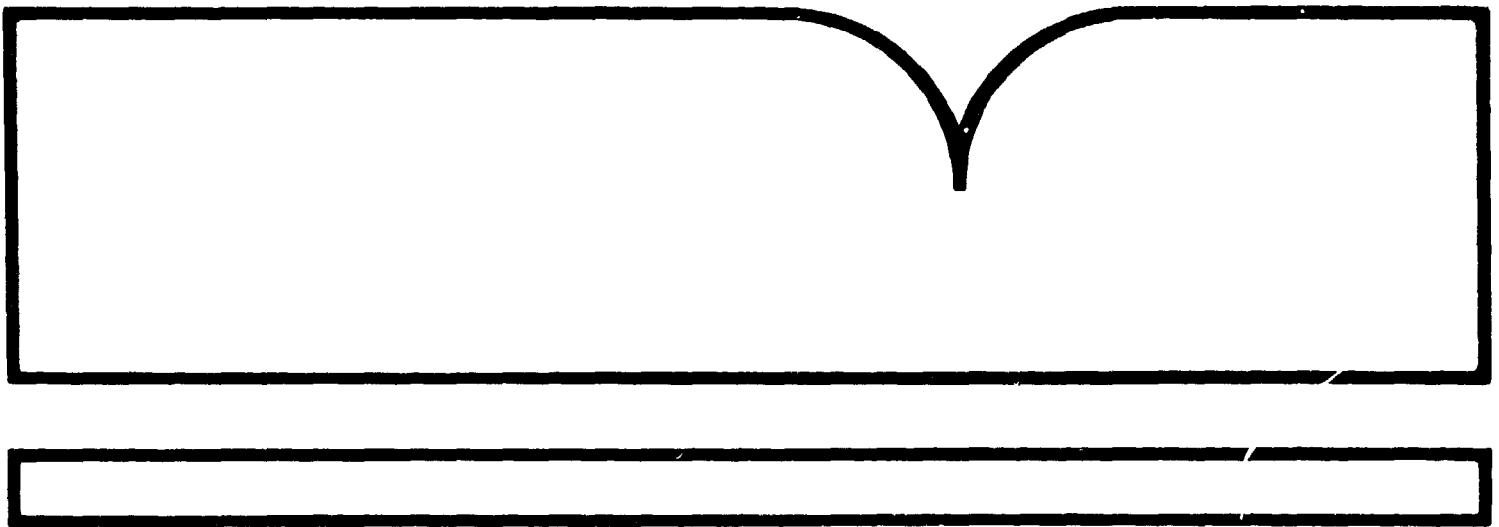AQUATIC FATE PROCESS DATA FOR
ORGANIC PRIORITY POLLUTANTS

SRI International
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Equilibrium and kinetic constants for evaluating the transformation and transport
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ships between water solubility, octonal-water partition coefficients, and partition
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AQUATIC FATE PROCESS DATA FOR ORGANIC PRIORITY POLLUTANTS

by

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FOREWORD

Effective regulatory action for toxic chemicals requires an understanding of the human and environmental risks associated with the manufacture, use, and disposal of a chemical. The assessment of risk requires the best scientific judgment about the probability of harm to the environment resulting from known or potential environmental concentrations. Environmental concentrations are a function of (1) the amount and form of the chemical released per unit time into the environment, (2) the geographic area, (3) prior accumulation, (4) time of measurement after release, and (5) the behavior of the chemical in the environment. The behavior, or fate and transport characteristics, of toxic pollutants in the environment depends on a variety of chemical, physical, and biological processes (e.g., photolysis, hydrolysis, oxidation, volatilization, sorption, biodegradation, biotransformation). These processes were placed into perspective and summarized for 129 chemical substances in a two-volume report entitled "Water-related Environmental Fate of 129 Priority Pollutants" (EPA-440/4-79-029a&b). Although this review contained literature data on some of the processes, data were incomplete for many of the processes affecting the 114 organic compounds.

This report takes data and information from the "129 report" as well as from other sources and puts it in a form for use in modeling the fate of the 114 organic priority pollutants.

Michael W. Slimak, Chief
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Office of Water Regulations and Standards

Note: This report was revised in late 1982 after review within EPA. Some values have been changed as a result of reexamination of information available.

