NATIONAL INSTITUTE OF PUBLIC HEALTH AND THE ENVIRONMENT
BILTHOVEN

Report no. 719101030

Prediction of environmental degradation rates for High Production Volume Chemicals (HPVC) using Quantitative Structure-Activity Relationships

E. Rorije, M. Müller* and W.J.G.M. Peijnenburg

May 1997

* Fraunhofer Institute for Environmental Chemistry and Ecotoxicology (IUCT), Schmallenberg, Germany

The work described in this report was carried out within the framework of the project "Fate and Activity Modelling of Environmental Pollutants using Structure-Activity Relationships" (FAME), financially supported by the Environmental Technologies RTD Programme (DG XII/D-1) of the Commission of the European Communities, under contract number ENV4-CT96-0221.

Laboratory for Ecotoxicology, National Institute of Public Health and the Environment,
P.O.Box 1, 3720 BA Bilthoven, Tel. 030-2749111, Fax 030-2744413.

MAILING LIST

1-2 Dr. C. Nolan, EU DG-XII/D-1, Brussels, Belgium

3 Dr. G. Vollmer, Head of the ECB, Joint Research Centre, Ispra, Italy

4 Dr. B. Hansen, ECB, Joint Research Centre, Ispra, Italy

5 Dr. W. Karcher, ECB, Joint Research Centre, Ispra, Italy

6 Dr. H. Barth, EU DG-XII/D-1, Brussels, Belgium

7 Directoraat-Generaal Milieubeheer, Directie Stoffen, Veiligheid en Straling

8 Plv. Directeur-Generaal Milieubeheer, Dr.Ir. B.C.J. Zoeteman

9 Directie RIVM, directeur Milieu Ir. N.D. van Egmond

10 Sectordirecteur Stoffen en Risico's, Dr.Ir. G. de Mik

11 Hoofd Centrum voor Stoffen en Risico's, Dr. H. Köneman

12 Hoofd Bureau voor Milieu- en Natuurverkenning, Drs. R.J.M. Maas

13 Hoofd Laboratorium voor Ecotoxicologie, Dr. H.J.P. Eijsackers

14 Dr. T. Carpanini, ECETOC, Brussels, Belgium

15 Dr. P. Masscheleyn, ECETOC / Proctor & Gamble, Antwerp, Belgium

16 Dr. K. Delbeke, LISEC, Genk, Belgium

17 Dr. B. Neven, CEBETOX, Brussels, Belgium

18 Dr. K. Hiromatsu, CITI, Fukuoka, Japan

19 Dr. M. Comber, ECETOC / Zeneca, Brixham, UK

20 Dr. D. Brown, CEFIC / Zeneca, Brixham, UK

21 Dr. J. Dearden, Liverpool John Moores University, Liverpool, UK

22 Dr. D. Brooke, Building Research Establishment, Garston, UK

23 Dr. C. Watts, WRC PLC Medmenham, UK

24 Dr. D. Riley, ECPA / Zeneca, Haslemere, Surrey, UK

25 Dr. T. Hayamizu, OECD, Paris, France

26 Dr. J. Devillers, CTIS, Lyon, France

27 Dr. M. Zeeman, US EPA, Washington, USA

28 Dr. Ph. Howard, EPA, Duluth, Minnesota, USA

29 Dr. Bradbury, EPA, Duluth, Minnesota, USA

30 Dr. Lipnick , EPA, Washington, USA

31 Dr. Boethling EPA, Washington, USA

32 Dr. D. Peterson, CONCAWE, Somerville, New Jersey, USA

33 Dr. M. Klein, Fraunhofer Institute (IUCT), Schmallenberg, Germany
34 Dr. A. Wenzel, EBÖ, Fraunhofer Institute (IUCT), Schmallenberg, Germany
35 Dr. K. Vormann, Umweltbundesamt, Berlin, Germany
36 Dr. H. Güsten, IMK, University of Karlsruhe, Germany
37 Dr. M. Nendza, Analytisches Laboratorium, Luhnstedt, Germany
38 Dr. A. Sabljiç, Institute Ruder Boskoviç, Zagreb, Croatia
39 Dr. J. Damborsky, Masaryk University, Brno, Czech Republic
40 Dr. J.V. Tarazona, Ministerio de Agricultura, Peca y Alimetacion, Madrid, Spain
41 Dr. J. Falck, National Chemicals Inspectorate (KEMI), Solna, Sweden
42 Dr. A. Lundgren, National Chemicals Inspectorate (KEMI), Solna, Sweden
43 Dr. L. Torstensson, Swedish University of Agricultureal Sciences, Uppsala, Sweden
44 Dr. L. Eriksson, UMETRI, Umeå, Sweden
45 Dr. M. Sjöström, University of Umeå, Umeå, Sweden
46 Dr. T. Madsen, VKI, Hørsholm, Denmark
47 Dr. H. Tyle, Miljøstyrelsen, Danish EPA, Copenhagen, Denmark
48 Dr. J. Niemelä, Miljøstyrelsen, Danish EPA, Copenhagen, Denmark
49 Dr. E. Nikunen, Finnish Environment Institute, Helsinki, Finland
50 Dr. E.A. Vik, Aquateam, Norwegian Water Technology Centre, Oslo, Norway
51 Dr. H. Govers, MTC, University of Amsterdam
52 Dr. F. Balk, BKH Consulting Engineers, Delft
53 Dr. H. Blok, BKH Consulting Engineers, Delft
54 Dr. J.L.M. Hermens, RITOX, University of Utrecht
55 Dr. H.J.M. Verhaar, RITOX, University of Utrecht
56 Drs. W. Vaas, RITOX, University of Utrecht
57 Drs. A. Freidig, RITOX, University of Utrecht
58 Drs E. Urrestarruzu, RITOX, University of Utrecht
59 Dr. P. van Beelen (RIVM/ECO)
60 Dr. C.W.M. Bodar (RIVM/CSR)
61 Dr. J.H.M. de Bruijn (RIVM/CSR)
62 Dr. G.H. Crommentuijn (RIVM/CSR)
63 Dr. J. Herremans (RIVM/CSR)
64 Dr. O. Klepper (RIVM/ECO)
65 Dr. C.J. van Leeuwen (RIVM/CSR)

66 Dr. H. Loonen, ECB, Joint Research Centre, Ispra, Italy (RIVM/ECO)

67 Dr.Ir. D. Van de Meent (RIVM/ECO)

68 Drs. E. van de Plassche (RIVM/CSR)

69 Ir. C. Roghair (RIVM/ECO)

70 Dr. J. Struijs (RIVM/ECO)

71 Dr. T.G. Vermeire (RIVM/CSR)

72-74 Authors

75 Head of Public Relations RIVM, Drs. J.A.M. Lijdsman-Schijvenaars

76 Depôt Nederlandse Publicaties en Nederlandse Bibliografie

77 Library RIVM, Bilthoven.

78 Report Registration Department

79-110 Extra copies for RIVM Report Sales department

CONTENTS

SAMENVATTING

In het kader van het EU-project "Fate and Activity Modelling of Environmental Pollutants using Structure-Activity Relationships" (FAME) zijn schattingen gemaakt van de (bio)degradatiesnelheden van 1073 stoffen in verschillende milieucompartimenten. Deze schattingen zijn uitgevoerd voor alle zuivere stoffen op de lijst van High Production Volume Chemicals (HPVC) lijst van de Europese Unie (4 Juni 1995). Met behulp van QSARs zijn geen schattingen te maken voor de grote groep van mengsels of slecht definieerbare substanties (> 50% van de HPVC). De gebruikte modellen zijn Quantitative Structure-Activity Relationships (QSARs) die in een eerder EU-project (contract nr. EV5V-CT92-0211 "QSARs for Predicting Fate and Effects of Chemicals in the Environment") zijn geselecteerd uit in de vakliteratuur gepubliceerde modellen. De nauwkeurigheid van de schattingen wordt in dit rapport gegeven aan de hand van eventuele validatiestudies en de statistische gegevens van de modellen. Gezien de grote hoeveelheid bestaande stoffen waarvoor nog geen of slechts enkele gegevens over de degradatie-kinetiek in het milieu beschikbaar zijn, kunnen deze schattingen dienen als aanvullende informatie voor prioritering van stoffen en voor de risico-evaluatie van bestaande stoffen in de EU die momenteel wordt uitgevoerd in het kader van de Europese "Regulation (EEC) 793/93 on existing chemical substances". Voor die eindpunten waarvoor meerdere modellen geschikt waren is een vergelijk gemaakt van de modelschattingen. Verscheidene modellen verschillen onderling voor aanzienlijke hoeveelheden stoffen, bijvoorbeeld voor biodegradatie wordt voor 19,5% van de HPV verbindingen een tegenstrijdige modelvoorspelling gedaan. Deze onzekerheden dienen zeker meegenomen te worden in de betrouwbaarheidsinschatting van de voorspellingen. De schattingen voor de HPVC en daarmee ook de geselecteerde QSAR modellen zullen in de toekomst worden gevalideerd met behulp van data van de Europese chemische industrie, die op dit moment verzameld worden door de EU.

SUMMARY

Estimates of (bio)degradation kinetics for 1073 compounds in various environmental compartments have been made as a part of the EU-project "Fate and Activity Modelling of Environmental Pollutants using Structure-Activity Relationships" (FAME). These estimates have been made for all single compounds on the High Production Volume Chemicals (HPVC) list of the European Union (as of June 4th 1995). No predictions can be made for the large amount (> 50%) of mixtures and ill-defined compounds on the HPVC-list. The models that have been applied are Quantitative Structure-Activity Relationships (QSARs), which were selected from literature. An indication of the precision of the estimates is given, either based on available validation studies of the models, and/or based on the statistical quality of the models. Given the large amount of compounds for which no or very few experimental degradation kinetics are available, these estimates can serve as supplementary information for the priority setting and the risk assessment of existing chemicals in the EU that is now being performed as a part of EU Regulation (EEC) 793/93 on existing chemical substances. For those endpoints for which more than one model has been selected an evaluation of the performance of the various models is given. The various models sometimes disagree for a substantial part of the HPVC. For example in biodegradation 19,5% of all predictions for the HPVC the biodegradation models disagreed. This information is important in the estimation of the precision of the prediction. In the future, the estimates, and therefore the selected QSAR models, will be validated using new data on the HPVC that are being collected by the EU at this moment, from the European industries.

1. INTRODUCTION

In 1993 the European Union has adopted the Regulation (EEC) 793/93 on existing chemical substances[1], as a first step towards managing the potential risks posed by chemicals to man and the environment. This regulation is divided in three main parts: data collection, priority setting and risk assessment. The data collection part is again divided into three phases, focusing first (Phase I and II) on the High Production Volume Chemicals (HPVC), i.e. those chemicals which have been imported or produced in quantities exceeding 1000 metric tonnes per year. The first two phases of data collection have been concluded June 4th 1995. In the third phase the focus will be on the whole European Inventory of Existing Chemical Substances (EINECS). Before the end of the data collection and even before the adoption of the Council Regulation it was already clear that large gaps in existing data would appear[2]. The enormous amount of existing chemicals -- the EINECS contains already well over 100.000 compounds -- makes clear that testing alone will not be sufficient to supply all the data needed for proper risk assessment within any appropriate time scale. It is therefore the intention of the European Commission to use Quantitative Structure-Activity Relationships (QSARs) in connection with the priority setting part, and in a smaller extent also for risk assessment within the framework of Council Regulation (EEC) 793/93. In order to fill the expected data gaps and to assess the applicability and suitability of QSARs for priority setting and risk assessment, selected relationships have now been applied to the HPVC list (phase II) as of June 4th, 1995 by the European Chemicals Bureau, Ispra, Italy. It is the intention that in the future these relationships will also be applied to the rest of the EINECS database.

STRUCTURE-ACTIVITY RELATIONSHIPS

Structure-Activity Relationships (SARs or QSARs) were originally developed within the pharmacological sciences. During the last decade, the number of QSAR studies in the field of toxicology as well as environmental chemistry and ecotoxicology is steadily growing[3-6]. QSARs are based on a relationship between some activity (chemical or biological) and the chemical structure or physico-chemical properties of a series of chemicals. The techniques to derive these relationships are manifold: from simple linear regression to multivariate data analysis and to the application of artificial neural networks and genetic algorithms. An example of a simple QSAR would be the relationship between the boiling point of a series of linear alkanes and the number of carbon atoms in the respective molecule. A graphical representation of this relationship is given in figure 1.

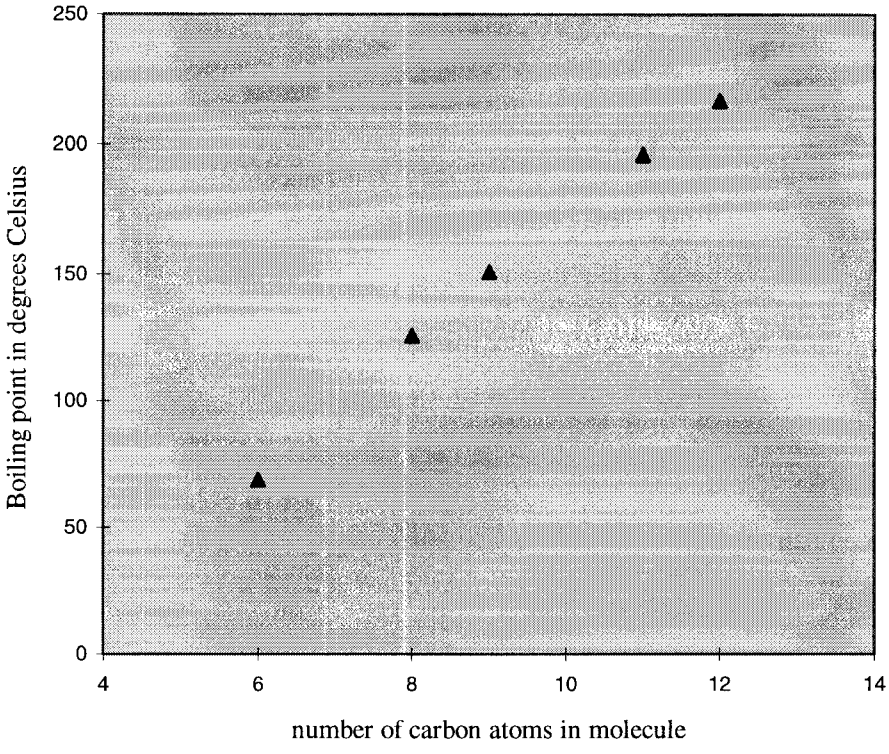


Figure 1. Relationship between boiling point and number of carbon atoms in a series of 5 linear alkanes.

When the property 'boiling point' would be fitted to the descriptor 'number of carbon atoms' using least squares linear regression, the QSAR would look like this:

$$[boiling\ point] = 24.4\ (\pm 0.96)\ x\ [\#\ of\ carbon\ atoms]\ -\ 73.1\ (\pm 9.0) \qquad (1)$$
$$r^2=0.995 \quad n=5 \quad s=4.57$$

in which r^2 is the goodness of fit, sometimes expressed as the percentage (r^2=99.5%) of variation in the dependent variable (in this case the boiling point) that can be explained by the descriptor variable (the number of carbon atoms in the molecule); n is the number of data points used to fit the model; and s is the standard deviation in the calculated dependent variable (the boiling point). The numbers between brackets give the standard error in the least squares regression coefficients. The better the relationship the smaller these standard errors will become. From the statistics of this relationship and the graphical representation we could conclude that this is a good, stable QSAR. One of the ways to look at the quality of a QSAR is to calculate Confidence Levels (C.L.). The C.L. are dependend on the standard error of prediction, s, the number of datapoints used to fit the relationship, and the level of confidence that is desired, i.e. 95% confidence. The calculated C.L. then gives the interval in which a predicted boiling point of a chemical lies with this specified certainty. In

this case the 95% C.L. interval will be quite narrow, becuase of the small values of the standard deviation and the standard errors in the coefficients. On the other hand only 5 datapoints have been used to fit the relationship, which increases the confidence interval. In figure 2 relationship (1) is given together with its 95% confidence interval, shown as the two dotted lines. Relationship (1) can now be used to make predictions of boiling points of other chemicals. At this point however we will have to restrict ourselves firmly.

RESTRICTIONS TO THE APPLICATION OF QSARs

If relationship (1) would be applied to the whole list of HPV chemicals large errors in the predictions would occur. The relationship is valid only for the *chemical domain* that it describes, in this case the linear alkanes. If the boiling point of for instance a primary alcohol would be predicted with this relationship the temperature would be largely underestimated for most of the alcohols. This is illustrated in figure 2 for four primary alcohols.

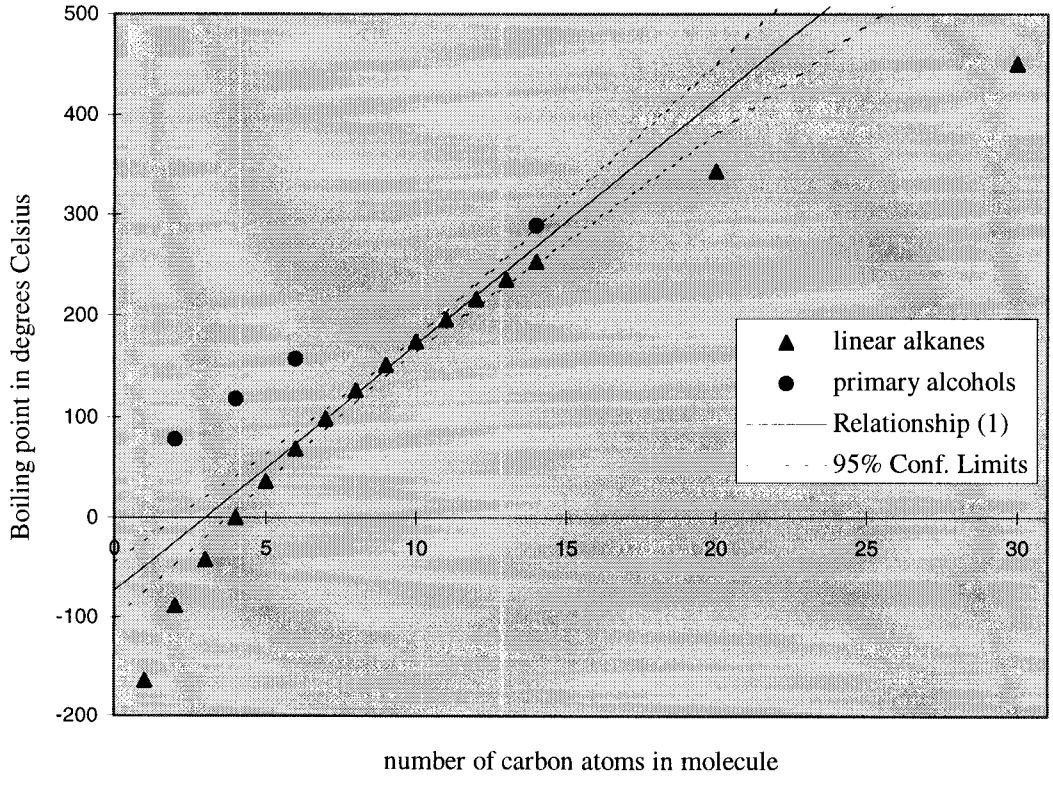


Figure 2. Relationship between the boiling point of linear alkanes, some primary alcohols and the number of carbon atoms in the molecule. Relationship (1) is given for comparison.

The reason for this deviating behaviour of the alcohols lies in their possibility to form hydrogen bonds. The *mechanistical background* of relationship (1) does not apply to the group of primary alcohols. However, even if relationship (1) would be applied to linear alkanes only, the model would give very poor predictions, as can be seen in figure 2, from the deviation of the data series of linear alkanes from the solid line representing relationship (1). The reason for these large deviations is that we have tried to extrapolate the model outside the boundaries of its chemical domain. Apparently the relationship between the number of carbon atoms and the boiling point of linear alkanes is not linear anymore, when the chemical domain is extended. This illustrates one of the main limitations of QSARs; they can only be (safely) applied within a properly specified chemical domain, and any extrapolation can lead to large errors in prediction. When a QSAR becomes more complicated, using more descriptor variables, or more advanced fitting techniques, the definition of the domain also becomes more complicated. In the application of QSARs we have to make sure the model is not extrapolated outside its domain.

The restrictions to the applicability of relationship (1) are very straightforward in this case. The model is only applicable to linear alkanes, with the number of carbon atoms between 6 and 12. The predictions we *can* safely make are for heptane and decane (nr. of carbon atoms is 7 and 10 respectively). This leads to:

Predicted boiling point of heptane	= 97.8 °C (± 9.3)	(experimental value 98.5)
Predicted boiling point of decane	= 174.1 °C (± 6.9)	(experimental value 174.1)

with the 95% Confidence Limits given in brackets behind the predicted values. The fact that the interval is larger for the prediction of the boiling point of heptane reflects the fact that this prediction is more towards the boundaries of the chemical domain of the QSAR. This is also graphically shown in figure two, where the interval of the Confidence Limits becomes larger when it is further away from the mean of the datapoints used for fitting the relationship.

SELECTION OF MODELS

Within the EU-DG XII/D-1 Project "QSAR for Prediction Fate and Effects of Chemicals in the Environment" a selection of qualitatively good and applicable QSARs from the scientific literature has been made, for various environmentally important endpoints: QSARs for ecotoxicity, soil sorption, chemical degradation in the gas phase, chemical degradation in the aqueous phase and QSARs for biodegradation. The literature search and the selection criteria are extensively described in the final report of this project[7]. The main selection criteria were statistical soundness of the model, reproducibility (which means that

the raw data has to be available) and preferably a mechanistical background that explains the success of a model. The selected models for the three degradation endpoints (atmospheric, aquatic and biodegradation) have now been applied to the list of HPV chemicals and the estimations are given in this report.

2. MATERIALS AND METHODS

Table I gives an overview of the selected models that were applied to the HPVC, showing the environmental degradation processes for which models have been selected and the chemical classes that are covered by the models, together with the type of input needed for each model.

TABLE I **Selected degradation QSAR models applied to the HPVC list, their chemical domain and the type of input needed**

log K_{ow} estimation	SMILES code [a]
Biodegradation	
1. BIODEG model - organic compounds	SMILES code [a]
2. OECD - acyclic organic compounds	SMILES code [a]
3. OECD - mono-aromatic compounds	SMILES code [a]
Degradation in the Gas Phase	
4. Atmospheric Oxidation Program - organic compounds	SMILES code [a]
5. MOOH-method - not N,S or P containing compounds	MO-calculation[b]
Degradation in the Aqueous Phase	
6. HYDROWIN, Hydrolysis of esters, epoxides, haloalkanes, carbamates and halomethanes	SMILES code [a]
7. hydrolysis of brominated alkanes	Taft substituent constants
8. hydrolysis of esters and carbamates	Hammett and Taft constants
9. hydrolysis of benzonitriles	Hammett substituent constant
10.oxidation of phenols by $^1O_2$	Energy of HOMO calculated[b]
11.oxidation of phenls by MnO_x	Energy of HOMO calculated[b]
12.oxidation of anilines by MnO_x	Energy of HOMO calculated[b]
13.reduction of halogenated aliphatics	Activation energy of reaction
14.reduction of halogenated aromatics	Hammett substituent constant
15.reduction of nitroaromatic compounds	Energy of LUMO in solution[b]

[a] More general: two-dimensional structure information; i.e. MOLfiles are possible as well as SMILES code

[b] Molecular Orbital calculations using semi-empirical quantum chemical methods (MOPAC/AM1).

As can be seen from this table, various types of descriptors were needed to produce predictions with the models. The various (literature) sources or calculation methods for these inputs are given in the following section.

SOURCES for QSAR INPUT

- SMILES code

When the chemical structure of a compound is known, the SMILES code can in principle be formulated by hand, using straightforward rules.[8-9] The SMILES codes for all 1047 single compounds on the HPVC list were provided by the Environmental Chemicals Bureau (ECB), Ispra, Italy, together with the compound's CAS-nr. and IUPAC name. The models using SMILES code as input are fragment contribution models, where the descriptors of the model are the number of certain substructures present in the molecule.

- Molecular orbital energy calculations

MO energy calculations for the determination of the energy of the Highest Occupied Molecular Orbital (E_{HOMO}) and the Lowest Unoccupied Orbital (E_{LUMO}) were carried out at the restricted Hartree-Fock level (RHF) using the AM1[10] semi-empirical SCF-MO method, as implemented in the MOPAC Version 6.00 program.[11-12] All structures were optimized and further refined using the Eigenvector Following algorithm with the PRECISE option. All optimized geometries were characterized as ground states by calculating the force-constants, and checking that these were all positive. From the calculation output, the energy level of the highest occupied molecular orbital (E_{HOMO}) and the lowest unoccupied molecular orbital (E_{LUMO}) were extracted. According to Koopmans' theorem these energies can be regarded as approximations of the compounds ionization potential (IP) and electron affinity (EA), respectively. For optimization of the chemicals geometry in solution the COSMO solvation model[13] was used as implemented in MOPAC93.

- Hammett and Taft constants

These were taken from the standard work by Hansch and Leo[14]. If a constant for a specific substructure was not found in this book, the compound containing the substructure has not been calculated.

- Activation Energy

For the calculation of activation energies of the reductive dehalogenation of aliphatic compounds the Gaussian92 *ab initio* quantum chemistry package[15] was used to calculate the unrestricted Hartree-Fock level (UHF) heats of formation for the RHF/STO-3G* geometry optimized ground states of all compounds. All geometry optimizations were followed by a frequency calculation to determine the zero-point vibrational energy and to ensure that the first six force constants were either zero, or small and positive, indicating a ground state local minimum.[16] Using the optimized geometries of the ground states, the transition states were subsequently constructed by placing a hydrogen atom at 1.5 Å distance from the halogen atom to be replaced. This hydrogen atom is used as a model for

the various non-specific enzymes and/or coenzymes that are responsible for the rate limiting step in the dehalogenation reaction under environmental conditions. Since we are only interested in the differences in dehalogenation reaction rates caused by variation in the structures of the aliphatic compounds, this simplification is justified, and results in necessary reduction of computer calculation time. The heats of formation for the transition states were then calculated at the UHF/STO-3G* level after a UHF/STO-3G* geometry optimization, with charge 0 and multiplicity 2 (a doublet state). These calculations were also followed by a frequency calculation to determine the zero-point vibrational energy and to ensure that the first force constant was negative (imaginary) and the second to sixth force constants were zero, or small and positive, indicating a saddle point in the energy surface, thus indicating a true transition state[16]. With these calculated energies we can determine the activation energy using the following equation:

$$E_{activation} = (E_{transition\ state} + E_{zero\ trans.}) - (E_{aliphatic} + E_{zero\ ground} + E_{hydrogen}) \quad (2)$$

MODEL DESCRIPTIONS

All the selected models are extensively described in the report of the EU-DG XII/D-1 project[17-19], giving the mathematical description and the statistical analysis of the model using a standard form. Here we will give a brief, textual description of the models, their input and output, and the importance of the modelled pathways in the environment. Added to the estimations of degradation in the environment is the estimation of the octanol water partitioning coefficient, log K_{OW}, and selected literature values of this coefficient, since it plays such an important role in the (bio)availability of chemicals in the environment, and the partioning of chemicals over different environmental compartments. The model used to calculate the estimated log K_{OW} values is SRC-KOWWIN for Microsoft Windows from Syracuse.[20] The estimation method has been described by Meylan & Howard.[21] This estimation method was preferred over the more generally known ClogP method because a recent evaluation[22] showed that KOWWIN gives comparable or even slightly better results than ClogP and moreover, ClogP failed to come up with an estimation due to missing or unrecognized fragments over 10 times more often than KOWWIN.

Biodegradation probability estimation

1. BIODEG linear and non-linear

Howard and co-workers have developed four fragment contribution models that can be used to estimate the probability of biodegradation of a chemical in the environment.[23-25] Two models are fitted to the judgement of an evaluation of various different biodegradation

test results from the Environmental Fate Data Base (EFDB)[26], one using linear regression and one using a form of non-linear fitting. The other two are fitted to an expert judgement of the average residence time of chemicals in the environment. Since this last endpoint is not of much use in the priority setting and risk assessment schemes from the EU these models have not been selected for use on the HPVC chemicals. The linear and non-linear fragment contribution models are thus applied in this report. These models use 36 fragments as descriptors with the molecular weight of the molecule as an added descriptor, and are fitted on the evaluated biodegradation data of a series of 295 organic chemicals. The output of the models, x, is a number that should be interpreted as follows:

$$\begin{aligned} x < 0.5 &= 0 \quad \textit{Chemical biodegrades slowly or not at all} \\ x > 0.5 &= 1 \quad \textit{Chemical biodegrades fast} \end{aligned} \qquad (3)$$

It is important to note that this number is not representing a smooth scale. Values of x close to 0.5 cannot be clearly interpreted. This is due to the fact that the 0/1 or yes/no output reflects experimental data for readily biodegradable compounds from standardized test. These tests typically produce 'biodegradable' (1) or 'non-biodegradable' (0) as a result.

2-3. OECD-models 75 and 78

Two other fragment contribution models developed for the OECD are also applied, namely models 75 and 78 of the OECD report on biodegradation models[27], developed by Degner.[28] These models use fewer fragments as descriptors (7 and 9 respectively) but are applicable only to well defined chemical classes. Model #75 is applicable to acyclic compounds, not a dithioether, a hydrazine or a compound with atoms other than C, N, H, O, P, S or halogen. Model #78 is applicable to monocyclic aromatic compounds, with (mono or multiple) substituents -OH, -COO-R, $-OCH_3$, $-SO_2$, $-NO_2$, $-NH_2$, -halogen, aliphatic chains with a non-terminal hetero-atom, branched alkyl chains. The models have been fitted to biodegradation test results from the MITI standardized test for ready biodegradability (65 and 60 compounds respectively). Again the result of the model is a number, x, that should be interpreted as a yes/no result. The interpretation of the model and the code given in Appendix I are as follows:

$$\begin{aligned} x < 0 \quad & \textit{Chemical biodegrades slowly or not at all} && = 0 \textit{ in Appendix I} \\ x > 0 \quad & \textit{Chemical biodegrades fast;} && = 1 \textit{ in Appendix I} \end{aligned} \qquad (4)$$

Chemical Degradation in the Gas-Phase

4. Atkinson's Group Contribution method

The Atkinson's group contribution method[29-31] and a recent update of the method[32] have been developed for the estimation of OH-radical reaction rate constants and is based on four possible reaction pathways. These pathways by which the hydroxyl radicals can react with organic compounds are: (i) hydrogen atom abstraction, (ii) hydroxyl radical addition to double and triple bonds, (iii) hydroxyl radical addition to aromatic rings, and (iv) reaction with nitrogen, sulphur and phosphorus containing groups. The mechanisms are modelled by an additive fragment contribution scheme to estimate the contribution of each reaction (13 parameters for reaction centers and 71 substituent constants). The group contribution scheme is based purely on statistical arguments (fitting to known data) and does not have a mechanistical background. It is very difficult to define the boundaries and the range of applicability of this method. At least one reaction center (of the 13 defined) has to be present in the molecule to be able to do a prediction, but otherwise the method does not give any restrictions to the user. The method does not give chemical classification rules, which would indicate when the method will give reliable estimates or when this method should not be used.

The model yields the second order reaction rate constant k for reaction with OH-radicals with units 10^{-12} cm^3/molecule-sec. The average OH-radical concentration in the atmosphere is assumed to be 1.5 x 10^6 molecules/cm^3 during day-time. Taking a yearly average of 12 hours of daylight the atmospheric half-life in days is then given by:

$$t_{1/2}\,(\text{days}) = \ln 2 / (k \times 1.5 \times 10^6 \times 12\text{hr.} \times 60\text{min.} \times 60\text{sec.}) \qquad (5)$$

Atkinson's method also provides a fragment contribution scheme for the reaction of unsaturated compounds (not aromatic) with ozone (O_3). For calculation of atmospheric half-lifes based on reaction with ozone an average O_3 concentration over a 24-hour day in the atmosphere is used of 7 x 10^{11} molecules/cm^3. The half-lifes in Appendix 2 are calculated by substituting this concentration for the OH-radical concentration in equation *(5)*, and substituting 12 hours with 24 hours. Because the OH-radical is not the only sink in the atmosphere (it is however the single most important), atmospheric half-lifes based on the estimated reaction rate with OH-radicals in the atmosphere will always give a worst case scenario. Sometimes the ozone reaction or reaction with nitrate-radicals (NO_3-radicals) during night-time, may contribute significantly to the removal of a chemical from the atmosphere. For compounds likely to react significantly with nitrate radicals an indication is given in Appendix 2.

5. MOOH-method

Klamt and co-workers have developed QSARs for three of the reaction routes of the OH-radical with organic compounds, (i) hydrogen atom abstraction, (ii) hydroxyl radical addition to double and triple bonds and (iii) hydroxyl radical addition to aromatic rings.[33] Reactions with oxygen containing compounds have been modeled in a later addition,[34] but reactions with other heteroatoms like nitrogen, sulphur and phosphorus are not taken into account. Instead of an additive group contribution scheme as used by Atkinson *et al.* these models are based on semi-empirical calculation of molecular orbital energies. To make a prediction the ground state of an organic molecule has to be structurally optimized using the AM1[10] parameterization in the MOPAC program.[11-12] From the atomic and molecular orbital coefficients various descriptors are then derived to make a prediction of the reactivity of the compound with OH-radicals in the different reaction routes. The derivation of the MO-based descriptors has a sound mechanistical basis, and in principle the predictive capabilities of this model are limited only by the semi-empirical parameterization of the AM1 scheme. The models give second order reaction rate constants which can be treated as mentioned above, using equation (*5*) to calculate atmospheric half-lifes.

Hydrolysis

6. HYDROWIN

The HYDROWIN program[35] from SRC incorporates models for the estimation of the rate of hydrolysis of esters, carbamates, alkyl halides and epoxides in the environment. These models have been described in an EPA-report[36], unfortunately the models have never been published in international journals, and were therefore not evaluated within the EU-QSAR-project. Since the data are not available these models could not be recalculated or evaluated. Only for the esters (part of) the data has been published.[37] Recalculation of the ester models proved to be very difficult because Hammett and Taft constants from different sources were mixed. Nevertheless, the estimates from the HYDROWIN program have been incorporated in this report, but they should be used with care. The results of the HYDROWIN calculations are expressed in Appendix 3 as half-lifes. The hydrolysis reactions are discussed in the following parts.

7. Hydrolysis of halogenated alkanes

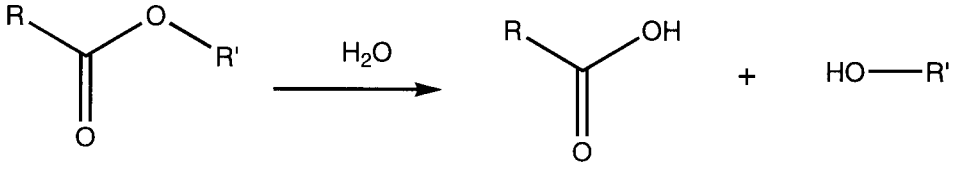
HYDROWIN provides estimates of the base catalyzed hydrolysis rates of halogenated alkanes. A selected model by Vogel & Reinhard[38] gives an estimation of the base catalyzed hydrolysis of brominated alkanes, yielding the subsequent alcohols:

$$R\text{-}Br + H_2O \rightleftharpoons R\text{-}OH + Br^- + H^+ \qquad (6)$$

The model uses Taft's polar constant σ_i as a descriptor for the pseudo first order hydrolysis rate constants. The influence of pH on the reactivity is therefore not taken into account. The environmental half-lifes as calculated with this model are therefore valid for pH 7. At lower pH values other hydrolysis mechanisms (neutral or acid catalyzed) may become more important than the base catalyzed reaction. This also holds for the HYDROWIN estimates. The estimation of the hydrolysis half-life in Appendix 3 thus gives a worst case approximation, leaving out the contribution of the two other hydrolysis mechanisms. The model is restricted to saturated linear and branched bromoalkanes, with substituents restricted to bromo and phenyl groups.

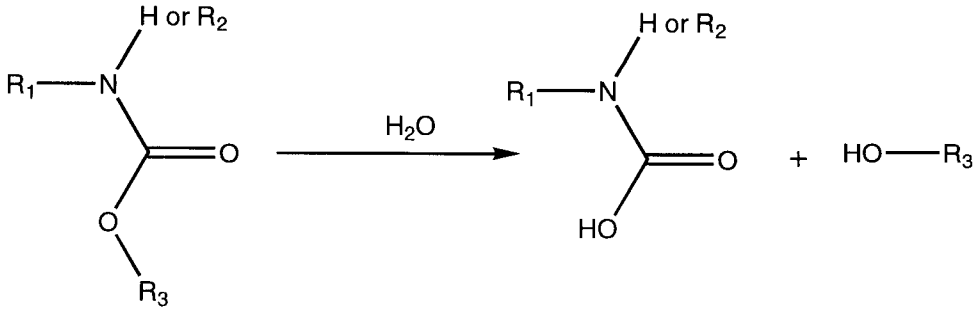
8. Hydrolysis of Esters and Carbamates

The base catalyzed hydrolysis of esters and carbamates is described by three Hammett and Taft substituent constant models by Drossman and co-workers,[37] and these models are also incorporated in the HYDROWIN program. The products of the hydrolysis of esters and carbamates are an acid and an alcohol. One model is for organic compounds containing the ester functionality:



(7)

The second and third model are for carbamates with either a hydrogen or a non-hydrogen substituent on the nitrogen atom respectively:



(8)

Recalculation of the models has been performed using Hammett and Taft substituent constants from the overview by Hansch & Leo,[14] since the original models mixed substitutent constants from different sources. The recalculation has lead to a model comparable to that published by Drossman *et al.*, only showing slightly worse statistics. All three models yield second order alkaline hydrolysis reaction rate constants. To arrive at an

environmental half-life, this reaction rate constant should be multiplied by the concentration of hydroxyl-ions in water. Half-lifes given in appendix 3 are calculated at pH 7. The estimated half-lifes are valid for the ester or carbamate moiety only when it is the fastest hydrolysing group in the molecule. When other easily hydrolysing groups are present in the molecule the half-life could be less. Restrictions in applicability of the models are defined by the availability of the Hammett and Taft substituent constants.

9. Hydrolysis of Benzonitriles, *para*-substituted

The model describes the neutral and base catalyzed hydrolysis of substituted benzonitriles to their corresponding benzoic acids in the aqueous environment[39], according to equation *(9)*. The experimental data is coming from elevated temperature experiments.

(9)

The model yields a first order rate constant for neutral hydrolysis at pH 7.7 and temperature of 85 degrees Celsius. To extrapolate these reactivities to environmentally relevant temperatures the Arrhenius equation is used (equation (10)):

$$ln(k) = ln(A) - E(act) / RT \qquad E(act) \text{ is determined to be } 40.7 \text{ KJ/Mol} \quad (10)$$

The half-lifes as given in Appendix 3 are calculated at 20°C.

