48E+01
Acifluorfen		279	6.2	1.06E+01	4.98E+00		5.29E+00	4.97E+00		4.25E+00
Acifluorfen sodium		2.05	31	1.52E+03	3.59E+02	77	1.36E+03	1.34E+02	>260	3.05E+02
Aclonifen		542	0.67	3.97E+00	2.06E+00	2.5	1.84E+00	2.35E+00	0.029	1.42E+00
Acrinathrin		5902	0.12	7.46E-01	5.42E-01	0.57	2.61E-01	9.95E-01	>0.82	1.75E-01
Acrolein		1.65	0.079	2.76E+02	6.31E+01	0.022	2.53E+02	2.26E+01	0.026	2.75E+02
Alachlor	39	84	1.8	2.60E+01	1.04E+01	10	1.50E+01	8.14E+00	0.11	1.29E+01
Alanycarb		164	1	1.98E+01	8.66E+00	>9.4	1.05E+01	7.78E+00		8.74E+00
Aldicarb	42	4.31	0.06	3.59E+02	9.40E+01	0.4	2.94E+02	4.08E+01		3.02E+02
Aldoxycarb		0.07	55.5	2.76E+04	4.01E+03		3.70E+04	7.52E+02		4.86E+04
Allethrin		3281	0.018	7.49E-01	5.01E-01	0.036	2.81E-01	8.18E-01		1.95E-01
Alloxydim sodium	4.5	0.13	2000	2.08E+04	3.34E+03	>4000	2.56E+04	7.25E+02	38	3.22E+04
Ametryn		68	5	2.71E+01	1.05E+01	28	1.61E+01	7.90E+00	0.0035	1.40E+01
Amidosulfuron		4.85	>320	6.19E+02	1.65E+02	36	5.00E+02	7.32E+01	47	5.10E+02
Amitraz	667	9441	0.45	2.53E-01	1.96E-01	0.035	8.37E-02	3.96E-01	0.67	5.46E-02
Amitrole		0.04		1.84E+04	2.47E+03	1.5	2.64E+04	4.13E+02	1.3	3.59E+04
Ancymidol		8.38	55	2.48E+02	7.15E+01		1.88E+02	3.54E+01		1.86E+02
Anilazine	210	396	0.15	5.65E+00	2.80E+00	0.07	2.72E+00	3.00E+00	1.02	2.14E+00
Asulam		0.20	>1700	9.31E+03	1.58E+03	63.4	1.09E+04	3.71E+02	13.5	1.34E+04
Asulam sodium		0.0001		2.69E+07	1.49E+06		8.02E+07	7.16E+04		1.57E+08
Atrazine	4.3	33	4.5	5.31E+01	1.86E+01	3.6	3.42E+01	1.21E+01	0.044	3.12E+01
Azaconazole		19	42	1.30E+02	4.20E+01	86	8.98E+01	2.44E+01		8.46E+01
Azamethiphos		1.56	0.2	1.69E+03	3.85E+02	6.70E-04	1.56E+03	1.36E+02		1.70E+03
Azinphos-ethyl		101	0.03	2.79E+01	1.14E+01	2.00E-04	1.58E+01	9.28E+00		1.34E+01
Azinphos-methyl	40	30	0.003	8.62E+01	2.97E+01	0.0011	5.62E+01	1.90E+01	3.61	5.15E+01
Benalaxyl		155	3.75	1.71E+01	7.42E+00	0.59	9.17E+00	6.58E+00	2.4	7.63E+00
Benazolin		2.75	27	7.21E+02	1.77E+02	233.4	6.22E+02	7.02E+01		6.56E+02
Benazolin ethyl	36	27	2.8	8.30E+01	2.81E+01	6.1	5.48E+01	1.75E+01	16	5.06E+01
Bendiocarb		5.74	0.86	3.16E+02	8.63E+01	0.16	2.50E+02	3.96E+01	1.71	2.53E+02
Benfluralin		6259	0.08	4.35E-01	3.19E-01	>0.1	1.51E-01	5.93E-01	4	1.01E-01
Benfuracarb		902	0.65	3.70E+00	2.06E+00	>10	1.62E+00	2.60E+00		1.21E+00
Benfuresate		22	12.28	9.34E+01	3.09E+01	35.36	6.30E+01	1.86E+01	3.8	5.87E+01
Benomyl		13	0.17	1.87E+02	5.69E+01	0.55	1.35E+02	3.06E+01	2	1.30E+02
Bensulfuron methyl		6.76	>150	4.93E+02	1.38E+02	>100	3.83E+02	6.53E+01		3.83E+02
Bensulide		741	1.1	4.36E+00	2.36E+00	0.58	1.95E+00	2.87E+00	1	1.48E+00
Bensultap		143	0.76	2.45E+01	1.05E+01	0.21	1.33E+01	9.19E+00	1	1.11E+01
Bentazone	21	0.08	635	2.41E+04	3.60E+03	125	3.15E+04	7.05E+02	47	4.08E+04
Bentazone sodium		0.66	1500	3.24E+03	6.51E+02		3.31E+03	1.94E+02	279	3.79E+03
Bifenox	83	1275	>0.18	2.18E+00	1.28E+00	0.66	9.14E-01	1.73E+00	130	6.72E-01
Bifenthrin	6000	1690000	0.00015	2.04E-03	3.29E-03	0.00016	3.66E-04	1.87E-02	>50	1.76E-04
Bioallethrin		1897	0.0099	1.30E+00	8.02E-01	0.0356	5.18E-01	1.17E+00		3.72E-01
Bioresmethrin		220000	0.00062	1.25E-02	1.51E-02	0.0008	2.85E-03	5.73E-02		
Bitertanol	175	532	2.1	5.16E+00	2.67E+00	2.79	2.40E+00	3.03E+00	0.31	1.85E+00
Brodifacoum		3350000	0.04	1.27E-03	2.26E-03	0.064	2.11E-04	1.48E-02		9.75E-05
Bromacil		7.75	71	2.74E+02	7.79E+01	119	2.09E+02	3.80E+01		2.07E+02
Bromacil lithium		0.4		5.48E+03	1.03E+03		5.94E+03	2.76E+02		7.02E+03
Bromadiolone		867	1.4	4.94E+00	2.74E+00	2	2.17E+00	3.43E+00		1.63E+00
Bromethalin		120000	0.006	3.91E-02	4.34E-02	0.0025	9.59E-03	1.46E-01		5.39E-03
Bromofenoxim		99	0.088	3.80E+01	1.55E+01	1.7	2.15E+01	1.25E+01	2.2	1.84E+01
Bromoxynil	1	58	23	3.87E+01	1.46E+01	12.5	2.33E+01	1.07E+01	44	2.05E+01

Name (ISO)	BCF	fish	Fish mg/l	LC50,96h		Daphnia mg/l	EC50, 48h		Algae mg/l	IC50,72h
	exp.	est.	exp.	est., np	est., pol.	exp.	est., np	est., pol.	exp.	est., np.