ABSTRACT

Equilibrium and kinetic constants for evaluating the transformation and transport in aquatic systems for 114 organic chemicals on EPA's priority pollutant list have been obtained from the literature and from theoretical or empirical calculation methods. Constants for selected physical properties and for partitioning, volatilization, photolysis, oxidation, hydrolysis, and biotransformation are listed for each chemical along with the source of the data. Values are reported in units suitable for use in a current aquatic fate model. A discussion of the empirical relationships between water solubility, octanol-water partition coefficients, and partition coefficients for sediment and biota is presented. The calculation of volatilization rates for organic chemicals in aqueous systems also is discussed.

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SECTION 1

INTRODUCTION

1.1 PURPOSE

The purpose of this report is to provide data for selected chemical, physical, and biological processes that occur in aquatic environments for organic chemicals on the EPA's list of priority pollutants. These data can be used with appropriate environmental parameters (e.g., pH, sediment loadings, bacterial populations, sunlight intensity) to calculate half-lives of chemicals in aquatic systems. The concentration of a chemical as a function of time or distance in a particular aquatic system may also be calculated from these data using computer models that include the hydrological properties of a water body. Some of the data in this report have been calculated or estimated using empirical or theoretical methods and are intended primarily for use by EPA's Office of Water Regulations and Standards (EPA-OWRS) in its assessment program. EPA-OWRS will use data from this report to obtain preliminary estimates of chemical concentrations in aquatic systems using aquatic fate models that incorporate the process modeling approach (see Section 2.2). As the needs for better process data are identified, laboratory or other studies will be conducted.

This report is published in recognition that these data are of interest to other environmental programs; users of these data must be responsible for how the definition, sources, limitations, and reliability of these data may be significant or inapplicable in the context of their own assessment programs. Users of the data in this report are encouraged always to seek more current data to confirm or supplant the data presented.

1.2 BACKGROUND

The Office of Water Regulations and Standards, U.S. EPA, is conducting a program to evaluate the environmental fates of 129 chemicals in aquatic systems; these chemicals are commonly referred to as priority

pollutants. A brief history of EPA's overall efforts on priority pollutants has been described by Keith and Telliard (1979). As part of the EPA program, EPA-OWRS has recently published a comprehensive literature review on the physico-chemical properties and the transformation and transport processes of priority pollutant chemicals for use in environmental exposure assessments (Callahan et al., 1979). Although the review contains literature data on some processes, the data were incomplete for most chemicals and often information was qualitative, of suspect reliability, or did not exist. However, some of these process data can be calculated or estimated by theoretical or empirical methods so that the significant transport and transformation processes can be identified, and provisional calculations of chemical concentrations in aquatic systems can be made for rough exposure assessments. These results can then be used to decide what process data must be upgraded in the context of the particular assessment.

This report takes data and information from the 1979 EPA-OWRS literature review (Callahan et al., 1979) as well as from other sources to provide data for use in modeling the fate of the individual organic priority pollutants. The data presented in this report are in units used in one particular aquatic fate model (known as EXAMS, the Exposure Analysis Modeling System, see Section 2.2), but may also be used in other fate assessments.

This report has five sections. The first three sections provide the data intended for use in aquatic fate modeling and include brief discussions of the processes or data for which values are given. These sections also describe the basic theory (including equations) related to the process and use of the data along with the estimation or calculation methods or sources of data. Sections 4 and 5 describe in detail the calculation methods for evaluating sorption and volatilization data, respectively.

The organic priority pollutant chemicals for which data are provided in this report are listed below according to the classes or groups of chemicals as listed in the 1979 EPA-OWRS report, "Water Related Environmental Fate of 129 Priority Pollutants," by Callahan et al. 1979.

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Pesticides

1. Acrolein
2. Aldrin
3. Chlordane (cis and trans isomers)
4. DDD
5. DDE
6. DDT
7. Dieldrin
8. Endosulfan (α and β isomers)
9. Endosulfan sulfate
10. Endrin
11. Endrin aldehyde
12. Heptachlor
13. Heptachlor epoxide
14. α-Hexachlorocyclohexane
15. β-Hexachlorocyclohexane
16. δ-Hexachlorocyclohexane
17. γ-Hexachlorocyclohexane (lindane)
18. Isophorone
19. TCDD
20. Toxaphene

PCBs and 2-Chloronaphthalene

21. Aroclor 1016
22. Aroclor 1221
23. Aroclor 1232
24. Aroclor 1242
25. Aroclor 1248
26. Aroclor 1254
27. Aroclor 1260
28. 2-Chloronaphthalene