Oxidation in the aqueous environment

10. Oxidation of phenols by $^1O_2$ and MnO_x

Singlet oxygen, $^1O_2$, the first excited state of oxygen, is produced by sunlight in surface waters and constitutes an important transformation pathway in the aquatic environment, although various other oxidants can play an important role. This is in contrast with tropospheric oxidant chemistry, where the main oxidation pathway is reaction with OH-radicals in the daytime. The rate-determining step in the oxidation reaction of phenols is thought to be a single-electron transfer from the phenolate anion to the oxidant:

(11)

The result is a phenoxide radical, which will rapidly be further oxidized by reaction with water, shifting the equilibrium to the right[40]. For the oxidation by manganese oxides, the same reaction mechanism is postulated. Manganese oxides constitute a minor oxidant in the environment, but the fact that reaction with both oxidants can be modelled using the same

descriptor, lends belief to the hypothesis that the same mechanism, and thus the same relative reactivity of the phenols, applies to most environmental oxidants. Oxidation in surface waters is not dominated by a single oxidation process; several oxidants are present at various steady-state concentrations. Some examples of environmental oxidants present in surface water are singlet oxygen, $^1O_2$, the hydroxyl radical, ·OH, or oxyradicals, RO_2· which can be formed under the influence of sunlight. Various other oxidants can be present, depending on the specific environmental conditions. This is in contrast to the tropospheric oxidant chemistry, where the main oxidation pathway is reaction with OH-radicals in the daytime, and with NO3-radicals in the night. Obviously, identification of the oxidant which plays a dominant role is needed in order to use QSAR correctly for predictive purposes. However, for a prediction, or better assessment, of the *relative* rate of oxidation, a measure of the susceptibility of a compound to degradation by any of these oxidants would satisfy. The models are described in detail in Rorije *et al.*[41] The calculated rate constants for reaction of the singlet oxygen with the dissociated and undissociated phenol are transformed to estimated environmental half-life given in Appendix 3 using the pKa of the phenol to calculate the fraction of the phenolate ion present at pH 7, and an average concentration of singlet oxygen in the first meter of surface water of 4 x 10^{-14} M is used.[40]

11. Oxidation of para-substituted anilines by MnO_2

The model describing the oxidation of para-substituted anilines by manganese oxides is based on the same hypotheses as the oxidation models for the phenols. Since manganese oxides do not constitute an important transformation pathway in the environment no half-lifes are estimated, but the pseudo-first order reaction rate constants are given in Appendix 3. The importance of these reaction rate constants is not their absolute value, but the relative reactivity in the environment. Based on what is said above for the phenols it is thought that the relative rates of reaction for most of the oxidation reactions in the environment will not change dramatically with a change of oxidant.

12. Oxidation of polychlorinated biphenyls by OH-radicals

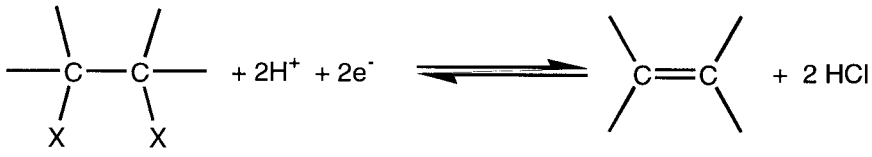
The model estimates the aqueous-phase oxidation of PCBs by OH-radicals in the aqueous phase using the number of non-chlorinated sites of the PCB as a descriptor. The model is described by Sedlak & Andren.[42] The chemical domain of the model is very clear, it is applicable only to PCB's. Since there are no PCBs on the HPVC list, this model has not been applied. Also the environmental significance of the oxidation of PCBs in the aqueous phase is very questionable since the environmental concentration of OH-radicals in the aqueous phase will be very low.

Reduction in the aqueous environment

13. Dehalogenation of halogenated aliphatic compounds

Two models are applied to estimate the rate of dehalogenation of halogenated aliphatics in an anaerobic sediment-water system. The two main dehalogenation reactions are given in equations 12 and 13:

(12)



(13)

Both reactions are thought to be rate limited by the transfer of an electron from some environmental donor to the halogen atom. Environmental reductors that have been shown to dehalogenate aliphatic compounds are a.o. porphyrins, vitamin B12. In general the availability of electron donors in the environment is related to the organic carbon content in the sediment.[43]

The two models yield two estimates of the reductive dehalogenation rates in the anaerobic environment. Both models are based on the same laboratory data, but use different parameters to describe the kinetics. The first model uses 36 physico-chemical or biological descriptors, fitted to the data using the PLS algorithm. This model is described by Eriksson *et al.*[44] A disadvantage of this model is that in order to do predictions one has to find most (preferably all) descriptors for that compound. Especially the biological descriptors are very hard to find. Therefore this model has not been applied to all halogenated aliphatic compounds on the HPVC list. The other model is based on a single descriptor, the *ab initio* calculated activation energy of the dehalogenation reaction. In principle this descriptor can be calculated for every compound that exists, but the calculations are rather time consuming. A description of the model is given by Rorije *et al.*[45] The calculated half-lifes in Appendix 3 are for the reaction in Vecht-sediment from Nieuwkoop, The Netherlands. However, the *relative* reactivity of the halogenated aliphatics is not thought to change dramatically when other sediment-water systems are used.

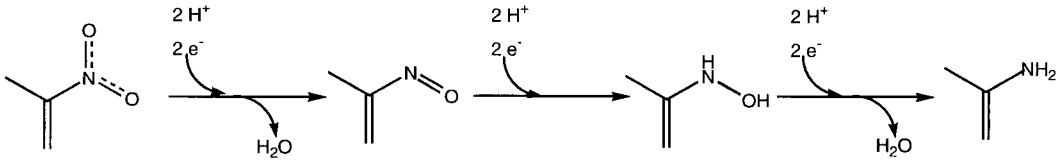
14. Dehalogenation of halogenated aromatic compounds

This model uses Hammett substituent constants to explain the differences in reactivity of substituted halogenated aromatic compounds in the dehalogenation reaction in anaerobic sediment-water systems. The reaction is given by equation 12. The model has been developed by Peijnenburg *et al.*[43,46] and is very well described to be restricted to halogenated benzenes, toluenes, anilines and phenols. The half-lifes calculated in Appendix

3 are for the reaction in Loosdrechtse Plassen sediment. To extrapolate to other sediments a relation with the organic carbon content of the sediment is given by Peijnenburg *et al.*[43,46] The sorption corrected order of reactivity will not change when the organic carbon content of the sediment is changed.

15. Reduction of nitro-aromatic compounds

Under anoxic conditions nitro-aromatic compounds are reduced in several steps to their respective anilines, equation *(14)*.



(14)

The reactivity of nitrobenzenes in anaerobic environments is described using the calculated energy of the Lowest Unoccupied Molecular Orbital of the parent compound. This makes sense because the nitrobenzene has to accept an electron from the environmental reductor. The model is described by Rorije *et al.*[18] In Appendix 3 the estimated reaction rate constants are given, since the data on which the model is based, is are not based on environmental systems.

3. RESULTS

The results of the log K_{OW} calculations and the biodegradation estimations are given in Appendix 1. The biodegradation probability is given according to calculations with the BIODEG linear and non-linear models by Howard *et al.*[24,25] and the models no. 75 and 78 introduced in the OECD Environment Monograph[27]. This probability is either 1, indicating rapid biodegradation, or 0, indicating slow or no biodegradation. In Appendix 2 the reactivities with the hydroxyl radical and ozone has been calculated according to Atkinson's model, and the reactivity with OH-radical as calculated with the MOOH method. All values are given as half-lifes in days. Both these appendices give the list of 1073 single compounds that are identified in the HPVC, and to which a SMILES code could be attributed. The complete HPVC list would contain 2413 compounds/mixtures. In Appendix 3 the calculated half-lifes for abiotic reactions in the aquous environment are given for those compounds for which an estimation was possible.

LOG K_{OW}

KOWWIN was able to make estimates of the octanol water partitioning coefficient for 996 of the 1074 compounds. Those compounds for which no estimation could be made were mainly inorganic, or metallo-organic. For 479 compounds a recommended literature value (logPstar) could be found. A plot of the predicted log K_{ow} values versus the literature values is given in figure 3.

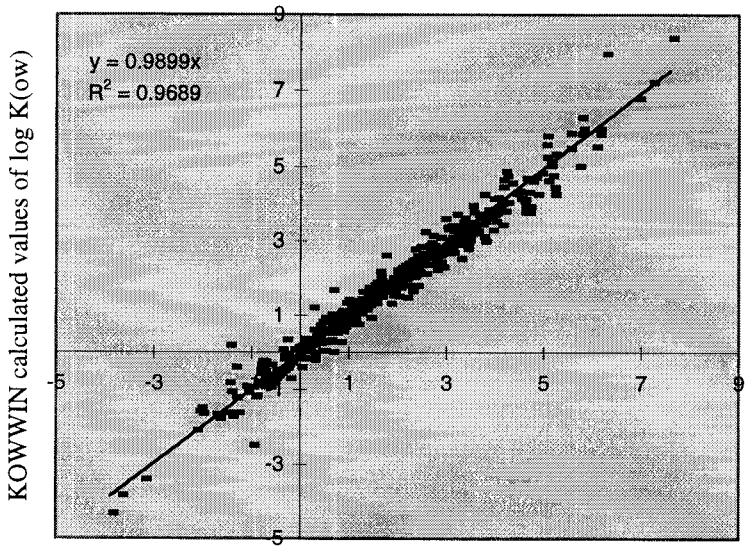


Figure 3 log K_{ow} calculated by KOWWIN versus recommended literature values for 479 compounds from the HPVC-list.

BIODEGRADATION

For 930 of the 1073 compounds on the HPVC list an estimate of the biodegradation probability could be produced using one or more of the four models, these are given in Appendix 1, together with the log K_{ow} values from literature and log K_{OW} estimated. For more than 50% (530 compounds) a prediction of ready biodegradability has been made.

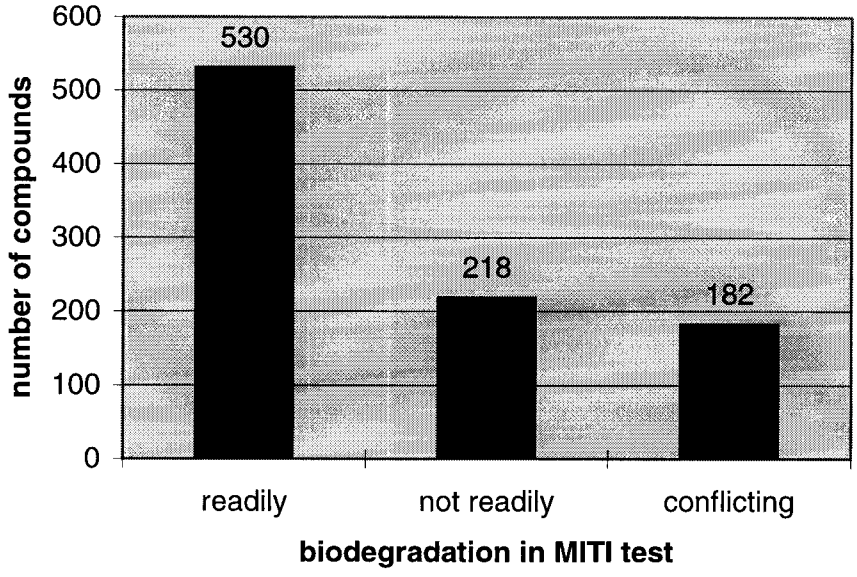


Figure 4. Number of compounds on the High Production Volume Chemicals List from the EU as a function of the estimated biodegradability in the ready biodegradation test.

218 compounds are predicted to be not readily biodegradable, and for 182 compounds the models give conflicting results. These conflicting results show the uncertainty of the biodegradability predictions. These numbers are shown in figure 4. The reliability of the different predictions given by different models is discussed in Chapter 4.

ATMOSPHERIC DEGRADATION

For 917 of the 1073 HPVC single compounds an estimation of the reaction rate constant for reaction with the OH-radical in the atmosphere could be calculated with Atkinson's fragment contribution method, and the MOOH method was applied to 864 compounds. To give an indication of the degradability of these compounds in the atmosphere as calculated with these to methods the results are graphically shown in figure 5.

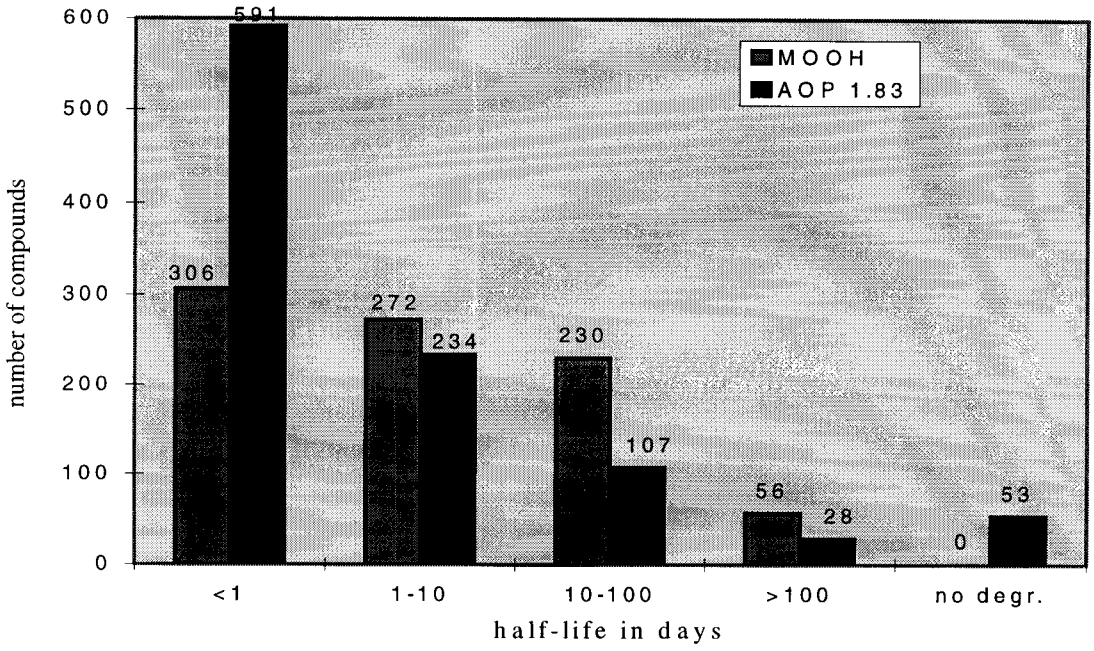


Figure 5. Number of compounds in the High Production Volume Chemicals List from the EU as a function of the estimated atmospheric half-life.

The contribution method by Atkinson predicts a reaction rate constant of 0 for reaction with OH-radical (no reactivity at all) for 53 compounds. Upon examination it turns out that this group consists mainly of inorganic compounds and a few perhalogenated aliphatic compounds, used as CFC's. The MOOH method does not give an estimate for inorganic compounds. AOP 1.83 and MOOH give very different results, especially for the number of compounds that is predicted to react very fast with OH-radicals in the atmosphere.

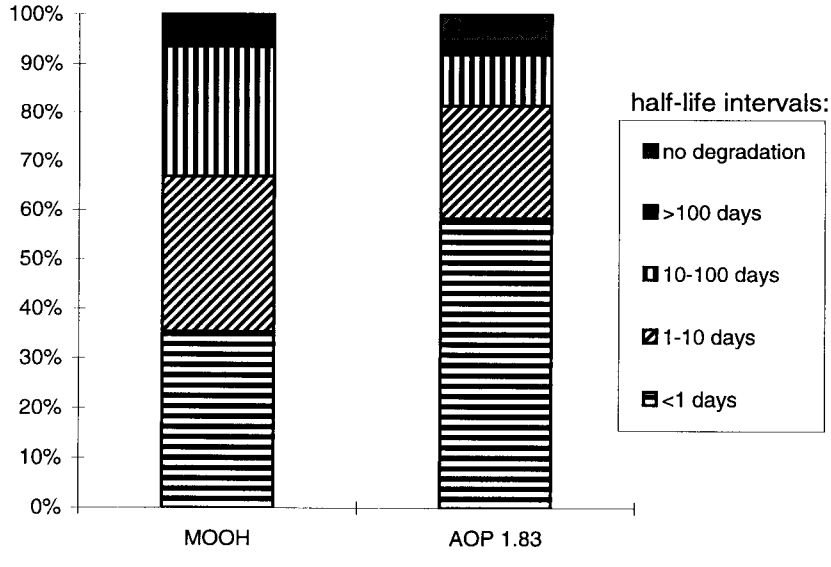


Figure 6 Predictied half-life intervals for reaction with OH-radical in the atmosphere, expressed as percentage of the total number of estimates for two methods.

This is clearly illustrated in figure 6, where the number of compounds are shown as a percentage of the total number of estimates from both methods. The estimation of the atmospheric half-life based solely on the reaction with OH-radicals will give us a worst case scenario, because other transformation pathways, although less important, do exist, like reaction with ozone and the nigh-time reaction with nitrate-radicals. All compounds for which a reaction rate constant with ozone could be estimated (organic aliphatic compounds with 1 or more double or triple bonds) are predicted to have a longer atmospheric half-life by at least a factor of two when compared to the estimated atmospheric half-life based on the reaction with OH-radicals.

ABIOTIC DEGRADATION

The selected QSAR models for abiotic degradation processes are all limited to certain chemical classes. This requires selection of the apropiate compounds from the list of HPVCs. In Table II an overview is given of the number of compounds that fitted into the chemical classes for which QSAR models were selected, together with the number of compounds for which a prediction could be made. This table shows that models relying on the tabulated Hammett and Taft substituent constants are not widely applicable because of a lack of constants for the more exotic substituents.

TABLE II **Number of compounds appropriate for the abiotic degradation models, and the number of predictions that could be made.**

Hydrolysis	HYDROWIN	1074	128	SMILES
	Brominated alkanes	4	4	Hammett/Taft
	esters	115	28	Hammett/Taft
	carbamates (2 models)	3	0	Hammett/Taft
	Benzonitriles	1	1	Hammett/Taft
Oxidation	subst'd phenols $^1O_2$	42	39	E(homo) calc'd
	subst'd phenols MnO_x	42	39	E(homo) calc'd
	PCBs	0	0	# of chlorine atoms
	subst'd anilines	12	12	E(homo) calc'd
Reduction	halogenated aliphatics E(act)	27	25	E(activation) calc'd
	halogenated aliphatics PLS		20	36 phys/chem. descr.
	halogenated aromatics	27	25	Hammett/Taft
	nitroaromatic compounds	35	34	E(lumo) calc'd

The lack of tabulated parameters is a problem that is not encountered with the calculated parameters. The proper calculation of these parameters on the other hand takes considerably more time.All compounds from the HPVC list (Appendix 1) for which one or more abiotic degradation endpoints are calculated are given in Appendix 3 (a total of 237 compounds, with a total of 355 estimated reaction rate constants).

4. DISCUSSION

To assess the value of the predictions as presented in this report it is most useful to look at external validations of the models. For those models which have been validated to some extent the results of this validation are given, for the other models a discussion of the quality of the predictions is based on the statistical quality of the model. The mathematical form of the models, and their statistical qualifications, including confidence intervals, can be found in the appropriate chapters of the EU report on QSARs.[17,18-19] Also some remarks about the applicability of the model to large datasets will be given, in view of the expected application of the models to the whole of the EINECS database.

LOG K_{OW}

The log K_{OW} estimation method employed by KOWWIN has been fitted on 2400 compounds, yilding a model with $r^2 = 0.98$ and $s = 0.22$ log units. An external validation of the model has been performed on a dataset of 8900 compounds[21], yielding an $Q^2 = 0.954$ and a standard deviation $s = 0.42$ log units. The results from the KOWWIN calculation on the HPVC-list are in agreement with these figures, yielding an $r^2 = 0.969$ and a standard deviation of $s = 0.317$ for the dataset of 478 compounds for which also literature values were found.

BIODEGRADATION

An external validation on the 4 biodegradation models applied in this report has been performed by Langenberg *et al.*[47] The main conclusions from this validation are that the models by Howard *et al.* perform rather poor overall, the OECD models are somewhat better, but the models by Howard *et al.* are especially reliable in predicting the non-biodegradability of a compounds; see Table III for details. In Table III the percentages of the correct predictions are given (overall), and the predictions are evalated separately for a prection of ready biodegradability and not-ready biodegradability. For risk-assessment purposes this is the most important information, since the only information on a compound to be reviewed will be the QSAR-predictions (as a worst case). Table III therefore gives the succes-percentages (and thus the probability of a correct prediction) for the different models separated by the prediction. From this information it is clear that the estimations from the BIODEG biodegradation models can best be used to indicate those chemicals which will probably biodegrade slowly or not at all in a ready-biodegradability test.

TABLE III Percentage of correct biodegradation predictions, with the number of compounds from a validation set of 488 MITI data[47]

	BIODEG linear	*non-linear*	*OECD #75*	*OECD #78*
Overall	56.1% (n=488)	62.5% (n=488)	91% (n=222)	85% (n=57)
predicted Biodegradable	36.4% (n=319)	39.9% (n=276)	93.7% (n=175)	75.0% (n=24)
predicted Non-Biodegradable	93.5% (n=169)	92.0% (n=212)	80.9% (n=47)	90.9% (n=33)

The prediction that a chemical is biodegradable has no more significance than stochastic correlation would give. The OECD models are more reliable for those cases for which a prediction "readily biodegradable" is given. The application of the models has been automated, the BIODEG models are incorporated in a PC-based program[24], and the OECD models have been incorporated in a computer program at the Fraunhofer Institute, Schmallenberg, Germany (UBA-SAR-System[48]). Therefore no difficulties should be encountered when doing predictions for larger datasets.

ATMOSPHERIC DEGRADATION

Both internal and external validation have been performed on Atkinson's atmospheric degradation model[31,49-50]. The internal validation (by Atkinson[31]) shows that 94% of the calculated reaction rate constants is within a factor of 2 of the experimental reaction rates. External validation on 369 chemicals estimates this to be within a factor of 3 for the majority of the compounds[50]. In these studies large deviations were found for several chemical classes: perhalogenated compounds, phosphates, small heterocyclic rings, nitroalkanes and aromatics which are not benzene derivatives. The half-life estimations for these classes of chemicals should be used with caution, because large deviations can occur An unpublished validation has been performed on both the AOP and the MOOH programs by Müller using a dataset of 460 compounds, that are partly included in both models. The conclusions from this evaluation were that it is difficult to give a 'true' external validation for the AOP program, since almost all known data on OH-radical reactivity has been used

to create the model. On the dataset of 460 organic chemicals the AOP program estimated the rate constants with a mean squared error of 0.051 log units, where the MOOH method gave a mean squared error of 0.609 log units. The AOP programs has a higher accuracy. However, the AOP-program underestimates as well as overestimates reaction rate constants, where the MOOH-method is more conservative and merely underestimates the rate constants. This is illustrated by figure 7, where the MOOH-predictions of the atmospheric half-lifes for reaction with OH-radicals have been plotted againts the AOP-predictions for the HPVC list. Most MOOH-predcitions lie above the line X=Y, indicating that for most predictions MOOH yields a longer half-life.. Application of both models is very straightforward since they have been automated.[48,51]

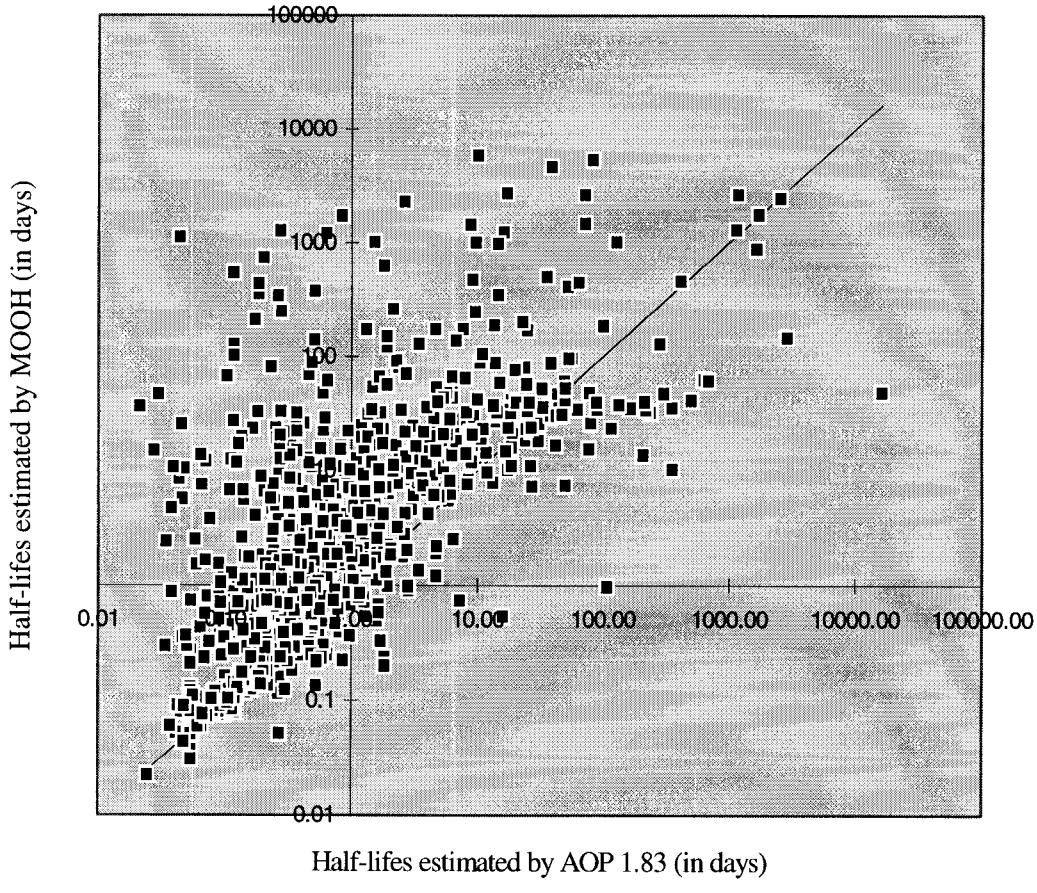


Figure 7 MOOH-estimates of atmospheric half-lifes for reaction with OH-radicals versus AOP-estimates for the HPV-chemicals.

ABIOTIC DEGRADATION

Hydrolysis

Those compounds for which two predictions of hydrolysis could be calculated are given in figure 8. Comparison the the different predictions shows that in general good agreement is observed between the HYDROWIN estimations and the recalculated model from Drossman *et al.* of hydrolysis half-lifes for esters. Only for four compounds the models differ more than a factor of 10. These four compounds should be evaluated more closely, and the prediction should be used with precautions. The four compounds are 2,6-dibromo-4-cyanophenyl octanoate, O-acetylsalicylic acid, vinyl-acetate and benzyl-salicylate. The reason for the different estimates from the two models has to lie in the use of different Hammett and Taft substituent constants.

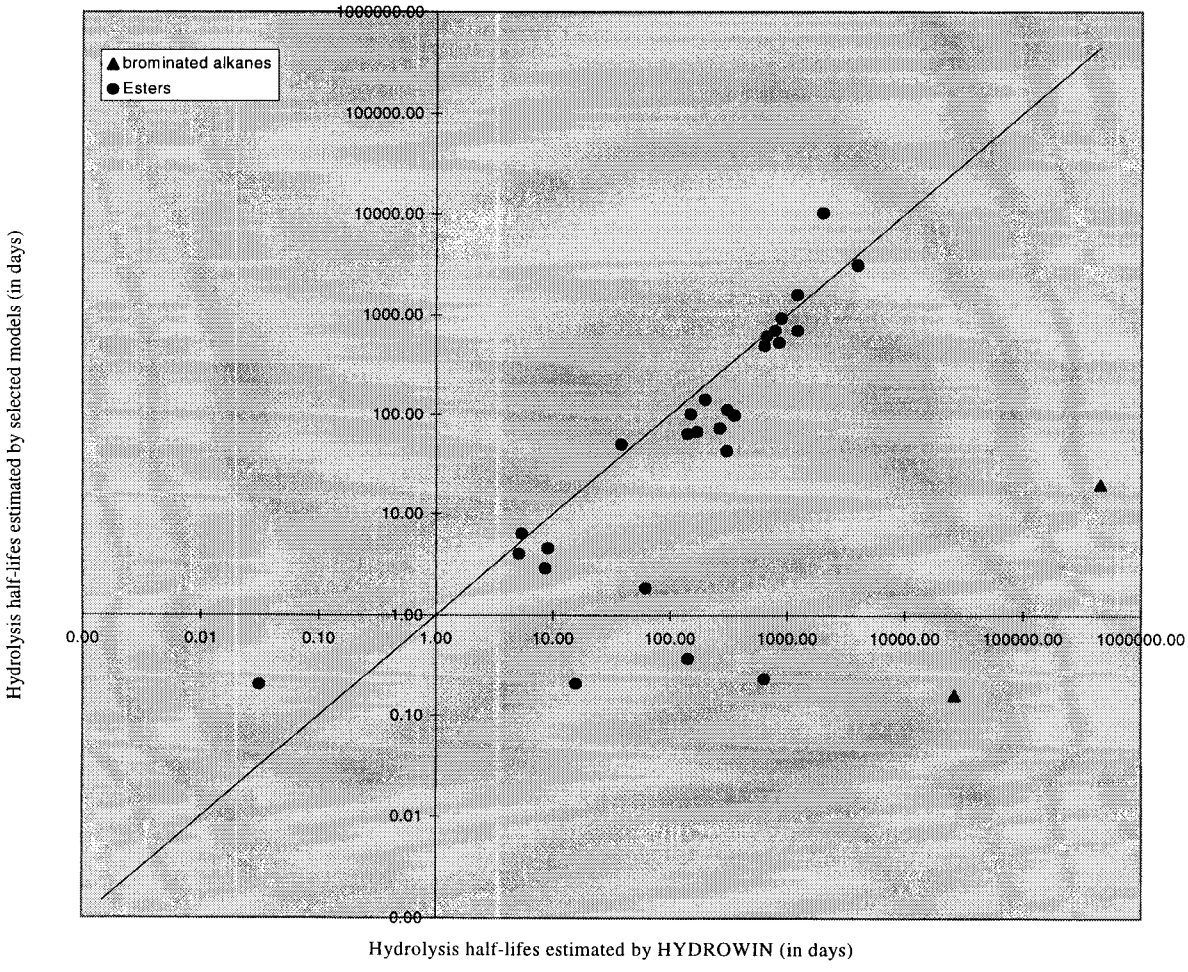


Figure 8 Hydrolysis half-lifes for esters and brominated alkanes estimated with the selected models from the EU-project on QSARs versus half-lifes estimated by the HYDROWIN program from Syracuse Inc.

The two brominated alkanes in figure 8, i.c. bromomethane and 1,2-dibromoethane, show large deviations between the two estimation methods. The HYDROWIN program estimates these compounds to be virtually unreactive, where the model by Vogel *et al.* predicts moderately fast hydrolysis. A review of QSARs for hydrolysis by Peijnenburg[52] gives an half-life interval for brominated alkanes from 10 seconds to 100 days. Therefore the estimates from HYDROWIN seem to be too conservative.

For the hydrolysis models no validations have been performed, so the judgement of the reliability of the predictions will have to be based on the statistical quality of the model, the quality of the data used, and comparison of the predictions from different models. The predictions for hydrolysis of brominated alkanes with the model from Vogel *et al.* should be seen as an indication of the order of magnitude of the reaction rate constants. The model is based on experimental data using water of relatively high ionic strength and high temperatures, therefore the extrapolation of the data to surface water conditions is dangerous. The relative order in reactivity will probably be predicted correctly. Since selection of the appropriate compounds for the model, and the calculation of the reaction rate constants have to be done by hand, large datasets will pose a problem for prediction. The selection of the right compounds for the model is the largest and most important problem in this respect.

For the prediction of hydrolysis rates for esters and carbamates one may have more faith in the selected models since their statistical quality is very good. However, the model does also use data that is extrapolated from elevated temperatures, and the model as incorporated in the HYDROWIN program (and given in the article by Drossman *et al.*[37] uses mixed Hammett and Taft substituent constants from various sources. The good performance of the substituent constants in predicting hydrolysis rate constants is explained by the high similarity between the hydrolysis reaction and the reaction(s) used for determining the substituent constants. The model for the hydrolysis of esters gives 60% of the values of the reactivity constant to within a factor of two of the measured values. The carbamate models are comparable to the ester model in quality. The half-lifes calculated this way are valid only for the ester/carbamate group in the compound. If another easily hydrolyzable group is present in the molecule, the predicted half-life will be an overestimation.

The model for hydrolysis of para-substituted benzonitriles has good accuracy, the standard deviation of the model is 0.284 log units. The model is also very well restricted in applicability. However, the rate constants are measured at elevated temperature, but the extrapolation to environmental temperatures has been performed very carefully, using the Arrhenius equation. For all models the same restrictions in applicability to large datasets apply as for the first hydrolysis model.

Oxidation in the aqueous environment

The models for predicting oxidation rates of phenols in the environment have a high statistical quality, and a good mechanistical basis. The standard error of prediction is 0.27 log units. The calculation of the environmental half-lifes is however subject to the estimation of the concentration of singlet oxygen in the (surface) water. This concentration is very dependent on the amount of sun light, and the depth at which the concentration of singlet oxygen is measured. The average concentration used to calculate the half-lifes given in Appendix 3 is based on a 12 hour day, and the concentration is measured in the first meter of the surface water, at 52° North latitude.

The predictions of the reactivity of anilines with manganese oxides are less precise, since the model is based on few compounds (n=6) and the standard error of prediction is as high as 0.74 log units. Calculations of orbital energies on the semi-empirical level, as required for these models, are executed in a timescale of minutes/compound on a modern PC. Therefore the predictions will not give large problems. The selection of the appropriate compounds for the model and the generation of the lowest energy structure as input for the semi-empirical calculations is however very laborious by hand.

Reduction in the aqueous environment

The models for dehalogenation of aliphatic compounds were both validated externally with 6 compounds. The PLS model, using 36 descriptors, can explain 77% of the variance in the reaction rate constants in the external validation set (Q^2=0.77). For the model based on the calculated activation energy of reaction this is 86%, with a standard error of prediction for the external validation set of 0.30 log units. For comparison of the two models the predictions for the HPVC-list have been plotted against each other in figure 9. In the predictions for the HPV-chemicals the models deviate significantly from each other for only one compound. *i.c.* hexachloroethane. When a larger set of predictions is compared, it turns out that this is not an isolated case. Apparently the PLS model estimates the group of (per)halogenated ethanes to be dehalogenated more rapidly than the activation energy model. Laboratory studies of hexachloroethane have shown that this compound is dehalogenated in minutes, en under not copletely anoxic conditions. Another group of compounds that stands out when we look at the larger set of predictions are the fluorinated alkanes. The general belief is that fluorinated compounds are resistant to dehalogenation in the anaerobic environments, since the carbon-fluoro bond is very inert. Therefore the predictions of the PLS model for fluorinated compounds are suspect.

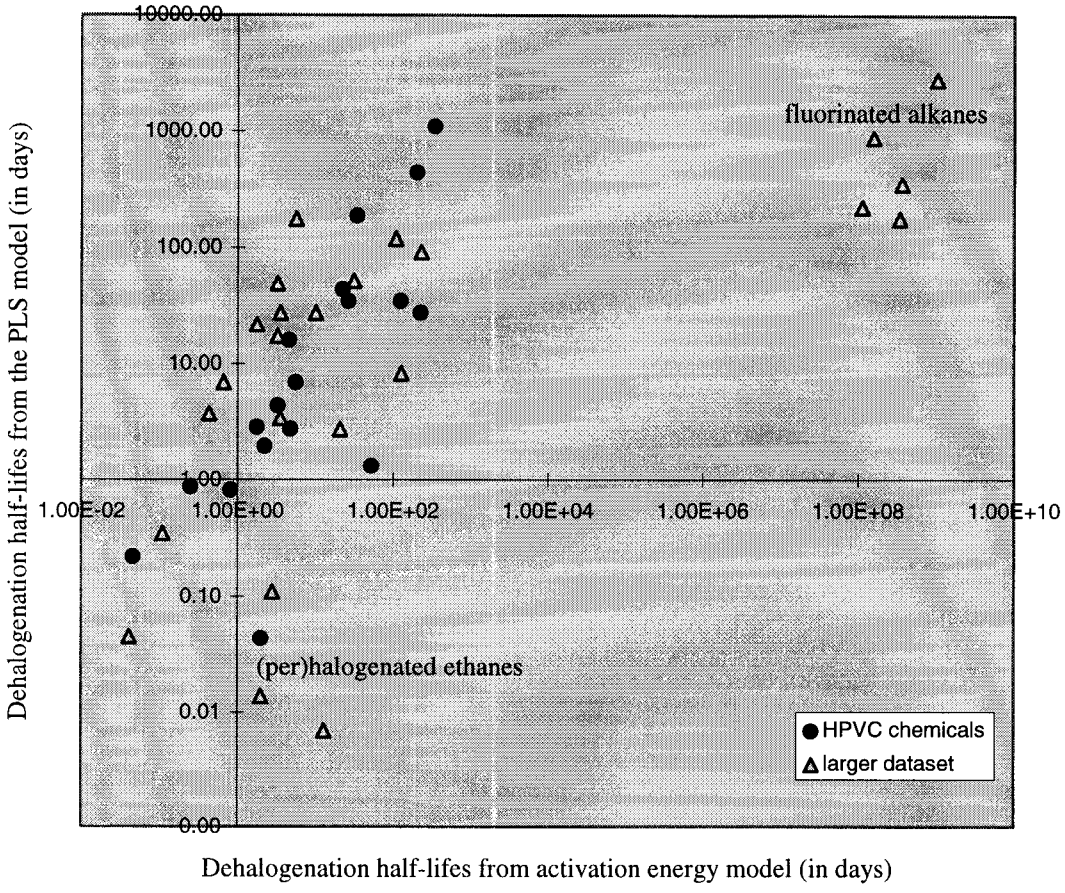


Figure 9 Predicted values for 41 halogenated aliphatic compounds (18 compounds from the HPVC). The estimations from the PLS model have been plotted against the estimations from the activation energy model. The line x=y is also drawn.

The predictions of the dehalogenation reaction for halogenated aromatic compounds are not validated, but the mechanistical background and the statistical quality of the model are high, with the calculated rate constants in the 90% Confidence Interval within 0.1 log units of the measured values. The model showed an r^2=0.966 and used 36 compounds for fitting the data. The calculation of the half-lifes given in Appendix 2 are dependent on the sediment system chosen. In this case (Loosdrechtse Plassen sediment from the Netherlands) the sediment does have extreme characteristics (organic carbon content of 33%) therefore calculated half-lifes can not be regarded to be generally applicable. If calculations should be performed for specific environmental conditions a model relating the rate constants to the organic carbon content of the sediments is available.[43]

The degradation of nitro-aromatic compounds under anoxic condition leads to the subsequent aniline. The model used in this report to calculate (relative) reaction rates uses laboratory data from reaction of nitroaromatic compounds with an artificial electron

mediator. In the environment various species ca act as electron carriers (catalysts). Therefore the rate constants cannot be regarded as absolute values, they show the relative reactivity of nitro-aromatic compounds only. The model used data on 11 nitromaromatic compounds, yielding a model with r^2=0.866, and stardard error of estimation s=0.456 log units. In most cases the aniline will be of greater environmental concern, because of the in general higher toxicity and resistance to further degradation.