Bromoxynil octanoate	100	7762	0.06	4.22E-01	3.19E-01	0.11	1.43E-01	6.19E-01	1.77	9.45E-02
Bromoxynil butyrate		412	0.03	6.84E+00	3.41E+00	0.2	3.28E+00	3.68E+00		2.57E+00
Bromoxynil potassium		0.3	5	9.57E+03	1.69E+03		1.09E+04	4.21E+02		1.31E+04
Bromuconazole	131	113	1.7	2.71E+01	1.13E+01	>5	1.51E+01	9.38E+00	2.1	1.28E+01
Bronopol		0.28	35.7	5.73E+03	1.02E+03	0.57	6.46E+03	2.57E+02	0.02	7.78E+03
Butylate		672	4.2	2.63E+00	1.41E+00		1.19E+00	1.67E+00		9.06E-01
Captafol		27.13	0.15	1.05E+02	3.55E+01	3.34	6.89E+01	2.22E+01		6.35E+01
Captan	140	19.84	0.034	1.23E+02	4.00E+01	0.5	8.42E+01	2.35E+01	0.45	7.91E+01
Carbaryl	<1	20.23	1.3	8.09E+01	2.64E+01	0.006	5.52E+01	1.56E+01		5.17E+01
Carbendazim	25	3.91	0.35	3.98E+02	1.03E+02	0.13	3.29E+02	4.37E+01	1.3	3.40E+02
Carbetamide		0.01	354	2.16E+05	2.37E+04	54	3.66E+05	2.98E+03	210	5.41E+05
Carbofuran	18	5.24	0.0073	3.43E+02	9.24E+01	0.015	2.74E+02	4.17E+01	7	2.79E+02
Carbosulfan		127	0.015	2.43E+01	1.03E+01	0.0015	1.33E+01	8.76E+00	20	1.12E+01
Carboxin		13	1.2	1.45E+02	4.46E+01	84.4	1.04E+02	2.42E+01	0.48	1.00E+02
Chinomethionate		326	0.0334	5.84E+00	2.82E+00	0.12	2.88E+00	2.90E+00		2.29E+00
Chloramben		8		2.04E+02	5.85E+01		1.55E+02	2.88E+01		1.53E+02
Chloramben sodium		0.01		1.75E+05	1.96E+04		2.90E+05	2.56E+03		4.25E+05
Chlordimeform hydrochloride		57		3.32E+01	1.25E+01		2.01E+01	9.11E+00		1.77E+01
Chlorfenvinphos		454	0.039	6.43E+00	3.25E+00	0.00025	3.04E+00	3.58E+00	1.6	2.38E+00
Chlorfenac sodium (Fenac)		0.2		1.25E+04	2.07E+03		1.49E+04	4.70E+02		1.85E+04
Chloridazon (Pyridazon)	12	2	20	8.79E+02	2.07E+02	50.1	7.86E+02	7.75E+01	1.9	8.43E+02
Chlorimuron ethyl		0.4	>100	8.35E+03	1.57E+03	1000	9.03E+03	4.23E+02		1.07E+04
Chlormequat chloride		0.01	525	1.66E+05	1.78E+04	7.4	2.86E+05	2.18E+03	>465	4.25E+05
Chlorobenzilate		2133	0.6	1.24E+00	7.80E-01		4.89E-01	1.17E+00		3.48E-01
Chloroneb		167	>4200	1.00E+01	4.41E+00		5.35E+00	3.98E+00		4.43E+00
Chloropicrin		11.93	0.168	1.12E+02	3.39E+01	0.91	8.14E+01	1.80E+01		7.87E+01
Chlorothalonil	187	57	0.044	3.79E+01	1.43E+01	0.07	2.29E+01	1.04E+01	0.21	2.02E+01
Chloroxuron		105	28	2.26E+01	9.28E+00	4.3	1.27E+01	7.61E+00	0.016	1.08E+01
Chlorpropham	61	140	3.02	1.24E+01	5.30E+00	8	6.72E+00	4.61E+00	3.3	5.62E+00
Chlorpyrifos	1850	1972	0.003	1.44E+00	8.99E-01	0.0017	5.75E-01	1.33E+00	0.58	4.12E-01
Chlorpyrifos methyl		801	0.3	3.27E+00	1.79E+00	0.02	1.45E+00	2.21E+00		1.09E+00
Chlorsulfuron		10	>50	2.91E+02	8.58E+01	370	2.16E+02	4.40E+01		2.11E+02
Chlorthal dimethyl (DCPA)		867	>4.7	3.11E+00	1.72E+00	>4.6	1.36E+00	2.16E+00		1.03E+00
Clethodim	3	727	56	4.02E+00	2.18E+00	>100	1.80E+00	2.63E+00	14.8	1.37E+00
Clofentezine		86	>0.015	2.86E+01	1.14E+01	>0.00145	1.65E+01	9.03E+00	>0.32	1.42E+01
Clomazone		27	19	7.32E+01	2.48E+01	5.2	4.84E+01	1.55E+01	2.1	4.46E+01
Cloprop (3-CPA)		21	21	7.60E+01	2.50E+01		5.15E+01	1.49E+01		4.81E+01
Cloprop ammonium		5		3.35E+02	8.92E+01		2.70E+02	3.96E+01		2.76E+02
Cloprop sodium		0.01		1.46E+05	1.68E+04		2.38E+05	2.25E+03		3.45E+05
Clopyralide	<1	4	103.5	3.72E+02	9.71E+01	225	3.06E+02	4.19E+01	7.1	3.14E+02
Clopyralid-olamine		0.004		4.97E+05	4.89E+04		9.21E+05	5.27E+03		1.42E+06
Coumatetralyl		174	48	1.36E+01	6.03E+00	>14	7.23E+00	5.47E+00	15.2	5.97E+00
Cyanazine	157	12	4.8	1.61E+02	4.88E+01	42	1.17E+02	2.60E+01	0.02	1.13E+02
Cyanophos		36	5	5.54E+01	1.96E+01	0.34	3.54E+01	1.29E+01		3.21E+01
Cycloate		396	4.5	4.42E+00	2.19E+00	2.6	2.12E+00	2.35E+00		1.67E+00
Cycloxidim		2.86	220	9.26E+02	2.29E+02	132	7.95E+02	9.14E+01	32	8.37E+02
Cyfluthrin	506	22777	0.0015	1.55E-01	1.36E-01	0.00016	4.63E-02	3.28E-01	>10	2.87E-02
Cyhalothrin		120226	0.00054	3.04E-02	3.38E-02	0.00038	7.47E-03	1.14E-01		4.20E-03
Cypermethrin	930	81283	0.00069	4.16E-02	4.38E-02	0.00015	1.07E-02	1.36E-01	>1.3	6.16E-03
alpha-Cypermethrin	4667	158000	0.00093	2.14E-02	2.47E-02	0.0002	5.09E-03	8.77E-02		2.81E-03
Cyproconazole		59	18.9	4.00E+01	1.52E+01	26	2.40E+01	1.11E+01	0.08	2.11E+01
Cyromazine	<1	0.23	>90	5.79E+03	1.01E+03	>9.1	6.68E+03	2.43E+02	124	8.14E+03
2,4-D		31	1.1	5.77E+01	2.00E+01	1.4	3.75E+01	1.29E+01	25-400	3.42E+01
2,4-D-dimethylammonium		0.7	100	3.04E+03	6.17E+02		3.07E+03	1.87E+02		3.51E+03
2,4-D methylester		58	0.9	3.28E+01	1.24E+01		1.98E+01	9.06E+00		1.74E+01
Dalapon sodium	2.5	1.03	>100	1.30E+03	2.78E+02	6	1.26E+03	9.06E+01	20	1.40E+03
Daminozide		0.01	149	1.21E+05	1.36E+04	98.5	2.00E+05	1.77E+03	160	2.91E+05

Name (ISO)	BCF	fish	Fish mg/l	LC50,96h		Daphnia mg/l	EC50, 48h		Algae mg/l	IC50,72h
	exp.	est.	exp.	est., np	est., pol.	exp.	est., np	est., pol.	exp.	est., np.