Halogenated Aliphatic Hydrocarbon

29. Chloromethane (methyl chloride)
30. Dichloromethane (methylene chloride)
31. Trichloromethane (chloroform)
32. Tetrachloromethane (carbon tetrachloride)
33. Chloroethane (ethyl chloride)
34. 1,1-Dichloroethane (ethylidine chloride)
35. 1,2-Dichloroethane (ethylene dichloride)
36. 1,1,1-Trichloroethane (methyl chloroform)
37. 1,1,2-Trichloroethane
38. 1,1,2,2-Tetrachloroethane
39. Hexachloroethane
40. Chloroethene (vinyl chloride)
41. 1,1-Dichloroethene (vinylidine chloride)
42. 1,2-trans-Dichloroethene
43. Trichloroethene
44. Tetrachloroethene (perchloroethylene)
45. 1,2-Dichloropropane

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46. 1,3-Dichloropropene
47. Hexachlorobutadiene
48. Hexachlorocyclopentadiene
49. Bromomethane (methyl bromide)
50. Bromodichloromethane
51. Dibromochloromethane
52. Tribromomethane (bromoform)
53. Dichlorodifluoromethane
54. Trichlorofluoromethane

Halogenated Ethers

55. Bis(chloromethyl)ether
56. Bis(2-chloroethyl)ether
57. Bis(2-chloroisopropyl)ether
58. 2-Chloroethyl vinyl ether
59. 4-Chlorophenyl phenyl ether
60. 4-Bromophenyl phenyl ether
61. Bis(2-chloroethoxy)methane

Monocyclic Aromatics

62. Benzene
63. Chlorobenzene
64. 1,2-Dichlorobenzene (o-dichlorobenzene)
65. 1,3-Dichlorobenzene (m-dichlorobenzene)
66. 1,4-Dichlorobenzene (p-dichlorobenzene)
67. 1,2,4-Trichlorobenzene
68. Hexachlorobenzene
69. Ethylbenzene
70. Nitrobenzene
71. Toluene
72. 2,4-Dinitrotoluene
73. 2,6-Dinitrotoluene
74. Phenol
75. 2-Chlorophenol
76. 2,4-Dichlorophenol
77. 2,4,6-Trichlorophenol
78. Pentachlorophenol
79. 2-Nitrophenol
80. 4-Nitrophenol
81. 2,4-Dinitrophenol
82. 2,4-Dimethyl phenol
83. p-Chloro-m-cresol
84. 4,6-Dinitro-o-cresol

Phthalate Esters

85. Dimethyl phthalate
86. Diethyl phthalate
87. Di-n-butyl phthalate
88. Di-n-octyl phthalate

89. Bis(2-ethylhexyl)phthalate
        90. Butyl benzyl phthalate

Polycyclic Aromatic Hydrocarbons

        91. Acenaphthene
        92. Acenaphthylene
        93. Anthracene
        94. Benzo(a)anthracene
        95. Benzo(b)fluoranthene
        96. Benzo(k)fluoranthene
        97. Benzo(ghi)perylene
        98. Benzo(a)pyrene
        99. Chrysene
       100. Dibenzo(a,h)anthracene
       101. Fluoranthene
       102. Fluorene
       103. Indeno(1,2,3-cd)pyrene
       104. Naphthalene
       105. Phenanthrene
       106. Pyrene

Nitrosamines and Other Nitrogen-containing Chemicals

       107. Dimethyl nitrosamine
       108. Diphenyl nitrosamine
       109. Di-n-propyl nitrosamine
       110. Benzidine
       111. 3,3'-Dichlorobenzidine
       112. 1,2-Diphenylhydrazine (hydrazobenzene)
       113. Acrylonitrile

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SECTION 2

ASSESSMENT OF CONCENTRATIONS AND HALF-LIVES OF
CHEMICALS IN AQUATIC ENVIRONMENTS

2.1 THE PROCESS MODELING APPROACH

A reliable and documented estimate of the concentration of a chemical in the environment is required for most chemical hazard evaluation programs. To predict such chemical concentrations, the fate of the chemical in the environment can be evaluated in terms of transport and transformation processes. The emphasis is then on the effects of the environment on the chemical, rather than the effects of the chemical on the environment as in ecological stuides (Baughman and Lassiter, 1978). Once the concentration of the chemical is estimated for the environments of concern, species population, toxicological data and other factors can be included to complete the hazard assessment.