REFERENCES

1. Council Regulation (EEC) No. 793/93/EEC On the evaluation and control of the risks of existing substances. Official Journal of European Communities L84/1 1993;March 23.

2. van der Zandt PGJ, van Leeuwen CJ. The Hague, The Netherlands: VROM, Directorate for Chemicals, External Safety and Radiation Protection; 1992.

3. Nirmalakhandan N, Speece RE. Structure-activity relationships: quantitative techniques for predicting the behavior of chemicals in the ecosystem. Environmental Science and Technology 1988;22:606-15.

4. Blum DJW, Speece RE. Determining chemical toxicity to aquatic species: The use of QSARs and surrogate organisms. Environmental Science and Technology 1990;24(3):284-93.

5. Hermens JLM. Quantitative Structure-Activity Relationships of environmental pollutants. in: Hutzinger O, Ed. Handbook of environmental chemistry. Volume 2E, Reactions and Processes. Berlin: Springer Verlag; 1989. p 111-62.

6. Peijnenburg WJGM. Structure-Activity relationships for biodegradation: A critical review. Pure and Applied Chemistry 1994;66(9):1931-41.

7. Hermens JLM. Part 1: General outline and procedure: EU-DG-XII; 1995. Report of the EU-DG-XII Project QSAR for Predicting Fate and Effects of Chemicals in the Environment, contract #EV5V-CT92-0211.

8. Weininger D. SMILES, a chemical and information system. 1. Introduction to methodology and encoding rules. J Chem Inf Comput Sci 1988;28(1):31-6.

9. Meylan WM. Syracuse, New York 13210, USA: Syracuse Research Corporation, Chemical Hazard Assessment Division, Environmental Chemistry Center; 1993.

10. Dewar MJS, Zoebisch EG, Healy EF, Stewart JJP. AM1: A new general pupose quantum mechanical molecular model. Journal of the American Chemical Society 1985;107(13):3902-9.

11. Stewart JJP, Coolidge MB. MOPAC 6.00 [A general molecular orbital package]Frank J. Seiler Research Laboratory, United States Air Force Academy CO 80840: QCPE #455; 1990.

12. Stewart JJP. MOPAC: A semiempirical molecular orbital program. J Comput Aided Mol Des 1990;4:1-105.

13. Klamt A, Schüürman G. COSMO: A new approach to dielectric screening in solvents with explicit expressions for the screening energy and its gradient. Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry 1993;799-805.

14. Hansch C, Leo AJ. Substituent constants for correlation analysis in chemistry and biology. New York, NY, USA: John Wiley & Sons; 1979.

15. Frisch MJ, Trucks GW, Head-Gordon M, Gill PMW, Wong MW, Foresman JB, Johnson BG, Schlegel HB, Robb MA, Replogle ES and others. Gaussian 92. Version Revision E.1. Pittsburgh, USA: Gaussian Inc.; 1992.

16. Foresman JB, Frisch A. Exploring chemistry with electronic structure methods: A guide to using Gaussian. 1 ed. Pittsburgh, USA: Gaussian, Inc.; 1993.

17. Güsten H, Sabljic A. Chapter IV: QSARs for chemical degradation in the gas phase. in: Hermens JLM. (ed.) Part 1: General outline and procedure: EU-DG-XII; 1995. Report of the EU-DG-XII Project QSAR for Predicting Fate and Effects of Chemicals in the Environment, contract #EV5V-CT92-0211. 1995.

18. Rorije E, Peijnenburg WJGM. Chapter V: QSARs for chemical degradation in the aqueous phase. in: Hermens JLM. (ed.) Part 1: General outline and procedure: EU-DG-XII; 1995. Report of the EU-DG-XII Project QSAR for Predicting Fate and Effects of Chemicals in the Environment, contract #EV5V-CT92-0211. 1995.

19. Rorije E, Langenberg JH, Peijnenburg WJGM. Chapter VI: QSARs for Biodegradation. in: Hermens JLM. (ed.) Part 1: General outline and procedure: EU-DG-XII; 1995. Report of the EU-DG-XII Project QSAR for Predicting Fate and Effects of Chemicals in the Environment, contract #EV5V-CT92-0211. 1995.

20. Meylan WM. SRC-KOWWIN for Microsoft Windows [KOWWIN]. Version 1.54. Syracuse, NY 13210 United States: Syracuse Reasearch Corporation; 1996.

21. Meylan WM, Howard PH. Atom/Fragment contribution method for estimateing octanol-water partitioning coefficients. Journal of Pharmaceutical Science 1995;84(1):83-92.

22. Müller M. Comparative evaluation of commercial $logP_{ow}$ estimation software. Poster presented at the 7th International Workshop on QSARs in Environmental Sciences; 1996 Jun 24-28,1996; Helsingør, Denmark. 1996.

23. Howard PH, Boethling RS, Stiteler WM, Hueber AE, Beauman JA, Larosche ME. Predictive model for aerobic biodegradability from a file of evaluated biodegradation data. Environmental Toxicology and Chemistry 1992;11:593-603.

24. Howard PH, Meylan WM. Biodegradation Probability Program. Version 3. Syracuse, NY 13210 United States: Syracuse Research Corporation; 1992.

25. Boethling RS, Howard PH, Meylan WM, Stiteler WM, Beauman JA, Tirado N. Group contribution method for predicting probability and rate of aerobic biodegradation. Environmental Science and Technology 1994;28(3):459-65.

26. Howard PH, Hueber AE, Boethling RS. Biodegradation data evaluation for structure/biodegradability relations. Environmental Toxicology and Chemistry 1987;6:1-10.

27. Degner P, Müller M, Nendza M, Klein W. Structure-activity relationships for biodegradation. OECD Environment Monographs No.68, OEDE/GD(93)126 ed. Paris, France: OECD Environment Directorate; 1993.

28. Degner P. Abschätzung der biologische Abbaubarkeit mittels SARs. Duisburg: University of Duisburg. 1992.

29. Atkinson R. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds under atmospheric conditions. Chemical Reviews 1986;86:69-201.

30. Atkinson R. A structure-activity relationship for the estimation of rate constants for the gas-phase reactions of OH radicals with organic compounds. International Journal of Chemical Kinetics 1987;19:799-828.

31. Atkinson R. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. Environmental Toxicology and Chemistry 1988;7:435-42.

32. Kwok ESC, Atkinson R. Estimation of hydroxyl radical reaction rate constants for gas-phase organic compounds using a structure-reactivity relationship: an update. Atmospheric Environment 1995;29(14):1685-95.

33. Klamt A. Estimation of gas-phase hydroxyl radical rate constants of organic compounds from molecular orbital calculations. Chemosphere 1993;26(7):1273-89.

34. Klamt A. Estimation of gas-phase hydroxyl radical rate constants of oxygenated compounds based on molecular orbital calculations. Chemosphere 1996;32(4):717-26.

35. Meylan WM. SRC-HYDROWIN for Microsoft Windows [HYDROWIN] Syracuse, NY 13210 United States: Syracuse Research Corporation; 1995.

36. Mill T, Haag W, Penwall P, Pettit T, Johnson H. Menlo Park, CA, United States: SRI International; 1987. EPA-contract No. 68-02-4254.

37. Drossman H, Johnson H, Mill T. Structure Activity Relationships for environmental processes 1: Hydrolysis of esters and carbamates. Chemosphere 1988;17(8):1509-30.

38. Vogel TM, Reinhard M. Reaction products and rates of disappearance of simple bromoalkanes, 1,2-dibromopropane, and 1,2-dibromoethane in water. Environmental Science and Technology 1986;20:992-7.

39. Masunaga S, Wolfe NL, Carriera L. Transformation of *para*-substituted benzonitriles in sediment and in sediment extract. Water Science and Technology 1994;28(8-9):123-32.

40. Tratnyek PG, Hoigné J. Oxidation of substituted phenols in the environment: A QSAR analysis of rate constants for reaction with singlet oxygen. Environmental Science and Technology 1991;25(9):1596-604.

41. Rorije E, Peijnenburg WJGM. QSARs for oxidation of phenols in the aqueous environments, suitable for risk assessment. Journal of Chemometrics 1996;10:79-93.

42. Sedlak DL, Andren AW. Aqueous-phase oxidation of polychlorinated biphenyls by hydroxyl radicals. Environmental Science and Technology 1991;25:1419-27.

43. Peijnenburg WJGM, 't Hart MJ, den Hollander HA, van de Meent D, Verboom HH, Wolfe NL. Reductive transformations of halogenated aromatic hydrocarbons

in anaerobic water-sediment systems: Kinetics, mechanisms and products. Environmental Toxicology and Chemistry 1992;11:289-300.

44. Eriksson L, Verboom HH, Peijnenburg WJGM. Multivariate QSAR Modelling of the rate of reductive dehalogenation. Journal of Chemometrics 1996.

45. Rorije E, Eriksson L, Verboom HH, Verhaar HJM, Hermens JLM, Peijnenburg WJGM. Predictiong reductive transformation rates of halogenated aliphatic compounds using different QSAR approaches. Environmental Science and Pollution Research 1997;2: in press.

46. Peijnenburg WJGM, 't Hart MJ, den Hollander HA, van de Meent D, Verboom HH, Wolfe NL. QSARs for predicting reductive transformation rate constants of halogenated aromatic hydrocarbons in anoxic sediment systems. Environmental Toxicology and Chemistry 1992;11:301-14.

47. Langenberg JH, Peijnenburg WJGM, Rorije E. On the usefulness and reliability of existing QSBRs for risk assessment and priority setting. SAR & QSAR in Environmental Research 1996;5:1-16.

48. Müller M. SAR-system: Estimating environmental relevant properties from chemical structureJochum C., ed. Software-development in Chemistry. Volume 8. Frankfurt am Main: Gesellschaft deutscher Chemiker; 1994.

49. Meylan WM. Syracuse, NY 13210, USA: Syracuse Research Corporation, Chemical Hazard Assessment Division, Environmental Chemistry Center; 1993.

50. Müller M, Klein W. Estimating atmospheric degradation processes by SARs. Sci Total Environ 1991;109/110:261-73.

51. Atmospheric Oxidation Program. Version 1.5. Syracuse, NY 13210 USA: Syracuse Research Corporation, Chemical Hazard Assessment Division, Environmental Chemistry Center; 1993.

52. Peijnenburg WJGM. The use of quantitative structure-activity relationships for predicting rates of environmental hydrolysis processes. Pure and Applied Chemistry 1991;63(11):1667-76.

References to the log K_{OW} values in Appendix 1:

a. Hansch, C. and A.J. Leo. 1985. MEDCHEM Project. Issue No. 26. Claremont, CA: Pomona College.

b. Sangster, J. 1993. LOGKOW Databank. A databank of evaluated octanol-water partition coefficients (Log P) on microcomputer diskette. Montreal, Quebec, Canada: Sangster Research Laboratories.

c. Hansch. C., A. Leo and D. Hoekman. 1995. Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Professional Reference Book. Washington, DC: American Chemical Society.

d. Sangster, J. 1994. LOGKOW Databank. A databank of evaluated octanol-water partition coefficients (Log P) on microcomputer diskette. Montreal, Quebec, Canada: Sangster Research Laboratories.

e. TSCATS. Toxic Substances Control Act Test Submissions Database. Manufacturer submissions (4, 8d, 8e, FYI) to the USEPA.

f. Chem Inspect Test Inst. 1992. Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan. compiled under the supervision of Chemical Products Safety Div, Basic Indust Bureau, Ministry of Intern Tade & Industry Japan (edited by Chemicals Inspection & Testing Institute Japan). Published by Japan Chemical Industry Ecology-Toxicology & Information Center. ISBN 4-89074-101-1.

g. Veith, G.D. et al. 1980. An evaluation of using partition coefficients and water solubility to estimate bioconcentration factors for organic chemicals in fish. ASTM STP 707. Aquatic Toxicology. Easton,J.G. et al. (editors). Amer. Soc . Test. Mater. pp.116-29; 1980.

h. Li, J. and E.M. Perdue. 1995. Physicochemical properties of selected monoterpenes. pre-print extended abstract, presented before the Division of Environmental Chemistry, Amer. Chem. Soc., Anaheim, CA, April 2-7, 1995.

i. Pomona. 1987. Pomona College Medicinal Chemistry Project, Claremont, CA 91711, Log P Database, (C. Hansch and A. Leo), July 1987 edition.

j. Nakagawa, Y., K. Izumi, N. Oikawa, T. Sotomatsu, M. Shigemura and T. Fujita. 1992. Analysis and prediction of hydrophobicity parameters of substituted

acetanilides, benzamides and related aromatic compounds. Environ. Toxicol. Chem. 11: 901-16.

k. Ilchmann, A., G. Wienke, T. Meyer and J. Gmehling, "Countercurrent liquid/liquid chromatography - a reliable method for the determination of partition coefficients", Chem.-Ing.-Tech., 65(1), 72-75 (1993).

l. Debnath, A.K., R.L. Lopez de Compadre, G. Debnath, A.J. Shusterman and C. Hansch, "Structure-activity relationship of mutagenic aromatic and heteroaromatic nitro compounds. Correlation with molecular orbital energies and hydrophobicity", J. Med. Chem., 34(2), 786-797 (1991).

m. Funasaki, N., S. Hada and S. Neya, "Prediction of retention times in reversed-phase high-performance liquid chromatography from the chemical structure", J. Chromatogr., 361, 33-45 (1986).

n. Sotomatsu, T., M. Shigemura, Y. Murata and T. Fujita, "Octanol/water partition coefficient of ortho-substituted aromatic solutes", J. Pharm. Sci., 82(8), 776-781 (1993).

o. Saito, H. et al. 1993. Cytotoxicity of 109 chemicals to goldfish gfs cells and relationships with 1-octanol/water partition coefficients. Chemosphere 26: 1015-28.

p. Deneer, J.W., T.L. Sinnige, W. Seinen and J.L.M. Hermens, "A quantitative structure-activity relationship for the acute toxicity of some epoxy compounds to the guppy", Aquatic Toxicol., 13(3), 195-204 (1988).

q. Tanii, H., H. Tsuji and K. Hashimoto, "Structure-toxicity relationship on monoketones", Toxicol. Lett., 30(1), 13-17 (1986).

r. Daniels, S.L. et al. 1985. Environmental exposure assessment: experience under the toxic substances control act. Environ. Toxicol. Chem. 4: 107-17.

s. Tewari, Y.B., M.M. Miller, S.P. Wasik and D.E. Martire, "Aqueous solubility and octanol-water partition coefficients of organic compounds at 298 K", J. Chem. Eng. Data, 27(4), 451-454 (1982).

t. Miller, M.M. et al. 1985. Relationships between octanol-water partition coefficient and aqueous solubility. Environ. Sci. Technol. 19: 522-9.

u. De Bruijn, J.F., Busser, W. Seinen and J. Hermens. 1989. Determination of octanol/water partition coefficients for hydrophobic organic chemicals with the "slow-stirring" method. Environ. Toxicol. Chem. 8: 499-512.

v. Okamoto, H., M. Hashida and H. Sezaki, "Effect of 1-alkyl- or 1-alkenylazacyclo-alkanone derivatives on the penetration of drugs with different lipophilicities through guinea pig skin", J. Pharm. Sci., 80(1), 39-45 (1991).

w. Coates, M., D.W. Connell and D.M. Barron, "Aqueous solubility and octan-1-ol to water partition coefficients of aliphatic hydrocarbons", Environ. Sci. Technol., 19(7), 628-632 (1985).

x. Sherblom, P.M. and R.P. Eganhouse, "Correlations between octanol-water partition coefficients and reversed-phase high-performance liquid chromatography capacity factors", J. Chromatogr., 454, 37-50 (1988).

y. Catz, P. and D.R. Friend, "Alkyl esters as skin permeation enhancers for indomethacin", Int. J. Pharm., 55(1), 17-23 (1989)

z. Dunn, W.J. III et al. 1983. Nonadditivity of 1-octanol/water partition coefficients of disubstituted benzenes: an explanation and its consideration of log P estimation. Quant. Struct-Act. Relat. 2: 156-63.

aa. De Voogt, P., G.A. Van Zijl, H. Govers and U.A.T. Brinkman, "Reversed-phase TLC and structure-activity relationships of polycyclic (hetero) aromatic hydrocarbons", J. Planar Chromatogr.-Mod. TLC, 3(1-2), 24-33 (1990).

ab. Tomlin, C. 1994. The Pesticide Manual, Tenth edition, Crop Protection Publications; British Crop Protection Council, 49 Downing St, Farnham, Survey GU9 7PH, United Kingdom.

ac. Niimi, A.J., H.B. Lee and G.P. Kisson, "Octanol/buffer partition coefficients and bioconcentration factors of chloronitrobenzenes in rainbow trout (Salmo gairdneri)", Environ. Toxicol. Chem., 8(9), 817-823 (1989).

ad. Sasaki, H., Y. Mori, J. Nakamura and J. Shibasaki, "Synthesis and anticonvulsant activity of 1-acyl-2-pyrrolidinone derivatives", J. Med. Chem., 34(2), 628-633 (1991).

ae. Rich, P.R., "Partition coefficients of quinones and their relation to biochemical reactivity", Highlights in Ubiquinone Research, Proc. Int. Symposium "Biochem., Bioener. Clin. Appl. Ubiquinone", 136-141 (1990).

af. Krawchuk, B.P. and Webster, G.R.B. 1987. Movement of pesticides to ground water in an irrigated soil. Water Poll. Res. J. Canada 22: 129-46.

ag. Braumann, T. and L.H. Grimme, "Determination of hydrophobic parameters for pyridazinone herbicides by liquid-liquid partition and reversed-phase high-performance liquid chromatography", J. Chromatogr., 206(1), 7-15 (1981).

ah. Schultz, T.W. and F.M. Applehans, "Correlations for the acute toxicity of multiple nitrogen-substituted aromatic molecules", Ecotoxicol. Environ. Saf., 10(1), 75-85 (1985).

ai. Pesticide Properties Database

aj. Chiari, M. et al. 1991. Capillary zone electrophoresis analysis of acrylamido buffers for isoelectroc focusing in immobilized pH gradients. J. Chromatogr 559: 119-31.

ak. Itokawa, H., N. Totsuka, K. Nakahara, M. Maezuru, K. Takeya, M. Kondo, M. Inamatsu and H. Morita, "A quantitative structure-activity relationship for antitumor activity of long-chain phenols from Ginkgo biloba L.", Chem. Pharm. Bull., 37(6), 1619-1621 (1989).

al. Baker, E.A., A.L. Hayes and R.C. Butler. 1992. Physicochemical properties of agrochemicals: their effect on foliar penetration. Pestic. Sci. 34: 167-82.

APPENDIX 1 - LOG K_{OW} AND BIODEGRADATION

Table of 1073 single compounds from the High Production Volume Chemicals list, European Chemicals Bureau, June 4th 1995, as part of the Regulation (EEC) 793/93) on existing chemical substances. The following properties are given:

- CAS-nr.
- EINECS nr.
- Name
- Log K_{ow} value from literature (ref. in Reference list of the report)
- Log K_{ow} estimates from KOWWIN program v. 1.54, SRC, Syracuse, NY, USA
- Biodegradation probability estimated using the BIODEG linear model version 1.5, SRC, Syracuse, NY, USA
- Biodegradation probability estimated using the BIODEG non-linear model version 1.5, SRC, Syracuse, NY, USA
- Biodegradation probability estimated using the OECD model for acyclic compounds (nr. 75)
- Biodegradation probability estimated using the OECD model for monoaromatic compounds (nr. 78)

All properties are adequately described in Section 2 Materials and Methods.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
50000	2000018	formaldehyde	0.35 [a]	0.35	1	1	1	-
50293	2000243	clofenotane	6.91 [a]	6.79	0	0	-	-
50782	2000641	O-acetylsalicylic acid	1.19 [a]	1.13	1	1	-	1
55389	2002319	fenthion	4.09 [a]	4.08	1	1	-	1
55630	2002408	glycerol trinitrate	1.62 [a]	1.51	1	0	-	-
56235	2002628	carbon tetrachloride	2.83 [a]	2.44	0	0	0	-
56359	2002680	bis(tributyltin) oxide	-	5.80	-	-	-	-
56382	2002717	parathion	3.83 [a]	3.73	1	1	-	0
56406	2002722	glycine--iron sulphate (1:1)	-3.21 [a]	-3.41	1	1	1	-
56815	2002895	glycerol	-1.76 [a]	-1.65	1	1	1	-
56848	2002916	aspartic acid	-3.89 [a]	-4.32	1	1	1	-
56860	2002937	glutamic acid	-3.69 [a]	-3.83	1	1	1	-
57136	2003155	urea	-2.11 [a]	-1.56	1	1	1	-
57487	2003333	fructose, pure	-	-1.46	1	1	0	-
57556	2003380	propane-1,2-diol	-0.92 [a]	-0.78	1	1	1	-
58082	2003621	caffeine	-0.07 [a]	0.16	1	1	-	-
58559	2003857	theophylline	-0.02 [a]	-0.39	1	1	-	-
58560	2003862	pyridoxine hydrochloride	-	-	-	-	-	-
58899	2004012	gamma-HCH or gamma-BHC	3.72 [a]	4.26	0	0	-	-
59507	2004316	chlorocresol	3.10 [a]	2.70	1	1	-	0
59676	2004410	nicotinic acid	0.36 [b]	0.69	1	1	-	-
60004	2004494	edetic acid	-	-3.86	0	0	0	-
60128	2004562	2-phenylethanol	1.36 [a]	1.57	1	1	-	-
60242	2004646	2-mercaptoethanol	-	-0.20	1	1	1	-
60297	2004672	diethyl ether	0.89 [a]	1.05	0	0	1	-
60515	2004803	dimethoate	0.78 [c]	0.28	1	1	1	-
60800	2004866	phenazone	0.38 [a]	0.59	1	1	-	-
61825	2005215	amitrole	-0.86 [d]	-0.47	0	0	-	-
62237	2005262	4-nitrobenzoic acid	1.89 [a]	1.69	1	1	-	0
62533	2005393	aniline	0.90 [a]	1.08	1	1	-	1
62566	2005435	thiourea	-	-0.21	1	1	-	-
64175	2005786	ethanol	-0.31 [a]	-0.14	1	1	1	-
64186	2005791	formic acid	-0.54 [a]	-0.46	1	1	1	-
64197	2005807	acetic acid	-0.17 [a]	0.09	1	1	1	-
64675	2005896	diethyl sulphate	1.14 [a]	1.14	1	1	1	-
65850	2006182	benzoic acid	1.87 [a]	1.87	1	1	-	1
67481	2006554	choline chloride	-	-	-	-	-	-
67561	2006596	methanol	-0.77 [a]	-0.63	1	1	1	-
67630	2006617	propan-2-ol	0.05 [a]	0.28	1	1	1	-
67641	2006622	acetone	-0.24 [a]	-0.24	1	1	1	-
67663	2006638	chloroform	1.97 [a]	1.52	0	0	0	-
67685	2006643	dimethyl sulfoxide	-1.35 [a]	-1.22	1	1	1	-
68111	2006774	mercaptoacetic acid	0.09 [a]	0.03	1	1	1	-
68122	2006795	N,N-dimethylformamide	-1.01 [a]	-0.93	1	1	1	-
68893	2006947	sodium [(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)methylamino]methanesulphonate	-	-3.08	1	1	-	1
69727	2007123	salicylic acid	2.26 [a]	2.24	1	1	-	1
71238	2007469	propan-1-ol	0.25 [a]	0.35	1	1	1	-
71363	2007516	butan-1-ol	0.88 [a]	0.84	1	1	1	-
71410	2007521	pentan-1-ol	1.51 [d]	1.33	1	1	1	-
71432	2007537	benzene	2.13 [a]	1.99	1	1	-	-
71556	2007563	1,1,1-trichloroethane	2.49 [a]	2.68	0	0	0	-
74317	2008064	N,N'-diphenyl-p-phenylenediamine	-	4.04	0	0	-	-
74828	2008127	methane in gaseus state	1.09 [a]	0.78	1	1	1	-
74839	2008132	bromomethane	1.19 [a]	1.18	1	0	1	-
74840	2008148	ethane	1.81 [a]	1.32	1	1	1	-
74851	2008153	ethylene, pure	1.13 [a]	1.27	1	1	-	-
74862	2008169	acetylene	0.37 [a]	0.50	1	1	-	-
74873	2008174	chloromethane	0.91 [a]	1.09	1	1	1	-
74895	2008200	methylamine, in aqueous solution	-0.57 [a]	-0.64	1	1	1	-
74908	2008216	hydrogen cyanide	-0.25 [a]	-0.69	1	1	-	-
74931	2008221	methanethiol	-	0.78	1	1	1	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
74986	2008279	propane liquefied	2.36 [a]	1.81	1	1	1	-
75003	2008305	chloroethane	1.43 [a]	1.58	1	1	1	-
75014	2008310	chloroethylene	-	1.62	1	1	1	-
75047	2008347	ethylamine	-0.13 [a]	-0.15	1	1	1	-
75058	2008352	acetonitrile	-0.34 [a]	-0.15	1	1	1	-
75070	2008368	acetaldehyde	-0.34 [e]	-0.17	1	1	1	-
75081	2008373	ethanethiol	-	1.27	1	1	1	-
75092	2008389	dichloromethane	1.25 [a]	1.34	0	0	0	-
75127	2008420	formamide	-1.51 [a]	-1.61	1	1	1	-
75150	2008436	carbon disulphide	1.94 [c]	1.94	1	1	-	-
75183	2008462	dimethyl sulphide	-	0.92	1	1	1	-
75218	2008499	ethylene oxide	-0.30 [a]	-0.05	0	0	-	-
75285	2008572	isobutane	2.76 [a]	2.23	1	1	1	-
75310	2008609	isopropylamine	0.26 [a]	0.27	1	1	1	-
75343	2008635	1,1-dichloroethane	1.79 [a]	1.76	0	0	0	-
75354	2008640	1,1-dichloroethylene	2.13 [a]	2.12	0	0	0	-
75365	2008656	acetyl chloride	-	-0.47	1	1	1	-
75387	2008677	1,1-difluoroethylene	1.24 [a]	1.24	1	1	0	-
75445	2008703	phosgene	-	-0.71	1	1	1	-
75456	2008719	chlorodifluoromethane	1.08 [a]	0.89	1	0	0	-
75503	2008750	trimethylamine, in aqueous solution	0.16 [a]	0.04	1	0	1	-
75525	2008766	nitromethane	-0.35 [a]	-0.04	1	1	1	-
75547	2008771	dichloro(methyl)silane	-	1.70	-	-	-	-
75569	2008792	methyloxirane	0.03 [a]	0.37	0	0	-	-
75638	2008876	bromotrifluoromethane	1.86 [a]	1.59	0	0	0	-
75650	2008897	2-methylpropan-2-ol	0.35 [a]	0.73	1	1	0	-
75683	2008918	1-chloro-1,1-difluoroethane	-	2.05	0	0	0	-
75694	2008923	trichlorofluoromethane	2.53 [a]	2.13	0	0	0	-
75718	2008939	dichlorodifluoromethane	2.16 [a]	1.82	0	0	0	-
75741	2008970	tetramethyllead	2.97 [c]	2.92	-	-	-	-
75752	2008986	methanesulphonic acid	-	-2.38	1	1	1	-
75774	2009005	chlorotrimethylsilane	-	2.48	-	-	-	-
75785	2009010	dichloro(dimethyl)silane	-	2.24	-	-	-	-
75796	2009026	trichloro(methyl)silane	-	2.01	-	-	-	-
75865	2009094	2-hydroxy-2-methylpropionitrile	-	-0.03	1	1	1	-
75876	2009115	trichloroacetaldehyde	0.99 [a]	1.19	0	1	0	-
75912	2009157	tert-butyl hydroperoxide	-	0.94	1	1	0	-
75945	2009178	trichloro(vinyl)silane	-	2.36	-	-	-	-
75978	2009204	3,3-dimethylbutanone	1.20 [c]	1.13	1	0	0	-
75989	2009225	pivalic acid	1.48 [f]	1.45	1	1	1	-
76039	2009272	trichloroacetic acid	1.33 [a]	1.44	0	0	0	-
76131	2009361	1,1,2-trichlorotrifluoroethane	3.16 [a]	3.09	0	0	0	-
76142	2009377	cryofluorane	2.82 [a]	2.78	0	0	0	-
76153	2009382	chloropentafluoroethane	-	2.47	0	0	0	-
77474	2010293	hexachlorocyclopentadiene	5.04 [a]	4.63	0	0	-	-
77736	2010529	3a,4,7,7a-tetrahydro-4,7-methanoindene	-	3.51	1	1	-	-
77781	2010581	dimethyl sulphate	-	0.16	1	1	1	-
77929	2010691	citric acid	-1.72 [a]	-1.67	1	1	1	-
77996	2010749	propylidynetrimethanol	-1.48 [e]	0.19	1	1	0	-
78002	2010754	tetraethyllead	-	4.88	-	-	-	-
78400	2011145	triethyl phosphate	0.80 [a]	0.87	1	1	1	-
78513	2011229	tris(2-butoxyethyl) phosphate	3.75 [f]	3.00	0	1	1	-
78591	2011260	3,5,5-trimethylcyclohex-2-enone	1.70 [g]	2.62	1	0	-	-
78706	2011344	linalool	2.97 [h]	3.38	0	0	0	-
78784	2011428	2-methylbutane	-	2.72	1	1	1	-
78795	2011433	isoprene	2.42 [f]	2.58	1	1	1	-
78831	2011480	2-methylpropan-1-ol	0.76 [a]	0.77	1	1	1	-
78842	2011496	isobutyraldehyde	-	0.74	1	1	1	-
78875	2011522	1,2-dichloropropane	-	2.25	0	0	0	-
78900	2011559	propylenediamine	-	-1.20	1	1	1	-
78922	2011585	butan-2-ol	0.61 [a]	0.77	1	1	1	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
78933	2011590	butanone	0.29 [a]	0.26	1	1	1	-
78966	2011627	1-aminopropan-2-ol	-0.96 [a]	-1.19	1	1	1	-
78988	2011648	pyruvaldehyde	-	-1.50	1	1	1	-
79005	2011669	1,1,2-trichloroethane	1.89 [i]	2.01	0	0	0	-
79016	2011674	trichloroethylene	2.42 [a]	2.47	0	0	0	-
79061	2011737	acrylamide	-0.67 [a]	-0.81	1	1	1	-
79094	2011763	propionic acid	0.33 [a]	0.58	1	1	1	-
79107	2011779	acrylic acid	0.35 [c]	0.44	1	1	1	-
79118	2011784	chloroacetic acid	0.22 [a]	0.34	1	1	1	-
79141	2011805	glycollic acid	-1.11 [a]	-1.07	1	1	1	-
79209	2011852	methyl acetate	0.18 [a]	0.37	1	1	1	-
79210	2011868	peracetic acid	-	-1.07	1	1	1	-
79312	2011957	isobutyric acid	0.94 [b]	1.00	1	1	1	-
79334	2011962	l-(+)-lactic acid	-0.72 [a]	-0.65	1	1	1	-
79345	2011978	1,1,2,2-tetrachloroethane	2.39 [a]	2.19	0	0	0	-
79390	2012023	methacrylamide	-	-0.26	1	1	1	-
79414	2012044	methacrylic acid	0.93 [a]	0.99	1	1	1	-
79469	2012091	2-nitropropane	0.93 [f]	0.87	1	1	1	-
79505	2012107	()-dihydro-3-hydroxy-4,4-dimethylfuran-2(3H)-one	-	-0.97	1	1	-	-
79776	2012243	(E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	-	4.42	0	0	-	-
79925	2012348	camphene	-	4.35	0	0	-	-
79947	2012369	2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol	-	7.20	0	0	-	-
80057	2012458	4,4'-isopropylidenediphenol	3.32 [a]	3.64	1	0	-	-
80159	2012547	alpha,alpha-dimethylbenzyl hydroperoxide	-	2.16	1	1	-	-
80433	2012793	bis(alpha,alpha-dimethylbenzyl) peroxide	5.50 [f]	5.88	1	0	-	-
80546	2012898	2-(4-tert-butylbenzyl)propionaldehyde	-	4.36	1	1	-	0
80568	2012919	pin-2(3)-ene	4.83 [h]	4.27	0	0	-	-
80626	2012971	methyl methacrylate	1.38 [a]	1.28	1	1	1	-
81049	2013179	naphthalene-1,5-disulphonic acid	-	-0.94	0	0	-	-
81118	2013252	4,4'-diaminostilbene-2,2'-disulphonic acid	-	-1.42	0	0	-	-
81163	2013315	2-aminonaphthalene-1-sulphonic acid	-1.16 [a]	-0.91	0	0	-	-
81641	2013687	1,4-dihydroxyanthraquinone	-	3.94	1	1	-	-
81845	2013802	naphthalene-1,8-dicarboxylic anhydride	-	3.24	1	1	-	-
82451	2014235	1-aminoanthraquinone	3.74 [f]	3.53	0	0	-	-
83329	2014696	acenaphthene	3.92 [a]	4.15	1	1	-	-
83567	2014874	naphthalene-1,5-diol	1.94 [a]	2.21	1	1	-	-
83625	2014895	1-amino-9,10-dihydro-9,10-dioxoanthracene-2-sulphonic acid	-	0.37	0	0	-	-
83885	2015071	riboflavin	-1.46 [a]	-1.05	1	1	-	1
84617	2015459	dicyclohexyl phthalate	-	6.20	1	1	-	-
84651	2015490	anthraquinone	3.39 [a]	3.34	1	0	-	-
84662	2015506	diethyl phthalate	2.47 [a]	2.65	1	1	-	1
84695	2015532	diisobutyl phthalate	4.11 [a]	4.46	1	1	-	-
84742	2015574	dibutyl phthalate	4.72 [a]	4.61	1	1	-	1
85405	2016028	1,2,3,6-tetrahydrophthalimide	-	0.30	1	1	-	-
85416	2016033	phthalimide	1.15 [a]	1.30	1	1	-	-
85427	2016049	cyclohexane-1,2-dicarboxylic anhydride	-	2.17	1	1	-	-
85438	2016054	1,2,3,6-tetrahydrophthalic anhydride	-	1.96	1	1	-	-
85449	2016075	phthalic anhydride	1.60 [i]	2.07	1	1	-	-
85563	2016159	2-(4-chlorobenzoyl)benzoic acid	-	3.33	1	0	-	-
85687	2016227	benzyl butyl phthalate	4.91 [a]	4.84	1	1	-	-
86500	2016761	azinphos-methyl	2.75 [a]	2.53	1	1	-	-
86577	2016845	1-nitronaphthalene	3.19 [a]	2.99	0	0	-	-
86748	2016960	carbazole	-	3.29	0	0	-	-
87569	2017524	mucochloric acid	-	1.37	1	1	0	-
87616	2017571	1,2,3-trichlorobenzene	4.05 [d]	3.93	0	0	-	0
87627	2017587	2,6-xylidine	-	2.17	1	1	-	0
87683	2017655	hexachlorobuta-1,3-diene	4.78 [a]	4.72	0	0	0	-
87901	2017828	symclosene	-	0.94	1	0	-	-
87990	2017880	xylitol	-	-2.56	1	1	0	-
88062	2017959	2,4,6-trichlorophenol	3.69 [a]	3.45	0	0	-	0
88120	2018004	1-vinyl-2-pyrrolidone	0.37 [a]	0.25	1	1	-	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
88448	2018313	4-aminotoluene-3-sulphonic acid	-	-1.53	0	0	-	0
88539	2018397	5-amino-2-chlorotoluene-4-sulphonic acid	-	-0.89	0	0	-	0
88664	2018491	1-chloro-2-(dichloromethyl)benzene	-	3.62	0	0	-	0
88722	2018533	2-nitrotoluene	2.30 [a]	2.36	0	0	-	0
88733	2018549	1-chloro-2-nitrobenzene	2.24 [a]	2.46	0	0	-	0
88744	2018554	2-nitroaniline	1.85 [a]	2.02	0	0	-	0
88755	2018575	2-nitrophenol	1.79 [a]	1.91	0	0	-	0
89258	2018910	3-methyl-1-phenyl-5-pyrazolone	-	2.56	1	1	-	1
89612	2019233	1,4-dichloro-2-nitrobenzene	3.09 [a]	3.10	0	0	-	0
89838	2019448	thymol	3.30 [a]	3.52	1	1	-	0
89872	2019474	4-nitro-m-xylene	-	2.91	0	0	-	0
89985	2019563	2-chlorobenzaldehyde	2.33 [a]	2.35	1	1	-	0
90040	2019631	o-anisidine	1.18 [a]	1.16	1	1	-	1
90051	2019647	guaiacol	1.32 [a]	1.34	1	1	-	1
90437	2019935	biphenyl-2-ol	3.09 [i]	3.28	1	1	-	-
90722	2020139	2,4,6-tris(dimethylaminomethyl)phenol	-	0.77	0	0	-	0
90802	2020165	D-glucono-1,5-lactone	-	-3.28	1	1	-	-
91156	2020448	phthalonitrile	0.99 [j]	1.09	1	1	-	-
91203	2020495	naphthalene, pure	3.30 [a]	3.17	1	1	-	-
91225	2020516	quinoline	2.03 [a]	2.14	1	1	-	-
91236	2020521	2-nitroanisole	1.73 [a]	1.89	1	1	-	0
91667	2020888	N,N-diethylaniline	3.31 [a]	3.15	1	1	-	0
91689	2020909	3-diethylaminophenol	-	2.32	1	0	-	0
91769	2020956	6-phenyl-1,3,5-triazine-2,4-diyldiamine	1.36 [a]	1.44	0	0	-	-
91941	2021090	3,3'-dichlorobenzidine	3.51 [a]	3.21	0	0	-	-
92524	2021635	biphenyl	3.98 [b]	3.76	1	1	-	-
92706	2021808	3-hydroxy-2-naphthoic acid	3.05 [b]	3.42	1	1	-	-
92842	2021965	phenothiazine	4.15 [a]	3.82	0	0	-	-
93652	2022644	2-(4-chloro-2-methylphenoxy)propionic acid	3.13 [k]	2.94	1	1	-	0
94360	2023276	dibenzoyl peroxide	3.46 [b]	3.43	1	1	-	-
94600	2023475	dimethyl cyclohexane-1,4-dicarboxylate	-	2.11	1	1	-	-
94688	2023543	N-ethyl-o-toluidine	-	2.66	1	0	-	0
94746	2023606	(4-chloro-2-methylphenoxy)acetic acid	3.25 [k]	2.52	1	1	-	0
94757	2023611	2,4-D	2.81 [a]	2.62	0	0	-	0
95169	2023962	benzothiazole	2.01 [a]	2.17	1	1	-	-
95318	2024091	N-tert-butylbenzothiazole-2-sulphenamide	-	2.56	0	0	-	-
95330	2024112	N-cyclohexylbenzothiazole-2-sulphenamide	-	3.47	1	0	-	-
95476	2024222	o-xylene	3.12 [a]	3.09	1	1	-	1
95487	2024238	o-cresol	1.95 [a]	2.06	1	1	-	1
95498	2024243	2-chlorotoluene	3.42 [a]	3.18	1	0	-	0
95501	2024259	1,2-dichlorobenzene	3.43 [c]	3.28	0	0	-	0
95512	2024264	2-chloroaniline	1.90 [a]	1.72	0	0	-	0
95534	2024290	o-toluidine	1.32 [a]	1.62	1	1	-	1
95545	2024306	o-phenylenediamine	0.15 [a]	0.16	0	0	-	0
95556	2024311	2-aminophenol	0.62 [a]	0.60	1	1	-	1
95578	2024332	2-chlorophenol	2.15 [a]	2.16	1	1	-	0
95636	2024369	1,2,4-trimethylbenzene	3.63 [c]	3.63	1	1	-	0
95749	2024463	3-chloro-p-toluidine	-	2.27	0	0	-	0
95761	2024484	3,4-dichloroaniline	2.69 [a]	2.37	0	0	-	0
95932	2024657	1,2,4,5-tetramethylbenzene	4.00 [a]	4.18	1	1	-	0
96106	2024772	diethylaluminium chloride	-	-	-	-	-	-
96184	2024861	1,2,3-trichloropropane	2.27 [f]	2.50	0	0	0	-
96220	2024903	pentan-3-one	0.99 [a]	0.75	1	1	1	-
96242	2024924	3-chloropropane-1,2-diol	-	-0.53	1	1	1	-
96297	2024966	butanone oxime	0.63 [f]	1.69	1	1	1	-
96311	2024987	1,3-dimethylurea	-0.49 [a]	-0.62	1	1	1	-
96333	2025006	methyl acrylate	0.80 [a]	0.73	1	1	1	-
96344	2025011	methyl chloroacetate	-	0.63	1	1	1	-
96480	2025095	gamma-butyrolactone	-0.64 [a]	-0.31	1	1	-	-
96764	2025320	2,4-di-tert-butylphenol	5.19 [f]	5.33	0	0	-	0
97007	2025514	1-chloro-2,4-dinitrobenzene	2.17 [l]	2.27	0	0	-	0