Dazomet		3.1	0.16	4.27E+02	1.07E+02	0.3	3.63E+02	4.33E+01	1.08	3.80E+02
2,4-DB		200	4	1.01E+01	4.57E+00	5	5.28E+00	4.26E+00		4.33E+00
2,4-DB butoxyethyl		4150	4	5.76E-01	3.98E-01		2.10E-01	6.82E-01		1.44E-01
Deltamethrin	772	1622	0.00059	2.53E+00	1.53E+00	0.0035	1.03E+00	2.18E+00	>9.1	7.47E-01
Desmedipham	0.8	152	1.7	1.61E+01	6.96E+00	0.59	8.65E+00	6.15E+00	1.05	7.20E+00
Desmetryn		21	2.2	8.24E+01	2.70E+01	45	5.60E+01	1.61E+01	0.004	5.24E+01
Diazinon	505	301	0.21	8.21E+00	3.92E+00	0.99	4.08E+00	3.97E+00	6.4	3.26E+00
Dicamba		15	135	1.19E+02	3.73E+01	110	8.41E+01	2.07E+01	>250	8.03E+01
Dicamba sodium		0.03		5.76E+04	7.63E+03		8.33E+04	1.26E+03		1.14E+05
Dichlobenil	56	42	5	3.29E+01	1.19E+01	6.2	2.05E+01	8.15E+00	2	1.84E+01
Dichlofluanid		279	0.03	9.72E+00	4.59E+00	0.42	4.87E+00	4.58E+00	>1	3.91E+00
1,3-Dichloropropene		11	1.8	8.02E+01	2.41E+01	3.1	5.87E+01	1.26E+01	8.2	5.69E+01
Dichlorprop (2,4-DP)		6	428	3.00E+02	8.30E+01	1300	2.34E+02	3.89E+01	220	2.35E+02
Dichlorprop butoxyethyl		1387		1.96E+00	1.16E+00		8.15E-01	1.60E+00		5.96E-01
Dichlorprop-P		164	100	1.16E+01	5.10E+00	1300	6.20E+00	4.58E+00	220	5.14E+00
Dichlorvos	7	1.9	0.225	9.30E+02	2.18E+02	0.00019	8.36E+02	8.03E+01	52.8	9.00E+02
Dicloran (DCNA)		6.8	1.6	2.49E+02	6.96E+01	2.07	1.94E+02	3.30E+01		1.94E+02
Dicofol	9000	3689	0.183	8.16E-01	5.55E-01	0.14	3.02E-01	9.28E-01	0.075	2.08E-01
Dicrotophos		0.08	200	2.52E+04	3.74E+03	0.6	3.32E+04	7.24E+02		4.32E+04
Dienochlor		2700000	0.05	1.43E-03	2.46E-03		2.43E-04	1.54E-02		1.14E-04
Diethatyl-ethyl		229	1.82	1.11E+01	5.08E+00	18.8	5.67E+00	4.87E+00		4.61E+00
Difenacoum		598000	0.1	6.04E-03	8.42E-03	0.5	1.23E-03	3.90E-02		6.28E-04
Difenoconazole	320	741	0.8	4.45E+00	2.41E+00	0.8	1.99E+00	2.93E+00	1.2	1.51E+00
Difenoxuron		29	5	8.09E+01	2.77E+01	79	5.30E+01	1.76E+01	0.3	4.86E+01
Difenzoquat methylsulfate	20	0.2	694	1.39E+05	1.72E+04	20	2.13E+05	2.58E+03	0.29	3.00E+05
Difethialone		44400000	0.05	8.86E-01	6.28E-01	0.004	3.17E-01	1.11E+00		2.15E-01
Diflubenzuron	320	396	137	6.37E+00	3.16E+00	0.0071	3.06E+00	3.38E+00		2.41E+00
Diflufenican	1100	2917	70	1.10E+00	7.22E-01	>10	4.18E-01	1.15E+00	>10	2.92E-01
Dimethachlor		14	3.9	1.49E+02	4.61E+01	14.2	1.06E+02	2.53E+01	0.13	1.02E+02
Dimethipin	3	0.14	8	1.19E+04	1.94E+03	20	1.46E+04	4.25E+02	5.12	1.83E+04
Dimethoate	<1	0.79	6.2	2.35E+03	4.86E+02	0.46	2.35E+03	1.50E+02	90.4	2.67E+03
Dinocap		1442	0.014	2.05E+00	1.22E+00	<0.05	8.48E-01	1.70E+00		6.19E-01
Dinoseb		211	0.04	9.22E+00	4.19E+00	0.68	4.77E+00	3.95E+00	31.5	3.90E+00
Dinoseb-olamin		0.4		6.82E+03	1.26E+03		7.48E+03	3.32E+02		8.89E+03
Dinoseb acetic acid		289		7.92E+00	3.76E+00		3.95E+00	3.78E+00		3.17E+00
Dinoterb		192	0.0034	1.02E+01	4.55E+00	0.47	5.32E+00	4.22E+00	7.4	4.37E+00
Diphenamid		54		3.61E+01	1.35E+01	56	2.20E+01	9.71E+00		1.95E+01
Dipropetryn		345	1.6	6.01E+00	2.92E+00		2.94E+00	3.04E+00		2.33E+00
Diquat dibromide	9	<1	4	1.14E+08	5.43E+06	2.5	3.86E+08	2.10E+05	0.011	8.07E+08
Disulfoton		454	0.039	4.91E+00	2.48E+00	0.013	2.32E+00	2.73E+00		1.81E+00
Dithianon		105	0.04	2.30E+01	9.46E+00	0.6	1.29E+01	7.76E+00	5.9	1.10E+01
Diuron		38	5.9	5.01E+01	1.78E+01	1.4	3.17E+01	1.19E+01	0.01	2.87E+01
DNOC		21	6	7.51E+01	2.47E+01	5.7	5.09E+01	1.47E+01	6	4.75E+01
Dodine		0.04	0.6	6.65E+04	8.73E+03		9.43E+04	1.45E+03		1.28E+05
Endosulfan	2755	359	0.002	9.20E+00	4.50E+00	0.075	4.48E+00	4.73E+00	1.44	3.54E+00
Endothal		8.38	77	1.80E+02	5.20E+01	92	1.37E+02	2.57E+01	15	1.35E+02
Endothal sodium		0.3	160	5.98E+03	1.08E+03		6.66E+03	2.77E+02		7.98E+03
EPTC	60	105	10	1.47E+01	6.04E+00	15.4	8.26E+00	4.96E+00	1.4	7.03E+00
Esfenvalerate	1934	38637	0.00034	8.83E-02	8.37E-02	0.00024	2.48E-02	2.24E-01	0.0065	1.49E-02
Ethalfluralin		4400	0.102	6.16E-01	4.29E-01	>0.365	2.23E-01	7.43E-01	0.009	1.52E-01
Ethametsulfuron-methyl		1.14	>600	2.93E+03	6.36E+02	34	2.80E+03	2.11E+02	2.4	3.11E+03
Ethephon	4	0.00	300	4.36E+05	4.04E+04	>500	8.51E+05	4.00E+03	21	1.35E+06
Ethiofencarb		11	12.8	1.69E+02	5.05E+01	0.22	1.24E+02	2.63E+01	7.4	1.21E+02
Ethion		4069	0.52	7.68E-01	5.29E-01	0.005	2.81E-01	9.03E-01		1.93E-01
Ethirimol		18	20	9.46E+01	3.03E+01	53	6.54E+01	1.75E+01	24	6.18E+01
Ethofumesate	125	39	15	5.91E+01	2.12E+01	295	3.73E+01	1.43E+01	0.06	3.36E+01
Ethoprophos		225	2.1	8.77E+00	4.02E+00	0.05	4.51E+00	3.84E+00	28.3	3.67E+00
Etridiazole		146	1.2	1.38E+01	5.94E+00	4.9	7.45E+00	5.21E+00	1.82	6.22E+00

Name (ISO)	BCF	fish	Fish mg/l	LC50,96h		Daphnia mg/l	EC50, 48h		Algae mg/l	IC50,72h
	exp.	est.	exp.	est., np	est., pol.	exp.	est., np	est., pol.	exp.	est., np.