One method for predicting the concentrations of chemicals in the environment is the process modeling approach in which it is assumed that the total rate of loss of the chemical is determined by the sum of rates of the individual chemical and biological transformation and physical transport processes that occur for the chemical in an environment (Baughman and Burns, 1980; Baughman and Lassiter, 1978, Mill, 1978; Smith et al. 1977, 1978). Data for the individual processes may be obtained in laboratory stuides, by structure-activity relationships for a class of chemicals, or from empirical correlations that apply to the chemical of concern. Combined with data for the appropriate environmental conditions (such as pH, sunlight flux, organism population) the process data can be used to calculate rates for the process in the particular environment. The rates for the processes in an environment may then be summed to estimate an overall rate for loss of chemical in the environment.

In this report, process data are defined as data relating to rate constants, equilibrium constants, or properties that describe the intrinsic processes the chemicals may undergo independent of environmental influences.

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The term _environmental parameter_ as used in this report refers to properties or data that describe (or are a function of) the environment.

The process modeling approach to predicting environmental concentrations of chemicals has several advantages over approaches such as field studies or, on a smaller scale, microcosms. Although both approaches have been considered representative of an environmental situation, the latter fails to identify which process or processes are important for transforming or transporting the chemical in the environment. Lack of such information may then make the observed loss rate unreliable and undocumentable as to whether the chemical generally may be expected to behave in a similar manner in the same or in different environments. The field study approach also has a drawback in that a hazard may actually be created in performing the experiment. The microcosm experiment has problems in extrapolating the data obtained to the real environment.

Although the process modeling approach should be verified by actual experience in aquatic systems, it does offer a flexible and documentable method for predicting environmental concentrations of a chemical. An indirect benefit of the process modeling approach is that attempts to verify the models will advance the understanding of how the individual processes operate in the environment and therefore guide efforts in research on these processes and suggest what new processes should be included in future modeling efforts.

The processes that can be important for transforming or transporting a chemical in an aquatic environment are shown in Figure 2.1. The following discussion summarizes the mathematical basis for the process modeling approach applied to such aquatic systems in three steps: (1) the evaluation of rates of loss of chemical due to transformations and volatilization processes, (2) the influence of sorption processes on the rates of loss of chemical, and (3) the prediction of concentration and half-life of chemical in the aquatic environment including terms for input of chemical, dilution, and finally flow out of the environment. This discussion assumes that return of the chemical from the atmosphere to the aquatic system is included in the term for the inflow of the chemical and that sorption to

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particulates in the environment is not kinetically controlled (i.e., sorption equilibrium is attained instantaneously).
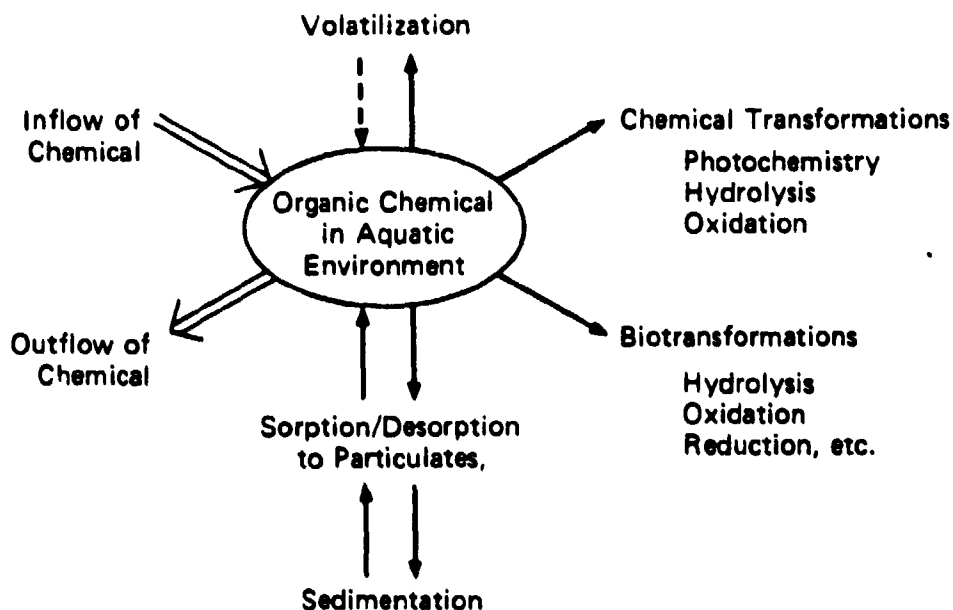
FIGURE 2.1   TRANSPORT AND TRANSFORMATION PROCESSES IN AQUATIC ENVIRONMENTS