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin	75	78
97029	2025535	2,4-dinitroaniline	-	1.84	0	0	-	0
97369	2025760	2',4'-dimethylacetoacetanilide	-	1.54	1	1	-	1
97654	2025996	itaconic acid	-	-0.34	1	1	1	-
97723	2026036	isobutyric anhydride	-	1.24	1	1	1	-
97745	2026057	tetramethylthiuram monosulphide	-	0.75	1	1	0	-
97778	2026078	disulfiram	3.88 [a]	3.67	1	0	-	-
97869	2026130	isobutyl methacrylate	2.66 [a]	2.67	1	1	1	-
97881	2026151	butyl methacrylate	2.88 [a]	2.75	1	1	1	-
97938	2026193	triethylaluminium	-	-	-	-	-	-
98000	2026261	furfuryl alcohol	0.28 [a]	0.45	1	1	-	-
98011	2026277	2-furaldehyde	0.41 [a]	0.83	1	1	-	-
98077	2026345	alpha,alpha,alpha-trichlorotoluene	-	3.90	0	0	-	-
98088	2026350	alpha,alpha,alpha-trifluorotoluene	3.01 [a]	2.96	0	0	-	-
98099	2026366	benzenesulphonyl chloride	-	2.94	1	1	-	-
98135	2026408	trichloro(phenyl)silane	-	3.60	-	-	-	-
98168	2026434	alpha,alpha,alpha-trifluoro-m-toluidine	2.29 [l]	2.04	0	0	-	1
98464	2026701	alpha,alpha,alpha-trifluoro-3-nitrotoluene	2.62 [a]	2.77	0	0	-	0
98511	2026759	4-tert-butyltoluene	5.17 [f]	4.45	1	0	-	0
98522	2026764	4-tert-butylcyclohexanol	3.09 [m]	3.42	1	1	-	-
98544	2026790	4-tert-butylphenol	3.31 [a]	3.42	1	1	-	0
98566	2026811	4-chloro-alpha,alpha,alpha-trifluorotoluene	-	3.60	0	0	-	0
98737	2026963	4-tert-butylbenzoic acid	3.85 [c]	3.78	1	1	-	0
98828	2027045	cumene	3.66 [a]	3.45	1	1	-	0
98839	2027050	2-phenylpropene	3.48 [c]	3.44	1	1	-	0
98862	2027087	acetophenone	1.58 [a]	1.67	1	1	-	1
98873	2027092	alpha,alpha-dichlorotoluene	-	2.97	1	0	-	-
98884	2027108	benzoyl chloride	-	1.44	1	1	-	-
98920	2027134	nicotinamide	-0.37 [a]	-0.45	1	1	-	-
98942	2027155	cyclohexyldimethylamine	-	2.31	0	0	-	-
98953	2027160	nitrobenzene	1.85 [a]	1.81	1	1	-	0
99081	2027286	3-nitrotoluene	2.45 [a]	2.36	0	0	-	0
99547	2027642	1,2-dichloro-4-nitrobenzene	3.12 [a]	3.10	0	0	-	0
99650	2027768	1,3-dinitrobenzene	1.49 [a]	1.63	0	0	-	0
99752	2027841	methyl p-toluate	2.70 [n]	2.38	1	1	-	1
99887	2027972	4-isopropylaniline	2.49 [d]	2.53	1	0	-	0
99990	2028080	4-nitrotoluene	2.37 [a]	2.36	0	0	-	0
100005	2028096	1-chloro-4-nitrobenzene	2.39 [a]	2.46	0	0	-	0
100016	2028101	4-nitroaniline	1.39 [a]	1.47	0	0	-	0
100027	2028117	4-nitrophenol	1.91 [a]	1.91	0	0	-	0
100209	2028295	terephthaloyl dichloride	-	0.88	1	1	-	-
100210	2028300	terephthalic acid	2.00 [a]	1.76	1	1	-	1
100298	2028379	4-nitrophenetole	2.53 [a]	2.38	0	1	-	0
100378	2028452	2-diethylaminoethanol	-	0.05	1	1	0	-
100403	2028489	4-vinylcyclohexene	3.93 [f]	3.73	1	1	-	-
100414	2028494	ethylbenzene	3.15 [a]	3.03	1	1	-	1
100425	2028515	styrene	2.95 [a]	2.89	1	1	-	-
100447	2028536	alpha-chlorotoluene	2.30 [a]	2.79	1	1	-	-
100470	2028557	benzonitrile	1.56 [a]	1.54	1	1	-	-
100516	2028599	benzyl alcohol	1.10 [a]	1.08	1	1	-	-
100527	2028604	benzaldehyde	1.48 [a]	1.71	1	1	-	1
100549	2028630	nicotinonitrile	0.36 [d]	0.35	1	1	-	-
100970	2029058	methenamine	-	-4.15	0	0	-	-
101020	2029084	triphenyl phosphite	-	6.62	1	1	-	-
101053	2029105	anilazine	3.88 [o]	3.64	0	0	-	0
101393	2029388	alpha-methylcinnamaldehyde	-	2.37	1	1	-	-
101542	2029519	N-(4-aminophenyl)aniline	-	1.82	0	0	-	-
101724	2029697	N-isopropyl-N'-phenyl-p-phenylenediamine	-	3.28	0	0	-	-
101779	2029744	4,4'-methylenedianiline	1.59 [a]	2.18	0	0	-	-
101837	2029807	dicyclohexylamine	-	4.37	1	1	-	-
101848	2029812	diphenyl ether	4.21 [a]	4.05	1	1	-	-
101860	2029833	alpha-hexylcinnamaldehyde	-	4.82	1	1	-	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
102012	2029964	acetoacetanilide	-	1.01	1	1	-	1
102067	2030021	1,3-diphenylguanidine	-	2.89	0	0	-	-
102090	2030058	diphenyl carbonate	3.28 [i]	3.21	1	1	-	-
102363	2030262	3,4-dichlorophenyl isocyanate	-	3.88	0	0	-	0
102716	2030498	2,2',2"-nitrilotriethanol	-1.00 [c]	-2.48	1	1	0	-
102761	2030519	triacetin	0.25 [i]	0.36	1	1	1	-
102772	2030524	2-(morpholinothio)benzothiazole	-	1.02	0	0	-	-
103015	2030702	N-phenylglycine	0.62 [a]	0.88	1	1	-	-
103117	2030807	2-ethylhexyl acrylate	-	4.09	1	1	1	-
103231	2030901	bis(2-ethylhexyl) adipate	-	8.12	1	1	1	-
103708	2031360	formanilide	1.15 [a]	1.13	1	1	-	-
103719	2031376	phenyl isocyanate	-	2.59	1	1	-	-
103822	2031486	phenylacetic acid	1.41 [a]	1.43	1	1	-	-
103844	2031507	acetanilide	1.16 [a]	1.10	1	1	-	1
103902	2031575	paracetamol	0.46 [d]	0.27	1	1	-	1
104154	2031800	toluene-4-sulphonic acid	-	-0.62	0	1	-	1
104552	2032139	cinnamaldehyde	1.90 [a]	1.82	1	1	-	-
104767	2032343	2-ethylhexan-1-ol	-	2.73	1	1	1	-
104881	2032474	4-chlorobenzaldehyde	2.10 [a]	2.35	1	1	-	0
104938	2032537	4-methylanisole	2.66 [c]	2.62	1	1	-	1
105384	2032935	vinyl propionate	-	1.22	1	1	1	-
105395	2032940	ethyl chloroacetate	-	1.12	1	1	1	-
105453	2032998	methyl acetoacetate	-	-0.69	1	1	1	-
105486	2033017	isopropyl chloroacetate	-	1.54	1	1	1	-
105533	2033059	diethyl malonate	0.96 [i]	0.90	1	1	1	-
105599	2033127	2,2'-methyliminodiethanol	-	-1.50	1	1	1	-
105602	2033132	epsilon-caprolactam	-	0.66	1	1	-	-
105624	2033153	1-methyl-1,2-ethanediyl dioleate	-	16.11	1	1	1	-
105760	2033284	dibutyl maleate	-	4.16	1	1	1	-
105997	2033504	dibutyl adipate	-	4.33	1	1	1	-
106241	2033771	geraniol	-	3.47	1	1	0	-
106252	2033787	nerol	-	3.47	1	1	0	-
106423	2033965	p-xylene	3.15 [a]	3.09	1	1	-	1
106434	2033970	4-chlorotoluene	3.33 [a]	3.18	1	0	-	0
106445	2033986	p-cresol	1.94 [a]	2.06	1	1	-	1
106467	2034005	1,4-dichlorobenzene	3.44 [c]	3.28	0	0	-	0
106489	2034026	4-chlorophenol	2.39 [a]	2.16	1	1	-	0
106490	2034031	p-toluidine	1.39 [a]	1.62	1	1	-	1
106503	2034047	p-phenylenediamine	-0.30 [c]	-0.39	0	0	-	0
106650	2034199	dimethyl succinate	0.35 [c]	0.40	1	1	1	-
106752	2034309	oxydiethylene bis(chloroformate)	-	-0.34	0	0	1	-
106887	2034382	1,2-epoxybutane	-	0.86	0	0	-	-
106898	2034398	1-chloro-2,3-epoxypropane	0.45 [p]	0.63	0	0	-	-
106934	2034445	1,2-dibromoethane	1.96 [c]	2.01	1	0	0	-
106978	2034487	butane, pure	2.89 [c]	2.31	1	1	1	-
106989	2034492	but-1-ene	2.40 [a]	2.17	1	1	1	-
106990	2034508	buta-1,3-diene	1.99 [a]	2.03	1	1	-	-
107017	2034529	butene, mixed -1- and -2- isomers	2.31 [a]	2.09	1	1	1	-
107028	2034534	acrylaldehyde	-0.01 [a]	0.19	1	1	1	-
107051	2034576	3-chloropropene	-	1.93	1	1	1	-
107062	2034581	1,2-dichloroethane	1.48 [a]	1.83	0	0	0	-
107073	2034597	2-chloroethanol	0.03 [a]	0.11	1	1	1	-
107131	2034665	acrylonitrile	0.25 [a]	0.21	1	1	-	-
107153	2034686	ethylenediamine	-2.04 [c]	-1.62	1	1	1	-
107186	2034707	allyl alcohol	0.17 [a]	0.21	1	1	1	-
107211	2034733	ethane-1,2-diol	-1.36 [a]	-1.20	1	1	1	-
107222	2034749	glyoxal	-	-1.66	1	1	1	-
107255	2034754	methyl vinyl ether	-	0.42	0	0	1	-
107313	2034817	methyl formate	0.03 [c]	-0.17	1	1	1	-
107415	2034890	2-methylpentane-2,4-diol	-	0.58	1	1	0	-
107437	2034906	betaine	-	-	-	-	-	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
107460	2034927	hexamethyldisiloxane	4.20 [d]	4.76	-	-	-	-
107642	2035082	dimethyldioctadecylammonium chloride	-	-	-	-	-	-
107868	2035276	3-methyl-2-butenal	-	1.15	1	1	1	-
107880	2035297	butane-1,3-diol	-	-0.29	1	1	1	-
107926	2035323	butyric acid	0.79 [a]	1.07	1	1	1	-
107982	2035391	1-methoxypropan-2-ol	-	-0.49	1	0	1	-
108010	2035428	2-dimethylaminoethanol	-	-0.94	1	1	1	-
108032	2035449	1-nitropropane	0.87 [a]	0.95	1	1	1	-
108054	2035454	vinyl acetate	0.73 [a]	0.73	1	1	1	-
108101	2035501	4-methylpentan-2-one	1.31 [q]	1.16	1	1	1	-
108112	2035517	4-methylpentan-2-ol	-	1.68	1	1	0	-
108189	2035585	diisopropylamine	1.40 [c]	1.64	1	1	0	-
108203	2035606	diisopropyl ether	1.52 [m]	1.88	0	0	0	-
108214	2035611	isopropyl acetate	-	1.28	1	1	1	-
108225	2035627	isopropenyl acetate	-	1.28	1	1	1	-
108247	2035648	acetic anhydride	-	-0.58	1	1	1	-
108316	2035716	maleic anhydride	-	1.62	1	1	-	-
108327	2035721	propylene carbonate	-0.41 [c]	0.08	1	1	-	-
108383	2035763	m-xylene	3.20 [a]	3.09	1	1	-	1
108394	2035779	m-cresol	1.96 [a]	2.06	1	1	-	1
108441	2035831	m-toluidine	1.40 [a]	1.62	1	1	-	1
108452	2035847	m-phenylenediamine	-0.33 [c]	-0.39	0	0	-	0
108463	2035852	resorcinol	0.80 [a]	1.03	1	1	-	1
108598	2035978	dimethyl malonate	-0.05 [c]	-0.09	1	1	1	-
108656	2036039	2-methoxy-1-methylethyl acetate	0.56 [r]	0.52	1	1	1	-
108689	2036065	3,5-xylenol	2.35 [a]	2.61	1	1	-	1
108770	2036149	2,4,6-trichloro-1,3,5-triazine	-	1.73	0	0	-	-
108781	2036154	melamine	-1.37 [c]	-0.38	0	0	-	-
108805	2036180	cyanuric acid	-	0.61	1	0	-	-
108838	2036201	2,6-dimethylheptan-4-one	-	2.56	1	1	0	-
108883	2036259	toluene	2.73 [a]	2.54	1	1	-	1
108907	2036285	chlorobenzene	2.84 [d]	2.64	1	1	-	0
108918	2036290	cyclohexylamine	1.49 [a]	1.63	1	1	-	-
108930	2036306	cyclohexanol	1.23 [a]	1.64	1	1	-	-
108941	2036311	cyclohexanone	0.81 [a]	1.13	1	1	-	-
108952	2036327	phenol	1.46 [a]	1.51	1	1	-	1
109068	2036437	2-methylpyridine	1.11 [a]	1.35	1	1	-	-
109535	2036788	isobutyl vinyl ether	-	1.82	0	0	1	-
109557	2036809	3-aminopropyldimethylamine	-	-0.45	1	1	1	-
109604	2036861	propyl acetate	1.24 [a]	1.36	1	1	1	-
109660	2036924	pentane	3.39 [a]	2.80	1	1	1	-
109693	2036966	1-chlorobutane	2.64 [a]	2.56	1	1	1	-
109706	2036971	1-bromo-3-chloropropane	2.18 [s]	2.41	1	0	0	-
109739	2036992	butylamine	0.97 [a]	0.83	1	1	1	-
109831	2037100	2-methylaminoethanol	-0.94 [c]	-1.15	1	1	1	-
109864	2037137	2-methoxyethanol	-0.77 [a]	-0.91	1	0	1	-
109897	2037163	diethylamine	0.58 [a]	0.81	1	1	1	-
109922	2037184	ethyl vinyl ether	1.04 [a]	0.91	0	0	1	-
109944	2037210	ethyl formate	0.23 [a]	0.32	1	1	1	-
109999	2037268	tetrahydrofuran	0.46 [a]	0.94	0	0	-	-
110010	2037289	tetrahydrothiophene	-	1.79	1	1	-	-
110054	2037336	di-tert-butyl peroxide	-	3.45	0	0	0	-
110123	2037378	5-methylhexan-2-one	1.88 [q]	1.66	1	1	1	-
110167	2037425	maleic acid	0.46 [c]	0.05	1	1	1	-
110178	2037430	fumaric acid	0.46 [c]	0.05	1	1	1	-
110190	2037451	isobutyl acetate	1.78 [c]	1.77	1	1	1	-
110214	2037472	1,1-hydrazoformamide	-	-2.37	1	1	-	-
110270	2037514	isopropyl myristate	-	7.17	1	1	1	-
110305	2037556	N,N'-ethylenedi(stearamide)	-	13.98	1	1	1	-
110338	2037577	dihexyl adipate	-	6.30	1	1	1	-
110429	2037666	methyl decanoate	4.41 [a]	4.30	1	1	1	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.
[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
110441	2037687	hexa-2,4-dienoic acid	1.33 [a]	1.62	1	1	1	-
110543	2037776	hexane	3.90 [a]	3.29	1	1	1	-
110634	2037865	butane-1,4-diol	-0.83 [c]	-0.22	1	1	1	-
110645	2037870	but-2-ene-1,4-diol	-0.81 [c]	-0.43	1	1	1	-
110656	2037886	but-2-yne-1,4-diol	-	-0.93	1	1	1	-
110805	2038041	2-ethoxyethanol	-0.32 [c]	-0.42	1	0	1	-
110827	2038062	cyclohexane	3.44 [a]	3.18	1	1	-	-
110850	2038083	piperazine	-1.50 [c]	-0.80	1	1	-	-
110883	2038125	1,3,5-trioxane	-0.43 [c]	-0.56	0	0	-	-
110918	2038151	morpholine	-0.86 [a]	-0.56	1	0	-	-
110930	2038167	6-methylhept-5-en-2-one	-	2.06	1	1	1	-
110974	2038209	1,1'-iminodipropan-2-ol	-0.82 [a]	-0.88	1	1	0	-
110985	2038214	1,1'-oxydipropan-2-ol	-	-0.64	1	0	0	-
111115	2038350	methyl octanoate	-	3.32	1	1	1	-
111148	2038387	heptanoic acid	2.42 [d]	2.54	1	1	1	-
111159	2038392	2-ethoxyethyl acetate	-	0.59	1	1	1	-
111273	2038523	hexan-1-ol	2.03 [a]	1.82	1	1	1	-
111295	2038544	pentane-1,5-diol	-	0.27	1	1	1	-
111308	2038565	glutaral	-	-0.18	1	1	1	-
111364	2038628	butyl isocyanate	-	2.26	1	1	1	-
111400	2038654	2,2'-iminodi(ethylamine)	-	-2.13	1	1	1	-
111411	2038675	2-(2-aminoethylamino)ethanol	-	-2.13	1	1	1	-
111422	2038680	2,2'-iminodiethanol	-1.43 [a]	-1.71	1	1	1	-
111466	2038722	2,2'-oxydiethanol	-	-1.47	1	1	1	-
111488	2038743	thiodiglycol	-0.63 [c]	-0.62	1	1	1	-
111659	2038921	octane	5.18 [t]	4.27	1	1	1	-
111660	2038937	oct-1-ene	4.57 [a]	4.13	1	1	1	-
111693	2038963	adiponitrile	-0.32 [q]	0.35	1	1	-	-
111717	2038984	heptanal	-	2.29	1	1	1	-
111762	2039050	2-butoxyethanol	0.83 [a]	0.57	1	1	1	-
111773	2039066	2-(2-methoxyethoxy)ethanol	-	-1.18	0	0	1	-
111820	2039113	methyl laurate	-	5.28	1	1	1	-
111875	2039176	octan-1-ol	3.00 [c]	2.81	1	1	1	-
111900	2039197	2-(2-ethoxyethoxy)ethanol	-0.54 [m]	-0.69	0	0	1	-
111911	2039202	bis(2-chloroethoxy)methane	-	1.30	0	0	0	-
111922	2039218	dibutylamine	2.83 [a]	2.77	1	1	1	-
111966	2039244	bis(2-methoxyethyl) ether	-0.36 [m]	-0.48	0	0	1	-
112050	2039312	nonanoic acid	3.42 [b]	3.52	1	1	1	-
112072	2039333	2-butoxyethyl acetate	-	1.57	1	1	1	-
112185	2039438	dodecyldimethylamine	-	5.44	1	0	1	-
112243	2039506	trientine	-	-2.65	1	1	1	-
112254	2039511	2-hexyloxyethanol	1.86 [m]	1.55	1	1	1	-
112276	2039532	2,2'-(ethylenedioxy)diethanol	-	-1.75	0	0	1	-
112301	2039569	decan-1-ol	4.57 [i]	3.79	1	1	1	-
112345	2039616	2-(2-butoxyethoxy)ethanol	0.56 [m]	0.29	0	0	1	-
112356	2039621	2-(2-(2-methoxyethoxy)ethoxy)ethanol	-	-1.46	0	0	1	-
112414	2039684	dodec-1-ene	-	6.10	1	1	1	-
112538	2039820	dodecan-1-ol	5.13 [a]	4.77	1	1	1	-
112572	2039862	3,6,9-triazaundecamethylenediamine	-	-3.16	1	1	1	-
112607	2039899	3,6,9-trioxaundecane-1,11-diol	-	-2.02	0	0	1	-
112629	2039925	methyl oleate	-	8.02	1	1	1	-
112721	2040003	tetradecanol	-	5.75	1	1	1	-
112765	2040045	stearoyl chloride	-	7.39	1	1	1	-
112845	2040092	(Z)-docos-13-enamide	-	8.44	1	1	1	-
112867	2040113	(Z)-docos-13-enoic acid	-	9.69	1	1	1	-
112889	2040129	octadec-1-ene	-	9.04	1	1	1	-
112903	2040155	(Z)-octadec-9-enylamine	-	7.50	1	1	1	-
112925	2040176	octadecan-1-ol	-	7.72	1	1	1	-
114261	2040438	propoxur	1.52 [c]	1.90	1	1	-	0
115071	2040621	propene, pure	1.77 [a]	1.68	1	1	1	-
115106	2040658	dimethyl ether	0.10 [a]	0.07	0	0	1	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
115117	2040663	2-methylpropene	2.34 [a]	2.23	1	1	1	-
115184	2040684	2-methylbut-3-en-2-ol	-	1.08	1	1	1	-
115195	2040705	2-methylbut-3-yn-2-ol	0.28 [i]	0.45	1	1	1	-
115297	2040794	endosulfan	3.83 [a]	3.84	0	0	-	-
115322	2040820	dicofol	5.02 [o]	5.81	0	0	-	-
115775	2041049	pentaerythritol	-1.69 [e]	-1.77	1	1	1	-
115866	2041122	triphenyl phosphate	4.59 [a]	4.70	1	1	-	-
115968	2041185	tris(2-chloroethyl) phosphate	1.44 [f]	1.63	1	1	0	-
116029	2041227	3,3,5-trimethylcyclohexanol	-	2.93	1	1	-	-
116143	2041269	tetrafluoroethylene	-	1.21	1	1	0	-
116154	2041274	hexafluoropropene	-	2.12	0	0	0	-
117793	2042084	2-aminoanthraquinone	-	2.43	0	0	-	-
117817	2042110	bis(2-ethylhexyl) phthalate	7.60 [u]	8.39	1	1	-	-
118332	2042461	6-aminonaphthalene-1,3-disulphonic acid	-	-1.85	0	0	-	-
118489	2042550	4H-3,1-benzoxazine-2,4(1H)-dione	-	2.60	1	1	-	1
118581	2042629	benzyl salicylate	-	4.31	1	1	-	-
118741	2042739	hexachlorobenzene	5.73 [u]	5.86	0	0	-	0
118821	2042791	2,2',6,6'-tetra-tert-butyl-4,4'-methylenediphenol	-	8.99	0	0	-	-
118967	2042896	2,4,6-trinitrotoluene	1.60 [a]	1.99	0	0	-	0
119368	2043177	methyl salicylate	2.55 [d]	2.60	1	1	-	1
119471	2043271	6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol	6.25 [f]	7.97	1	0	-	-
119619	2043376	benzophenone	3.18 [a]	3.15	1	1	-	-
119642	2043402	1,2,3,4-tetrahydronaphthalene	3.49 [c]	3.96	1	1	-	1
119802	2043528	2,2'-dithiodi(benzoic acid)	-	3.38	1	1	-	-
120127	2043711	anthracene, pure	4.45 [a]	4.35	1	1	-	-
120183	2043753	naphthalene-2-sulphonic acid	0.63 [a]	0.01	0	0	-	-
120365	2043905	dichlorprop	3.43 [k]	3.03	0	0	-	0
120514	2044029	benzyl benzoate	3.97 [a]	3.54	1	1	-	-
120616	2044118	dimethyl terephthalate	2.25 [a]	1.66	1	1	-	1
120785	2044249	di(benzothiazol-2-yl) disulphide	-	4.66	1	0	-	-
120809	2044275	pyrocatechol	0.88	1.03	1	1	-	1
120821	2044280	1,2,4-trichlorobenzene	4.02 [c]	3.93	0	0	-	0
120832	2044296	2,4-dichlorophenol	3.06 [c]	2.80	0	0	-	0
120923	2044359	cyclopentanone	-	0.63	1	1	-	-
121039	2044453	4-nitrotoluene-2-sulphonic acid	-	-0.80	0	0	-	0
121142	2044500	2,4-dinitrotoluene	1.98 [a]	2.18	0	0	-	0
121335	2044652	vanillin	1.21 [a]	1.05	1	1	-	1
121448	2044694	triethylamine	1.45 [a]	1.51	0	0	0	-
121471	2044736	3-aminobenzenesulphonic acid	-	-2.08	0	0	-	0
121573	2044825	sulphanilic acid	-2.16 [v]	-2.08	0	0	-	0
121697	2044935	N,N-dimethylaniline	2.31 [a]	2.17	1	1	-	0
121733	2044961	1-chloro-3-nitrobenzene	2.46 [c]	2.46	0	0	-	0
121755	2044977	malathion	2.36 [a]	2.29	1	1	1	-
121824	2045001	perhydro-1,3,5-trinitro-1,3,5-triazine	0.87 [b]	0.68	1	0	-	-
121868	2045017	2-chloro-4-nitrotoluene	-	3.00	0	0	-	0
121879	2045022	2-chloro-4-nitroaniline	-	2.12	0	0	-	0
121915	2045064	isophthalic acid	1.66 [a]	1.76	1	1	-	1
122349	2045352	simazine	2.18 [a]	2.40	0	0	-	-
122394	2045394	diphenylamine	3.50 [a]	3.29	1	1	-	-
122510	2045504	triethyl orthoformate	1.20 [c]	1.45	0	0	1	-
122521	2045525	triethyl phosphite	-	2.80	1	1	1	-
122996	2045897	2-phenoxyethanol	1.16 [a]	1.10	1	1	-	-
123057	2045965	2-ethylhexanal	-	2.71	1	1	1	-
123308	2046162	4-aminophenol	0.04 [a]	0.24	1	1	-	1
123319	2046178	hydroquinone	0.59 [a]	1.03	1	1	-	1
123353	2046225	7-methyl-3-methyleneocta-1,6-diene	4.17 [f]	4.88	1	1	1	-
123386	2046230	propionaldehyde	0.59 [a]	0.33	1	1	1	-
123422	2046267	4-hydroxy-4-methylpentan-2-one	-	-0.34	1	0	1	-
123513	2046335	3-methylbutan-1-ol	1.16 [c]	1.26	1	1	1	-
123546	2046340	pentane-2,4-dione	0.40 [c]	0.05	1	1	1	-
123728	2046466	butyraldehyde	0.88 [a]	0.82	1	1	1	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
123773	2046508	C,C'-azodi(formamide)	-	-3.89	1	1	1	-
123864	2046581	n-butyl acetate	1.78 [c]	1.85	1	1	1	-
123911	2046618	1,4-dioxane	-0.27 [a]	-0.32	0	0	-	-
124049	2046733	adipic acid	0.08 [a]	0.23	1	1	1	-
124072	2046775	octanoic acid	3.05 [a]	3.03	1	1	1	-
124094	2046796	hexamethylenediamine	-	0.35	1	1	1	-
124107	2046801	methyl myristate	-	6.27	1	1	1	-
124174	2046859	2-(2-butoxyethoxy)ethyl acetate	-	1.30	0	0	1	-
124185	2046864	decane	5.01 [w]	5.25	1	1	1	-
124301	2046953	octadecylamine	-	7.71	1	1	1	-
124389	2046969	carbon dioxide	-	0.83	1	1	1	-
124403	2046974	dimethylamine, in aqueous solution	-0.38 [a]	-0.17	1	1	1	-
124630	2047061	methanesulphonyl chloride	-	1.27	1	1	1	-
124685	2047098	2-amino-2-methylpropanol	-	-0.74	1	1	1	-
125122	2047276	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acetate	-	3.86	0	1	-	-
126307	2047810	2,2-dimethylpropane-1,3-diol	-	0.16	1	1	0	-
126330	2047831	tetrahydrothiophene 1,1-dioxide	-0.77 [a]	-0.24	1	1	-	-
126716	2047983	triisobutyl phosphate	-	3.60	1	1	0	-
126738	2048002	tributyl phosphate	4.00 [a]	3.82	1	1	1	-
126998	2048180	2-chlorobuta-1,3-diene	-	2.53	1	0	1	-
127184	2048259	tetrachloroethylene	3.40 [a]	2.97	0	0	0	-
127195	2048264	N,N-dimethylacetamide	-0.77 [a]	-0.49	1	1	1	-
127479	2048442	retinyl acetate	-	8.63	1	1	-	-
128370	2048814	2,6-di-tert-butyl-p-cresol	5.10 [e]	5.03	0	0	-	0
128392	2048840	2,6-di-tert-butylphenol	-	4.48	0	0	-	0
131099	2050100	2-chloroanthraquinone	-	3.99	0	0	-	-
131113	2050116	dimethyl phthalate	1.56 [a]	1.66	1	1	-	1
133493	2051078	pentachlorobenzenethiol	-	5.91	0	0	-	0
134327	2051387	1-naphthylamine	2.25 [a]	2.25	0	0	-	-
135193	2051827	2-naphthol	2.70 [a]	2.69	1	1	-	-
135988	2052270	sec-butylbenzene	4.57 [x]	3.94	1	1	-	0
136232	2052328	zinc bis(dibutyldithiocarbamate)	-	5.54	-	-	-	-
137268	2052862	thiram	-	1.70	1	0	-	-
140114	2053997	benzyl acetate	1.96 [a]	2.08	1	1	-	-
140294	2054105	phenylacetonitrile	1.56 [a]	1.56	1	1	-	-
140318	2054110	2-piperazin-1-ylethylamine	-	-1.57	1	1	-	-
140669	2054262	4-(1,1,3,3-tetramethylbutyl)phenol	-	5.28	0	0	-	0
140885	2054388	ethyl acrylate	1.32 [a]	1.22	1	1	1	-
140954	2054440	1,3-bis(hydroxymethyl)urea	-	-3.15	1	1	1	-
141059	2054519	diethyl maleate	-	2.20	1	1	1	-
141106	2054571	6,10-dimethylundeca-3,5,9-trien-2-one	-	4.43	1	0	0	-
141322	2054807	butyl acrylate	2.36 [a]	2.20	1	1	1	-
141435	2054833	2-aminoethanol	-1.31 [a]	-1.61	1	1	1	-
141786	2055004	ethyl acetate	0.73 [a]	0.86	1	1	1	-
141979	2055161	ethyl acetoacetate	0.25 [y]	-0.20	1	1	1	-
142165	2055245	bis(2-ethylhexyl) maleate	-	7.94	1	1	1	-
142223	2055287	diallyl 2,2'-oxydiethyl dicarbonate	-	1.54	0	0	1	-
142789	2055601	N-(2-hydroxyethyl)dodecanamide	-	3.24	1	1	1	-
142825	2055638	heptane	4.66 [t]	3.78	1	1	1	-
142847	2055659	dipropylamine	1.67 [a]	1.79	1	1	1	-
142905	2055706	dodecyl methacrylate	-	6.68	1	1	1	-
142916	2055711	isopropyl palmitate	-	8.16	1	1	1	-
143226	2055926	2-(2-(2-butoxyethoxy)ethoxy)ethanol	-	0.02	0	0	1	-
143339	2055994	sodium cyanide	-	-1.69	-	-	-	-
144627	2056343	oxalic acid	-	-1.74	1	1	1	-
149304	2057368	benzothiazole-2-thiol	2.42 [e]	2.86	1	1	-	-
149575	2057436	2-ethylhexanoic acid	2.64 [b]	2.96	1	1	1	-
149735	2057457	trimethyl orthoformate	0.25 [a]	-0.03	0	0	1	-
150787	2057719	1,4-dimethoxybenzene	2.04 [z]	2.15	1	1	-	1
151508	2057923	potassium cyanide	-	-1.69	-	-	-	-
151564	2057939	aziridine	-	-0.28	1	1	-	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
156434	2058555	p-phenetidine	1.24 [a]	1.65	1	1	-	0
287923	2060166	cyclopentane	3.00 [a]	2.68	1	1	-	-
288324	2060192	imidazole	-0.08 [a]	0.06	1	1	-	-
288880	2060229	1,2,4-triazole	-0.58 [c]	-0.76	1	1	-	-
294622	2060339	cyclododecane	-	6.12	1	1	-	-
298000	2060501	parathion-methyl	2.86 [a]	2.75	1	1	-	0
298066	2060559	O,O-diethyl hydrogen phosphorodithioate	-	2.24	1	1	1	-
298124	2060585	glyoxylic acid	-	-1.40	1	1	1	-
301020	2061039	oleamide	-	6.48	1	1	1	-
302012	2061149	hydrazine	-2.07 [c]	-1.47	-	-	-	-
328847	2063371	3,4-dichloro-alpha,alpha,alpha-trifluorotoluene	-	4.24	0	0	-	0
329011	2063413	alpha,alpha,alpha-trifluoro-3-tolyl isocyanate	-	3.56	0	0	-	-
330541	2063544	diuron	2.68 [c]	2.67	0	0	-	0
330552	2063565	linuron	3.20 [a]	2.91	0	0	-	0
333415	2063738	diazinon	3.81 [a]	3.86	1	1	-	-
334485	2063764	decanoic acid	4.09 [a]	4.02	1	1	1	-
353593	2065379	bromochlorodifluoromethane	-	1.90	0	0	0	-
366187	2066744	2,2'-bipyridyl	1.50 [aa]	1.38	0	0	-	-
393759	2068893	4-chloro-3,5-dinitro-alpha,alpha,alpha-trifluorotoluene	2.50 [i]	3.24	0	0	-	0
420042	2069923	cyanamide	-0.82 [ab]	-0.81	1	1	-	-
461585	2073128	cyanoguanidine	-	-1.34	1	1	-	-
463514	2073369	ketene	-	-0.52	1	1	1	-
473552	2074671	2,6,6-trimethylbicyclo[3.1.1]heptane	-	4.35	0	0	-	-
482893	2075869	2-(1,3-dihydro-3-oxo-2H-indazol-2-ylidene)-1,2-dihydro-3H-indol-3-one	3.72 [i]	3.11	0	0	-	-
497392	2078477	4,6-di-tert-butyl-m-cresol	-	5.88	0	0	-	0
502443	2079381	hexan-6-olide	-	0.68	1	1	-	-
502692	2079507	6,10,14-trimethylpentadecan-2-one	-	6.91	1	0	0	-
504609	2079952	penta-1,3-diene	2.44 [d]	2.45	1	1	1	-
505328	2080088	3,7,11,15-tetramethylhexadec-1-en-3-ol	-	8.23	0	0	0	-
505657	2080156	1,3-dioxepane	-	0.67	0	0	-	-
513359	2081563	2-methylbut-2-ene	-	2.64	1	1	1	-
526954	2084014	D-gluconic acid	-	-1.87	1	1	0	-
533744	2085767	dazomet	1.40 [ab]	0.94	1	0	-	-
538932	2087062	isobutylbenzene	4.68 [x]	3.94	1	1	-	0
540841	2087591	2,2,4-trimethylpentane	-	4.09	1	0	0	-
541731	2087921	1,3-dichlorobenzene	3.53 [c]	3.28	0	0	-	0
542756	2088265	1,3-dichloropropene	2.03 [ab]	2.29	0	0	0	-
544638	2088752	myristic acid, pure	6.11 [b]	5.98	1	1	1	-
551166	2089934	6-aminopenicillanic acid	-	0.60	1	1	-	-
552307	2090080	benzene-1,2,4-tricarboxylic acid 1,2-anhydride	-	1.95	1	1	-	1
553264	2090363	4,4'-bipyridyl	1.28 [aa]	1.38	0	0	-	-
556672	2091367	octamethylcyclotetrasiloxane	5.10 [e]	5.09	-	-	-	-
556821	2091414	3-methylbut-2-en-1-ol	-	1.17	1	1	1	-
563473	2092512	3-chloro-2-methylpropene	-	2.48	1	0	1	-
563780	2092622	2,3-dimethylbut-1-ene	-	3.13	1	1	1	-
576261	2094001	2,6-xylenol	2.36 [a]	2.61	1	1	-	1
583915	2095230	2-hydroxy-4-(methylthio)butyric acid	-	-0.07	1	1	1	-
590863	2096915	isovaleraldehyde	-	1.23	1	1	1	-
591275	2097112	3-aminophenol	0.21 [c]	0.24	1	1	-	1
592358	2097510	butyl carbamate	0.85 [a]	0.96	1	1	1	-
592416	2097531	hex-1-ene	3.39 [a]	3.15	1	1	1	-
593817	2098100	trimethylammonium chloride	-	-	-	-	-	-
594423	2098404	trichloromethanesulphenyl chloride	-	3.47	0	0	0	-
598561	2099408	ethyldimethylamine	0.70 [a]	0.53	1	0	1	-
598787	2099523	2-chloropropionic acid	-	0.76	1	1	1	-
599042	2099633	alpha-hydroxy-beta,beta-dimethyl-gamma-butyrolactone	-	-0.97	1	1	-	-
603350	2100360	triphenylphosphine	5.69 [c]	5.02	1	1	-	-
609143	2101799	ethyl 2-methylacetoacetate	-	0.21	1	1	1	-
611063	2102483	1,3-dichloro-4-nitrobenzene	3.07 [ac]	3.10	0	0	-	0
613901	2103597	benzoyl cyanide	-	0.20	1	1	-	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
616386	2104784	dimethyl carbonate	-	0.23	1	1	1	-
616455	2104831	2-pyrrolidone	-0.85 [ad]	-0.32	1	1	-	-
620677	2106472	propane-1,2,3-triyl trisheptanoate	-	9.20	1	1	1	-
624486	2108485	dimethyl maleate	0.22 [c]	1.21	1	1	1	-
624920	2108710	dimethyl disulphide	1.77 [a]	1.87	1	1	-	-
627703	2110096	acetone azine	-	4.36	1	1	-	-
627838	2110143	ethylene distearate	-	16.12	1	1	1	-
627930	2110206	dimethyl adipate	1.03 [c]	1.39	1	1	1	-
628966	2110630	ethylene dinitrate	1.16 [a]	1.17	1	1	-	-
629118	2110740	hexane-1,6-diol	-	0.76	1	1	1	-
629505	2110934	tridecane	-	6.73	1	1	1	-
629594	2110960	tetradecane	7.20 [a]	7.22	1	1	1	-
629732	2111058	hexadec-1-ene	-	8.06	1	1	1	-
629969	2111194	icosan-1-ol	-	8.70	1	1	1	-
630080	2111283	carbon monoxide	-	-	-	-	-	-
637923	2113097	2-ethoxy-2-methylpropane	-	1.92	0	0	0	-
645625	2114483	2-ethylhex-2-enal	-	2.62	1	1	1	-
661198	2115466	docosan-1-ol	-	9.68	1	1	1	-
674828	2116171	but-3-en-3-olide	-	-0.39	1	1	-	-
682097	2116611	2,2-bis(allyloxymethyl)butan-1-ol	-	1.87	0	0	1	-
683181	2116700	dibutyltin dichloride	-	1.89	-	-	-	-
691372	2117201	4-methylpent-1-ene	-	3.08	1	1	1	-
693232	2117463	dodecanedioic acid	-	3.17	1	1	1	-
700130	2118383	2,3,5-trimethylhydroquinone	-	2.67	1	1	-	0
709988	2119146	propanil	3.07 [a]	2.88	0	0	-	0
756809	2120539	O,O-dimethyl hydrogen dithiophosphate	-	1.26	1	1	1	-
760236	2120790	3,4-dichlorobut-1-ene	-	2.60	0	0	0	-
760678	2120811	2-ethylhexanoyl chloride	-	2.40	1	1	1	-
763326	2121108	3-methylbut-3-en-1-ol	-	1.25	1	1	1	-
763699	2121129	ethyl 3-ethoxypropionate	-	1.08	1	1	1	-
764410	2121218	1,4-dichlorobut-2-ene	-	2.60	0	0	0	-
791286	2123388	triphenylphosphine oxide	2.83 [a]	3.10	1	1	-	-
793248	2123440	N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine	-	4.68	0	0	-	-
811972	2123770	norflurane	-	1.68	0	0	0	-
818611	2124549	2-hydroxyethyl acrylate	-0.21 [a]	-0.25	1	1	1	-
822060	2124858	hexamethylene diisocyanate	-	3.20	1	1	1	-
822366	2124973	4-methylimidazole	0.23 [a]	0.61	1	1	-	-
826368	2125542	2,2,6,6-tetramethyl-4-piperidone	-	0.43	0	0	-	-
830137	2125956	cyclododecanone	4.10 [a]	4.07	1	0	-	-
834128	2126347	ametryn	2.98 [a]	3.32	0	0	-	-
836306	2126462	4-nitro-N-phenylaniline	3.74 [c]	3.69	0	0	-	-
838880	2126588	4,4'-methylenedi-o-toluidine	-	3.28	0	0	-	-
839907	2126609	tris(2-hydroxyethyl)-1,3,5-triazinetrione	-	0.07	1	1	-	-
868779	2127822	2-hydroxyethyl methacrylate	0.47 [a]	0.30	1	1	1	-
868859	2127838	dimethyl phosphonate	-	-1.13	1	1	1	-
872059	2128192	dec-1-ene	-	5.12	1	1	1	-
872504	2128281	1-methyl-2-pyrrolidone	-0.38 [ad]	-0.11	1	1	-	-
875741	2128763	D-(-)-alpha-phenylglycine	-1.70 [c]	-1.77	1	1	-	-
924425	2131032	N-(hydroxymethyl)acrylamide	-	-1.81	1	1	1	-
926578	2131383	1,3-dichlorobut-2-ene	-	2.84	0	0	0	-
928687	2131797	6-methylheptan-2-one	-	2.15	1	1	1	-
929066	2131954	2-(2-aminoethoxy)ethanol	-	-1.89	1	1	1	-
931884	2132455	cyclooctene	-	3.94	1	1	-	-
935922	2133092	2,3,6-trimethyl-p-benzoquinone	1.82 [ae]	1.89	1	0	-	-
947046	2134248	dodecane-12-lactam	2.92 [f]	3.61	1	1	-	-
994058	2136114	2-methoxy-2-methylbutane	-	1.92	0	0	0	-
999815	2136664	chlormequat chloride	-	-	-	-	-	-
999973	2136685	1,1,1,3,3,3-hexamethyldisilazane	-	2.62	-	-	-	-
1070004	2139644	trioctylaluminium	-	-	-	-	-	-
1071836	2139974	glyphosate	-	-4.47	1	1	1	-
1085989	2141187	dichlofluanid	-	2.72	0	0	-	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
1115204	2142222	3-hydroxy-2,2-dimethylpropyl 3-hydroxy-2,2-dimethylpropionate	-	1.07	1	1	0	-
1116707	2142400	tributylaluminium	-	-	-	-	-	-
1119400	2142772	dimethyl glutarate	0.62 [c]	0.90	1	1	1	-
1120361	2143069	tetradec-1-ene	-	7.08	1	1	1	-
1120496	2143121	didecylamine	-	8.67	1	1	1	-
1151140	2145663	2-(4-ethylbenzoyl)benzoic acid	-	3.72	1	1	-	-
1163195	2146049	bis(pentabromophenyl) ether	-	12.11	0	0	-	-
1191157	2147299	diisobutylaluminium hydride	-	-	-	-	-	-
1203174	2148685	1,1,2,3,3-pentamethylindan	-	5.63	0	0	-	0
1217089	2149343	beta,1,1,2,3,3-hexamethylindan-5-ethanol	-	5.62	0	0	-	0
1222055	2149469	1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno[5,6-c]pyran	-	6.26	0	0	-	0
1241947	2149872	2-ethylhexyl diphenyl phosphate	5.73 [a]	6.30	1	1	-	-
1302427	2151001	aluminium sodium dioxide	-	-	-	-	-	-
1303862	2151258	diboron trioxide	-	-0.22	-	-	-	-
1305620	2151373	calcium dihydroxide	-	-	-	-	-	-
1305788	2151389	calcium oxide	-	-	-	-	-	-
1306190	2151462	cadmium oxide	-	-	-	-	-	-
1306383	2151504	cerium dioxide	-	-	-	-	-	-
1308141	2151588	dichromium trioxide hydrate	-	-	-	-	-	-
1309360	2151677	Pyrite (FeS2)	-	-	-	-	-	-
1309428	2151703	magnesium hydroxide	-	-	-	-	-	-
1309484	2151719	magnesium oxide	-	-	-	-	-	-
1310583	2151813	potassium hydroxide	-	-3.88	-	-	-	-
1310652	2151834	lithium hydroxide	-	-3.88	-	-	-	-
1310732	2151855	sodium hydroxide	-	-3.88	-	-	-	-
1313139	2152026	manganese dioxide, ore of Chapter 26	-	-	-	-	-	-
1313275	2152047	molybdenum trioxide	-	-	-	-	-	-
1313822	2152115	disodium sulphide	-	-4.23	-	-	-	-
1313991	2152157	nickel monoxide	-	-0.57	-	-	-	-
1314132	2152225	zinc oxide	-	-	-	-	-	-
1314234	2152272	zirconium dioxide	-	-	-	-	-	-
1314983	2152513	zinc sulphide	-	-	-	-	-	-
1317335	2152639	molybdenum disulphide	-	-	-	-	-	-
1317380	2152691	copper oxide	-	-0.57	-	-	-	-
1317391	2152707	dicopper oxide	-	-2.63	-	-	-	-
1317426	2152733	cobalt sulphide	-	-	-	-	-	-
1317700	2152801	Anatase (TiO2)	-	-	-	-	-	-
1317802	2152822	Rutile (TiO2)	-	-	-	-	-	-
1318236	2152843	Boehmite (Al(OH)O)	-	-	-	-	-	-
1333740	2156057	hydrogen	-	-	-	-	-	-
1333820	2156078	chromium trioxide	-	-	-	-	-	-
1338392	2156633	sorbitan laurate	-	3.15	1	1	-	-
1338416	2156649	sorbitan stearate	-	6.10	1	1	-	-
1338438	2156654	sorbitan oleate	-	5.89	1	1	-	-
1459934	2159519	dimethyl isophthalate	-	1.66	1	1	-	1
1461252	2159608	tetrabutyltin	-	9.37	-	-	-	-
1477550	2160325	m-phenylenebis(methylamine)	-	0.15	1	1	-	-
1490046	2160744	DL-menthol	3.30 [f]	3.38	1	1	-	-
1506021	2161334	1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-1-one	-	6.35	0	0	-	0
1552121	2162914	(Z,Z)-cycloocta-1,5-diene	3.16 [a]	3.73	1	1	-	-
1559348	2163221	3,6,9,12-tetraoxahexadecan-1-ol	-	-0.26	0	0	1	-
1569024	2163745	1-ethoxypropan-2-ol	-	0.00	1	0	1	-
1570645	2163813	4-chloro-o-cresol	2.63 [c]	2.70	1	1	-	0
1634044	2166531	tert-butyl methyl ether	0.94 [c]	1.43	0	0	0	-
1653196	2167210	2,3-dichlorobuta-1,3-diene	-	3.02	0	0	0	-
1663394	2167687	tert-butyl acrylate	-	2.09	1	1	1	-
1675543	2168235	2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bisoxirane	-	3.84	0	0	-	-
1689992	2168853	2,6-dibromo-4-cyanophenyl octanoate	6.10 [af]	5.86	1	1	-	0