Etrimfos	336	127	0.253	1.87E+01	7.89E+00	0.0038	1.03E+01	6.73E+00	2.9	8.63E+00
Fenamiphos		127	0.0096	1.94E+01	8.18E+00	0.0019	1.06E+01	6.98E+00	3.5	8.95E+00
Fenarimol		273	0.91	9.85E+00	4.64E+00	6.8	4.95E+00	4.61E+00	1.9	3.98E+00
Fenbuconazole		111	0.68	2.47E+01	1.02E+01		1.38E+01	8.48E+00		1.17E+01
Fenbutatin oxide	733	5248	0.27	1.63E+00	1.16E+00	0.05	5.79E-01	2.09E+00		3.91E-01
Fenitrothion	114	164	1.7	1.37E+01	6.01E+00	0.00158	7.32E+00	5.40E+00	3.9	6.07E+00
Fenoxaprop		699		3.88E+00	2.09E+00		1.75E+00	2.50E+00		1.33E+00
Fenoxaprop-ethyl		634	0.31	4.64E+00	2.46E+00	1.9	2.11E+00	2.89E+00	0.36	1.62E+00
Fenoxaprop-P-ethyl	510	867	0.46	3.39E+00	1.88E+00	2.7	1.49E+00	2.35E+00	0.51	1.12E+00
Fenoxycarb		902	1.6	2.72E+00	1.51E+00	0.4	1.19E+00	1.91E+00		8.89E-01
Fenpiclonil	346	381	0.8	5.06E+00	2.50E+00	1.3	2.44E+00	2.65E+00	0.22	1.93E+00
Fenpropathrin	300	13963	0.002	2.03E-01	1.67E-01	0.0005	6.43E-02	3.64E-01		4.11E-02
Fenpropidin	160	32	1.93	7.01E+01	2.43E+01	0.54	4.53E+01	1.57E+01	0.0025	4.14E+01
Fenpropimorph	1073	610	3.16	4.05E+00	2.13E+00	2.39	1.85E+00	2.49E+00	0.29	1.42E+00
Fenthion		598	0.87	3.78E+00	1.99E+00	0.0052	1.73E+00	2.31E+00	0.05	1.33E+00
Fentin acetate		164	0.32	2.03E+01	8.88E+00	0.00032	1.08E+01	7.97E+00	0.002	8.96E+00
Fentin hydroxide	4300	164	0.042	1.82E+01	7.96E+00	0.0165	9.69E+00	7.14E+00	0.002	8.03E+00
Fenvalerate	1664	3618	0.00064	9.43E-01	6.40E-01	0.0003	3.50E-01	1.07E+00		2.42E-01
Ferbam		0.95		3.54E+03	7.51E+02	0.04	3.46E+03	2.41E+02	2.4	3.89E+03
Flamprop methyl		71	4.7	3.86E+01	1.50E+01		2.27E+01	1.14E+01		1.98E+01
Flamprop-M isopropyl	120	273	2.4	1.08E+01	5.10E+00	18.6	5.44E+00	5.06E+00	6.8	4.37E+00
Flocoumafen		1972	0.15	2.24E+00	1.39E+00	0.66	8.90E-01	2.05E+00	1.1	6.37E-01
Fluazifob		101	117	2.64E+01	1.08E+01	240	1.49E+01	8.79E+00		1.27E+01
Fluazifop-butyl		1333	0.53	2.34E+00	1.38E+00	1	9.74E-01	1.88E+00		7.14E-01
Fluazifop-P-butyl	320	1333	1.07	2.34E+00	1.38E+00	>1	9.74E-01	1.88E+00	>1.8	7.14E-01
Flucythrinate		12	0.00032	3.14E+02	9.47E+01	0.0083	2.28E+02	5.01E+01		2.21E+02
Flumetralin		8560	>0.0032	4.00E-01	3.07E-01	>0.0028	1.34E-01	6.07E-01	>0.85	8.81E-02
Fluometuron		16	47	1.20E+02	3.78E+01	54	8.46E+01	2.12E+01		8.05E+01
Flurenol-butyl		26	12.5	8.97E+01	3.02E+01		5.95E+01	1.87E+01		5.51E+01
Fluridone		97	11.7	2.76E+01	1.12E+01	6.3	1.57E+01	9.08E+00		1.34E+01
Fluroxypyr		6	>100	3.45E+02	9.47E+01	>100	2.71E+02	4.39E+01	49.8	2.73E+02
Fluroxypyr-meptyl		1414	>0.7	2.11E+00	1.25E+00	>5	8.74E-01	1.73E+00	3.8	6.38E-01
Flurprimidol	33	138	17.2	1.84E+01	7.88E+00	11.8	1.00E+01	6.83E+00	0.84	8.41E+00
Flusilazole	250	301	1.2	8.51E+00	4.06E+00	3.4	4.23E+00	4.12E+00	6.6	3.38E+00
tau-Fluvalinate	354	834	0.0027	4.90E+00	2.70E+00	0.00085	2.16E+00	3.36E+00		1.63E+00
Folpet	56	88	0.0655	2.75E+01	1.10E+01	0.02	1.58E+01	8.72E+00	0.15	1.36E+01
Fomesafen		58	680	6.13E+01	2.32E+01		3.69E+01	1.69E+01		3.25E+01
Fomesafen sodium		20	170	1.89E+02	6.14E+01		1.29E+02	3.61E+01		1.21E+02
Fonofos		446	0.028	4.49E+00	2.27E+00	0.001	2.13E+00	2.48E+00	1.5	1.67E+00
Formetanate hydrochloride		0.85	2.76	2.47E+03	5.14E+02	0.093	2.44E+03	1.61E+02	1.5	2.76E+03
Formothion		0.07	38.3	3.20E+04	4.64E+03	16.1	4.28E+04	8.70E+02	42.3	5.63E+04
Fosamine ammonium		<1	278	5.01E+07	2.43E+06	1524	1.67E+08	9.62E+04		3.47E+08
Fosetyl-aluminium		<1	161	2.85E+06	2.29E+05	189	6.22E+06	1.87E+04	21.9	1.05E+07
Fuberidazole		37	2.5	4.03E+01	1.43E+01	5.6	2.56E+01	9.55E+00	0.49	2.32E+01
Furathiocarb	92	1622	0.0095	1.92E+00	1.16E+00	0.0018	7.81E-01	1.65E+00	381	5.66E-01
Glufosinate ammonium		<1	320	9.90E+07	4.45E+06	560	3.52E+08	1.59E+05	>1000	7.53E+08
Glyphosate	2	<1	38	2.70E+06	1.97E+05	281	6.39E+06	1.40E+04	1	1.12E+07
Glyphosate isopropylammonium		<1	>1000	1.81E+07	1.06E+06	930	5.19E+07	5.44E+04	73	9.96E+07
Glyphosate trimesium		<1	385	2.51E+07	1.41E+06	12	7.40E+07	6.91E+04	19	1.44E+08
Guazatine		<1	0.54	1.74E+08	7.85E+06		6.18E+08	2.81E+05		1.32E+09
Guazatine acetates		0.04	19			0.15			0.0135	
Haloxyfop	8.7	2.75	548	1.07E+03	2.63E+02	96.4	9.23E+02	1.04E+02	106.5	9.74E+02
Haloxyfop ethoxyethyl	12	956	0.28	3.69E+00	2.07E+00	4.64	1.60E+00	2.65E+00	80.7	1.19E+00
Hexaconazole		412	3.4	6.20E+00	3.09E+00	2.9	2.97E+00	3.34E+00	1.7	2.33E+00
Hexazinone	7	1.56	274	1.32E+03	2.99E+02	35	1.21E+03	1.06E+02	0.02	1.32E+03
Hexythiazox	>100	28.22	3.7	1.02E+02	3.47E+01	1.2	6.67E+01	2.19E+01	250	6.13E+01
Hydramethylnon		18.34	0.1	2.19E+02	7.04E+01	1.14	1.51E+02	4.08E+01		1.43E+02

Name (ISO)	BCF	fish	Fish mg/l	LC50,96h		Daphnia mg/l	EC50, 48h		Algae mg/l	IC50,72h
	exp.	est.	exp.	est., np	est., pol.	exp.	est., np	est., pol.	exp.	est., np.