Evaluation of Chemical Loss Rates. The rate of loss of a chemical due to the above transformation processes plus volatilization, R_T, is given by the sum of the rates of the individual processes, R_i, according to the equation

$$R_T = \Sigma R_i = \Sigma k_i'[E_i][C] \tag{2.1}$$

where k_i' is the rate constant for the i-th process, $[E_i]$ is an environmental parameter that is kinetically important for the i-th process, and $[C]$ is the concentration of the chemical. The calculations of R_i for individual processes from environmental parameter and process data are discussed in Sections 2.3.6 through 2.3.10 and in Sections 4 and 5 and therefore will not be discussed here. The important environmental parameters

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for each process have been reviewed and the use of the parameters in the calculations of environmental transformation rates has been discussed in detail by Baughman and Burns (1980), Mill (1978), and Smith et al. (1977).

The above expression for R_T assumes that the loss of chemical is first order in the chemical concentration, as certainly must be the case at the highly dilute concentrations expected in the environment. Equation (2.1) also requires that the rate of loss of chemical due to any one process R_i, is first order in the environmental parameter term F_i; R_i is then considered as following overall second-order kinetic behavior. If it is assumed that the low concentration of chemical in the environment has no significant effect on the environment (i.e., does not change pH, biomass, dissolved oxygen, etc.) and that the environmental parameter, E_i, is constant over a specific region and time period, the term k_i' $[E_i]$ can be expressed as a simple pseudo-first-order rate constant, k_i, and then

$$R_T = [\Sigma k_i][C] = k_T[C] \qquad (2.2)$$

or

$$k_T = \Sigma k_i \qquad (2.3)$$

where k_T is the overall pseudo-first-order rate constant for loss of chemical due to transformation and volatilization. The half-life for loss of chemical due to these processes is then given by

$$t_{\frac{1}{2}} = \ell n2/k_T \qquad (2.4)$$

Influence of Sorption. In addition to losses of chemicals due to these transformation and volatilization processes, sorption to particulates can also reduce the concentrations of chemicals in aquatic systems. These particulates may be either suspended sediments or biotic in origin, and may eventually be deposited into benthic sediments. The suspended or benthic sediment may later serve as a source of chemical from sorption-desorption equilibrium as the chemical in solution is lost due to volatilization or undergoes transformation in the water column. If biotransformation does not occur in biota (such as bacteria, algae, fish), the chemical may be released back into solution when the organism dies and decomposes. The understanding of chemical transformation when sorbed onto particulates is

inadequate to predict or measure the rates of such reactions for use in modeling efforts. Therefore, the following discussion assumes that no transformations occur on particulates and that sorption is completely reversible and rapid in comparison with transformations that occur in solution.

The partitioning of a chemical between particulates (sediment or biota) and water at the low concentrations of chemicals usually found in the environment can be expressed as a partition coefficient K_p

$$K_p = \frac{C_s}{C_w} \qquad (2.5)$$

where C_s and C_w are the equilibrium concentrations of chemical on sediment and in water, respectively* (Baughman and Lassiter, 1978; Smith and Bomberger, 1980). For a chemical in aqueous solution containing particulates, the chemical is equilibrated between the water and particulate (P) according to the equation

$$C + P \rightleftharpoons (C\text{-}P)$$

and the partition coefficient can be rewritten as

$$K_p = \frac{[C\text{-}P]}{[C_w][P]} \qquad (2.6)$$

where [C-P] is the mass of sorbed chemical per unit solution volume and [P] is the mass of sorbing particulate per unit solution volume. The mass balance of chemical in the solution-sediment system is given by

$$[C_T] = [C\text{-}P] + [C_w] \qquad (2.7)$$

where $[C_T]$ is the total mass of chemical in a unit solution volume of water containing [P] grams of particulate. Combination of equations (2.6)

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*By convention, K_p is unitless when C_s is in units that are equivalent to C_w (i.e., C_s is in µg chemical per g particulate and C_w is in µg chemical per g water). In this discussion, $[C_w]$ will be defined in these weight units and [C] will be defined in molecular units (moles liter^{-1}); since 1 g water is approximately 1 ml, it follows that $[C] = 10^3 [C_w][MW]^{-1}$ where MW is the molecular weight of chemical. Note that [C] and $[C_w]$ can be used interchangeably in expressions such as equation (2.2) since first-order rate constants are concentration independent, but the rate of loss term, R, is of course defined in units corresponding to $[C_w]$ or [C].

and (2.7) then gives the fraction of the total chemical dissolved in solution:

$$\frac{[C_w]}{[C_T]} = \frac{1}{K_p[P] + 1}$$ (2.8)

Baughman and Lassiter (1978) have pointed out that, given the relationship shown in equation (2.8), the fraction of chemical in solution may be quite high inspite of a large K_p value because the sediment or biota loading, [P], is often low in aquatic systems (i.e., $K_p[P]<1$).