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
1698539	2169176	4,5-dichloro-2,3-dihydro-2-phenylpyridazin-3-one	-	2.66	1	0	-	1
1698608	2169202	chloridazon	1.14 [ag]	0.76	1	1	-	1
1724396	2170312	cyclododecanol	-	4.58	1	1	-	-
1738256	2170904	3-dimethylaminopropiononitrile	-	-0.45	1	1	1	-
1758732	2171578	aminoiminomethanesulphinic acid	-	-3.37	1	1	1	-
1761713	2171688	4,4'-methylenebis(cyclohexylamine)	-	3.26	1	1	-	-
1762272	2171709	diethyldimethylplumbane	-	3.90	-	-	-	-
1762954	2171756	ammonium thiocyanate	-	-	-	-	-	-
1817476	2173266	p-nitrocumene	3.45 [c]	3.27	0	0	-	0
1836755	2174060	nitrofen	4.64 [d]	4.32	0	0	-	-
1843056	2174212	octabenzone	-	6.96	1	1	-	-
1854268	2174516	4,5-dihydroxy-1,3-bis(hydroxymethyl)imidazolidin-2-one	-	-5.91	1	1	-	-
1912249	2176178	atrazine	2.61 [c]	2.82	0	0	-	-
1928434	2176733	2-ethylhexyl 2,4-dichlorophenoxyacetate	-	6.27	1	1	-	0
2082793	2182160	octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	-	13.41	1	0	-	0
2100427	2182679	1-chloro-2,5-dimethoxybenzene	2.69 [j]	2.80	1	1	-	0
2157199	2184676	1,4,5,6,7,7-hexachlorobicyclo[2.2.1]hept-5-ene-2,3-dimethanol	-	3.68	0	0	-	-
2186927	2185774	p-(dimethoxymethyl)anisole	-	1.52	0	0	-	1
2243621	2188178	1,5-naphthylenediamine	0.89 [ah]	1.34	0	0	-	-
2303175	2189627	tri-allate	4.29 [ai]	4.57	0	0	0	-
2310170	2189962	phosalone	4.38 [c]	4.29	1	1	-	0
2312358	2190061	propargite	5.00 [o]	5.57	1	0	-	0
2402791	2192839	2,3,5,6-tetrachloropyridine	3.32 [a]	3.38	0	0	-	-
2403885	2192912	2,2,6,6-tetramethylpiperidin-4-ol	-	0.94	1	0	-	-
2409554	2193146	2-tert-butyl-p-cresol	-	3.97	1	1	-	0
2416946	2193303	2,3,6-trimethylphenol	2.67 [b]	3.15	1	1	-	0
2431507	2193979	2,3,4-trichlorobut-1-ene	-	3.10	0	0	0	-
2432997	2194176	11-aminoundecanoic acid	-	-0.16	1	1	1	-
2439352	2194600	2-(dimethylamino)ethyl acrylate	-	0.42	1	1	1	-
2494895	2196697	2-[(p-aminophenyl)sulphonyl]ethyl hydrogensulphate	-	-4.33	0	0	-	1
2517433	2197418	3-methoxybutan-1-ol	-	0.00	1	0	1	-
2524030	2197549	O,O-dimethyl phosphorochloridothioate	-	1.39	1	1	0	-
2524041	2197554	O,O-diethyl phosphorochloridothioate	-	2.37	1	1	0	-
2551624	2198542	sulphur hexafluoride	1.68 [c]	1.64	-	-	0	-
2634335	2201209	1,2-benzisothiazol-3(2H)-one	-	0.64	1	1	-	-
2809214	2205528	etidronic acid	-	-0.81	0	0	0	-
2835065	2206081	DL-alpha-phenylglycine	-1.70 [c]	-1.77	1	1	-	-
2855132	2206668	3-aminomethyl-3,5,5-trimethylcyclohexylamine	-	1.90	1	0	-	-
2867472	2206888	2-dimethylaminoethyl methacrylate	-	0.97	1	1	1	-
3033770	2212210	2,3-epoxypropyltrimethylammonium chloride	-	-	-	-	-	-
3048644	2212598	5-vinylnorborn-2-ene	-	3.62	1	1	-	-
3081014	2213743	N-(1,4-dimethylpentyl)-N'-phenylbenzene-1,4-diamine	-	5.17	0	0	-	-
3120749	2214967	4-(methylthio)-m-cresol	-	2.66	1	1	-	1
3173726	2216414	1,5-naphthylene diisocyanate	-	4.37	1	1	-	-
3194556	2216959	1,2,5,6,9,10-hexabromocyclodecane	-	7.74	0	0	-	-
3268493	2218825	3-(methylthio)propionaldehyde	-	0.41	1	1	1	-
3282302	2219216	pivaloyl chloride	-	0.89	1	0	0	-
3302101	2219750	3,5,5-trimethylhexanoic acid	-	3.34	1	0	0	-
3319311	2220200	tris(2-ethylhexyl) benzene-1,2,4-tricarboxylate	-	11.59	1	1	-	-
3327228	2220483	(3-chloro-2-hydroxypropyl)trimethylammonium chloride	-	-	-	-	-	-
3452979	2223767	3,5,5-trimethylhexan-1-ol	-	3.11	1	1	0	-
3542367	2225832	dichlorodioctylstannane	-	5.82	-	-	-	-
3590849	2227337	tetraoctyltin	-	17.23	-	-	-	-
3622842	2228236	N-butylbenzenesulphonamide	-	2.31	1	1	-	-
3648202	2228849	diundecyl phthalate	-	11.49	1	1	-	1
3687465	2229816	decyl oleate	-	12.44	1	1	1	-
3845769	2233424	N-[3-(dimethylamino)propyl]acrylamide	0.00 [aj]	-0.15	1	1	1	-
3982910	2236226	thiophosphoryl trichloride	-	1.85	1	1	-	-
4035896	2237188	1,3,5-tris(6-isocyanatohexyl)biuret	-	7.58	1	0	1	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
4098719	2238616	3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	-	4.75	0	0	-	-
4116103	2239075	2-chloro-N-methyl-3-oxobutyramide	-	-0.28	1	1	1	-
4170303	2240300	crotonaldehyde	-	0.60	1	1	1	-
4435534	2246449	3-methoxybutyl acetate	-	1.01	1	1	1	-
4445072	2246847	octadecylbenzene	-	10.89	1	1	-	1
4454051	2246983	3,4-dihydro-2-methoxy-2H-pyran	-	0.88	0	0	-	-
4553622	2249235	2-methylglutaronitrile	-	0.28	1	1	1	-
4618182	2250277	lactulose	-	-4.67	1	0	-	-
4685147	2251417	1,1'-dimethyl-4,4'-bipyridinium	-	-	-	-	-	-
4904614	2255338	cyclododeca-1,5,9-triene	5.50 [b]	5.48	1	1	-	-
4979322	2256258	N,N-dicyclohexylbenzothiazole-2-sulphenamide	-	5.95	1	0	-	-
5039781	2257335	[2-(methacryloyloxy)ethyl]trimethylammonium chloride	-	-	-	-	-	-
5064313	2257686	trisodium nitrilotriacetate	-	-3.81	1	1	0	-
5102830	2258229	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]	-	8.11	0	0	-	-
5205936	2260023	N-[3-(dimethylamino)propyl]methacrylamide	-	0.39	1	1	1	-
5208935	2260065	3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3-ol	-	5.45	0	0	-	-
5216251	2260091	alpha,alpha,alpha,4-tetrachlorotoluene	-	4.54	0	0	-	0
5234684	2260311	carboxin	2.14 [a]	1.49	1	1	-	1
5321313	2261818	(2-chloro-2-oxo-1-phenylethyl)ammonium chloride	-	-	-	-	-	-
5329146	2262188	sulphamidic acid	-	-4.34	-	-	1	-
5333426	2262429	2-octyldodecan-1-ol	-	8.63	1	1	1	-
5392405	2263946	citral	-	3.45	1	1	1	-
5435643	2266030	3,5,5-trimethylhexanal	-	3.09	1	1	0	-
5567157	2269398	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-chloro-2,5-dimethoxyphenyl)-3-oxobutyramide]	-	7.94	0	0	-	-
6104309	2280558	N,N''-(isobutylidene)diurea	-	-1.68	1	1	1	-
6284408	2285069	meglumine	-	-3.15	1	1	0	-
6358641	2287820	4-chloro-2,5-dimethoxyaniline	-	1.88	1	1	-	0
6358856	2287878	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-N-phenylbutyramide]	-	7.05	0	0	-	-
6386385	2289854	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	-	5.06	1	1	-	0
6419198	2291465	nitrilotrimethylenetris(phosphonic acid)	-	-4.55	0	0	0	-
6846500	2299349	1-isopropyl-2,2-dimethyltrimethylene diisobutyrate	-	4.91	1	1	0	-
6864375	2299621	2,2'-dimethyl-4,4'-methylenebis(cyclohexylamine)	-	4.10	1	1	-	-
6923224	2300427	monocrotophos	-	-1.31	1	1	0	-
6940530	2300867	1-chloro-2,5-dimethoxy-4-nitrobenzene	-	2.62	0	0	-	0
7397628	2309917	butyl glycollate	-	0.38	1	1	1	-
7434404	2310812	ethane-1,2-diylbis(oxyethane-2,1-diyl) bisheptanoate	-	4.77	0	1	1	-
7439896	2310964	iron	-	-	-	-	-	-
7439987	2311072	molybdenum	-	-	-	-	-	-
7440020	2311114	nickel	-	-0.57	-	-	-	-
7440031	2311135	niobium	-	-	-	-	-	-
7440224	2311313	silver	-	-	-	-	-	-
7440337	2311439	tungsten	-	-	-	-	-	-
7440473	2311575	chromium	-	-	-	-	-	-
7440484	2311580	cobalt	-	-	-	-	-	-
7440508	2311596	copper	-	-0.57	-	-	-	-
7440611	2311706	uranium	-	-	-	-	-	-
7440622	2311711	vanadium	-	-	-	-	-	-
7446095	2311952	sulphur dioxide	-	-2.20	-	-	-	-
7446119	2311973	sulphur trioxide	-	0.23	-	-	-	-
7446700	2312081	aluminium chloride	-	-	-	-	-	-
7447407	2312118	potassium chloride	-	-0.46	-	-	-	-
7447418	2312123	lithium chloride	-	-0.46	-	-	-	-
7550450	2314419	titanium tetrachloride	-	-	-	-	-	-
7631869	2315454	silicon dioxide, chemically prepared	-	0.53	-	-	-	-
7637072	2315695	boron trifluoride	-	0.22	-	-	-	-
7646788	2315889	tin tetrachloride	-	-1.53	-	-	0	-
7646857	2315920	zinc chloride	-	-	-	-	-	-
7647010	2315957	hydrogen chloride	-	0.54	-	-	-	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
7647145	2315983	sodium chloride	-	-0.46	-	-	-	-
7647156	2315999	sodium bromide	-	-0.37	-	-	-	-
7659861	2316264	2-ethylhexyl mercaptoacetate	-	3.68	1	1	1	-
7664393	2316348	hydrogen fluoride	-	0.23	-	-	1	-
7664417	2316353	ammonia, anhydrous	-	0.23	-	-	-	-
7664939	2316395	sulphuric acid	-	-2.20	-	-	1	-
7681494	2316678	sodium fluoride	-	-0.77	-	-	-	-
7697372	2317142	nitric acid	-	0.21	-	-	1	-
7699436	2317179	zirconium dichloride oxide	-	-	-	-	-	-
7705080	2317294	iron trichloride	-	-	-	-	-	-
7718549	2317430	nickel dichloride	-	0.05	-	-	0	-
7719097	2317488	thionyl dichloride	-	0.92	-	-	-	-
7719122	2317493	phosphorus trichloride	-	2.01	-	-	-	-
7722841	2317650	hydrogen peroxide	-	-1.57	-	-	1	-
7726956	2317781	bromine	-	1.03	-	-	0	-
7758023	2318303	potassium bromide	-	-0.37	-	-	-	-
7758943	2318434	iron dichloride	-	-	-	-	-	-
7778394	2319019	arsenic acid	-	-3.14	-	-	-	-
7782447	2319569	oxygen	-	-1.03	-	-	-	-
7782505	2319595	chlorine	-	0.85	-	-	-	-
7783064	2319773	hydrogen sulphide	-	0.23	-	-	-	-
7784181	2320511	aluminium fluoride	-	-	-	-	-	-
7786303	2320946	magnesium chloride	-	-	-	-	-	-
7789233	2321515	potassium fluoride	-	-0.77	-	-	-	-
7789415	2321646	calcium bromide	-	-	-	-	-	-
7789755	2321887	calcium fluoride	-	-	-	-	-	-
7790945	2322346	chlorosulphuric acid	-	0.00	-	-	-	-
7791255	2322456	sulphuryl dichloride	-	1.04	-	-	-	-
8000417	2322681	Terpineol	2.98 [h]	3.33	0	0	-	-
10024972	2330320	dinitrogen oxide	-	-	-	-	-	-
10025679	2330362	disulphur dichloride	-	4.26	-	-	-	-
10025782	2330425	trichlorosilane	-	1.46	-	-	0	-
10025873	2330467	phosphoryl trichloride	-	0.09	1	1	-	-
10026047	2330540	silicon tetrachloride	-	1.77	-	-	0	-
10026138	2330603	phosphorus pentachloride	-	-3.47	-	-	-	-
10035106	2331130	hydrogen bromide	-	0.63	-	-	1	-
10043353	2331392	boric acid	-	-0.22	-	-	-	-
10043524	2331408	calcium chloride	-	-	-	-	-	-
10049146	2331701	uranium tetrafluoride	-	-	-	-	-	-
10101527	2332527	zirconium orthosilicate	-	-	-	-	-	-
10265926	2336060	methamidophos	-0.66 [a]	-0.93	1	1	1	-
10361372	2337881	barium chloride	-	-	-	-	-	-
10420334	2338974	dimethyl acetylsuccinate	-	-0.74	1	1	1	-
10543574	2341238	N,N'-ethylenebis[N-acetylacetamide]	-	-2.36	1	0	1	-
10544726	2341264	dinitrogen tetraoxide	-	-	-	-	-	-
10545990	2341290	sulphur dichloride	-	1.87	-	-	-	-
10584982	2341861	2-ethylhexyl 4,4-dibutyl-10-ethyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate	-	11.43	-	-	-	-
10605217	2342320	carbendazim	1.52 [a]	1.55	1	1	-	-
12018018	2346304	chromium dioxide	-	-	-	-	-	-
12071839	2351340	propineb	-	-0.94	-	-	-	-
13150000	2360910	sodium 2-[2-[2-(dodecyloxy)ethoxy]ethoxy]ethyl sulphate	-	2.20	0	0	1	-
13463677	2366755	titanium dioxide	-	-	-	-	-	-
13547701	2369206	1-chloro-3,3-dimethylbutan-2-one	-	1.38	0	0	0	-
13674845	2371587	tris(2-chloro-1-methylethyl) phosphate	2.59 [f]	2.89	1	1	0	-
13674878	2371592	tris[2-chloro-1-(chloromethyl)ethyl] phosphate	3.65 [f]	3.65	0	1	0	-
13684634	2371990	phenmedipham	3.59 [ab]	3.27	1	1	-	-
13705050	2372397	2,4-dichloro-6-(methylthio)-1,3,5-triazine	-	2.23	0	0	-	-
13825746	2375230	titanium oxide sulphate	-	-	-	-	-	-
13940948	2377217	4-chloro-1-(dichloromethyl)benzene	-	3.62	0	0	-	0
14324551	2382709	zinc bis(diethyldithiocarbamate)	-	1.61	-	-	-	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
14475639	2384727	zirconium tetrahydroxide	-	-	-	-	-	-
14542235	2385757	Fluorite (CaF2)	-	-	-	-	-	-
14808607	2388784	Quartz (SiO2)	-	0.53	-	-	-	-
14861177	2389327	4-(2,4-dichlorophenoxy)aniline	-	3.58	0	0	-	-
14940682	2390196	zircon	-	-	-	-	-	-
15206550	2392633	methyl benzoylformate	-	1.49	1	1	-	-
15214898	2392680	2-acrylamido-2-methylpropanesulphonic acid	-	-2.19	1	1	1	-
15545489	2395922	chlorotoluron	2.41 [a]	2.58	1	0	-	0
15571581	2396224	2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate	-	15.35	-	-	-	-
15625895	2397013	2-ethyl-2-[[(1-oxoallyl)oxy]methyl]-1,3-propanediyl diacrylate	-	2.86	1	1	1	-
15687271	2397846	ibuprofen	3.50 [b]	3.79	1	1	-	0
15827608	2399314	[[(phosphonomethyl)imino]bis[ethane-2,1-diylnitrilobis(methylene)]]tetrakisphosphonic acid	-	-8.22	0	0	0	-
15894709	2400324	N,N'''-1,6-hexanediylbis[N'-cyanoguanidine]	-	-0.12	1	0	-	-
16219753	2403477	5-ethylidene-8,9,10-trinorborn-2-ene	3.82 [f]	3.67	1	1	-	-
16721805	2407780	sodium hydrogensulphide	-	-2.47	-	-	-	-
16883833	2409201	benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate	-	7.00	1	1	-	-
16954691	2410259	N-methylbenzothiazol-2-amine	-	2.55	0	0	-	-
17194002	2412345	barium hydroxide	-	-	-	-	-	-
17321470	2413422	O,O-dimethyl thiophosphoramidate	-	1.48	1	1	1	-
17639939	2416245	methyl 2-chloropropionate	-	1.04	1	1	1	-
17700093	2417055	4-nitro-1,2,3-trichlorobenzene	3.61 [a]	3.74	0	0	-	0
17796826	2417741	N-(cyclohexylthio)phthalimide	-	3.76	1	0	-	-
17976431	2418944	cyclo-di-mu-oxo(mu-phthalato)trilead	-	1.06	-	-	-	-
18297637	2421779	1,3-bis(trimethylsilyl)urea	-	2.17	-	-	-	-
18467771	2423488	diprogulic acid	1.35 [ab]	1.76	0	0	-	-
18479497	2423582	3,7-dimethyloct-1-en-3-ol	-	3.47	0	0	0	-
18691979	2425050	methabenzthiazuron	2.64 [ab]	2.65	1	0	-	-
19438609	2430720	hexahydro-4-methylphthalic anhydride	-	2.59	1	1	-	-
20030302	2434730	2,5,6-trimethylcyclohex-2-en-1-one	-	2.58	1	1	-	-
20120336	2435289	dimethyl [3-[(hydroxymethyl)amino]-3-oxopropyl]phosphonate	-	-3.09	1	1	1	-
20292084	2436979	2-ethylhexyl laurate	-	8.65	1	1	1	-
20306756	2437239	N-methyl-3-oxobutyramide	-	-0.79	1	1	1	-
20344494	2437464	iron hydroxide oxide	-	-	-	-	-	-
21109955	2442144	barium sulphide	-	-	-	-	-	-
21645512	2444927	aluminium hydroxide	-	-	-	-	-	-
22224926	2448481	fenamiphos	3.23 [a]	3.29	1	0	-	1
22839470	2452613	aspartame	-	0.07	1	1	-	-
23783428	2458835	3,6,9,12-tetraoxotridecanol	-	-1.73	0	0	1	-
24310405	2461518	3-(hydroxymethyl)-1,2,3-benzotriazin-4(3H)-one	-	0.09	1	1	-	-
24549062	2463096	6-ethyl-2-toluidine	-	2.66	1	1	-	0
24602866	2463473	tridemorph	-	6.38	0	0	-	-
24800440	2464660	[(methylethylene)bis(oxy)]dipropanol	-	-0.28	0	0	1	-
25013154	2465622	vinyltoluene	3.48 [c]	3.44	1	1	-	0
25103097	2466139	isooctyl mercaptoacetate	-	3.68	1	1	1	-
25103520	2466170	isooctanoic acid	-	2.85	1	0	0	-
25103586	2466191	tert-dodecanethiol	-	6.07	0	0	1	-
25154523	2466720	nonylphenol	5.76 [ak]	5.99	1	1	-	1
25167708	2466909	2,4,4-trimethylpentene	4.55 [f]	4.08	1	0	0	-
25168052	2466982	chlorotoluene	2.30 [a]	2.79	1	1	-	-
25265718	2467703	oxydipropanol	-	-0.49	1	0	1	-
25265774	2467719	isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol	-	3.00	1	1	0	-
25311711	2468141	isofenphos	4.12 [a]	4.65	1	1	-	1
25339177	2468691	isodecyl alcohol	-	3.71	1	1	1	-
25377735	2469171	dodecenylsuccinic anhydride	-	6.63	1	1	-	-
25550985	2470983	diisodecyl phenyl phosphite	-	11.78	1	0	-	-
26140603	2474773	terphenyl	6.03 [b]	5.52	1	1	-	-
26225796	2475253	ethofumesate	2.70 [ab]	2.89	0	0	-	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.

[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

CAS-nr.	EINECS-nr.	NAME	log Kow [1]		BIODEG [2]		OECD models [2]	
			literature	estimate	linear	non-lin.	75	78
26272764	2475777	N-[2-(2-heptadecyl-4,5-dihydro-1H-imidazol-1-yl)ethyl]stearamide	-	15.52	1	1	-	-
26401354	2476608	diisotridecyl adipate	-	13.03	1	1	1	-
26489010	2477376	()-3,7-dimethyloct-6-en-1-ol	-	3.56	1	1	0	-
26544230	2477774	isodecyl diphenyl phosphite	-	9.20	1	1	-	-
26760645	2479750	2-methylbutene	-	2.58	1	1	1	-
26761400	2479771	di-"isodecyl" phthalate	-	10.36	1	1	-	-
26761455	2479792	2,3-epoxypropyl neodecanoate	-	3.62	0	0	-	-
26896184	2480923	isononanoic acid	-	3.45	1	1	1	-
27178161	2482999	diisodecyl adipate	-	10.08	1	1	1	-
27247967	2483636	2-ethylhexyl nitrate	-	4.12	1	1	1	-
27375526	2484336	N-[4-[(2-hydroxyethyl)sulphonyl]phenyl]acetamide	-	-0.45	1	1	-	1
27458920	2484692	isotridecan-1-ol	-	5.19	1	1	1	-
27458942	2484713	isononyl alcohol	-	3.22	1	1	1	-
27554263	2485235	diisooctyl phthalate	-	8.39	1	1	-	-
28479223	2490507	3-chloro-p-tolyl isocyanate	-	3.78	1	0	-	0
28553120	2490795	di-"isononyl" phthalate	-	9.37	1	1	-	-
29171208	2494826	3,7-dimethyloct-6-en-1-yn-3-ol	-	2.75	0	0	0	-
29387868	2495987	butoxypropan-1-ol	-	0.98	1	1	1	-
29797408	2498548	dichloromethylbenzene	-	2.97	1	0	-	-
29911282	2499515	1-(2-butoxy-1-methylethoxy)propan-2-ol	-	1.13	0	0	0	-
30399849	2501780	isooctadecanoic acid	-	7.87	1	0	1	-
31570044	2507096	tris(2,4-ditert-butylphenyl) phosphite	-	18.08	0	0	-	-
32210234	2509549	4-tert-butylcyclohexyl acetate	-	4.42	1	1	-	-
32588764	2511186	N,N'-ethylenebis(3,4,5,6-tetrabromophthalimide)	-	9.80	0	0	-	-
33703081	2516467	diisononyl adipate	-	9.10	1	1	1	-
34123596	2518354	3-(4-isopropylphenyl)-1,1-dimethylurea	2.87 [a]	2.84	1	1	-	0
34590948	2521042	(2-methoxymethylethoxy)propanol	-	-0.35	0	0	0	-
34893920	2522769	1,3-dichloro-5-isocyanatobenzene	-	3.88	0	0	-	0
36653824	2531490	hexadecan-1-ol	-	6.73	1	1	1	-
36734197	2531789	3-(3,5-dichlorophenyl)-2,4-dioxo-N-isopropylimidazolidine-1-carboxamide	3.00 [ab]	2.85	0	0	-	0
37971361	2537335	2-phosphonobutane-1,2,4-tricarboxylic acid	-	0.14	1	0	1	-
38051104	2537602	2,2-bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phosphate)	-	3.31	0	1	0	-
38861788	2541598	1-[4-(2-methylpropyl)phenyl]ethan-1-one	-	3.62	1	1	-	0
40372723	2548965	4,4,15,15-tetraethoxy-3,16-dioxa-8,9,10,11-tetrathia-4,15-disilaoctadecane	-	2.97	-	-	-	-
40843730	2551061	4-(2,4-dichlorophenoxy)phenol	-	4.02	1	0	-	-
42576023	2558947	methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	4.48 [c]	4.15	0	0	-	-
44992010	2561766	[2-(acryloyloxy)ethyl]trimethylammonium chloride	-	-	-	-	-	-
46948725	2562890	6-[methyl(phenylsulphonyl)amino]hexanoic acid	-	2.27	1	1	-	-
50849473	2567988	5-nonylsalicylaldehyde oxime	-	5.86	1	1	-	1
52722868	2581321	4-hydroxy-2,2,6,6-tetramethylpiperidine-1-ethanol	-	0.59	0	0	-	-
56107041	2599962	3-(p-tert-butylphenyl)-2-methylpropanol	-	4.38	1	1	-	0
56966520	2604804	5-chloro-2-(2,4-dichlorophenoxy)aniline	-	4.23	0	0	-	-
57219644	2606335	[.mu.-[carbonato(2-)-O:O']]dihydroxydioxodizirconium	-	-	-	-	-	-
57966957	2610430	2-cyano-N-[(ethylamino)carbonyl]-2-(methoxyimino)acetamide	-	4.24	1	1	1	-
61260557	2626791	N,N'-bis(2,2,6,6-tetramethylpiperidin-4-yl)hexane-1,6-diamine	-	4.43	0	0	-	-
63589253	2643471	4-diazo-3,4-dihydro-7-nitro-3-oxonaphthalene-1-sulphonic acid	-	-1.27	0	0	-	-
67747095	2669945	N-propyl-N-[2-(2,4,6-trichlorophenoxy)ethyl]-1H-imidazole-1-carboxamide	4.10 [ab]	3.44	0	0	-	-
67846688	2673820	dimethylbis[2-[(1-oxooctadecyl)oxy]ethyl]ammonium chloride	-	-	-	-	-	-
68134269	2687388	2-(2-heptadecyl-4,5-dihydro-1H-imidazol-1-yl)ethyl stearate	-	16.59	1	1	-	-
68298964	2695870	2-[(2-hydroxyethyl)amino]ethyl dihydrogen orthoborate	-	-2.27	-	-	-	-

[1] log K_{ow} values from literature, see Section References. log K_{ow} estimates from the KOWWIN program v. 1.54, see text.
[2] Biodegradation probability, 1=biodegrades fast, 0=biodegrades slowly or not at all. See text for details.

APPENDIX 2 - ATMOSPHERIC DEGRADATION

Table of 1073 single compounds from the High Production Volume Chemicals list, European Chemicals Bureau, June 4th 1995, as part of the Regulation (EEC) 793/93) on existing chemical substances. The following properties are given:

- CAS-nr.
- Name
- Atmospheric degradation half-lifes by reaction with OH-radicals,

  estimated using the Atmospheric Oxidation Program v. 1.83, SRC, Syracuse, USA
- Atmospheric degradation half-lifes by reaction with Ozone (O_3),

  estimated using the Atmospheric Oxidation Program v. 1.83, SRC, Syracuse, USA
- Atmospheric degradation half-lifes by reaction with OH-radicals,

  estimated with the MOOH-method from Klamt *et al.*

All properties are adequately described in Section 2 Materials and Methods.