Hymexazol		0.49	165	1.64E+03	3.16E+02	12.7	1.73E+03	8.88E+01	0.22	2.02E+03
Imazalil	64	352	2.05	6.86E+00	3.35E+00	3.5	3.34E+00	3.50E+00	5	2.65E+00
Imazamethabenz-methyl (m)		7.03	280	3.33E+02	9.36E+01	220	2.58E+02	4.47E+01	127	2.57E+02
Imazamethabenz-methyl (p)		4.06	280	5.77E+02	1.50E+02	220	4.75E+02	6.42E+01	127	4.90E+02
Imazapyr		2.54	>100	8.36E+02	2.03E+02	>100	7.28E+02	7.93E+01		7.71E+02
Imazaquin		0.39	280	6.52E+03	1.22E+03	280	7.08E+03	3.26E+02		8.38E+03
Imazaquin ammonium		0.22		1.24E+04	2.12E+03		1.44E+04	5.06E+02		1.76E+04
Imazethapyr		3.69	240	6.38E+02	1.64E+02	<1000	5.32E+02	6.87E+01		5.51E+02
Imidacloprid		0.61	211	3.41E+03	6.79E+02	85	3.52E+03	1.99E+02	>10	4.05E+03
4-Indol-3-ylbutyric acid		18		9.18E+01	2.94E+01		6.35E+01	1.70E+01		6.00E+01
Ioxynil		192	8.4	1.57E+01	7.03E+00	3.9	8.22E+00	6.51E+00	10	6.75E+00
Ioxynil octanoate		31768	4	1.27E-01	1.17E-01		3.65E-02	3.01E-01		2.22E-02
Iprodione	90	86	3.1	3.12E+01	1.25E+01	0.25	1.79E+01	9.83E+00	1.9/0.048	1.54E+01
Isazofos		352	0.008	7.24E+00	3.53E+00	0.0014	3.53E+00	3.69E+00		2.80E+00
Isofenphos	240	634	1.8	4.43E+00	2.35E+00	0.0039	2.02E+00	2.76E+00	6.8	1.54E+00
Isopropalin		17000	>0.1	1.48E-01	1.25E-01		4.57E-02	2.83E-01		2.89E-02
Isoproturon		54.89	9	3.05E+01	1.15E+01	507	1.85E+01	8.27E+00	0.03	1.64E+01
Isoxaben		34.99	>1.1	7.72E+01	2.72E+01	>1.3	4.94E+01	1.79E+01	>1.4	4.48E+01
Lactofen		2446		1.53E+00	9.84E-01		5.96E-01	1.52E+00		4.21E-01
Lambda-Cyhalothrin	2000	177800	0.00021	2.06E-02	2.42E-02	0.00036	4.82E-03	8.77E-02	>0.3	2.65E-03
Lenacil		18	10	1.04E+02	3.34E+01	33	7.17E+01	1.93E+01	0.014	6.76E+01
Lindane (Gamma HCH)	1300	284	0.022	8.32E+00	3.94E+00	1.6	4.16E+00	3.95E+00	1	3.34E+00
Linuron		71	0.89	2.86E+01	1.11E+01	0.12	1.68E+01	8.44E+00		1.47E+01
Malathion	39	43	0.04	6.21E+01	2.25E+01	0.0022	3.88E+01	1.55E+01	100/1	3.48E+01
Maleic hydrazide		0.004	1435	2.12E+05	2.09E+04	>1000	3.90E+05	2.28E+03	>8	6.02E+05
Maleic hydrazide potassium		0.0001	>1000	1.57E+07	8.79E+05	>1000	4.64E+07	4.29E+04	>100	9.05E+07
Mancozeb		2.8	1.5			13.6			2.2	
Maneb		6.1	0.22			0.52			0.43	
MCPA	<1	1.1	97	1.49E+03	3.22E+02	160	1.43E+03	1.06E+02	220	1.59E+03
MCPA octyl ester		40200		6.33E-02	6.03E-02		1.77E-02	1.63E-01		1.06E-02
MCPA dimethylammonium		0.85	>180	2.35E+03	4.90E+02		2.33E+03	1.53E+02		2.63E+03
MCPB		47	5.6	3.96E+01	1.45E+01		2.45E+01	1.02E+01		2.18E+01
MCPB sodium		0.11		1.87E+04	2.92E+03		2.36E+04	6.06E+02		3.01E+04
Mecoprop (MCPP)		91	100	1.91E+01	7.71E+00	420	1.09E+01	6.15E+00	220	9.37E+00
Mecoprop dimethylamine		1.9		1.09E+03	2.56E+02		9.83E+02	9.44E+01		1.06E+03
Mecoprop-P		91	150	1.91E+01	7.71E+00	420	1.09E+01	6.15E+00	220	9.37E+00
Mecoprop-P dimethylamine		2		1.09E+03	2.56E+02		9.83E+02	9.44E+01		1.06E+03
Mepiquat chloride		<1	4300	1.35E+06	1.07E+05	68.5	3.00E+06	8.53E+03	268	5.07E+06
Mepronil		268	8	8.17E+00	3.84E+00	>10	4.11E+00	3.80E+00	>10	3.31E+00
Metalaxyl		6	>100	3.70E+02	1.02E+02	610	2.91E+02	4.74E+01	42	2.93E+02
Metaldehyde		0.25	7.3	5.63E+03	9.90E+02	>190	6.43E+03	2.44E+02	73	7.80E+03
Metam (metham) sodium		0.03	0.079	3.19E+04	4.20E+03		4.63E+04	6.86E+02		6.33E+04
Metamitron		1.01	326	1.62E+03	3.47E+02	101.7	1.58E+03	1.12E+02	0.22	1.76E+03
Methabenzthiazuron		35	15.9	5.14E+01	1.81E+01	30.6	3.29E+01	1.19E+01	0.119	2.99E+01
Methamidophos		0.04	25	2.75E+04	3.75E+03	0.27	3.89E+04	6.42E+02		5.24E+04
Methazole		32	4	6.69E+01	2.32E+01		4.33E+01	1.50E+01		3.95E+01
Methidathion		15	0.002	1.66E+02	5.18E+01	0.0072	1.18E+02	2.87E+01	11	1.12E+02
Methiocarb (Mercaptodimethur)	93	61	0.436	3.03E+01	1.15E+01	0.019	1.81E+01	8.46E+00	1.2	1.60E+01
Methomyl		0.65	0.9	2.04E+03	4.09E+02	0.0317	2.09E+03	1.21E+02	60	2.40E+03
Methoxychlor		4150	0.052	6.77E-01	4.68E-01	0.00078	2.47E-01	8.01E-01		1.69E-01
Methylarsonate, sodium hydrogen		0.20	>51	6.60E+03	1.12E+03	77.5	7.75E+03	2.63E+02		9.53E+03
Methyl Bromide		2.05	0.8	3.77E+02	8.89E+01	1.7	3.36E+02	3.32E+01	3.2	3.61E+02