The concentration of chemical in solution $[C_w]$ in the presence of a particulate-water system is then given by

$$[C_w] = \frac{[C_T]}{[P]K_p + 1}$$ (2.9)

Substitution of equation (2.9) into equation (2.2) for the rate of loss of chemical then gives

$$R_T = \frac{k_T C_T}{[P]K_p + 1}$$ (2.10)

This relationship shows that, unless transformation on particulate is as rapid (or faster) than in solution, the net effect of sorption will be to reduce the overall rate of loss of chemical from the aquatic system. From equation (2.10), it also follows that the half-life of the chemical is given by

$$t_{\frac{1}{2}} = \frac{([P]K_p + 1)\ln 2}{k_T}$$ (2.11)

Steady-state Concentrations. These equations describe the fate of a chemical in a water body with no inflow or outflow. In a real aquatic system, there is of course a rate of introduction of the chemical into the water body, R_I. The rate of loss of chemical in the environment R_L is the sum of R_T (as defined above) and the rates of dilution and flow out of the system (R_D and R_0, respectively). In a given segment of the water body, a steady-state concentration of chemical is attained when R_L equals R_I (Mill, 1978),

$$R_I = R_L = R_T + R_D + R_0$$ (2.12)

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or

$$R_I = \left[\frac{k_T}{K_p[P] + 1}\right] C_T + R_O + R_D \qquad (2.13)$$

The steady-state concentration of chemical is then

$$[C_T]_{SS} = \frac{[R_I - R_O - R_D](K_p[P] + 1)}{k_T} \qquad (2.14)$$

The preceding discussion shows that along with the rate constant k_T, other factors such as initial concentrations, sorption, and dilution will determine the final concentration of chemical in an aquatic environment. The persistence of the chemical, however, is often described in terms of a half-life where $t_{\frac{1}{2}} = \ln 2/k_T$. The half-life is simply the time at which one-half of the init al concentration remains (or is lost), and is not concentration dependent for the first-order processes assumed in most calculations or environmental models. Table 2.1 shows the relationship between the percentage of a chemical remaining as a function of time in terms of half-lives. From these data it is clear that a short half-life of a chemical may not be a sufficient argument for the safe discharge of the chemical if the initial concentration must be substantially reduced by environmental processes.

Table 2.1

PERCENT CHEMICAL REMAINING AS A FUNCTION
OF HALF-LIVES

% Chemical Remaining	Number of Half-Lives Elapsed
75	0.42
50	1.0
25	2.0
10	3.3
5	4.3
1	6.6
0.1	10
0.01	13

From the above discussion and equations, it is obvious that although the half-lives and concentrations of chemicals in aquatic environments can be predicted by manual calculations, the time required and the chances for calculational errors may be overwhelming in some assessments. Therefore, a computer program for executing these calculations is useful. The use of process data and environmental parameters in calculating half-lives and concentrations of chemicals for different types of assessments using manual computations and several existing computer programs is discussed in Section 2.2.

2.2 APPLICATIONS OF PROCESS MODELING

The process modeling approach for predicting the persistence and concentrations of chemicals in an aquatic environment can be applied to many types of assessments. According to the scope of an assessment, each evaluation can be performed within limitations of time, cost, and the availability (or reliability) of data. The process approach is the only economical way in which sensitivity analyses can be performed to determine the relative importance of environmental parameter and process data variables for chemicals in aquatic environments.

"Worst case" or other scenarios can also be easily evaluated using a process modeling approach; the worst case situation may be defined in terms of environmental conditions least likely to transform a chemical or in terms of the availability (or reliability) of process data where in- complete data do not permit all processes to be included in the assessment. The purpose of such assessments may range from simply establishing priorities for future research to actually predicting environmental concentrations of chemicals for regulatory/control strategy decisions.