CAS-nr.	EINECS-nr.	NAME	Half-life in	AOP 1.83 OH radical [1] (cis)	(trans)	AOP 1.83 Ozone [1] (cis)	(trans)	MOOH [1] OH-radical
50000	2000018	formaldehyde		1.45	-	-	-	-
50293	2000243	clofenotane		2.96	-	-	-	12.27
50782	2000641	O-acetylsalicylic acid		9.11	-	-	-	24.92
55389	2002319	fenthion		0.14	-	-	-	0.62
55630	2002408	glycerol trinitrate		88.99	-	-	-	1002.50
56235	2002628	carbon tetrachloride		>99999	-	-	-	-
56359	2002680	bis(tributyltin) oxide		-	-	-	-	-
56382	2002717	parathion		0.12	-	-	-	27.45
56406	2002722	glycine--iron sulphate (1:1)		0.40	-	-	-	3.06
56815	2002895	glycerol		0.60	-	-	-	5.37
56848	2002916	aspartic acid		0.27	-	-	-	1282.58
56860	2002937	glutamic acid		0.26	-	-	-	341.86
57136	2003155	urea		0.45	-	-	-	-
57487	2003333	fructose, pure		0.19	-	-	-	8.36
57556	2003380	propane-1,2-diol		0.89	-	-	-	6.86
58082	2003621	caffeine		0.20	-	-	-	0.53
58559	2003857	theophylline		0.20	-	-	-	0.41
58560	2003862	pyridoxine hydrochloride		-	-	-	-	-
58899	2004012	gamma-HCH or gamma-BHC		7.89	-	-	-	41.61
59507	2004316	chlorocresol		0.39 *	-	-	-	0.89
59676	2004410	nicotinic acid		19.96	-	-	-	35.50
60004	2004494	edetic acid		0.06	-	-	-	1.53
60128	2004562	2-phenylethanol		1.08	-	-	-	3.76
60242	2004646	2-mercaptoethanol		0.24	-	-	-	4.72
60297	2004672	diethyl ether		0.93	-	-	-	1.65
60515	2004803	dimethoate		0.12	-	-	-	2.64
60800	2004866	phenazone		0.09	-	9.40	-	-
61825	2005215	amitrole		0.05	-	-	-	2.25
62237	2005262	4-nitrobenzoic acid		22.86	-	-	-	34.29
62533	2005393	aniline		0.08	-	-	-	0.08
62566	2005435	thiourea		0.21	-	-	-	740.26
64175	2005786	ethanol		3.48	-	-	-	4.61
64186	2005791	formic acid		26.74	-	-	-	-
64197	2005807	acetic acid		21.00	-	-	-	2735.73
64675	2005896	diethyl sulphate		5.44	-	-	-	22.36
65850	2006182	benzoic acid		9.30	-	-	-	26.11
67481	2006554	choline chloride		-	-	-	-	-
67561	2006596	methanol		20.35	-	-	-	10.27
67630	2006617	propan-2-ol		1.61	-	-	-	53.90
67641	2006622	acetone		48.87	-	-	-	411.41
67663	2006638	chloroform		106.54	-	-	-	185.71
67685	2006643	dimethyl sulfoxide		0.17	-	-	-	209.66
68111	2006774	mercaptoacetic acid		0.29	-	-	-	248.82
68122	2006795	N,N-dimethylformamide		0.06	-	-	-	6.66
68893	2006947	sodium [(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)methylamino]methanesulphonate		-	-	-	-	0.44
69727	2007123	salicylic acid		0.79 *	-	-	-	16.46
71238	2007469	propan-1-ol		2.15	-	-	-	6.42
71363	2007516	butan-1-ol		1.68	-	-	-	4.91
71410	2007521	pentan-1-ol		1.38	-	-	-	1.90
71432	2007537	benzene		5.24	-	-	-	7.01
71556	2007563	1,1,1-trichloroethane		822.82	-	-	-	1296.57
74317	2008064	N,N'-diphenyl-p-phenylenediamine		0.03	-	-	-	0.06
74828	2008127	methane in gaseus state		1273.42	-	-	-	-
74839	2008132	bromomethane		247.61	-	-	-	127.51
74840	2008148	ethane		37.14	-	-	-	30.40
74851	2008153	ethylene, pure		1.26	-	61.12	-	0.78
74862	2008169	acetylene		13.12	-	3565.57	-	-
74873	2008174	chloromethane		195.55	-	-	-	13.69
74895	2008200	methylamine, in aqueous solution		0.50	-	-	-	1.96
74908	2008216	hydrogen cyanide		356.56	-	-	-	-
74931	2008221	methanethiol		0.33	-	-	-	20.02
74986	2008279	propane liquefied		8.84	-	-	-	8.36
75003	2008305	chloroethane		26.71	-	-	-	11.01
75014	2008310	chloroethylene		2.03	-	427.44	-	1.00
75047	2008347	ethylamine		0.37	-	-	-	1.73
75058	2008352	acetonitrile		529.54	-	-	-	457.52
75070	2008368	acetaldehyde		0.66	-	-	-	1208.67
75081	2008373	ethanethiol		0.28	-	-	-	3.38
75092	2008389	dichloromethane		88.40	-	-	-	26.13

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).
* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	Half-life in	AOP 1.83 OH radical [1] (cis)	(trans)	AOP 1.83 Ozone [1] (cis)	(trans)	MOOH [1] OH-radical
75127	2008420	formamide		0.06	-	-	-	-
75150	2008436	carbon disulphide		>99999	-	-	-	-
75183	2008462	dimethyl sulphide		2.33 *	-	-	-	9.15
75218	2008499	ethylene oxide		47.71	-	-	-	86.85
75285	2008572	isobutane		4.48	-	-	-	9.25
75310	2008609	isopropylamine		0.28	-	-	-	12.78
75343	2008635	1,1-dichloroethane		30.89	-	-	-	52.26
75354	2008640	1,1-dichloroethylene		5.20	-	2988.74	-	1.21
75365	2008656	acetyl chloride		148.57	-	-	-	2628.19
75387	2008677	1,1-difluoroethylene		1.30	-	382.03	-	1.93
75445	2008703	phosgene		>99999	-	-	-	-
75456	2008719	chlorodifluoromethane		1573.05	-	-	-	876.06
75503	2008750	trimethylamine, in aqueous solution		0.17	-	-	-	0.73
75525	2008766	nitromethane		413.00	-	-	-	5348.36
75547	2008771	dichloro(methyl)silane		-	-	-	-	1475.41
75569	2008792	methyloxirane		19.71	-	-	-	28.33
75638	2008876	bromotrifluoromethane		>99999	-	-	-	-
75650	2008897	2-methylpropan-2-ol		18.03	-	-	-	66.28
75683	2008918	1-chloro-1,1-difluoroethane		2971.31	-	-	-	2436.61
75694	2008923	trichlorofluoromethane		>99999	-	-	-	-
75718	2008939	dichlorodifluoromethane		>99999	-	-	-	-
75741	2008970	tetramethyllead		-	-	-	-	-
75752	2008986	methanesulphonic acid		59.43	-	-	-	4630.61
75774	2009005	chlorotrimethylsilane		-	-	-	-	80.01
75785	2009010	dichloro(dimethyl)silane		-	-	-	-	502.67
75796	2009026	trichloro(methyl)silane		-	-	-	-	2615.33
75865	2009094	2-hydroxy-2-methylpropionitrile		26.25	-	-	-	472.47
75876	2009115	trichloroacetaldehyde		7.38	-	-	-	-
75912	2009157	tert-butyl hydroperoxide		2.35	-	-	-	80.90
75945	2009178	trichloro(vinyl)silane		-	-	-	-	6.53
75978	2009204	3,3-dimethylbutanone		5.32	-	-	-	48.35
75989	2009225	pivalic acid		11.17	-	-	-	88.07
76039	2009272	trichloroacetic acid		26.74	-	-	-	-
76131	2009361	1,1,2-trichlorotrifluoroethane		>99999	-	-	-	-
76142	2009377	cryofluorane		>99999	-	-	-	-
76153	2009382	chloropentafluoroethane		>99999	-	-	-	-
77474	2010293	hexachlorocyclopentadiene		19.10	-	31553.73	-	7.26
77736	2010529	3a,4,7,7a-tetrahydro-4,7-methanoindene		0.09	-	0.27	-	0.08
77781	2010581	dimethyl sulphate		92.85	-	-	-	95.94
77929	2010691	citric acid		3.72	-	-	-	1016.80
77996	2010749	propylidynetrimethanol		0.86	-	-	-	1.85
78002	2010754	tetraethyllead		-	-	-	-	-
78400	2011145	triethyl phosphate		0.20	-	-	-	8.83
78513	2011229	tris(2-butoxyethyl) phosphate		0.09	-	-	-	0.49
78591	2011260	3,5,5-trimethylcyclohex-2-enone		0.13	-	1.45	-	0.32
78706	2011344	linalool		0.09 *	-	0.25	-	0.09
78784	2011428	2-methylbutane		2.67	-	-	-	4.24
78795	2011433	isoprene		0.10 *	-	7.64	-	0.11
78831	2011480	2-methylpropan-1-ol		1.66	-	-	-	6.10
78842	2011496	isobutyraldehyde		0.46	-	-	-	70.01
78875	2011522	1,2-dichloropropane		16.21	-	-	-	18.61
78900	2011559	propylenediamine		0.14	-	-	-	1.82
78922	2011585	butan-2-ol		1.12	-	-	-	12.29
78933	2011590	butanone		7.75	-	-	-	64.76
78966	2011627	1-aminopropan-2-ol		0.27	-	-	-	9.28
78988	2011648	pyruvaldehyde		0.87	-	-	-	1725.28
79005	2011669	1,1,2-trichloroethane		32.21	-	-	-	44.83
79016	2011674	trichloroethylene		15.39	-	20892.02	-	7.86
79061	2011737	acrylamide		0.30	-	61.12	-	2.08
79094	2011763	propionic acid		8.75	-	-	-	173.39
79107	2011779	acrylic acid		0.44	-	61.12	-	3.92
79118	2011784	chloroacetic acid		16.66	-	-	-	188.09
79141	2011805	glycollic acid		4.11	-	-	-	129.05
79209	2011852	methyl acetate		49.52	-	-	-	35.86
79210	2011868	peracetic acid		2.67	-	-	-	2300.37
79312	2011957	isobutyric acid		4.95	-	-	-	173.62
79334	2011962	l-(+)-lactic acid		2.00	-	-	-	626.64
79345	2011978	1,1,2,2-tetrachloroethane		35.51	-	-	-	95.37
79390	2012023	methacrylamide		0.18	-	9.40	-	0.88
79414	2012044	methacrylic acid		0.23	-	9.40	-	1.46

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).
* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1] Half-life in (cis)	(trans)	AOP 1.83 Ozone [1] (cis)	(trans)	MOOH [1] OH-radical
79469	2012091	2-nitropropane	25.73	-	-	-	447.00
79505	2012107	()-dihydro-3-hydroxy-4,4-dimethylfuran-2(3H)-one	6.27	-	-	-	21.88
79776	2012243	(E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one	0.05	-	0.12	-	0.08
79925	2012348	camphene	0.18	-	9.40	-	0.20
79947	2012369	2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol	3.70 *	-	-	-	6.78
80057	2012458	4,4'-isopropylidenediphenol	0.12 *	-	-	-	0.18
80159	2012547	alpha,alpha-dimethylbenzyl hydroperoxide	1.20	-	-	-	13.01
80433	2012793	bis(alpha,alpha-dimethylbenzyl) peroxide	1.09	-	-	-	1.30
80546	2012898	2-(4-tert-butylbenzyl)propionaldehyde	0.32	-	-	-	3.66
80568	2012919	pin-2(3)-ene	0.12 *	-	0.25	-	0.08
80626	2012971	methyl methacrylate	0.23	-	9.40	-	1.07
81049	2013179	naphthalene-1,5-disulphonic acid	10.32	-	-	-	22.29
81118	2013252	4,4'-diaminostilbene-2,2'-disulphonic acid	0.08	0.07	0.85	0.42	0.65
81163	2013315	2-aminonaphthalene-1-sulphonic acid	0.17	-	-	-	2.47
81641	2013687	1,4-dihydroxyanthraquinone	1.62 *	-	-	-	2.93
81845	2013802	naphthalene-1,8-dicarboxylic anhydride	2.01	-	-	-	22.56
82451	2014235	1-aminoanthraquinone	0.22	-	-	-	0.36
83329	2014696	acenaphthene	0.16	-	-	-	0.13
83567	2014874	naphthalene-1,5-diol	0.05 *	-	-	-	0.08
83625	2014895	1-amino-9,10-dihydro-9,10-dioxoanthracene-2-sulphonic acid	0.40	-	-	-	12.73
83885	2015071	riboflavin	0.09	-	-	-	8.56
84617	2015459	dicyclohexyl phthalate	0.45	-	-	-	0.77
84651	2015490	anthraquinone	10.61	-	-	-	14.69
84662	2015506	diethyl phthalate	3.53	-	-	-	6.11
84695	2015532	diisobutyl phthalate	1.21	-	-	-	2.99
84742	2015574	dibutyl phthalate	1.23	-	-	-	2.46
85405	2016028	1,2,3,6-tetrahydrophthalimide	0.12	-	0.53	-	0.44
85416	2016033	phthalimide	0.87	-	-	-	32.50
85427	2016049	cyclohexane-1,2-dicarboxylic anhydride	2.40	-	-	-	23.00
85438	2016054	1,2,3,6-tetrahydrophthalic anhydride	0.18	-	0.53	-	0.67
85449	2016075	phthalic anhydride	21.22	-	-	-	33.04
85563	2016159	2-(4-chlorobenzoyl)benzoic acid	5.77	-	-	-	14.90
85687	2016227	benzyl butyl phthalate	0.99	-	-	-	1.50
86500	2016761	azinphos-methyl	0.07	-	-	-	12.14
86577	2016845	1-nitronaphthalene	4.02	-	-	-	16.43
86748	2016960	carbazole	0.04	-	-	-	0.13
87569	2017524	mucochloric acid	0.61	-	18667.92	-	48.43
87616	2017571	1,2,3-trichlorobenzene	36.78	-	-	-	29.28
87627	2017587	2,6-xylidine	0.05	-	-	-	0.08
87683	2017655	hexachlorobuta-1,3-diene	477.53	-	>99999	-	10.23
87901	2017828	symclosene	0.30	-	-	-	-
87990	2017880	xylitol	0.28	-	-	-	4.22
88062	2017959	2,4,6-trichlorophenol	20.57 *	-	-	-	14.01
88120	2018004	1-vinyl-2-pyrrolidone	0.30	-	61.12	-	0.14
88448	2018313	4-aminotoluene-3-sulphonic acid	0.21	-	-	-	1.49
88539	2018397	5-amino-2-chlorotoluene-4-sulphonic acid	0.28	-	-	-	3.22
88664	2018491	1-chloro-2-(dichloromethyl)benzene	8.98	-	-	-	16.43
88722	2018533	2-nitrotoluene	13.29	-	-	-	27.08
88733	2018549	1-chloro-2-nitrobenzene	60.67	-	-	-	34.48
88744	2018554	2-nitroaniline	0.31	-	-	-	3.69
88755	2018575	2-nitrophenol	2.42 *	-	-	-	33.31
89258	2018910	3-methyl-1-phenyl-5-pyrazolone	0.72	-	-	-	0.39
89612	2019233	1,4-dichloro-2-nitrobenzene	209.74	-	-	-	40.02
89838	2019448	thymol	0.09 *	-	-	-	0.16
89872	2019474	4-nitro-m-xylene	5.28	-	-	-	22.76
89985	2019563	2-chlorobenzaldehyde	0.65	-	-	-	26.10
90040	2019631	o-anisidine	0.09	-	-	-	0.12
90051	2019647	guaiacol	0.34 *	-	-	-	0.38
90437	2019935	biphenyl-2-ol	0.37 *	-	-	-	0.40
90722	2020139	2,4,6-tris(dimethylaminomethyl)phenol	0.05 *	-	-	-	0.09
90802	2020165	D-glucono-1,5-lactone	0.37	-	-	-	17.38
91156	2020448	phthalonitrile	233.04	-	-	-	32.50
91203	2020495	naphthalene, pure	0.50	-	-	-	0.40
91225	2020516	quinoline	1.65	-	-	-	3.86
91236	2020521	2-nitroanisole	2.89	-	-	-	14.12
91667	2020888	N,N-diethylaniline	0.13	-	-	-	0.06
91689	2020909	3-diethylaminophenol	0.11 *	-	-	-	0.04
91769	2020956	6-phenyl-1,3,5-triazine-2,4-diyldiamine	0.24	-	-	-	8.49

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).
* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1] Half-life in (cis)	(trans)	AOP 1.83 Ozone [1] (cis)	(trans)	MOOH [1] OH-radical
91941	2021090	3,3'-dichlorobenzidine	0.15	-	-	-	0.16
92524	2021635	biphenyl	1.50	-	-	-	1.12
92706	2021808	3-hydroxy-2-naphthoic acid	0.45 *	-	-	-	0.34
92842	2021965	phenothiazine	0.04	-	-	-	0.11
93652	2022644	2-(4-chloro-2-methylphenoxy)propionic acid	0.62	-	-	-	4.92
94360	2023276	dibenzoyl peroxide	3.57	-	-	-	13.88
94600	2023475	dimethyl cyclohexane-1,4-dicarboxylate	1.78	-	-	-	4.91
94688	2023543	N-ethyl-o-toluidine	0.09	-	-	-	0.21
94746	2023606	(4-chloro-2-methylphenoxy)acetic acid	0.85	-	-	-	11.01
94757	2023611	2,4-D	1.72	-	-	-	23.38
95169	2023962	benzothiazole	1.53	-	-	-	3.57
95318	2024091	N-tert-butylbenzothiazole-2-sulphenamide	0.10	-	-	-	0.56
95330	2024112	N-cyclohexylbenzothiazole-2-sulphenamide	0.07	-	-	-	0.49
95476	2024222	o-xylene	1.55	-	-	-	0.68
95487	2024238	o-cresol	0.24 *	-	-	-	0.34
95498	2024243	2-chlorotoluene	5.62	-	-	-	6.58
95501	2024259	1,2-dichlorobenzene	25.81	-	-	-	22.05
95512	2024264	2-chloroaniline	0.20	-	-	-	0.18
95534	2024290	o-toluidine	0.07	-	-	-	0.08
95545	2024306	o-phenylenediamine	0.05	-	-	-	0.07
95556	2024311	2-aminophenol	0.11 *	-	-	-	0.12
95578	2024332	2-chlorophenol	1.03 *	-	-	-	3.43
95636	2024369	1,2,4-trimethylbenzene	0.60	-	-	-	0.25
95749	2024463	3-chloro-p-toluidine	0.09	-	-	-	0.12
95761	2024484	3,4-dichloroaniline	0.25	-	-	-	0.34
95932	2024657	1,2,4,5-tetramethylbenzene	0.49	-	-	-	0.14
96106	2024772	diethylaluminium chloride	-	-	-	-	-
96184	2024861	1,2,3-trichloropropane	18.16	-	-	-	18.39
96220	2024903	pentan-3-one	4.21	-	-	-	21.73
96242	2024924	3-chloropropane-1,2-diol	1.22	-	-	-	6.07
96297	2024966	butanone oxime	7.36	-	-	-	0.74
96311	2024987	1,3-dimethylurea	0.43	-	-	-	1.36
96333	2025006	methyl acrylate	0.44	-	61.12	-	2.66
96344	2025011	methyl chloroacetate	74.28	-	-	-	47.07
96480	2025095	gamma-butyrolactone	4.43	-	-	-	18.22
96764	2025320	2,4-di-tert-butylphenol	0.20 *	-	-	-	0.17
97007	2025514	1-chloro-2,4-dinitrobenzene	492.94	-	-	-	41.36
97029	2025535	2,4-dinitroaniline	0.49	-	-	-	43.57
97369	2025760	2',4'-dimethylacetoacetanilide	0.33	-	-	-	3.41
97654	2025996	itaconic acid	0.22	-	9.40	-	3.17
97723	2026036	isobutyric anhydride	14.40	-	-	-	47.86
97745	2026057	tetramethylthiuram monosulphide	0.08	-	-	-	0.64
97778	2026078	disulfiram	0.03	-	-	-	15.06
97869	2026130	isobutyl methacrylate	0.21	-	9.40	-	0.91
97881	2026151	butyl methacrylate	0.21	-	9.40	-	0.84
97938	2026193	triethylaluminium	-	-	-	-	-
98000	2026261	furfuryl alcohol	0.10 *	-	-	-	0.28
98011	2026277	2-furaldehyde	0.29 *	-	-	-	5.53
98077	2026345	alpha,alpha,alpha-trichlorotoluene	28.96	-	-	-	25.35
98088	2026350	alpha,alpha,alpha-trifluorotoluene	26.38	-	-	-	28.30
98099	2026366	benzenesulphonyl chloride	24.79	-	-	-	28.72
98135	2026408	trichloro(phenyl)silane	-	-	-	-	27.51
98168	2026434	alpha,alpha,alpha-trifluoro-m-toluidine	0.29	-	-	-	3.58
98464	2026701	alpha,alpha,alpha-trifluoro-3-nitrotoluene	214.36	-	-	-	34.32
98511	2026759	4-tert-butyltoluene	1.50	-	-	-	0.50
98522	2026764	4-tert-butylcyclohexanol	0.52	-	-	-	1.09
98544	2026790	4-tert-butylphenol	0.25 *	-	-	-	0.31
98566	2026811	4-chloro-alpha,alpha,alpha-trifluorotoluene	37.60	-	-	-	32.66
98737	2026963	4-tert-butylbenzoic acid	4.08	-	-	-	15.50
98828	2027045	cumene	1.51	-	-	-	1.98
98839	2027050	2-phenylpropene	0.20	-	0.78	-	0.17
98862	2027087	acetophenone	6.66	-	-	-	20.04
98873	2027092	alpha,alpha-dichlorotoluene	4.51	-	-	-	14.95
98884	2027108	benzoyl chloride	7.15	-	-	-	28.04
98920	2027134	nicotinamide	0.89	-	-	-	34.25
98942	2027155	cyclohexyldimethylamine	0.11	-	-	-	0.58
98953	2027160	nitrobenzene	42.58	-	-	-	30.37
99081	2027286	3-nitrotoluene	17.69	-	-	-	30.02
99547	2027642	1,2-dichloro-4-nitrobenzene	209.74	-	-	-	40.08
99650	2027768	1,3-dinitrobenzene	346.17	-	-	-	35.63

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).

* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1]		AOP 1.83 Ozone [1]		MOOH [1]
		Half-life in	(cis)	(trans)	(cis)	(trans)	OH-radical
99752	2027841	methyl p-toluate	5.17	-	-	-	10.60
99887	2027972	4-isopropylaniline	0.07	-	-	-	0.08
99990	2028080	4-nitrotoluene	13.29	-	-	-	30.80
100005	2028096	1-chloro-4-nitrobenzene	60.67	-	-	-	34.60
100016	2028101	4-nitroaniline	0.31	-	-	-	10.82
100027	2028117	4-nitrophenol	2.42 *	-	-	-	34.25
100209	2028295	terephthaloyl dichloride	21.22	-	-	-	32.99
100210	2028300	terephthalic acid	10.67	-	-	-	32.59
100298	2028379	4-nitrophenetole	1.25	-	-	-	25.07
100378	2028452	2-diethylaminoethanol	0.12	-	-	-	0.88
100403	2028489	4-vinylcyclohexene	0.12	-	0.50	-	0.10
100414	2028494	ethylbenzene	1.74	-	-	-	2.07
100425	2028515	styrene	0.38	-	5.09	-	0.27
100447	2028536	alpha-chlorotoluene	4.41	-	-	-	6.09
100470	2028557	benzonitrile	30.06	-	-	-	25.94
100516	2028599	benzyl alcohol	1.34	-	-	-	1.35
100527	2028604	benzaldehyde	0.62	-	-	-	22.77
100549	2028630	nicotinonitrile	165.84	-	-	-	35.29
100970	2029058	methenamine	0.01	-	-	-	36.75
101020	2029084	triphenyl phosphite	0.94	-	-	-	0.98
101053	2029105	anilazine	0.10	-	-	-	23.87
101393	2029388	alpha-methylcinnamaldehyde	0.26	-	4.90	-	0.34
101542	2029519	N-(4-aminophenyl)aniline	0.04	-	-	-	0.05
101724	2029697	N-isopropyl-N'-phenyl-p-phenylenediamine	0.03	-	-	-	0.05
101779	2029744	4,4'-methylenedianiline	0.04	-	-	-	0.04
101837	2029807	dicyclohexylamine	0.08	-	-	-	0.67
101848	2029812	diphenyl ether	0.55	-	-	-	1.52
101860	2029833	alpha-hexylcinnamaldehyde	0.23	-	4.90	-	0.29
102012	2029964	acetoacetanilide	0.42	-	-	-	15.45
102067	2030021	1,3-diphenylguanidine	0.05	-	-	-	0.99
102090	2030058	diphenyl carbonate	2.54	-	-	-	9.18
102363	2030262	3,4-dichlorophenyl isocyanate	23.51	-	-	-	23.18
102716	2030498	2,2',2''-nitrilotriethanol	0.10	-	-	-	1.28
102761	2030519	triacetin	1.37	-	-	-	15.82
102772	2030524	2-(morpholinothio)benzothiazole	0.05	-	-	-	0.74
103015	2030702	N-phenylglycine	0.10	-	-	-	0.87
103117	2030807	2-ethylhexyl acrylate	0.31	-	61.12	-	1.23
103231	2030901	bis(2-ethylhexyl) adipate	0.44	-	-	-	1.27
103708	2031360	formanilide	0.05	-	-	-	4.34
103719	2031376	phenyl isocyanate	4.77	-	-	-	-
103822	2031486	phenylacetic acid	2.41	-	-	-	13.10
103844	2031507	acetanilide	0.43	-	-	-	0.22
103902	2031575	paracetamol	0.35 *	-	-	-	0.30
104154	2031800	toluene-4-sulphonic acid	8.14	-	-	-	28.24
104552	2032139	cinnamaldehyde	0.33	0.31	63.67	31.84	0.54
104767	2032343	2-ethylhexan-1-ol	0.83	-	-	-	1.73
104881	2032474	4-chlorobenzaldehyde	0.65	-	-	-	29.06
104938	2032537	4-methylanisole	0.37	-	-	-	0.25
105384	2032935	vinyl propionate	0.40	-	61.12	-	0.46
105395	2032940	ethyl chloroacetate	10.45	-	-	-	21.94
105453	2032998	methyl acetoacetate	32.87	-	-	-	76.06
105486	2033017	isopropyl chloroacetate	4.86	-	-	-	28.93
105533	2033059	diethyl malonate	3.71	-	-	-	14.91
105599	2033127	2,2'-methyliminodiethanol	0.12	-	-	-	0.70
105602	2033132	epsilon-caprolactam	0.43	-	-	-	9.87
105624	2033153	1-methyl-1,2-ethanediyl dioleate	0.07 *	0.06	0.41	0.27	-
105760	2033284	dibutyl maleate	0.19	0.17	122.25	61.12	2.70
105997	2033504	dibutyl adipate	0.94	-	-	-	3.63
106241	2033771	geraniol	0.06 *	-	0.12	-	0.07
106252	2033787	nerol	0.06 *	-	0.12	-	0.06
106423	2033965	p-xylene	1.55	-	-	-	0.58
106434	2033970	4-chlorotoluene	5.62	-	-	-	5.54
106445	2033986	p-cresol	0.24 *	-	-	-	0.34
106467	2034005	1,4-dichlorobenzene	25.81	-	-	-	24.09
106489	2034026	4-chlorophenol	1.03 *	-	-	-	2.13
106490	2034031	p-toluidine	0.07	-	-	-	0.08
106503	2034047	p-phenylenediamine	0.05	-	-	-	0.06
106650	2034199	dimethyl succinate	24.76	-	-	-	30.14
106752	2034309	oxydiethylene bis(chloroformate)	0.65	-	-	-	11.07
106887	2034382	1,2-epoxybutane	6.31	-	-	-	13.02

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).
* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1] Half-life in		AOP 1.83 Ozone [1]		MOOH [1]
			(cis)	(trans)	(cis)	(trans)	OH-radical
106898	2034398	1-chloro-2,3-epoxypropane	18.81	-	-	-	21.09
106934	2034445	1,2-dibromoethane	37.32	-	-	-	35.43
106978	2034487	butane, pure	4.22	-	-	-	4.22
106989	2034492	but-1-ene	0.39	-	8.91	-	0.32
106990	2034508	buta-1,3-diene	0.16	-	13.21	-	0.13
107017	2034529	butene, mixed -1- and -2- isomers	0.19 *	0.17	0.82	0.53	0.16
107028	2034534	acrylaldehyde	0.47	-	382.03	-	1.71
107051	2034576	3-chloropropene	0.53	-	67.92	-	0.63
107062	2034581	1,2-dichloroethane	29.47	-	-	-	16.75
107073	2034597	2-chloroethanol	5.17	-	-	-	6.26
107131	2034665	acrylonitrile	2.71	-	1222.48	-	1.81
107153	2034686	ethylenediamine	0.17	-	-	-	0.95
107186	2034707	allyl alcohol	0.37	-	8.91	-	0.29
107211	2034733	ethane-1,2-diol	1.44	-	-	-	5.77
107222	2034749	glyoxal	0.44	-	-	-	-
107255	2034754	methyl vinyl ether	0.31	-	61.12	-	0.26
107313	2034817	methyl formate	49.52	-	-	-	60.47
107415	2034890	2-methylpentane-2,4-diol	1.06	-	-	-	6.42
107437	2034906	betaine	-	-	-	-	-
107460	2034927	hexamethyldisiloxane	-	-	-	-	-
107642	2035082	dimethyldioctadecylammonium chloride	-	-	-	-	-
107868	2035276	3-methyl-2-butenal	0.27	-	9.04	-	0.38
107880	2035297	butane-1,3-diol	0.80	-	-	-	4.77
107926	2035323	butyric acid	4.30	-	-	-	36.30
107982	2035391	1-methoxypropan-2-ol	0.68	-	-	-	2.03
108010	2035428	2-dimethylaminoethanol	0.14	-	-	-	0.61
108032	2035449	1-nitropropane	16.93	-	-	-	170.33
108054	2035454	vinyl acetate	0.41	-	61.12	-	0.48
108101	2035501	4-methylpentan-2-one	1.14	-	-	-	19.78
108112	2035517	4-methylpentan-2-ol	0.86	-	-	-	3.25
108189	2035585	diisopropylamine	0.11	-	-	-	6.86
108203	2035606	diisopropyl ether	0.46	-	-	-	3.74
108214	2035611	isopropyl acetate	3.43	-	-	-	24.71
108225	2035627	isopropenyl acetate	0.21	-	9.40	-	0.42
108247	2035648	acetic anhydride	>99999	-	-	-	1019.71
108316	2035716	maleic anhydride	4.77	-	61.12	-	53.29
108327	2035721	propylene carbonate	2.48	-	-	-	91.53
108383	2035763	m-xylene	0.74	-	-	-	0.56
108394	2035779	m-cresol	0.11 *	-	-	-	0.30
108441	2035831	m-toluidine	0.05	-	-	-	0.06
108452	2035847	m-phenylenediamine	0.04	-	-	-	0.04
108463	2035852	resorcinol	0.05 *	-	-	-	0.27
108598	2035978	dimethyl malonate	24.76	-	-	-	39.79
108656	2036039	2-methoxy-1-methylethyl acetate	0.96	-	-	-	1.80
108689	2036065	3,5-xylenol	0.05 *	-	-	-	0.13
108770	2036149	2,4,6-trichloro-1,3,5-triazine	2971.31	-	-	-	144.94
108781	2036154	melamine	0.18	-	-	-	1235.19
108805	2036180	cyanuric acid	68.35 *	-	-	-	201.60
108838	2036201	2,6-dimethylheptan-4-one	0.58	-	-	-	8.88
108883	2036259	toluene	1.94	-	-	-	2.08
108907	2036285	chlorobenzene	7.47	-	-	-	15.16
108918	2036290	cyclohexylamine	0.19	-	-	-	0.91
108930	2036306	cyclohexanol	0.62	-	-	-	1.46
108941	2036311	cyclohexanone	0.85	-	-	-	8.04
108952	2036327	phenol	0.30 *	-	-	-	0.88
109068	2036437	2-methylpyridine	9.58	-	-	-	12.49
109535	2036788	isobutyl vinyl ether	0.22	-	61.12	-	0.23
109557	2036809	3-aminopropyldimethylamine	0.10	-	-	-	0.65
109604	2036861	propyl acetate	3.70	-	-	-	7.90
109660	2036924	pentane	2.72	-	-	-	2.81
109693	2036966	1-chlorobutane	4.66	-	-	-	5.98
109706	2036971	1-bromo-3-chloropropane	10.62	-	-	-	14.42
109739	2036992	butylamine	0.32	-	-	-	5.21
109831	2037100	2-methylaminoethanol	0.14	-	-	-	0.88
109864	2037137	2-methoxyethanol	0.96	-	-	-	2.12
109897	2037163	diethylamine	0.14	-	-	-	0.78
109922	2037184	ethyl vinyl ether	0.27	-	61.12	-	0.24
109944	2037210	ethyl formate	7.41	-	-	-	28.26
109999	2037268	tetrahydrofuran	0.58	-	-	-	0.79
110010	2037289	tetrahydrothiophene	0.54 *	-	-	-	1.91

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).
* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1]		AOP 1.83 Ozone [1]		MOOH [1]
		Half-life in	(cis)	(trans)	(cis)	(trans)	OH-radical
110054	2037336	di-tert-butyl peroxide	9.60	-	-	-	19.10
110123	2037378	5-methylhexan-2-one	1.27	-	-	-	9.33
110167	2037425	maleic acid	0.23	0.20	122.25	61.12	31.79
110178	2037430	fumaric acid	0.23	0.20	122.25	61.12	19.83
110190	2037451	isobutyl acetate	2.46	-	-	-	10.88
110214	2037472	1,1-hydrazoformamide	0.23	-	-	-	-
110270	2037514	isopropyl myristate	0.58	-	-	-	0.93
110305	2037556	N,N'-ethylenedi(stearamide)	0.13	-	-	-	-
110338	2037577	dihexyl adipate	0.63	-	-	-	1.65
110429	2037666	methyl decanoate	1.09	-	-	-	1.92
110441	2037687	hexa-2,4-dienoic acid	0.09	-	2.03	-	0.25
110543	2037776	hexane	2.01	-	-	-	1.75
110634	2037865	butane-1,4-diol	1.05	-	-	-	2.47
110645	2037870	but-2-ene-1,4-diol	0.17 *	0.15	0.82	0.53	0.31
110656	2037886	but-2-yne-1,4-diol	0.31	-	3565.57	-	-
110805	2038041	2-ethoxyethanol	0.67	-	-	-	1.53
110827	2038062	cyclohexane	1.28	-	-	-	0.63
110850	2038083	piperazine	0.07	-	-	-	0.43
110883	2038125	1,3,5-trioxane	0.70	-	-	-	1.53
110918	2038151	morpholine	0.07	-	-	-	0.70
110930	2038167	6-methylhept-5-en-2-one	0.12 *	-	0.25	-	0.14
110974	2038209	1,1'-iminodipropan-2-ol	0.11	-	-	-	0.82
110985	2038214	1,1'-oxydipropan-2-ol	0.36	-	-	-	3.05
111115	2038350	methyl octanoate	1.51	-	-	-	3.26
111148	2038387	heptanoic acid	1.60	-	-	-	5.15
111159	2038392	2-ethoxyethyl acetate	0.77	-	-	-	2.04
111273	2038523	hexan-1-ol	1.17	-	-	-	2.76
111295	2038544	pentane-1,5-diol	0.92	-	-	-	4.14
111308	2038565	glutaral	0.23	-	-	-	80.88
111364	2038628	butyl isocyanate	2.86	-	-	-	2.04
111400	2038654	2,2'-iminodi(ethylamine)	0.07	-	-	-	0.82
111411	2038675	2-(2-aminoethylamino)ethanol	0.09	-	-	-	0.86
111422	2038680	2,2'-iminodiethanol	0.12	-	-	-	0.88
111466	2038722	2,2'-oxydiethanol	0.52	-	-	-	2.03
111488	2038743	thiodiglycol	0.37 *	-	-	-	2.25
111659	2038921	octane	1.32	-	-	-	1.47
111660	2038937	oct-1-ene	0.33	-	8.91	-	0.28
111693	2038963	adiponitrile	7.73	-	-	-	58.78
111717	2038984	heptanal	0.35	-	-	-	5.40
111762	2039050	2-butoxyethanol	0.46	-	-	-	1.20
111773	2039066	2-(2-methoxyethoxy)ethanol	0.44	-	-	-	0.98
111820	2039113	methyl laurate	0.85	-	-	-	1.53
111875	2039176	octan-1-ol	0.90	-	-	-	1.83
111900	2039197	2-(2-ethoxyethoxy)ethanol	0.37	-	-	-	1.01
111911	2039202	bis(2-chloroethoxy)methane	1.12	-	-	-	4.18
111922	2039218	dibutylamine	0.12	-	-	-	0.62
111966	2039244	bis(2-methoxyethyl) ether	0.38	-	-	-	0.60
112050	2039312	nonanoic acid	1.13	-	-	-	2.95
112072	2039333	2-butoxyethyl acetate	0.51	-	-	-	1.61
112185	2039438	dodecyldimethylamine	0.12	-	-	-	0.39
112243	2039506	trientine	0.05	-	-	-	0.36
112254	2039511	2-hexyloxyethanol	0.41	-	-	-	1.02
112276	2039532	2,2'-(ethylenedioxy)diethanol	0.32	-	-	-	1.08
112301	2039569	decan-1-ol	0.73	-	-	-	1.37
112345	2039616	2-(2-butoxyethoxy)ethanol	0.30	-	-	-	0.71
112356	2039621	2-(2-(2-methoxyethoxy)ethoxy)ethanol	0.28	-	-	-	0.65
112414	2039684	dodec-1-ene	0.28	-	8.91	-	0.25
112538	2039820	dodecan-1-ol	0.61	-	-	-	1.08
112572	2039862	3,6,9-triazaundecamethylenediamine	0.03	-	-	-	0.30
112607	2039899	3,6,9-trioxaundecane-1,11-diol	0.23	-	-	-	0.71
112629	2039925	methyl oleate	0.15 *	0.13	0.82	0.53	0.14
112721	2040003	tetradecanol	0.53	-	-	-	0.88
112765	2040045	stearoyl chloride	0.43	-	-	-	0.91
112845	2040092	(Z)-docos-13-enamide	0.11 *	0.10	0.82	0.53	0.12
112867	2040113	(Z)-docos-13-enoic acid	0.13 *	0.12	0.82	0.53	0.13
112889	2040129	octadec-1-ene	0.23	-	8.91	-	0.21
112903	2040155	(Z)-octadec-9-enylamine	0.10 *	0.09	0.82	0.53	0.13
112925	2040176	octadecan-1-ol	0.41	-	-	-	0.65
114261	2040438	propoxur	0.26	-	-	-	0.70
115071	2040621	propene, pure	0.40	-	8.91	-	0.33