Methyl isothiocyanate		2.91	0.37	2.04E+02	5.06E+01	0.06	1.75E+02	2.03E+01		1.84E+02
Metiram		0.37	1.1	2.37E+04	4.40E+03	2.55	2.59E+04	1.17E+03	0.27	3.07E+04
Metolachlor		91.31	2	2.53E+01	1.02E+01	25	1.44E+01	8.13E+00	0.07	1.24E+01
Metoxuron		4.94	19.8	3.76E+02	1.00E+02	215.6	3.03E+02	4.48E+01	0.06	3.08E+02

Name (ISO)	BCF	fish	Fish mg/l	LC50,96h		Daphnia mg/l	EC50, 48h		Algae mg/l	IC50,72h
	exp.	est.	exp.	est., np	est., pol.	exp.	est., np	est., pol.	exp.	est., np.
Metribuzin		4.31	59	4.04E+02	1.06E+02	4.5	3.31E+02	4.59E+01	0.0078	3.40E+02
Metsulfuron-methyl	0.9	14.79	>150	2.10E+02	6.54E+01	>150	1.48E+02	3.63E+01	2.9	1.42E+02
Mevinphos		0.26	0.012	7.08E+03	1.25E+03	0.00016	8.07E+03	3.07E+02		9.78E+03
Monocrotophos		0.02	7	1.18E+05	1.40E+04	0.023	1.88E+05	1.96E+03		2.68E+05
Monolinuron		15	56	1.18E+02	3.68E+01	32.5	8.35E+01	2.04E+01	0.001	7.98E+01
Muscalure		598	>1000	4.39E+00	2.31E+00	0.266	2.01E+00	2.68E+00		1.54E+00
Naled		3	2	1.04E+03	2.59E+02	0.005	8.91E+02	1.04E+02		9.35E+02
2-(1-Naphthyl)acetamide		6		2.60E+02	7.11E+01		2.06E+02	3.27E+01		2.08E+02
2-(1-Naphthyl)acetic acid		16	57	9.46E+01	2.98E+01	360	6.64E+01	1.68E+01		6.31E+01
2-(1-Naphthyl)acetate, ethyl-ester		307		5.67E+00	2.71E+00		2.81E+00	2.76E+00		2.24E+00
2-(1-Naphthyl)acetate sodium		0.04		4.39E+04	5.91E+03		6.26E+04	9.97E+02		8.48E+04
Napropamide		127	16.6	1.73E+01	7.32E+00	14.3	9.52E+00	6.25E+00	4.5	8.01E+00
Naptalam		157	76.1	1.18E+04	2.00E+03	118.5	1.38E+04	4.70E+02		1.70E+04
Naptalam sodium		0.09		2.74E+04	4.17E+03		3.52E+04	8.40E+02		4.53E+04
Nitrapyrin		133	5.8	1.40E+01	5.98E+00	>10	7.67E+00	5.15E+00		6.44E+00
Norflurazon		18	>200	1.37E+02	4.40E+01		9.49E+01	2.54E+01		8.96E+01
Nuarimol		100	5.6	2.56E+01	1.05E+01	8	1.45E+01	8.50E+00	2.5	1.24E+01
1,4,4a,5a,6,9,9a,9b-Octahydro-dibenzofuran-4a-carbaldehyde		4	18.1	4.33E+02	1.12E+02		3.60E+02	4.73E+01		3.72E+02
Oryzalin		295	2.88	9.53E+00	4.54E+00	1.7	4.74E+00	4.58E+00		3.80E+00
Oxadiazon		2399	1.2	1.17E+00	7.48E-01	>2.4	4.55E-01	1.15E+00		3.22E-01
Oxadixyl		0.83	360	2.72E+03	5.64E+02	530	2.70E+03	1.76E+02	45.7	3.05E+03
Oxamyl	2	0.08	4.2	2.11E+04	3.18E+03	5.7	2.75E+04	6.27E+02	3.3	3.56E+04
Oxycarboxin		0.90	19.9	2.41E+03	5.07E+02	69.1	2.37E+03	1.61E+02		2.67E+03
Oxydemeton-methyl		0.05	1.9	4.31E+04	5.96E+03	0.11	6.01E+04	1.04E+03	>100	8.06E+04
Oxyfluorfen		1257	0.2	2.34E+00	1.37E+00	1.5	9.81E-01	1.84E+00		7.22E-01
Paclobutrazol		105	27.8	2.28E+01	9.38E+00	33.2	1.28E+01	7.69E+00	7.2	1.09E+01
Paraquat dichloride		<1	2.5	7.00E+07	3.43E+06	<1	2.32E+08	1.38E+05		4.79E+08
Parathion ethyl	40	359	0.57	6.59E+00	3.22E+00	0.0025	3.20E+00	3.38E+00	0.03	2.54E+00
Parathion methyl		54	2.7	3.97E+01	1.49E+01	0.0073	2.42E+01	1.07E+01	5.3	2.14E+01
Pebulate		359	6.25	4.60E+00	2.25E+00	5.9	2.24E+00	2.36E+00		1.77E+00
Penconazole	90	290	1.3	7.97E+00	3.78E+00	6.75	3.98E+00	3.81E+00	2.98	3.19E+00
Pencycuron	154	1897	5	1.41E+00	8.72E-01	0.27	5.64E-01	1.28E+00	0.71	4.05E-01
Pendimethalin	1446	5047	0.14	4.53E-01	3.22E-01	0.04	1.62E-01	5.73E-01	0.055	1.09E-01
Permethrin	300	66834	0.0011	4.76E-02	4.87E-02	0.0006	1.25E-02	1.45E-01	0.0125	7.29E-03
Phenmedipham	165	225	1.4	1.09E+01	4.98E+00	3.2	5.59E+00	4.76E+00	0.13	4.55E+00
Phorate		212	0.013	9.99E+00	4.54E+00		5.17E+00	4.29E+00		4.22E+00
Phosalone	180	902	0.11	3.32E+00	1.85E+00	0.0012	1.45E+00	2.33E+00	0.68	1.09E+00
Phosmet		46	0.07	5.60E+01	2.05E+01	0.0085	3.47E+01	1.43E+01		3.10E+01
Phosphamidon		0.94	3.2	2.60E+03	5.50E+02	0.02	2.55E+03	1.75E+02	240	2.86E+03
Phoxim		149	0.22	1.63E+01	7.03E+00	0.000648	8.78E+00	6.19E+00	0.65	7.32E+00
Picloram		2.9	19.3	6.87E+02	1.70E+02	50.7	5.90E+02	6.78E+01	36.9	6.21E+02
Picloram potassium		0.002	24	1.15E+06	1.02E+05	68.3	3.24E+06	9.51E+03	52.6	3.77E+06
Piperalin		919	0.2	2.92E+00	1.63E+00		1.27E+00	2.07E+00		9.52E-01
Piperonyl butoxide		2175	5.3	1.26E+00	7.98E-01	3	4.98E-01	1.20E+00	0.24	3.54E-01