Although the process modeling approach should be verified by actual experience in the environment, it is explicit as to what processes and environmental conditions are (and are not) used in any assessment and therefore has potential for rational modifications and additions of new processes. Three examples of the application of the process approach are described below to demonstrate the utility of the process data and the flexibility of the approach.

The simplest level of application of the process modeling approach
is the manual calculation of rate or partitioning constants for a specific
environment. Thus, if the hydrolysis rate constant of a chemical is very
rapid within the time concern of an assessment, no other work need be con-
ducted even if other reactions are, in fact, faster but the data are less
reliable or not available. If several processes appear to be equally
important, the overall first-order rate constant, k_T for loss of chemical
is given by the sum of individual constants

$$k_T = \Sigma k_i \qquad (2.3)$$

and the half-life is then

$$t_{\frac{1}{2}} = \frac{\ell n 2}{\Sigma k_i} \qquad (2.15)$$

Partitioning data may be used to calculate manually the fraction of chemical
in water or in biota and sediments for assessments. The K_p value may be
also used in equation (2.11) for the half-life of the chemical to include
the influence of partitioning of the chemical to aquatic particulates.
Manual calculations may then be used for a number of simple aquatic fate
assessments in a cost-effective manner that does not require computer
facilities or personnel.

A higher level of sophistication for the process model approach is
an application in which manual calculations of the first-order rate constants
k_i and of partition coefficients are integrated using a computer model that
allows for transformations and transport in and among several compartments
of a water body. The computer calculates solutions of the differential
equation for loss of chemical to obtain the concentration of chemical as
a function of time. Application of such a model has been used by Smith
et al. (1978) in estimating concentrations of chemicals in several types
of aquatic environments. Such an aquatic fate assessment requires the
participation of persons knowledgeable in the evaluation and use of the
individual process data and environmental parameters and yet is relatively
inexpensive in terms of the computer time required.

A more sophisticated level of application of the process approach
currently in use is a computer model that uses process data and environmental

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parameters to calculate the concentrations and half-lives of chemicals in aquatic environments. One multicompartment model, known as the Exposure Analysis Modeling System (EXAMS), has been applied to evaluate the transport and transformation of phthalate esters in aquatic systems (Wolfe et al., 1980).

The EXAMS model can calculate rate and partitioning constants as a function of temperature if suitable temperature-dependence data are available. EXAMS can also include transformation processes in sediment and biota if such process data are available. EXAMS requires less chemical and biological expertise for manual calculations than the model described by Smith et al. (1978), but is more expensive in terms of computer time. Data presented in Section 3 of this report are in the units used in the EXAMS model. Since EXAMS is a steady state model, it is limited to applications of constant pollutant input, and more dynamic models would closely simulate environmental situations.

In summary, the process modeling approach is a flexible procedure that can be tailored to the needs of an individual assessment. Computer manipulation of data is easily applied to these assessments, but manual calculations are also practical if persons with suitable expertise are available. It is certain that the iterative process involving the use, verification, and subsequent modification of the process modeling approach will allow better process models to evolve and contribute to an overall better understanding of the environmental fate of chemicals.

2.3 DEFINITIONS OF PROCESSES AND SOURCES OF DATA

2.3.1 Basis for Derivation of Data

The data on organic priority pollutants given in this report were
obtained from the literature and from calculations based on theory, structure-
activity relationships (SAR), or empirical calculations. In general, the
physical properties of a chemical are functions of the molecular structure
as an entity; that is, the elemental composition, spatial relationships
and size, molecular weight, and functional groups of the molecule all may
contribute to the property of the chemical. By contrast, the chemical or
biological reactivity of a molecule is usually due to selected functional
groups in the molecular structure, and the functional group may undergo
transformation with sometimes only minor changes in the total structure of
the molecule. The toxicity of a chemical may also be due, in part, to
functional groups on a chemical structure, although physical properties
will certainly be important in the transport, accumulation, and excretion
of the chemical in an organism.

Although many of the data on toxicity and concentration of chemicals
in the environment are expressed in terms of weight units (i.e., ppm), the
toxic impact and dynamic aspects of transport and transformations of the
chemical actually occur on a molecular level. Therefore, kinetic/equilibrium
units and concentrations are better expressed as molecular units (i.e., moles
liter^{-1} or M), especially when relative reactivities or properties of chemicals
are compared to provide estimates or calculations of fate data.