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).
* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1]		AOP 1.83 Ozone [1]		MOOH [1]
		Half-life in	(cis)	(trans)	(cis)	(trans)	OH-radical
115106	2040658	dimethyl ether	6.09	-	-	-	2.55
115117	2040663	2-methylpropene	0.21	-	8.91	-	0.20
115184	2040684	2-methylbut-3-en-2-ol	0.40	-	61.12	-	0.50
115195	2040705	2-methylbut-3-yn-2-ol	1.57	-	3565.57	-	173.59
115297	2040794	endosulfan	0.13	-	2988.74	-	-
115322	2040820	dicofol	3.08	-	-	-	12.64
115775	2041049	pentaerythritol	0.72	-	-	-	2.50
115866	2041122	triphenyl phosphate	0.94	-	-	-	2.36
115968	2041185	tris(2-chloroethyl) phosphate	0.32	-	-	-	10.90
116029	2041227	3,3,5-trimethylcyclohexanol	0.59	-	-	-	2.89
116143	2041269	tetrafluoroethylene	3.80	-	2387.66	-	7.46
116154	2041274	hexafluoropropene	1.52	-	955.06	-	87.44
117793	2042084	2-aminoanthraquinone	0.22	-	-	-	0.89
117817	2042110	bis(2-ethylhexyl) phthalate	0.49	-	-	-	0.74
118332	2042461	6-aminonaphthalene-1,3-disulphonic acid	0.36	-	-	-	3.10
118489	2042550	4H-3,1-benzoxazine-2,4(1H)-dione	0.24	-	-	-	33.37
118581	2042629	benzyl salicylate	0.60 *	-	-	-	3.77
118741	2042739	hexachlorobenzene	625.54	-	-	-	62.36
118821	2042791	2,2',6,6'-tetra-tert-butyl-4,4'-methylenediphenol	0.28 *	-	-	-	-
118967	2042896	2,4,6-trinitrotoluene	73.47	-	-	-	48.13
119368	2043177	methyl salicylate	0.92 *	-	-	-	10.26
119471	2043271	6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol	0.25 *	-	-	-	0.12
119619	2043376	benzophenone	3.57	-	-	-	9.46
119642	2043402	1,2,3,4-tetrahydronaphthalene	0.96	-	-	-	0.37
119802	2043528	2,2'-dithiodi(benzoic acid)	0.05	-	-	-	5.67
120127	2043711	anthracene, pure	0.10	-	-	-	0.05
120183	2043753	naphthalene-2-sulphonic acid	2.32	-	-	-	16.70
120365	2043905	dichlorprop	0.97	-	-	-	22.41
120514	2044029	benzyl benzoate	1.52	-	-	-	2.68
120616	2044118	dimethyl terephthalate	18.63	-	-	-	16.00
120785	2044249	di(benzothiazol-2-yl) disulphide	0.04	-	-	-	2.44
120809	2044275	pyrocatechol	0.44 *	-	-	-	0.32
120821	2044280	1,2,4-trichlorobenzene	36.78	-	-	-	30.82
120832	2044296	2,4-dichlorophenol	3.54 *	-	-	-	8.59
120923	2044359	cyclopentanone	1.20	-	-	-	9.25
121039	2044453	4-nitrotoluene-2-sulphonic acid	33.47	-	-	-	36.51
121142	2044500	2,4-dinitrotoluene	47.48	-	-	-	38.58
121335	2044652	vanillin	0.40 *	-	-	-	2.51
121448	2044694	triethylamine	0.12	-	-	-	0.74
121471	2044736	3-aminobenzenesulphonic acid	0.24	-	-	-	12.86
121573	2044825	sulphanilic acid	0.24	-	-	-	11.81
121697	2044935	N,N-dimethylaniline	0.04	-	-	-	0.12
121733	2044961	1-chloro-3-nitrobenzene	87.04	-	-	-	34.59
121755	2044977	malathion	0.16	-	-	-	-
121824	2045001	perhydro-1,3,5-trinitro-1,3,5-triazine	0.04	-	-	-	1115.40
121868	2045017	2-chloro-4-nitrotoluene	31.92	-	-	-	35.96
121879	2045022	2-chloro-4-nitroaniline	0.44	-	-	-	13.46
121915	2045064	isophthalic acid	9.94	-	-	-	32.69
122349	2045352	simazine	0.08	-	-	-	1.24
122394	2045394	diphenylamine	0.04	-	-	-	0.08
122510	2045504	triethyl orthoformate	0.13	-	-	-	1.13
122521	2045525	triethyl phosphite	0.20	-	-	-	1.84
122996	2045897	2-phenoxyethanol	0.32	-	-	-	1.10
123057	2045965	2-ethylhexanal	0.31	-	-	-	5.23
123308	2046162	4-aminophenol	0.11 *	-	-	-	0.15
123319	2046178	hydroquinone	0.44 *	-	-	-	0.29
123353	2046225	7-methyl-3-methyleneocta-1,6-diene	0.06 *	-	0.24	-	0.05
123386	2046230	propionaldehyde	0.49	-	-	-	88.26
123422	2046267	4-hydroxy-4-methylpentan-2-one	7.99	-	-	-	70.13
123513	2046335	3-methylbutan-1-ol	1.36	-	-	-	2.56
123546	2046340	pentane-2,4-dione	15.22	-	-	-	348.65
123728	2046466	butyraldehyde	0.42	-	-	-	26.44
123773	2046508	C,C'-azodi(formamide)	0.45	-	-	-	-
123864	2046581	n-butyl acetate	2.50	-	-	-	7.77
123911	2046618	1,4-dioxane	0.41	-	-	-	2.27
124049	2046733	adipic acid	2.04	-	-	-	121.73
124072	2046775	octanoic acid	1.33	-	-	-	6.84
124094	2046796	hexamethylenediamine	0.16	-	-	-	1.15
124107	2046801	methyl myristate	0.69	-	-	-	1.08
124174	2046859	2-(2-butoxyethoxy)ethyl acetate	0.31	-	-	-	1.25

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).

* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1]		AOP 1.83 Ozone [1]		MOOH [1]
		Half-life in	(cis)	(trans)	(cis)	(trans)	OH-radical
124185	2046864	decane	0.98	-	-	-	1.11
124301	2046953	octadecylamine	0.20	-	-	-	0.45
124389	2046969	carbon dioxide	>99999	-	-	-	-
124403	2046974	dimethylamine, in aqueous solution	0.17	-	-	-	0.91
124630	2047061	methanesulphonyl chloride	8.25	-	-	-	5845.20
124685	2047098	2-amino-2-methylpropanol	0.44	-	-	-	5.35
125122	2047276	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acetate	1.23	-	-	-	2.11
126307	2047810	2,2-dimethylpropane-1,3-diol	1.37	-	-	-	4.46
126330	2047831	tetrahydrothiophene 1,1-dioxide	2.40	-	-	-	61.61
126716	2047983	triisobutyl phosphate	0.12	-	-	-	-
126738	2048002	tributyl phosphate	0.13	-	-	-	-
126998	2048180	2-chlorobuta-1,3-diene	0.51	-	92.35	-	0.25
127184	2048259	tetrachloroethylene	60.78	-	>99999	-	53.10
127195	2048264	N,N-dimethylacetamide	0.82	-	-	-	3.01
127479	2048442	retinyl acetate	0.03	-	0.23	-	0.02
128370	2048814	2,6-di-tert-butyl-p-cresol	0.55 *	-	-	-	0.24
128392	2048840	2,6-di-tert-butylphenol	0.20 *	-	-	-	0.14
131099	2050100	2-chloroanthraquinone	12.47	-	-	-	16.45
131113	2050116	dimethyl phthalate	18.63	-	-	-	11.04
133493	2051078	pentachlorobenzenethiol	67.23	-	-	-	15.52
134327	2051387	1-naphthylamine	0.05	-	-	-	0.05
135193	2051827	2-naphthol	0.05 *	-	-	-	0.12
135988	2052270	sec-butylbenzene	1.23	-	-	-	1.63
136232	2052328	zinc bis(dibutyldithiocarbamate)	-	-	-	-	2.55
137268	2052862	thiram	0.03	-	-	-	47.03
140114	2053997	benzyl acetate	1.68	-	-	-	3.10
140294	2054105	phenylacetonitrile	5.10	-	-	-	16.72
140318	2054110	2-piperazin-1-ylethylamine	0.05	-	-	-	0.30
140669	2054262	4-(1,1,3,3-tetramethylbutyl)phenol	0.24 *	-	-	-	0.28
140885	2054388	ethyl acrylate	0.42	-	61.12	-	2.04
140954	2054440	1,3-bis(hydroxymethyl)urea	0.22	-	-	-	15.00
141059	2054519	diethyl maleate	0.22	0.19	122.25	61.12	4.87
141106	2054571	6,10-dimethylundeca-3,5,9-trien-2-one	0.04 *	-	0.08	-	0.05
141322	2054807	butyl acrylate	0.38	-	61.12	-	2.02
141435	2054833	2-aminoethanol	0.31	-	-	-	1.82
141786	2055004	ethyl acetate	7.41	-	-	-	13.77
141979	2055161	ethyl acetoacetate	6.89	-	-	-	43.57
142165	2055245	bis(2-ethylhexyl) maleate	0.16	0.14	122.25	61.12	1.42
142223	2055287	diallyl 2,2'-oxydiethyl dicarbonate	0.15	-	4.46	-	0.29
142789	2055601	N-(2-hydroxyethyl)dodecanamide	0.29	-	-	-	0.97
142825	2055638	heptane	1.59	-	-	-	1.74
142847	2055659	dipropylamine	0.13	-	-	-	0.67
142905	2055706	dodecyl methacrylate	0.17	-	9.40	-	0.51
142916	2055711	isopropyl palmitate	0.51	-	-	-	0.84
143226	2055926	2-(2-(2-butoxyethoxy)ethoxy)ethanol	0.22	-	-	-	0.51
143339	2055994	sodium cyanide	-	-	-	-	-
144627	2056343	oxalic acid	13.37	-	-	-	-
149304	2057368	benzothiazole-2-thiol	0.23	-	-	-	3.72
149575	2057436	2-ethylhexanoic acid	1.33	-	-	-	5.69
149735	2057457	trimethyl orthoformate	0.15	-	-	-	1.94
150787	2057719	1,4-dimethoxybenzene	0.50	-	-	-	0.22
151508	2057923	potassium cyanide	-	-	-	-	-
151564	2057939	aziridine	0.18	-	-	-	66.62
156434	2058555	p-phenetidine	0.08	-	-	-	0.12
287923	2060166	cyclopentane	1.92	-	-	-	1.33
288324	2060192	imidazole	0.30	-	-	-	0.12
288880	2060229	1,2,4-triazole	1.07	-	-	-	0.97
294622	2060339	cyclododecane	0.64	-	-	-	0.49
298000	2060501	parathion-methyl	0.17	-	-	-	33.20
298066	2060559	O,O-diethyl hydrogen phosphorodithioate	0.09	-	-	-	127.10
298124	2060585	glyoxylic acid	0.85	-	-	-	-
301020	2061039	oleamide	0.12 *	0.11	0.82	0.53	0.15
302012	2061149	hydrazine	-	-	-	-	-
328847	2063371	3,4-dichloro-alpha,alpha,alpha-trifluorotoluene	129.97	-	-	-	37.85
329011	2063413	alpha,alpha,alpha-trifluoro-3-tolyl isocyanate	24.03	-	-	-	33.65
330541	2063544	diuron	0.31	-	-	-	0.68
330552	2063565	linuron	0.32	-	-	-	1.11
333415	2063738	diazinon	0.11	-	-	-	12.59
334485	2063764	decanoic acid	0.99	-	-	-	2.14
353593	2065379	bromochlorodifluoromethane	>99999	-	-	-	-

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).

* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1]		AOP 1.83 Ozone [1]		MOOH [1]
		Half-life in	(cis)	(trans)	(cis)	(trans)	OH-radical
366187	2066744	2,2'-bipyridyl	8.29	-	-	-	7.58
393759	2068893	4-chloro-3,5-dinitro-alpha,alpha,alpha-trifluorotoluene	17827.86	-	-	-	48.31
420042	2069923	cyanamide	0.53	-	-	-	-
461585	2073128	cyanoguanidine	0.13	-	-	-	377.98
463514	2073369	ketene	0.21	-	1222.48	-	0.38
473552	2074671	2,6,6-trimethylbicyclo[3.1.1]heptane	2.76	-	-	-	0.63
482893	2075869	2-(1,3-dihydro-3-oxo-2H-indazol-2-ylidene)-1,2-dihydro-3H-indol-3-one	0.05	-	61.12	-	0.69
497392	2078477	4,6-di-tert-butyl-m-cresol	0.08 *	-	-	-	0.11
502443	2079381	hexan-6-olide	1.84	-	-	-	16.72
502692	2079507	6,10,14-trimethylpentadecan-2-one	0.43	-	-	-	0.80
504609	2079952	penta-1,3-diene	0.10 *	-	2.03	-	0.08
505328	2080088	3,7,11,15-tetramethylhexadec-1-en-3-ol	0.22	-	61.12	-	0.28
505657	2080156	1,3-dioxepane	0.38	-	-	-	2.26
513359	2081563	2-methylbut-2-ene	0.12 *	-	0.25	-	0.11
526954	2084014	D-gluconic acid	0.26	-	-	-	19.25
533744	2085767	dazomet	0.04	-	-	-	0.89
538932	2087062	isobutylbenzene	1.20	-	-	-	1.76
540841	2087591	2,2,4-trimethylpentane	2.28	-	-	-	3.24
541731	2087921	1,3-dichlorobenzene	10.64	-	-	-	23.19
542756	2088265	1,3-dichloropropene	1.21	1.07	949.89	474.95	0.80
544638	2088752	myristic acid, pure	0.65	-	-	-	1.17
551166	2089934	6-aminopenicillanic acid	0.12	-	-	-	67.21
552307	2090080	benzene-1,2,4-tricarboxylic acid 1,2-anhydride	18.28	-	-	-	37.43
553264	2090363	4,4'-bipyridyl	8.29	-	-	-	14.94
556672	2091367	octamethylcyclotetrasiloxane	-	-	-	-	11.99
556821	2091414	3-methylbut-2-en-1-ol	0.12 *	-	0.25	-	0.14
563473	2092512	3-chloro-2-methylpropene	0.27	-	10.45	-	0.37
563780	2092622	2,3-dimethylbut-1-ene	0.20	-	8.91	-	0.20
576261	2094001	2,6-xylenol	0.20 *	-	-	-	0.21
583915	2095230	2-hydroxy-4-(methylthio)butyric acid	0.51 *	-	-	-	6.14
590863	2096915	isovaleraldehyde	0.36	-	-	-	29.99
591275	2097112	3-aminophenol	0.05 *	-	-	-	0.05
592358	2097510	butyl carbamate	0.67	-	-	-	10.28
592416	2097531	hex-1-ene	0.36	-	8.91	-	0.29
593817	2098100	trimethylammonium chloride	-	-	-	-	-
594423	2098404	trichloromethanesulphenyl chloride	5.35	-	-	-	-
598561	2099408	ethyldimethylamine	0.15	-	-	-	0.67
598787	2099523	2-chloropropionic acid	10.58	-	-	-	245.68
599042	2099633	alpha-hydroxy-beta,beta-dimethyl-gamma-butyrolactone	6.27	-	-	-	21.88
603350	2100360	triphenylphosphine	1.75	-	-	-	0.24
609143	2101799	ethyl 2-methylacetoacetate	4.89	-	-	-	11.97
611063	2102483	1,3-dichloro-4-nitrobenzene	86.47	-	-	-	39.95
613901	2103597	benzoyl cyanide	7.15	-	-	-	28.44
616386	2104784	dimethyl carbonate	24.76	-	-	-	57.26
616455	2104831	2-pyrrolidone	0.54	-	-	-	1.66
620677	2106472	propane-1,2,3-triyl trisheptanoate	0.38	-	-	-	-
624486	2108485	dimethyl maleate	0.23	0.20	122.25	61.12	11.99
624920	2108710	dimethyl disulphide	0.05	-	-	-	10.57
627703	2110096	acetone azine	14.40	-	-	-	0.54
627838	2110143	ethylene distearate	0.24	-	-	-	-
627930	2110206	dimethyl adipate	3.32	-	-	-	13.25
628966	2110630	ethylene dinitrate	118.20	-	-	-	982.25
629118	2110740	hexane-1,6-diol	0.82	-	-	-	3.33
629505	2110934	tridecane	0.71	-	-	-	0.82
629594	2110960	tetradecane	0.65	-	-	-	0.75
629732	2111058	hexadec-1-ene	0.24	-	8.91	-	0.22
629969	2111194	icosan-1-ol	0.37	-	-	-	0.57
630080	2111283	carbon monoxide	-	-	-	-	-
637923	2113097	2-ethoxy-2-methylpropane	1.39	-	-	-	1.56
645625	2114483	2-ethylhex-2-enal	0.25	-	9.04	-	0.31
661198	2115466	docosan-1-ol	0.34	-	-	-	0.51
674828	2116171	but-3-en-3-olide	0.21	-	9.40	-	1.55
682097	2116611	2,2-bis(allyloxymethyl)butan-1-ol	0.13	-	4.46	-	0.14
683181	2116700	dibutyltin dichloride	-	-	-	-	-
691372	2117201	4-methylpent-1-ene	0.36	-	8.91	-	0.29
693232	2117463	dodecanedioic acid	0.79	-	-	-	3.64
700130	2118383	2,3,5-trimethylhydroquinone	0.05 *	-	-	-	0.11

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).
* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1]		AOP 1.83 Ozone [1]		MOOH [1]
		Half-life in	(cis)	(trans)	(cis)	(trans)	OH-radical
709988	2119146	propanil	0.68	-	-	-	0.91
756809	2120539	O,O-dimethyl hydrogen dithiophosphate	0.12	-	-	-	358.71
760236	2120790	3,4-dichlorobut-1-ene	0.40	-	8.91	-	0.96
760678	2120811	2-ethylhexanoyl chloride	0.83	-	-	-	7.15
763326	2121108	3-methylbut-3-en-1-ol	0.19	-	8.91	-	0.23
763699	2121129	ethyl 3-ethoxypropionate	0.78	-	-	-	2.74
764410	2121218	1,4-dichlorobut-2-ene	0.32	0.29	150.92	75.46	0.68
791286	2123388	triphenylphosphine oxide	1.75	-	-	-	0.20
793248	2123440	N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine	0.03	-	-	-	0.09
811972	2123770	norflurane	1725.28	-	-	-	1762.23
818611	2124549	2-hydroxyethyl acrylate	0.37	-	61.12	-	1.65
822060	2124858	hexamethylene diisocyanate	1.38	-	-	-	-
822366	2124973	4-methylimidazole	0.11	-	-	-	0.09
826368	2125542	2,2,6,6-tetramethyl-4-piperidone	0.17	-	-	-	23.57
830137	2125956	cyclododecanone	0.51	-	-	-	-
834128	2126347	ametryn	0.07	-	-	-	1.55
836306	2126462	4-nitro-N-phenylaniline	0.04	-	-	-	7.57
838880	2126588	4,4'-methylenedi-o-toluidine	0.04	-	-	-	0.04
839907	2126609	tris(2-hydroxyethyl)-1,3,5-triazinetrione	0.18	-	-	-	8.44
868779	2127822	2-hydroxyethyl methacrylate	0.20	-	9.40	-	1.11
868859	2127838	dimethyl phosphonate	1.86	-	-	-	56.86
872059	2128192	dec-1-ene	0.30	-	8.91	-	0.26
872504	2128281	1-methyl-2-pyrrolidone	0.52	-	-	-	1.41
875741	2128763	D-(-)-alpha-phenylglycine	0.27	-	-	-	19.05
924425	2131032	N-(hydroxymethyl)acrylamide	0.22	-	61.12	-	2.13
926578	2131383	1,3-dichlorobut-2-ene	0.78	-	73.07	-	0.47
928687	2131797	6-methylheptan-2-one	1.09	-	-	-	4.27
929066	2131954	2-(2-aminoethoxy)ethanol	0.14	-	-	-	1.77
931884	2132455	cyclooctene	0.17	-	0.53	-	0.15
935922	2133092	2,3,6-trimethyl-p-benzoquinone	0.07	-	1.25	-	0.82
947046	2134248	dodecane-12-lactam	0.32	-	-	-	1.51
994058	2136114	2-methoxy-2-methylbutane	1.74	-	-	-	1.86
999815	2136664	chlormequat chloride	-	-	-	-	-
999973	2136685	1,1,1,3,3,3-hexamethyldisilazane	-	-	-	-	9.67
1070004	2139644	trioctylaluminium	-	-	-	-	-
1071836	2139974	glyphosate	0.14	-	-	-	19.86
1085989	2141187	dichlofluanid	0.08	-	-	-	7.52
1115204	2142222	3-hydroxy-2,2-dimethylpropyl 3-hydroxy-2,2-dimethylpropionate	1.09	-	-	-	2.57
1116707	2142400	tributylaluminium	-	-	-	-	-
1119400	2142772	dimethyl glutarate	5.86	-	-	-	19.92
1120361	2143069	tetradec-1-ene	0.26	-	8.91	-	0.22
1120496	2143121	didecylamine	0.10	-	-	-	0.35
1151140	2145663	2-(4-ethylbenzoyl)benzoic acid	1.92	-	-	-	10.25
1163195	2146049	bis(pentabromophenyl) ether	61.44	-	-	-	23.51
1191157	2147299	diisobutylaluminium hydride	-	-	-	-	-
1203174	2148685	1,1,2,3,3-pentamethylindan	1.22	-	-	-	0.54
1217089	2149343	beta,1,1,2,3,3-hexamethylindan-5-ethanol	0.47	-	-	-	0.57
1222055	2149469	1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno[5,6-c]pyran	0.27	-	-	-	0.22
1241947	2149872	2-ethylhexyl diphenyl phosphate	0.22	-	-	-	1.63
1302427	2151001	aluminium sodium dioxide	-	-	-	-	-
1303862	2151258	diboron trioxide	-	-	-	-	-
1305620	2151373	calcium dihydroxide	-	-	-	-	-
1305788	2151389	calcium oxide	-	-	-	-	-
1306190	2151462	cadmium oxide	-	-	-	-	-
1306383	2151504	cerium dioxide	-	-	-	-	-
1308141	2151588	dichromium trioxide hydrate	-	-	-	-	-
1309360	2151677	Pyrite (FeS2)	-	-	-	-	-
1309428	2151703	magnesium hydroxide	-	-	-	-	-
1309484	2151719	magnesium oxide	-	-	-	-	-
1310583	2151813	potassium hydroxide	-	-	-	-	-
1310652	2151834	lithium hydroxide	-	-	-	-	-
1310732	2151855	sodium hydroxide	-	-	-	-	-
1313139	2152026	manganese dioxide	-	-	-	-	-
1313275	2152047	molybdenum trioxide	-	-	-	-	-
1313822	2152115	disodium sulphide	-	-	-	-	-
1313991	2152157	nickel monoxide	-	-	-	-	-
1314132	2152225	zinc oxide	-	-	-	-	-
1314234	2152272	zirconium dioxide	-	-	-	-	-

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).

* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1]		AOP 1.83 Ozone [1]		MOOH [1]
		Half-life in	(cis)	(trans)	(cis)	(trans)	OH-radical
1314983	2152513	zinc sulphide	-	-	-	-	-
1317335	2152639	molybdenum disulphide	-	-	-	-	-
1317380	2152691	copper oxide	-	-	-	-	-
1317391	2152707	dicopper oxide	-	-	-	-	-
1317426	2152733	cobalt sulphide	-	-	-	-	-
1317700	2152801	Anatase (TiO2)	-	-	-	-	-
1317802	2152822	Rutile (TiO2)	-	-	-	-	-
1318236	2152843	Boehmite (Al(OH)O)	-	-	-	-	-
1333740	2156057	hydrogen	-	-	-	-	-
1333820	2156078	chromium trioxide	-	-	-	-	-
1338392	2156633	sorbitan laurate	0.17	-	-	-	1.12
1338416	2156649	sorbitan stearate	0.15	-	-	-	-
1338438	2156654	sorbitan oleate	0.09 *	0.08	0.82	0.53	-
1459934	2159519	dimethyl isophthalate	16.73	-	-	-	14.82
1461252	2159608	tetrabutyltin	-	-	-	-	-
1477550	2160325	m-phenylenebis(methylamine)	0.15	-	-	-	0.96
1490046	2160744	DL-menthol	0.44	-	-	-	0.76
1506021	2161334	1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-1-one	0.66	-	-	-	0.83
1552121	2162914	(Z,Z)-cycloocta-1,5-diene	0.09	-	0.27	-	0.09
1559348	2163221	3,6,9,12-tetraoxahexadecan-1-ol	0.17	-	-	-	0.41
1569024	2163745	1-ethoxypropan-2-ol	0.52	-	-	-	2.15
1570645	2163813	4-chloro-o-cresol	0.83 *	-	-	-	0.87
1634044	2166531	tert-butyl methyl ether	3.79	-	-	-	2.20
1653196	2167210	2,3-dichlorobuta-1,3-diene	1.98	-	645.78	-	0.33
1663394	2167687	tert-butyl acrylate	0.41	-	61.12	-	2.00
1675543	2168235	2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bisoxirane	0.15	-	-	-	0.24
1689992	2168853	2,6-dibromo-4-cyanophenyl octanoate	1.55	-	-	-	4.48
1698539	2169176	4,5-dichloro-2,3-dihydro-2-phenylpyridazin-3-one	0.54	-	459.86	-	2.41
1698608	2169202	chloridazon	0.22	-	65.76	-	0.78
1724396	2170312	cyclododecanol	0.42	-	-	-	0.71
1738256	2170904	3-dimethylaminopropiononitrile	0.16	-	-	-	0.98
1758732	2171578	aminoiminomethanesulphinic acid	0.13	-	-	-	140.73
1761713	2171688	4,4'-methylenebis(cyclohexylamine)	0.09	-	-	-	0.72
1762272	2171709	diethyldimethylplumbane	-	-	-	-	-
1762954	2171756	ammonium thiocyanate	-	-	-	-	-
1817476	2173266	p-nitrocumene	3.82	-	-	-	21.97
1836755	2174060	nitrofen	5.36	-	-	-	18.19
1843056	2174212	octabenzone	0.05 *	-	-	-	0.37
1854268	2174516	4,5-dihydroxy-1,3-bis(hydroxymethyl)imidazolidin-2-one	0.11	-	-	-	17.40
1912249	2176178	atrazine	0.07	-	-	-	2.48
1928434	2176733	2-ethylhexyl 2,4-dichlorophenoxyacetate	0.84	-	-	-	3.36
2082793	2182160	octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	0.25 *	-	-	-	-
2100427	2182679	1-chloro-2,5-dimethoxybenzene	0.68	-	-	-	0.75
2157199	2184676	1,4,5,6,7,7-hexachlorobicyclo[2.2.1]hept-5-ene-2,3-dimethanol	0.63	-	2988.74	-	4.52
2186927	2185774	p-(dimethoxymethyl)anisole	0.26	-	-	-	0.29
2243621	2188178	1,5-naphthylenediamine	0.04	-	-	-	0.03
2303175	2189627	tri-allate	0.33	-	3216.09	-	3.30
2310170	2189962	phosalone	0.06	-	-	-	25.75
2312358	2190061	propargite	0.09	-	3565.57	-	0.16
2402791	2192839	2,3,5,6-tetrachloropyridine	703.73	-	-	-	60.94
2403885	2192912	2,2,6,6-tetramethylpiperidin-4-ol	0.14	-	-	-	5.62
2409554	2193146	2-tert-butyl-p-cresol	0.20 *	-	-	-	0.18
2416946	2193303	2,3,6-trimethylphenol	0.08 *	-	-	-	0.12
2431507	2193979	2,3,4-trichlorobut-1-ene	0.99	-	65.76	-	1.65
2432997	2194176	11-aminoundecanoic acid	0.25	-	-	-	2.39
2439352	2194600	2-(dimethylamino)ethyl acrylate	0.11	-	61.12	-	0.64
2494895	2196697	2-[(p-aminophenyl)sulphonyl]ethyl hydrogensulphate	0.14	-	-	-	13.71
2517433	2197418	3-methoxybutan-1-ol	0.52	-	-	-	2.82
2524030	2197549	O,O-dimethyl phosphorochloridothioate	0.18	-	-	-	436.24
2524041	2197554	O,O-diethyl phosphorochloridothioate	0.12	-	-	-	101.51
2551624	2198542	sulphur hexafluoride	-	-	-	-	-
2634335	2201209	1,2-benzisothiazol-3(2H)-one	0.45	-	-	-	2.85
2809214	2205528	etidronic acid	29.24	-	-	-	1449.42
2835065	2206081	DL-alpha-phenylglycine	0.27	-	-	-	19.05

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).

* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1]		AOP 1.83 Ozone [1]		MOOH [1]
		Half-life in	(cis)	(trans)	(cis)	(trans)	OH-radical
2855132	2206668	3-aminomethyl-3,5,5-trimethylcyclohexylamine	0.12	-	-	-	0.72
2867472	2206888	2-dimethylaminoethyl methacrylate	0.09	-	9.40	-	0.43
3033770	2212210	2,3-epoxypropyltrimethylammonium chloride	-	-	-	-	-
3048644	2212598	5-vinylnorborn-2-ene	0.12	-	0.50	-	0.11
3081014	2213743	N-(1,4-dimethylpentyl)-N'-phenylbenzene-1,4-diamine	0.03	-	-	-	0.04
3120749	2214967	4-(methylthio)-m-cresol	0.18 *	-	-	-	0.73
3173726	2216414	1,5-naphthylene diisocyanate	0.72	-	-	-	-
3194556	2216959	1,2,5,6,9,10-hexabromocyclodecane	1.75	-	-	-	10.06
3268493	2218825	3-(methylthio)propionaldehyde	0.18 *	-	-	-	6.62
3282302	2219216	pivaloyl chloride	5.63	-	-	-	138.49
3302101	2219750	3,5,5-trimethylhexanoic acid	1.67	-	-	-	6.84
3319311	2220200	tris(2-ethylhexyl) benzene-1,2,4-tricarboxylate	0.33	-	-	-	-
3327228	2220483	(3-chloro-2-hydroxypropyl)trimethylammonium chloride	-	-	-	-	-
3452979	2223767	3,5,5-trimethylhexan-1-ol	1.04	-	-	-	1.82
3542367	2225832	dichlorodioctylstannane	-	-	-	-	-
3590849	2227337	tetraoctyltin	-	-	-	-	-
3622842	2228236	N-butylbenzenesulphonamide	0.14	-	-	-	3.67
3648202	2228849	diundecyl phthalate	0.38	-	-	-	-
3687465	2229816	decyl oleate	0.12 *	0.11	0.82	0.53	-
3845769	2233424	N-[3-(dimethylamino)propyl]acrylamide	0.09	-	61.12	-	0.45
3982910	2236226	thiophosphoryl trichloride	0.19	-	-	-	-
4035896	2237188	1,3,5-tris(6-isocyanatohexyl)biuret	0.16	-	-	-	-
4098719	2238616	3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate	1.21	-	-	-	3.09
4116103	2239075	2-chloro-N-methyl-3-oxobutyramide	0.83	-	-	-	7.48
4170303	2240300	crotonaldehyde	0.35	0.33	117.55	58.77	0.61
4435534	2246449	3-methoxybutyl acetate	0.58	-	-	-	2.91
4445072	2246847	octadecylbenzene	0.38	-	-	-	0.41
4454051	2246983	3,4-dihydro-2-methoxy-2H-pyran	0.12	-	9.40	-	0.13
4553622	2249235	2-methylglutaronitrile	8.85	-	-	-	104.88
4618182	2250277	lactulose	0.07	-	-	-	3.82
4685147	2251417	1,1'-dimethyl-4,4'-bipyridinium	-	-	-	-	-
4904614	2255338	cyclododeca-1,5,9-triene	0.06	-	0.18	-	0.06
4979322	2256258	N,N-dicyclohexylbenzothiazole-2-sulphenamide	0.06	-	-	-	0.25
5039781	2257335	[2-(methacryloyloxy)ethyl]trimethylammonium chloride	-	-	-	-	-
5064313	2257686	trisodium nitrilotriacetate	0.13	-	-	-	11.83
5102830	2258229	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]	0.16	-	-	-	-
5205936	2260023	N-[3-(dimethylamino)propyl]methacrylamide	0.08	-	9.40	-	0.37
5208935	2260065	3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta 1,4-dien-3-ol	0.04	-	0.31	-	0.06
5216251	2260091	alpha,alpha,alpha,4-tetrachlorotoluene	41.27	-	-	-	30.73
5234684	2260311	carboxin	0.05	-	9.40	-	0.12
5321313	2261818	(2-chloro-2-oxo-1-phenylethyl)ammonium chloride	-	-	-	-	-
5329146	2262188	sulphamidic acid	-	-	-	-	-
5333426	2262429	2-octyldodecan-1-ol	0.36	-	-	-	0.61
5392405	2263946	citral	0.08 *	-	0.24	-	0.10
5435643	2266030	3,5,5-trimethylhexanal	0.31	-	-	-	8.62
5567157	2269398	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-chloro-2,5-dimethoxyphenyl)-3-oxobutyramide]	0.15	-	-	-	-
6104309	2280558	N,N''-(isobutylidene)diurea	0.12	-	-	-	5.81
6284408	2285069	meglumine	0.09	-	-	-	1.56
6358641	2287820	4-chloro-2,5-dimethoxyaniline	0.05	-	-	-	0.21
6358856	2287878	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-N-phenylbutyramide]	0.20	-	-	-	-
6386385	2289854	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	0.54 *	-	-	-	0.62
6419198	2291465	nitrilotrimethylenetris(phosphonic acid)	0.13	-	-	-	544.09
6846500	2299349	1-isopropyl-2,2-dimethyltrimethylene diisobutyrate	1.07	-	-	-	2.12
6864375	2299621	2,2'-dimethyl-4,4'-methylenebis(cyclohexylamine)	0.09	-	-	-	0.51
6923224	2300427	monocrotophos	0.11	-	9.40	-	0.66
6940530	2300867	1-chloro-2,5-dimethoxy-4-nitrobenzene	3.09	-	-	-	16.38
7397628	2309917	butyl glycollate	2.48	-	-	-	7.17
7434404	2310812	ethane-1,2-diylbis(oxyethane-2,1-diyl) bisheptanoate	0.26	-	-	-	0.98

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).
* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1]		AOP 1.83 Ozone [1]		MOOH [1]
		Half-life in	(cis)	(trans)	(cis)	(trans)	OH-radical
7439896	2310964	iron	-	-	-	-	-
7439987	2311072	molybdenum	-	-	-	-	-
7440020	2311114	nickel	-	-	-	-	-
7440031	2311135	niobium	-	-	-	-	-
7440224	2311313	silver	-	-	-	-	-
7440337	2311439	tungsten	-	-	-	-	-
7440473	2311575	chromium	-	-	-	-	-
7440484	2311580	cobalt	-	-	-	-	-
7440508	2311596	copper	-	-	-	-	-
7440611	2311706	uranium	-	-	-	-	-
7440622	2311711	vanadium	-	-	-	-	-
7446095	2311952	sulphur dioxide	-	-	-	-	-
7446119	2311973	sulphur trioxide	-	-	-	-	-
7446700	2312081	aluminium chloride	-	-	-	-	-
7447407	2312118	potassium chloride	-	-	-	-	-
7447418	2312123	lithium chloride	-	-	-	-	-
7550450	2314419	titanium tetrachloride	-	-	-	-	-
7631869	2315454	silicon dioxide, chemically prepared	-	-	-	-	-
7637072	2315695	boron trifluoride	-	-	-	-	-
7646788	2315889	tin tetrachloride	-	-	-	-	-
7646857	2315920	zinc chloride	-	-	-	-	-
7647010	2315957	hydrogen chloride	-	-	-	-	-
7647145	2315983	sodium chloride	-	-	-	-	-
7647156	2315999	sodium bromide	-	-	-	-	-
7659861	2316264	2-ethylhexyl mercaptoacetate	0.26	-	-	-	2.68
7664393	2316348	hydrogen fluoride	-	-	-	-	-
7664417	2316353	ammonia, anhydrous	-	-	-	-	-
7664939	2316395	sulphuric acid	-	-	-	-	-
7681494	2316678	sodium fluoride	-	-	-	-	-
7697372	2317142	nitric acid	-	-	-	-	-
7699436	2317179	zirconium dichloride oxide	-	-	-	-	-
7705080	2317294	iron trichloride	-	-	-	-	-
7718549	2317430	nickel dichloride	-	-	-	-	-
7719097	2317488	thionyl dichloride	-	-	-	-	-
7719122	2317493	phosphorus trichloride	-	-	-	-	-
7722841	2317650	hydrogen peroxide	-	-	-	-	-
7726956	2317781	bromine	-	-	-	-	-
7758023	2318303	potassium bromide	-	-	-	-	-
7758943	2318434	iron dichloride	-	-	-	-	-
7778394	2319019	arsenic acid	-	-	-	-	-
7782447	2319569	oxygen	-	-	-	-	-
7782505	2319595	chlorine	-	-	-	-	-
7783064	2319773	hydrogen sulphide	-	-	-	-	-
7784181	2320511	aluminium fluoride	-	-	-	-	-
7786303	2320946	magnesium chloride	-	-	-	-	-
7789233	2321515	potassium fluoride	-	-	-	-	-
7789415	2321646	calcium bromide	-	-	-	-	-
7789755	2321887	calcium fluoride	-	-	-	-	-
7790945	2322346	chlorosulphuric acid	-	-	-	-	-
7791255	2322456	sulphuryl dichloride	-	-	-	-	-
8000417	2322681	Terpineol	0.11 *	-	0.25	-	0.10
10024972	2330320	dinitrogen oxide	-	-	-	-	-
10025679	2330362	disulphur dichloride	-	-	-	-	-
10025782	2330425	trichlorosilane	-	-	-	-	-
10025873	2330467	phosphoryl trichloride	>99999	-	-	-	-
10026047	2330540	silicon tetrachloride	-	-	-	-	-
10026138	2330603	phosphorus pentachloride	-	-	-	-	-
10035106	2331130	hydrogen bromide	-	-	-	-	-
10043353	2331392	boric acid	-	-	-	-	-
10043524	2331408	calcium chloride	-	-	-	-	-
10049146	2331701	uranium tetrafluoride	-	-	-	-	-
10101527	2332527	zirconium orthosilicate	-	-	-	-	-
10265926	2336060	methamidophos	0.39	-	-	-	21.98
10361372	2337881	barium chloride	-	-	-	-	-
10420334	2338974	dimethyl acetylsuccinate	19.76	-	-	-	40.35
10543574	2341238	N,N'-ethylenebis[N-acetylacetamide]	0.32	-	-	-	17.32
10544726	2341264	dinitrogen tetraoxide	-	-	-	-	-
10545990	2341290	sulphur dichloride	-	-	-	-	-
10584982	2341861	2-ethylhexyl 4,4-dibutyl-10-ethyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate	-	-	-	-	-

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).

* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1]		AOP 1.83 Ozone [1]		MOOH [1]
		Half-life in	(cis)	(trans)	(cis)	(trans)	OH-radical
10605217	2342320	carbendazim	0.05	-	-	-	0.74
12018018	2346304	chromium dioxide	-	-	-	-	-
12071839	2351340	propineb	-	-	-	-	-
13150000	2360910	sodium 2-[2-[2-(dodecyloxy)ethoxy]ethoxy]ethyl sulphate	0.14	-	-	-	0.46
13463677	2366755	titanium dioxide	-	-	-	-	-
13547701	2369206	1-chloro-3,3-dimethylbutan-2-one	4.99	-	-	-	20.79
13674845	2371587	tris(2-chloro-1-methylethyl) phosphate	0.17	-	-	-	7.71
13674878	2371592	tris[2-chloro-1-(chloromethyl)ethyl] phosphate	0.28	-	-	-	8.15
13684634	2371990	phenmedipham	0.06	-	-	-	0.24
13705050	2372397	2,4-dichloro-6-(methylthio)-1,3,5-triazine	3.24	-	-	-	42.33
13825746	2375230	titanium oxide sulphate	-	-	-	-	-
13940948	2377217	4-chloro-1-(dichloromethyl)benzene	8.98	-	-	-	20.83
14324551	2382709	zinc bis(diethyldithiocarbamate)	-	-	-	-	13.84
14475639	2384727	zirconium tetrahydroxide	-	-	-	-	-
14542235	2385757	Fluorite (CaF2)	-	-	-	-	-
14808607	2388784	Quartz (SiO2)	-	-	-	-	-
14861177	2389327	4-(2,4-dichlorophenoxy)aniline	0.10	-	-	-	0.35
14940682	2390196	zircon	-	-	-	-	-
15206550	2392633	methyl benzoylformate	6.25	-	-	-	21.04
15214898	2392680	2-acrylamido-2-methylpropanesulphonic acid	0.28	-	61.12	-	1.60
15545489	2395922	chlorotoluron	0.17	-	-	-	0.24
15571581	2396224	2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate	-	-	-	-	-
15625895	2397013	2-ethyl-2-[[(1-oxoallyl)oxy]methyl]-1,3-propanediyl diacrylate	0.14	-	20.37	-	0.70
15687271	2397846	ibuprofen	0.90	-	-	-	3.29
15827608	2399314	[[(phosphonomethyl)imino]bis[ethane-2,1-diylnitrilobis(methylene)]]tetrakisphosphonic acid	0.04	-	-	-	4.71
15894709	2400324	N,N'''-1,6-hexanediylbis[N'-cyanoguanidine]	0.04	-	-	-	1.68
16219753	2403477	5-ethylidene-8,9,10-trinorborn-2-ene	0.07 *	-	0.17	-	0.07
16721805	2407780	sodium hydrogensulphide	-	-	-	-	-
16883833	2409201	benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate	0.65	-	-	-	-
16954691	2410259	N-methylbenzothiazol-2-amine	0.05	-	-	-	0.57
17194002	2412345	barium hydroxide	-	-	-	-	-
17321470	2413422	O,O-dimethyl thiophosphoramidate	0.29	-	-	-	150.91
17639939	2416245	methyl 2-chloropropionate	47.31	-	-	-	39.79
17700093	2417055	4-nitro-1,2,3-trichlorobenzene	298.79	-	-	-	47.41
17796826	2417741	N-(cyclohexylthio)phthalimide	0.22	-	-	-	1.33
17976431	2418944	cyclo-di-mu-oxo(mu-phthalato)trilead	-	-	-	-	-
18297637	2421779	1,3-bis(trimethylsilyl)urea	-	-	-	-	7.38
18467771	2423488	diprogulic acid	0.15	-	-	-	4.11
18479497	2423582	3,7-dimethyloct-1-en-3-ol	0.32	-	61.12	-	0.39
18691979	2425050	methabenzthiazuron	0.33	-	-	-	1.36
19438609	2430720	hexahydro-4-methylphthalic anhydride	1.79	-	-	-	34.61
20030302	2434730	2,5,6-trimethylcyclohex-2-en-1-one	0.11	-	1.45	-	0.28
20120336	2435289	dimethyl [3-[(hydroxymethyl)amino]-3-oxopropyl]phosphonate	0.31	-	-	-	32.09
20292084	2436979	2-ethylhexyl laurate	0.46	-	-	-	0.80
20306756	2437239	N-methyl-3-oxobutyramide	0.82	-	-	-	2.60
20344494	2437464	iron hydroxide oxide	-	-	-	-	-
21109955	2442144	barium sulphide	-	-	-	-	-
21645512	2444927	aluminium hydroxide	-	-	-	-	-
22224926	2448481	fenamiphos	0.10	-	-	-	1.12
22839470	2452613	aspartame	0.18	-	-	-	8.93
23783428	2458835	3,6,9,12-tetraoxotridecanol	0.21	-	-	-	0.49
24310405	2461518	3-(hydroxymethyl)-1,2,3-benzotriazin-4(3H)-one	0.44	-	-	-	22.39
24549062	2463096	6-ethyl-2-toluidine	0.05	-	-	-	0.08
24602866	2463473	tridemorph	0.08	-	-	-	0.33
24800440	2464660	[(methylethylene)bis(oxy)]dipropanol	0.23	-	-	-	0.82
25013154	2465622	vinyltoluene	0.20	-	0.78	-	0.17
25103097	2466139	isooctyl mercaptoacetate	0.26	-	-	-	3.10
25103520	2466170	isooctanoic acid	2.18	-	-	-	11.23
25103586	2466191	tert-dodecanethiol	0.21	-	-	-	1.13
25154523	2466720	nonylphenol	0.20 *	-	-	-	0.29
25167708	2466909	2,4,4-trimethylpentene	0.20	-	8.91	-	0.18
25168052	2466982	chlorotoluene	4.41	-	-	-	6.09
25265718	2467703	oxydipropanol	0.35	-	-	-	1.59

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).

* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

CAS-nr.	EINECS-nr.	NAME	AOP 1.83 OH radical [1]		AOP 1.83 Ozone [1]		MOOH [1]
		Half-life in	(cis)	(trans)	(cis)	(trans)	OH-radical
25265774	2467719	isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol	0.69	-	-	-	6.61
25311711	2468141	isofenphos	0.07	-	-	-	10.75
25339177	2468691	isodecyl alcohol	0.72	-	-	-	1.60
25377735	2469171	dodecenylsuccinic anhydride	0.70	-	-	-	1.87
25550985	2470983	diisodecyl phenyl phosphite	0.14	-	-	-	-
26140603	2474773	terphenyl	1.11	-	-	-	0.87
26225796	2475253	ethofumesate	0.17	-	-	-	0.47
26272764	2475777	N-[2-(2-heptadecyl-4,5-dihydro-1H-imidazol-1-yl)ethyl]stearamide	0.07	-	-	-	-
26401354	2476608	diisotridecyl adipate	0.29	-	-	-	-
26489010	2477376	()-3,7-dimethyloct-6-en-1-ol	0.11 *	-	0.25	-	0.11
26544230	2477774	isodecyl diphenyl phosphite	0.24	-	-	-	0.71
26760645	2479750	2-methylbutene	0.19 *	0.16	0.82	0.53	0.16
26761400	2479771	di-"isodecyl" phthalate	0.42	-	-	-	-
26761455	2479792	2,3-epoxypropyl neodecanoate	1.85	-	-	-	4.23
26896184	2480923	isononanoic acid	1.12	-	-	-	6.71
27178161	2482999	diisodecyl adipate	0.38	-	-	-	-
27247967	2483636	2-ethylhexyl nitrate	1.66	-	-	-	7.11
27375526	2484336	N-[4-[(2-hydroxyethyl)sulphonyl]phenyl]acetamide	0.54	-	-	-	11.38
27458920	2484692	isotridecan-1-ol	0.56	-	-	-	1.08
27458942	2484713	isononyl alcohol	0.80	-	-	-	1.87
27554263	2485235	diisooctyl phthalate	0.53	-	-	-	0.98
28479223	2490507	3-chloro-p-tolyl isocyanate	5.79	-	-	-	8.18
28553120	2490795	di-"isononyl" phthalate	0.47	-	-	-	-
29171208	2494826	3,7-dimethyloct-6-en-1-yn-3-ol	0.11 *	-	0.25	-	0.10
29387868	2495987	butoxypropan-1-ol	0.39	-	-	-	1.17
29797408	2498548	dichloromethylbenzene	4.51	-	-	-	14.95
29911282	2499515	1-(2-butoxy-1-methylethoxy)propan-2-ol	0.22	-	-	-	0.75
30399849	2501780	isooctadecanoic acid	0.48	-	-	-	0.87
31570044	2507096	tris(2,4-ditert-butylphenyl) phosphite	0.42	-	-	-	-
32210234	2509549	4-tert-butylcyclohexyl acetate	0.73	-	-	-	0.92
32588764	2511186	N,N'-ethylenebis(3,4,5,6-tetrabromophthalimide)	0.33	-	-	-	20.57
33703081	2516467	diisononyl adipate	0.42	-	-	-	-
34123596	2518354	3-(4-isopropylphenyl)-1,1-dimethylurea	0.13	-	-	-	0.14
34590948	2521042	(2-methoxymethylethoxy)propanol	0.29	-	-	-	1.12
34893920	2522769	1,3-dichloro-5-isocyanatobenzene	16.97	-	-	-	23.86
36653824	2531490	hexadecan-1-ol	0.46	-	-	-	0.74
36734197	2531789	3-(3,5-dichlorophenyl)-2,4-dioxo-N-isopropylimidazolidine-1-carboxamide	0.23	-	-	-	15.69
37971361	2537335	2-phosphonobutane-1,2,4-tricarboxylic acid	2.48	-	-	-	261.09
38051104	2537602	2,2-bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phosphate)	0.12	-	-	-	6.78
38861788	2541598	1-[4-(2-methylpropyl)phenyl]ethan-1-one	1.40	-	-	-	6.58
40372723	2548965	4,4,15,15-tetraethoxy-3,16-dioxa-8,9,10,11-tetrathia-4,15-disilaoctadecane	-	-	-	-	-
40843730	2551061	4-(2,4-dichlorophenoxy)phenol	0.40 *	-	-	-	1.67
42576023	2558947	methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	8.33	-	-	-	14.08
44992010	2561766	[2-(acryloyloxy)ethyl]trimethylammonium chloride	-	-	-	-	-
46948725	2562890	6-[methyl(phenylsulphonyl)amino]hexanoic acid	0.14	-	-	-	3.59
50849473	2567988	5-nonylsalicylaldehyde oxime	0.16 *	-	-	-	0.34
52722868	2581321	4-hydroxy-2,2,6,6-tetramethylpiperidine-1-ethanol	0.12	-	-	-	1.29
56107041	2599962	3-(p-tert-butylphenyl)-2-methylpropanol	0.73	-	-	-	0.75
56966520	2604804	5-chloro-2-(2,4-dichlorophenoxy)aniline	0.13	-	-	-	0.41
57219644	2606335	[.mu.-[carbonato(2-)-O:O']]dihydroxydioxodizirconium	-	-	-	-	-
57966957	2610430	2-cyano-N-[(ethylamino)carbonyl]-2-(methoxyimino)acetamide	0.39	-	-	-	17.33
61260557	2626791	N,N'-bis(2,2,6,6-tetramethylpiperidin-4-yl)hexane-1,6-diamine	0.03	-	-	-	-
63589253	2643471	4-diazo-3,4-dihydro-7-nitro-3-oxonaphthalene-1-sulphonic acid	4.05	-	-	-	31.10
67747095	2669945	N-propyl-N-[2-(2,4,6-trichlorophenoxy)ethyl]-1H-imidazole-1-carboxamide	0.14	-	-	-	0.18
67846688	2673820	dimethylbis[2-[(1-oxooctadecyl)oxy]ethyl]ammonium chloride	-	-	-	-	-
68134269	2687388	2-(2-heptadecyl-4,5-dihydro-1H-imidazol-1-yl)ethyl stearate	0.09	-	-	-	-
68298964	2695870	2-[(2-hydroxyethyl)amino]ethyl dihydrogen orthoborate	-	-	-	-	1.06

[1] Half-lifes in days, calculated with [OH] = 1.5 x 10^6 molecules/cm^3 12-hour day), [O_3] = 7 x 10^{11} molecules/cm^3 (24 hour day).
* An asterisk indicates probable importance of (night-time) reaction with NO_3-radicals.

APPENDIX 3 - ABIOTIC DEGRADATION

Table of 153 compounds from Appendix I for which one or more selected QSARs for abiotic degradation in the aquatic environment could be applied. The processes and chemical classes for which appropriate QSARs were selected are numbered according to table 1 in the report, as follows:

- 6. Hydrolysis of halogenated alkanes, esters, carbamates and epoxides estimated by the HYDROWIN program v. 1.00 from SRC.
- 7. Hydrolysis of brominated alkanes
- 8. Hydrolysis of esters and carbamates
- 9. Hydrolysis of *para*-substituted benzonitriles
- 10 Oxidation of substituted phenols by singlet oxygen
- 11. Oxidation of substituted phenols by manganese oxides
- 12. Oxidation of *para*-substituted anilines by manganese oxides
- 13. Reductive dehalogenation of halogenated aliphatic compounds
- 14. Reductive dehalogenation of halogenated aromatic compounds
- 15. Reduction of the nitro-group in nitro-aromatic compounds.

CAS-nr.	Name	HYDROWIN (in days)	Hydrolysis models half-life in days			Oxidation models (days)	log(k)	log(k)	Reduction models half-life in days			log(k)
		6	7	8	9	10	11	12	13 (PLS)	13 (Eact)	14	15
50782	O-acetylsalicylic acid	61.43	-	1.84	-	-	-	-	-	-	-	-
56235	carbon tetrachloride	-	-	-	-	-	-	-	0.82	0.80	-	-
56382	parathion	-	-	-	-	-	-	-	-	-	-	7.18
58899	gamma-HCH or gamma-BHC	1.30E+13	-	-	-	-	-	-			-	-
59507	chlorocresol	-	-	-	-	25.84	2.03	-	-	-	196.00	-
62237	4-nitrobenzoic acid	-	-	-	-	-	-	-	-	-	-	1.82
62533	aniline	-	-	-	-	-	-	1.95	-	-	-	-
67663	chloroform	1.24E+06	-	-	-	-	-	-	15.99	4.51	-	-
69727	salicylic acid	-	-	-	-	83.61	0.74	-	-	-	-	-
71556	1,1,1-trichloroethane	1.08E+10	-	-	-	-	-	-	4.37	3.24	-	-
74839	bromomethane	4.47E+05	19.62	-	-	-	-	-	174.11	5.54	-	-
74873	chloromethane	8.20E+06	-	-	-	-	-	-	1098.56	339.02	-	-
75003	chloroethane	6.86E+12	-	-	-	-	-	-	437.35	199.72	-	-
75092	dichloromethane	1.57E+10	-	-	-	-	-	-	185.71	33.78	-	-
75218	ethylene oxide	4669.69	-	-	-	-	-	-	-	-	-	-
75343	1,1-dichloroethane	8.76E+10	-	-	-	-	-	-	43.73	22.23	-	-
75456	chlorodifluoromethane	88.95	-	-	-	-	-	-	34.74	26.24	-	-
75569	methyloxirane	1042.02	-	-	-	-	-	-	-	-	-	-
75638	bromotrifluoromethane	-	0.00	-	-	-	-	-	0.87	0.25	-	-
75683	1-chloro-1,1-difluoroethane	3.43E+10	-	-	-	-	-	-	-	19.74	-	-
75694	trichlorofluoromethane	-	-	-	-	-	-	-	2.86	1.75	-	-
75718	dichlorodifluoromethane	-	-	-	-	-	-	-	2.76	4.69	-	-
76131	1,1,2-trichlorotrifluoroethane	-	-	-	-	-	-	-	0.04	1.98	-	-
76142	cryofluorane	-	-	-	-	-	-	-	0.01	12.69	-	-
76153	chloropentafluoroethane	-	-	-	-	-	-	-	-	16.33	-	-
78875	1,2-dichloropropane	2.11E+08	-	-	-	-	-	-	-	184.55	-	-
79005	1,1,2-trichloroethane	4276.40	-	-	-	-	-	-	6.93	5.49	-	-
79209	methyl acetate	627.25	-	-	-	-	-	-	-	-	-	-
79210	peracetic acid	0.35	-	-	-	-	-	-	-	-	-	-
79345	1,1,2,2-tetrachloroethane	54.61	-	-	-	-	-	-	2.76	20.38	-	-
79947	2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol	-	-	-	-	2.71	1.25	-	-	-		-
80626	methyl methacrylate	23574.89	-	-	-	-	-	-	-	-	-	-
84617	dicyclohexyl phthalate	4260.51	-	-	-	-	-	-	-	-	-	-
84662	diethyl phthalate	1062.45	-	-	-	-	-	-	-	-	-	-
84695	diisobutyl phthalate	1948.64	-	-	-	-	-	-	-	-	-	-
84742	dibutyl phthalate	1251.96	-	-	-	-	-	-	-	-	-	-
85687	benzyl butyl phthalate	506.15	-	-	-	-	-	-	-	-	-	-
87616	1,2,3-trichlorobenzene	-	-	-	-	-	-	-	-	-	21.09	-
88062	2,4,6-trichlorophenol	-	-	-	-	3.49	0.96	-	-	-	22.65	-
88722	2-nitrotoluene	-	-	-	-	-	-	-	-	-	-	-1.26
88733	1-chloro-2-nitrobenzene	-	-	-	-	-	-	-	-	-	-	-1.11
88744	2-nitroaniline	-	-	-	-	-	-	-	-	-	-	-2.13
88755	2-nitrophenol	-	-	-	-	-	-	-	-	-	-	-0.62
89612	1,4-dichloro-2-nitrobenzene	-	-	-	-	-	-	-	-	-	-	-0.50
89838	thymol	-	-	-	-	17.07	2.61	-	-	-	-	-
89872	4-nitro-m-xylene	-	-	-	-	-	-	-	-	-	-	-0.99
89985	2-chlorobenzaldehyde	-	-	-	-	-	-	-	-	-	4292.03	-
90051	guaiacol	-	-	-	-	10.05	3.17	-	-	-	-	-

Environmental half-lifes in days are given for those models for which this has significance. Otherwise the pseudo-first order reaction rate constant, log k, is given. See Section 2 for details.

CAS-nr.	Name	HYDROWIN (in days)	Hydrolysis models half-life in days			Oxidation models (days)	log(k)	log(k)	Reduction models half-life in days			log(k)
		6	7	8	9	10	11	12	13 (PLS)	13 (Eact)	14	15
90437	2-phenylphenol	-	-	-	-	11.28	3.05	-	-	-	-	-
90722	2,4,6-tris(dimethylaminomethyl)phenol	-	-	-	-	12.37	2.60	-	-	-	-	-
91236	2-nitroanisole	-	-	-	-	-	-	-	-	-	-	-1.01
91689	3-diethylaminophenol	-	-	-	-	28.99	1.95	-	-	-	-	-
94360	dibenzoyl peroxide	0.00	-	-	-	-	-	-	-	-	-	-
94600	dimethyl cyclohexane-1,4-dicarboxylate	3310.99	-	-	-	-	-	-	-	-	-	-
95487	o-cresol	-	-	-	-	21.49	2.32	-	-	-	-	-
95498	2-chlorotoluene	-	-	-	-	-	-	-	-	-	1883.92	-
95501	1,2-dichlorobenzene	-	-	-	-	-	-	-	-	-	114.56	-
95512	2-chloroaniline	-	-	-	-	-	-	-	-	-	413.87	-
95556	2-aminophenol	-	-	-	-	4.92	3.33	-	-	-	-	-
95578	2-chlorophenol	-	-	-	-	24.67	1.38	-	-	-	88.44	-
95749	3-chloro-p-toluidine	-	-	-	-	-	-	-	-	-	836.11	-
95761	3,4-dichloroaniline	-	-	-	-	-	-	-	-	-	19.31	-
96184	1,2,3-trichloropropane	8.54E+07	-	-	-	-	-	-	1.32	51.75	-	-
96333	methyl acrylate	3105.90	-	-	-	-	-	-	-	-	-	-
96344	methyl chloroacetate	8.56	-	2.88	-	-	-	-	-	-	-	-
96764	2,4-di-tert-butylphenol	-	-	-	-	13.25	2.91	-	-	-	-	-
97007	1-chloro-2,4-dinitrobenzene	-	-	-	-	-	-	-	-	-	-	2.61
97029	2,4-dinitroaniline	-	-	-	-	-	-	-	-	-	-	-1.01
97723	isobutyric anhydride	0.02	-	-	-	-	-	-	-	-	-	-
97869	isobutyl methacrylate	45790.72	-	-	-	-	-	-	-	-	-	-
97881	butyl methacrylate	29418.90	-	-	-	-	-	-	-	-	-	-
98464	alpha,alpha,alpha-trifluoro-3-nitrotoluene	-	-	-	-	-	-	-	-	-	-	-0.04
98544	4-tert-butylphenol	-	-	-	-	17.88	2.53	-	-	-	-	-
98953	nitrobenzene	-	-	-	-	-	-	-	-	-	-	-1.08
99081	3-nitrotoluene	-	-	-	-	-	-	-	-	-	-	-1.08
99547	1,2-dichloro-4-nitrobenzene	-	-	-	-	-	-	-	-	-	-	0.89
99650	1,3-dinitrobenzene	-	-	-	-	-	-	-	-	-	-	1.10
99752	methyl p-toluate	3950.04	-	3092.69	-	-	-	-	-	-	-	-
99887	4-isopropylaniline	-	-	-	-	-	-	0.22	-	-	-	-
99990	4-nitrotoluene	-	-	-	-	-	-	-	-	-	-	-0.80
100005	1-chloro-4-nitrobenzene	-	-	-	-	-	-	-	-	-	-	0.14
100016	4-nitroaniline	-	-	-	-	-	-	-1.97	-	-	-	-1.75
100027	4-nitrophenol	-	-	-	-	64.90	-1.19	-	-	-	-	-1.75
100298	4-nitrophenetole	-	-	-	-	-	-	-	-	-	-	-0.92
100470	benzonitrile	-	-	-	339.50	-	-	-	-	-	-	-
101542	N-(4-aminophenyl)aniline	-	-	-	-	-	-	4.52	-	-	-	-
101779	4,4'-methylenedianiline	-	-	-	-	-	-	3.10	-	-	-	-
102761	triacetin	129.98	-	-	-	-	-	-	-	-	-	-
103117	2-ethylhexyl acrylate	6031.98	-	-	-	-	-	-	-	-	-	-
103231	bis(2-ethylhexyl) adipate	1174.26	-	-	-	-	-	-	-	-	-	-
104881	4-chlorobenzaldehyde	-	-	-	-	-	-	-	-	-	3102.15	-
105384	vinyl propionate	167.73	-	66.53	-	-	-	-	-	-	-	-
105395	ethyl chloroacetate	9.06	-	4.55	-	-	-	-	-	-	-	-
105453	methyl acetoacetate	140.65	-	63.24	-	-	-	-	-	-	-	-
105486	isopropyl chloroacetate	12.06	-	-	-	-	-	-	-	-	-	-
105533	diethyl malonate	16.20	-	-	-	-	-	-	-	-	-	-

Environmental half-lifes in days are given for those models for which this has significance. Otherwise the pseudo-first order reaction rate constant, log k, is given. See Section 2 for details.

CAS-nr.	Name	HYDROWIN (in days)	Hydrolysis models half-life in days			Oxidation models (days)	log(k)	log(k)	Reduction models half-life in days			log(k)
		6	7	8	9	10	11	12	13 (PLS)	13 (Eact)	14	15
105760	dibutyl maleate	122.13	-	-	-	-	-	-	-	-	-	-
105997	dibutyl adipate	754.71	-	-	-	-	-	-	-	-	-	-
106434	4-chlorotoluene	-	-	-	-	-	-	-	-	-	1299.16	-
106445	p-cresol	-	-	-	-	17.47	2.57	-	-	-	-	-
106467	1,4-dichlorobenzene	-	-	-	-	-	-	-	-	-	486.00	-
106489	4-chlorophenol	-	-	-	-	30.36	1.80	-	-	-	279.17	-
106490	p-toluidine	-	-	-	-	-	-	2.83	-	-	-	-
106503	p-phenylenediamine	-	-	-	-	-	-	5.15	-	-	-	-
106650	dimethyl succinate	848.59	-	524.38	-	-	-	-	-	-	-	-
106887	1,2-epoxybutane	1113.31	-	-	-	-	-	-	-	-	-	-
106898	1-chloro-2,3-epoxypropane	1.27E+05	-	-	-	-	-	-	-	-	-	-
106934	1,2-dibromoethane	26459.55	0.16	-	-	-	-	-	1.97	2.20	-	-
107062	1,2-dichloroethane	1.71E+08	-	-	-	-	-	-	34.82	123.36	-	-
107313	methyl formate	5.11	-	4.02	-	-	-	-	-	-	-	-
108054	vinyl acetate	141.59	-	0.37	-	-	-	-	-	-	-	-
108214	isopropyl acetate	883.34	-	913.56	-	-	-	-	-	-	-	-
108225	isopropenyl acetate	301.37	-	42.74	-	-	-	-	-	-	-	-
108247	acetic anhydride	0.03	-	0.20	-	-	-	-	-	-	-	-
108394	m-cresol	-	-	-	-	27.06	2.06	-	-	-	-	-
108463	resorcinol	-	-	-	-	30.36	1.80	-	-	-	-	-
108598	dimethyl malonate	21.79	-	-	-	-	-	-	-	-	-	-
108656	2-methoxy-1-methylethyl acetate	883.34	-	-	-	-	-	-	-	-	-	-
108689	3,5-xylenol	-	-	-	-	21.99	2.29	-	-	-	-	-
108907	chlorobenzene	-	-	-	-	-	-	-	-	-	1894.36	-
108952	phenol	-	-	-	-	32.53	1.83	-	-	-	-	-
109604	propyl acetate	782.69	-	-	-	-	-	-	-	-	-	-
109693	1-chlorobutane	2.81E+14	-	-	-	-	-	-	27.59	221.31	-	-
109706	1-bromo-3-chloropropane	2.37E+08	-	-	-	-	-	-	-	-	-	-
109944	ethyl formate	5.41	-	6.34	-	-	-	-	-	-	-	-
110190	isobutyl acetate	1217.93	-	694.45	-	-	-	-	-	-	-	-
110270	isopropyl myristate	3747.10	-	-	-	-	-	-	-	-	-	-
110338	dihexyl adipate	754.71	-	-	-	-	-	-	-	-	-	-
110429	methyl decanoate	2659.99	-	-	-	-	-	-	-	-	-	-
111115	methyl octanoate	1209.31	-	1576.15	-	-	-	-	-	-	-	-
111159	2-ethoxyethyl acetate	304.81	-	111.60	-	-	-	-	-	-	-	-
111820	methyl laurate	2659.99	-	-	-	-	-	-	-	-	-	-
112072	2-butoxyethyl acetate	304.81	-	-	-	-	-	-	-	-	-	-
112629	methyl oleate	742.83	-	-	-	-	-	-	-	-	-	-
114261	propoxur	17.14	-	-	-	-	-	-	-	-	-	-
117817	bis(2-ethylhexyl) phthalate	1948.64	-	-	-	-	-	-	-	-	-	-
118581	benzyl salicylate	634.69	-	0.23	-	-	-	-	-	-	-	-
118741	hexachlorobenzene	-	-	-	-	-	-	-	-	-	1.41	-
118967	2,4,6-trinitrotoluene	-	-	-	-	-	-	-	-	-	-	3.19
119368	methyl salicylate	2006.64	-	10128.00	-	67.96	0.97	-	-	-	-	-
119471	6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol	-	-	-	-	14.53	2.81	-	-	-	-	-
120514	benzyl benzoate	634.69	-	488.34	-	-	-	-	-	-	-	-
120616	dimethyl terephthalate	264.33	-	72.17	-	-	-	-	-	-	-	-
120809	pyrocatechol	-	-	-	-	12.95	2.84	-	-	-	-	-

Environmental half-lifes in days are given for those models for which this has significance. Otherwise the pseudo-first order reaction rate constant, log k, is given. See Section 2 for details.

CAS-nr.	Name	HYDROWIN (in days)	Hydrolysis models half-life in days			Oxidation models (days)	log(k)	log(k)	Reduction models half-life in days			log(k)
		6	7	8	9	10	11	12	13 (PLS)	13 (Eact)	14	15
120821	1,2,4-trichlorobenzene	-	-	-	-	-	-	-	-	-	64.48	-
120832	2,4-dichlorophenol	-	-	-	-	12.37	1.34	-	-	-	51.73	-
121039	4-nitrotoluene-2-sulphonic acid	-	-	-	-	-	-	-	-	-	-	0.30
121142	2,4-dinitrotoluene	-	-	-	-	-	-	-	-	-	-	-1.05
121573	sulphanilic acid	-	-	-	-	-	-	-2.37	-	-	-	-
121733	1-chloro-3-nitrobenzene	-	-	-	-	-	-	-	-	-	-	-0.36
121868	2-chloro-4-nitrotoluene	-	-	-	-	-	-	-	-	-	-	-0.10
121879	2-chloro-4-nitroaniline	-	-	-	-	-	-	-	-	-	-	-1.50
123308	4-aminophenol	-	-	-	-	3.33	4.50	3.28	-	-	-	-
123319	hydroquinone	-	-	-	-	10.53	3.06	-	-	-	-	-
123864	n-butyl acetate	782.69	-	694.45	-	-	-	-	-	-	-	-
124107	methyl myristate	2659.99	-	-	-	-	-	-	-	-	-	-
124174	2-(2-butoxyethoxy)ethyl acetate	304.81	-	-	-	-	-	-	-	-	-	-
125122	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acetate	840.23	-	-	-	-	-	-	-	-	-	-
127479	retinyl acetate	231.40	-	-	-	-	-	-	-	-	-	-
128370	2,6-di-tert-butyl-p-cresol	-	-	-	-	8.75	3.39	-	-	-	-	-
128392	2,6-di-tert-butylphenol	-	-	-	-	14.53	2.80	-	-	-	-	-
131113	dimethyl phthalate	1003.44	-	-	-	-	-	-	-	-	-	-
140114	benzyl acetate	198.23	-	140.26	-	-	-	-	-	-	-	-
140669	4-(1,1,3,3-tetramethylbutyl)phenol	-	-	-	-	17.88	2.52	-	-	-	-	-
140885	ethyl acrylate	3287.92	-	-	-	-	-	-	-	-	-	-
141059	diethyl maleate	103.62	-	-	-	-	-	-	-	-	-	-
141322	butyl acrylate	3873.75	-	-	-	-	-	-	-	-	-	-
141786	ethyl acetate	664.12	-	605.46	-	-	-	-	-	-	-	-
141979	ethyl acetoacetate	148.90	-	99.88	-	-	-	-	-	-	-	-
142165	bis(2-ethylhexyl) maleate	190.11	-	-	-	-	-	-	-	-	-	-
142905	dodecyl methacrylate	66029.09	-	-	-	-	-	-	-	-	-	-
142916	isopropyl palmitate	3747.10	-	-	-	-	-	-	-	-	-	-
156434	p-phenetidine	-	-	-	-	-	-	3.79	-	-	-	-
298000	parathion-methyl	-	-	-	-	-	-	-	-	-	-	6.34
328847	3,4-dichloro-alpha,alpha,alpha-trifluorotoluene	-	-	-	-	-	-	-	-	-	-5.45	-
353593	bromochlorodifluoromethane	-	0.00	-	-	-	-	-		3.67	-	-
393759	4-chloro-3,5-dinitro-alpha,alpha,alpha-trifluorotoluene	-	-	-	-	-	-	-	-	-	-	2.17
497392	4,6-di-tert-butyl-m-cresol	-	-	-	-	16.68	2.63	-	-	-	-	-
541731	1,3-dichlorobenzene	-	-	-	-	-	-	-	-	-	729.51	-
576261	2,6-xylenol	-	-	-	-	17.88	2.56	-	-	-	-	-
591275	3-aminophenol	-	-	-	-	2.97	3.55	-	-	-	-	-
592358	butyl carbamate	1.22E+06	-	-	-	-	-	-	-	-	-	-
609143	ethyl 2-methylacetoacetate	1835.40	-	-	-	-	-	-	-	-	-	-
611063	1,3-dichloro-4-nitrobenzene	-	-	-	-	-	-	-	-	-	-	0.02
616386	dimethyl carbonate	-	-	0.02	-	-	-	-	-	-	-	-
624486	dimethyl maleate	119.42	-	-	-	-	-	-	-	-	-	-
627930	dimethyl adipate	604.56	-	-	-	-	-	-	-	-	-	-
700130	2,3,5-trimethylhydroquinone	-	-	-	-	5.92	3.80	-	-	-	-	-
763699	ethyl 3-ethoxypropionate	1028.27	-	-	-	-	-	-	-	-	-	-
811972	norflurane	3.03E+08	-	-	-	-	-	-	-	3.24E+07	-	-
818611	2-hydroxyethyl acrylate	3287.92	-	-	-	-	-	-	-	-	-	-
868779	2-hydroxyethyl methacrylate	24961.22	-	-	-	-	-	-	-	-	-	-

Environmental half-lifes in days are given for those models for which this has significance. Otherwise the pseudo-first order reaction rate constant, log k, is given. See Section 2 for details.

CAS-nr.	Name	HYDROWIN (in days)	Hydrolysis models half-life in days			Oxidation models (days)	log(k)	log(k)	Reduction models half-life in days			log(k)
		6	7	8	9	10	11	12	13 (PLS)	13 (Eact)	14	15
1115204	3-hydroxy-2,2-dimethylpropyl 3-hydroxy-2,2-dimethylpropionate	41524.51	-	-	-	-	-	-	-	-	-	-
1119400	dimethyl glutarate	604.56	-	-	-	-	-	-	-	-	-	-
1338392	sorbitan laurate	2816.90	-	-	-	-	-	-	-	-	-	-
1459934	dimethyl isophthalate	352.17	-	97.09	-	-	-	-	-	-	-	-
1570645	4-chloro-o-cresol	-	-	-	-	23.56	2.17	-	-	-	255.90	-
1663394	tert-butyl acrylate	8618.04	-	-	-	-	-	-	-	-	-	-
1675543	2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bisoxirane	45634.44	-	-	-	-	-	-	-	-	-	-
1689992	2,6-dibromo-4-cyanophenyl octanoate	15.80	-	0.21	-	-	-	-	-	-	-	-
1817476	p-nitrocumene	-	-	-	-	-	-	-	-	-	-	-0.77
1836755	nitrofen	-	-	-	-	-	-	-	-	-	-	-0.52
1928434	2-ethylhexyl 2,4-dichlorophenoxyacetate	35.00	-	-	-	-	-	-	-	-	-	-
2100427	1-chloro-2,5-dimethoxybenzene	-	-	-	-	-	-	-	-	-	41.48	-
2409554	2-tert-butyl-p-cresol	-	-	-	-	12.65	2.95	-	-	-	-	-
2416946	2,3,6-trimethylphenol	-	-	-	-	15.57	2.72	-	-	-	-	-
2439352	2-(dimethylamino)ethyl acrylate	2480.68	-	-	-	-	-	-	-	-	-	-
2494895	2-[(p-aminophenyl)sulphonyl]ethyl hydrogensulphate	-	-	-	-	-	-	-2.22	-	-	-	-
2867472	2-dimethylaminoethyl methacrylate	18836.66	-	-	-	-	-	-	-	-	-	-
3120749	4-(methylthio)-m-cresol	-	-	-	-	1.24	5.48	-	-	-	-	-
3194556	1,2,5,6,9,10-hexabromocyclodecane	6.83E+08	-	-	-	-	-	-	-	-	-	-
4435534	3-methoxybutyl acetate	782.69	-		-	-	-	-	-	-	-	-
6358641	4-chloro-2,5-dimethoxyaniline	-	-	-	-	-	-	-	-	-	4.32	-
6386385	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	942.16	-	-	-	-	-	-	-	-	-	-
6846500	1-isopropyl-2,2-dimethyltrimethylene diisobutyrate	5384.25	-	-	-	-	-	-	-	-	-	-
6940530	1-chloro-2,5-dimethoxy-4-nitrobenzene	-	-	-	-	-	-	-	-	-	-	0.69
7397628	butyl glycollate	38.18	-	49.35	-	-	-	-	-	-	-	-
7434404	ethane-1,2-diylbis(oxyethane-2,1-diyl) bisheptanoate	293.87	-	-	-	-	-	-	-	-	-	-
7659861	2-ethylhexyl mercaptoacetate	92.72	-	-	-	-	-	-	-	-	-	-
10420334	dimethyl acetylsuccinate	1251.18	-	-	-	-	-	-	-	-	-	-
10605217	carbendazim	3.07E+05	-	-	-	-	-	-	-	-	-	-
13684634	phenmedipham	0.23	-	-	-	-	-	-	-	-	-	-
13940948	4-chloro-1-(dichloromethyl)benzene	-	-	-	-	-	-	-	-	-	1367.77	-
14861177	4-(2,4-dichlorophenoxy)aniline	-	-	-	-	-	-	2.48	-	-	-	-
15625895	2-ethyl-2-[[(1-oxoallyl)oxy]methyl]-1,3-propanediyl diacrylate	3313.73	-		-	-	-	-	-	-	-	-
17639939	methyl 2-chloropropionate	16.13	-	-	-	-	-	-	-	-	-	-
17700093	4-nitro-1,2,3-trichlorobenzene	-	-	-	-	-	-	-	-	-	-	0.38
20292084	2-ethylhexyl laurate	5165.83	-	-	-	-	-	-	-	-	-	-
22839470	aspartame	1733.48	-	-	-	-	-	-	-	-	-	-
25103097	isooctyl mercaptoacetate	59.56	-	-	-	-	-	-	-	-	-	-
25265774	isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol	5548.09	-	-	-	-	-	-	-	-	-	-
25311711	isofenphos	2826.83	-	-	-	-	-	-	-	-	-	-
26761455	2,3-epoxypropyl neodecanoate	1.73E+05	-	-	-	-	-	-	-	-	-	-
27554263	diisooctyl phthalate	1251.96	-	-	-	-	-	-	-	-	-	-
32210234	4-tert-butylcyclohexyl acetate	2661.76	-	-	-	-	-	-	-	-	-	-
40843730	4-(2,4-dichlorophenoxy)phenol	-	-	-	-	21.00	2.37	-	-	-	-	-
42576023	methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	599.14	-	-	-	-	-	-	-	-	-	-

Environmental half-lifes in days are given for those models for which this has significance. Otherwise the pseudo-first order reaction rate constant, log k, is given. See Section 2 for details.