Pirimicarb	24	5.56	29	3.48E+02	9.46E+01	0.019	2.77E+02	4.32E+01	140	2.80E+02
Pirimiphos-ethyl		2645	0.02	1.02E+00	6.64E-01	0.0003	3.94E-01	1.04E+00		2.77E-01
Pirimiphos-methyl		741	0.64	3.35E+00	1.81E+00	1.4	1.50E+00	2.20E+00		1.13E+00
Primisulfuron-methyl		0.22	70	1.70E+04	2.93E+03	260	1.97E+04	7.03E+02	0.024	2.40E+04
Prochloraz	393	610	2.2	5.02E+00	2.65E+00	2.6	2.30E+00	3.09E+00	0.073	1.76E+00
Profenofos		1186	0.08	2.56E+00	1.48E+00		1.08E+00	1.98E+00		7.99E-01
Prometon		69	12	2.64E+01	1.02E+01		1.56E+01	7.73E+00		1.36E+01
Prometryn		192	2.5	1.02E+01	4.57E+00	12.66	5.35E+00	4.24E+00	0.02	4.39E+00
Propachlor	42	14	0.17	1.21E+02	3.75E+01	7.8	8.60E+01	2.06E+01	0.029	8.24E+01
Propamocarb hydrochloride	54	<1	163	1.97E+06	1.57E+05	284	4.35E+06	1.25E+04	301	7.34E+06
Propaquizafop	583	2307	0.19	1.56E+00	9.95E-01	>2.1	6.11E-01	1.52E+00	>2.1	4.34E-01

Name (ISO)	BCF	fish	Fish mg/l	LC50,96h		Daphnia mg/l	EC50, 48h		Algae mg/l	IC50,72h
	exp.	est.	exp.	est., np	est., pol.	exp.	est., np	est., pol.	exp.	est., np.
Propargite		3548	0.04	8.03E-01	5.43E-01	0.092	2.98E-01	9.01E-01		2.06E-01
Propazine		62	17.5	3.02E+01	1.15E+01	17.7	1.81E+01	8.52E+00	0.24	1.59E+01
Propetamphos		352	4.6	6.49E+00	3.17E+00	0.0145	3.16E+00	3.31E+00		2.51E+00
Propham (IPC)		32	32	4.50E+01	1.57E+01	23	2.91E+01	1.02E+01	26	2.65E+01
Propiconazole	52	290	5.3	9.60E+00	4.56E+00	1.7	4.79E+00	4.58E+00	0.68	3.84E+00
Propineb		0.12	0.5	1.96E+04	3.10E+03	4.7	2.45E+04	6.57E+02	0.49	3.11E+04
Propoxur		4.23	6.2	4.02E+02	1.05E+02	0.15	3.30E+02	4.54E+01	5.3	3.39E+02
Propyzamide	155	105	54	1.99E+01	8.17E+00	>5.6	1.12E+01	6.71E+00	2.9	9.52E+00
Prosulfocarb	570	1789	1.7	1.14E+00	7.01E-01	1.3	4.60E-01	1.01E+00	0.09	3.31E-01
Prosulfuron		0.13	100	2.58E+04	4.13E+03	>120	3.18E+04	8.92E+02		4.01E+04
Pyrazophos	360	339	0.016	8.96E+00	4.35E+00	0.00018	4.39E+00	4.51E+00	65.5	3.48E+00
Pyrethrins (extract)		33700	0.0052	7.92E-02	7.36E-02	0.012	2.26E-02	1.92E-01		1.37E-02
Pyrethrins I (chrysanthemates)		6902		3.87E-01	2.87E-01		1.33E-01	5.45E-01		8.84E-02
Pyrethrins II (pyrethrates)		332		9.11E+00	4.41E+00		4.47E+00	4.56E+00		3.56E+00
Pyridate	7238	14808	48	2.08E-01	1.72E-01	0.83	6.53E-02	3.80E-01	82	4.15E-02
Pyriproxyfen		10411		2.51E-01	1.97E-01		8.21E-02	4.06E-01		5.33E+02
Quintozene (PCNB)		1754	0.1	1.37E+00	8.38E-01	0.77	5.52E-01	1.21E+00		3.98E-01
Quizalofop-ethyl		867	2.8	3.50E+00	1.94E+00	2.1	1.53E+00	2.42E+00	>3.2	1.15E+00
Rimsulfuron		0.01	110	3.12E+05	3.53E+04	>360	5.14E+05	4.66E+03	1.6	7.50E+05
Rotenone		610	0.023	5.26E+00	2.77E+00	0.008	2.40E+00	3.24E+00		1.84E+00
Sethoxydim		5	38	5.28E+02	1.41E+02	1.5	4.24E+02	6.33E+01		4.32E+02
Siduron		84	18	2.24E+01	8.92E+00	18	1.29E+01	7.01E+00	0.25	1.11E+01
Simazine		14	49	1.15E+02	3.57E+01	92.1	8.20E+01	1.97E+01	0.042	7.85E+01
Sulfometuron methyl		0.07	>12.5	4.02E+04	5.93E+03	>12.5	5.31E+04	1.14E+03		6.92E+04
Sulprofos		9078	11	2.89E-01	2.23E-01	0.001	9.60E-02	4.46E-01	64	6.29E-02
2,4,5-T		130	350	1.60E+01	6.78E+00	5	8.77E+00	5.80E+00	50	7.37E+00
2,4,5-T trihydroxyethyl-ammonium		0.002		2.15E+06	1.84E+05		4.48E+06	1.62E+04		7.35E+06
2,3,6-TBA		40	>100	4.57E+01	1.64E+01		2.87E+01	1.11E+01		2.59E+01
TCA-sodium		0.002	2500	7.81E+05	6.89E+04	1428	1.58E+06	6.39E+03		2.56E+06
Tebuconazole	78	278	5.9	8.98E+00	4.24E+00	4.2	4.50E+00	4.23E+00	0.11	3.62E+00
Tebuthiuron		6	112	2.83E+02	7.86E+01	297	2.20E+02	3.71E+01	0.05	2.21E+02
Tefluthrin	3000	66834	0.00006	5.09E-02	5.21E-02	0.00007	1.34E-02	1.56E-01	>1.8	7.80E-03
Temephos		23227	8	1.63E-01	1.44E-01	0.5	4.86E-02	3.48E-01		3.01E-02
Terbacil	4	8.4	46.2	2.10E+02	6.05E+01	68	1.59E+02	2.99E+01	0.3	1.57E+02
Terbufos		1282	0.004	1.83E+00	1.07E+00	0.003	7.66E-01	1.45E+00	1.4	5.62E-01
Terbutryn		301	3	6.51E+00	3.11E+00	2.66	3.23E+00	3.15E+00	0.0034	2.59E+00
Terbutylazine		77	1.8	2.44E+01	9.59E+00	21.2	1.42E+01	7.39E+00	0.02	1.23E+01
Tetrachlorvinphos		199	0.3	1.49E+01	6.71E+00	0.0035	7.76E+00	6.26E+00		6.36E+00
Tetradifon	190	1653	>10	1.75E+00	1.06E+00	>2	7.11E-01	1.51E+00	>0.2	5.15E-01
Thiabendazole	199	19	0.56	8.61E+01	2.78E+01	0.45	5.92E+01	1.62E+01	9	5.57E+01
Thidiazuron		6.2	>1000	2.89E+02	7.96E+01	970	2.26E+02	3.71E+01		2.28E+02
Thifensulfuron methyl	1	0.21	360	1.52E+04	2.59E+03	970	1.77E+04	6.12E+02	14.5	2.18E+04
Thiobencarb		161	3.6	1.30E+01	5.68E+00	0.1	6.95E+00	5.08E+00	0.02	5.77E+00
2-(Thiocyanomethylthio)-benzothiazol (TCMTB)	250	111	0.024	1.74E+01	7.23E+00	0.022	9.74E+00	6.00E+00	0.03	8.26E+00
Thiodicarb		6	1.21	5.18E+02	1.41E+02	0.053	4.12E+02	6.42E+01		4.16E+02
Thiofanox		14	0.13	1.30E+02	4.00E+01		9.27E+01	2.19E+01		8.89E+01
Thiometon		174	8	1.15E+01	5.08E+00	8.2	6.09E+00	4.61E+00	12.8	5.03E+00
Thiophanate-methyl		4	1.07	7.40E+02	1.90E+02	12.7	6.16E+02	8.03E+01	0.8	6.38E+02
Thiram		6	0.16	3.31E+02	9.08E+01	0.21	2.61E+02	4.19E+01	1	2.64E+02
Tolclofos-methyl	700	1500	0.87	1.63E+00	9.77E-01	2.4	6.71E-01	1.37E+00	5.6	4.88E-01
Tolylfluanid		412	0.06	6.85E+00	3.42E+00	0.57	3.28E+00	3.69E+00	1.45	2.57E+00
Camphechlor (Toxaphene)		9440	0.0011	3.56E-01	2.77E-01	0.015	1.18E-01	5.58E-01	0.38	7.71E-02
Tralomethrin		3548	0.0016	1.50E+00	1.01E+00	0.000038	5.58E-01	1.68E+00		3.86E-01
Triadimefon	7.1	88	6.9	2.72E+01	1.09E+01	11.3	1.56E+01	8.64E+00	0.9	1.34E+01
Triadimenol		58	15	4.13E+01	1.56E+01	2.5	2.49E+01	1.14E+01	3.7	2.19E+01
Triallate	2040	1824	1.2	1.36E+00	8.36E-01	0.43	5.46E-01	1.21E+00	0.12	3.92E-01

Name (ISO)	BCF	fish	Fish mg/l	LC50,96h		Daphnia mg/l	EC50, 48h		Algae mg/l	IC50,72h
	exp.	est.	exp.	est., np	est., pol.	exp.	est., np	est., pol.	exp.	est., np.
Triasulfuron	0.4	0.06	>100	5.19E+04	7.49E+03	>100	6.99E+04	1.39E+03	0.77	9.21E+04
Triazamate		39	0.43	6.62E+01	2.36E+01	0.048	4.19E+01	1.59E+01	240	3.78E+01
Tribenuron methyl		0.08	>1000	3.84E+04	5.77E+03	720	5.00E+04	1.14E+03	7	6.47E+04
S,S,S-tributyl phosphorotrithioate (Tribufos)		111	0.72	2.30E+01	9.54E+00	0.12	1.29E+01	7.92E+00		1.09E+01
Trichlorfon		0.54	0.52	3.87E+03	7.56E+02	0.00096	4.04E+03	2.16E+02	>10	4.68E+03
Triclopyr		0.08	117	2.52E+04	3.78E+03	133	3.29E+04	7.43E+02	45	4.26E+04
Triclopyr-butotyl		511		5.67E+00	2.92E+00	10.1	2.65E+00	3.29E+00		2.05E+00
Triclopyr-triethylammonium		0.9		3.23E+03	6.78E+02		3.18E+03	2.15E+02		3.58E+03
Tridemorph		741	3.5	3.26E+00	1.77E+00	1.3	1.46E+00	2.15E+00	0.26	1.11E+00
Tridiphane		5046		5.16E-01	3.67E-01		1.84E-01	6.53E-01		1.25E-01
Trifluralin	1580	6019	0.02	4.53E-01	3.30E-01	0.24	1.58E-01	6.08E-01	0.085	1.06E-01
Triflusulfuron methyl		1.32	730	3.04E+03	6.74E+02	460	2.86E+03	2.30E+02	0.5	3.15E+03
Triforine	<1	11	>100	3.27E+02	9.76E+01	117	2.40E+02	5.08E+01	380	2.34E+02
Trimethacarb		36		4.32E+01	1.53E+01		2.75E+01	1.02E+01		2.49E+01
Trinexapac ethyl	6	4.6	35	4.49E+02	1.19E+02	142	3.65E+02	5.20E+01	0.4	3.73E+02
Vernolate		366	4.6	4.51E+00	2.21E+00		2.19E+00	2.33E+00		1.73E+00
Vinclozolin	6.5	72	32.5	3.22E+01	1.26E+01	4	1.89E+01	9.57E+00	16	1.65E+01
Zineb	20	0.005	2	4.54E+05	4.57E+04	0.97	8.24E+05	5.12E+03	1.8	1.26E+06
Ziram		1.7	0.47	1.49E+03	3.41E+02	0.36	1.36E+03	1.22E+02	1.2	1.48E+03
Total number	115	409	371	409	409	341	409	409	249	409

List of abbreviations used in the tables 1 to 4.

A	Acaricide
B	Bactericide
CA	Contact action
Cell div. inh	Cell division inhibitor
CSA	Contact and stomach action
CSRA	Contact, stomach and respiration action
dev.	Development
Exp.	Experimental value
Est.	Estimated value
F	Fungicide
H	Herbicide
hf	QSAR on hydrophobic substances
I	Insecticide
inh.	inhibitor
I rep	Insect repellent
Lyman	cf. reference Lyman ***et al.*** 1982
MW	Molecular weight
N	Nematicide
nhf	QSAR on non-hydrophobic substances
np	non-polar
PGR	Plant growth regulator
pol	polar
Prot.synt.inh	Protein syntesis inhibitor
R	Rodenticide
SA	Systemic action
Synt.	Synthesis
Syst.	Systemic
TGD	cf. reference TGD 1996
Vit. K inh.	Vitamin K inhibitor (anticoagulant)