The individual processes that chemicals may undergo can then be
classified and evaluated either according to specific physical properties
or according to the reactive functional groups that these chemicals may
have in common. The basis for the empirical correlations between K_{ow}, K_{oc},
S_w, and K_b are discussed in Section 4 and will not be discussed here except
to point out that all these constants describe equilibrium processes for the
chemical between water and a second (organic) phase. Similarly, the volatil-
ization of a chemical can be evaluated in terms of Henry's constants, which
are functions of vapor pressure and water solubility (see Section 5).

The reactivity of a chemical may be classified according to select functional groups in the molecular structure. For evaluations of hydrolysis reactions, chemicals are classified as carboxylic acid esters ($-CO_2R$), carboxylic acid amides ($-CONH_2$), alkyl halides ($R-X$), phosphoric acid esters ($(RO)_3PO$), to name only a few. Data for hydrolysis of a chemical can often be estimated by analogy to another chemical with a similar functional group or calculated by more formal procedures using linear-free energy relationships such as the Taft equations, Hammett equation, or other such correlations (Mill, 1979; Wolfe et al., 1978 and 1980).

Chemical oxidation rate constants can be calculated by evaluating the reaction of an oxidant at a particular type of carbon-hydrogen bond (i.e., hydrogen abstraction process) or at an olefinic bond (see Section 2.3.8).

No structure-activity relationship (SAR) or correlation method is now available for predicting a direct photolysis rate constant except by analogy to other chemicals, which is ofter unreliable because of the complex chemistry of photoexcited states. When absorption spectral data are available, a maximum rate constant (ie., fastest reaction possible) may be calculated if a reaction quantum yield of unity is assumed. The maximum rate constant is useful for comparison with other rate constants to determine whether photolysis may be an important process, but probably will overestimate the photolysis rate because the reaction quantum yield is usually less than unity. The use of SAR and correlation procedures in environmental assessments has been discussed by Mill (1979), by Wolfe et al. (1980), and in Sections 4 and 5 of this report.

In using the theoretical equations, SARs, and empirical correlations, it is important to remember that the scientific basis for understanding these relationships is still being developed and verified. The situation of the several empirical correlations between S_w and K_{oc} is a good example of such problems, in that different groups of chemicals have been used to establish empirical correlations that, not surprisingly, give different equations. Recognition of the influence of sediment particle size on K_{oc} measurements has also redefined the K_{oc} data base, which changed the correlation equations (see Section 4 and Karickhoff et al., 1979). Thus

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the existence of several SARs or empirical correlations for individual 'properties, reactivities, or processes should not be considered a problem or contradiction, but rather a reflection of the developing understanding and increased data base available for such data prediction methods.

For this report, data obtained from calculations involving theory, SARs, or empirical correlations have been clearly identified so that the user can recognize the source of such data and can recalculate data using more current or improved procedures as they become available.

The following sections contain descriptions of environmental processes and the process data important in aquatic fate assessments. The process data are discussed in the order that they appear on the data sheets in Section 3. The sources of the process data are also discussed.

2.3.2 Chemical Name and Molecular Weight

The names of the chemicals used on the data sheets in Section 3 are those used by Callahan et al. (1979); alternative names are also given in that report. The Toxic Substances List[*] (TSL) number is given in that report to provide an unambiguous reference to toxicological data.

The molecular weight is not used for environmental assessments in itself, but is required for conversion of units from ppm to molar units (M). The molecular weight has also been used to calculate the oxygen re-aeration rate ratio (see Section 5.)

2.3.3 Melting and Boiling Point

These data are not used directly in aquatic fate assessments, but they show in which phase (gas, liquid, solid) the pure chemical is found under environmental conditions. If the heat of vaporization, ΔH_{vap}, of a chemical is not available, it may be estimated from Trouton's rule

$$\Delta H_{vap} = 21 T_{BP} \tag{2.16}$$

where the boiling point, T_{BP}, is given in degrees Kelvin ($= °C + 273$); Trouton's Rule is discussed in most physical chemistry textbooks. A value of ΔH_{vap} can then be used to calculate vapor pressure values at any

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[*] Registry of Toxic Effects of Chemical Substances, published yearly by the National Institute of Occupational Safety and Health.

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temperature using the Clausius-Clapeyron equation, which is also found in
chemistry textbooks. The melting point should be used in the calculation
of water solubility from K_{ow} data for compounds that are solids above 25°C
(see Section 4).

Most melting point and boiling point data were taken from Callahan
et al. (1979) and are reliable within several degrees. Boiling point data
are usually cited for 760 torr (or 1 atmosphere) unless otherwise noted.

2.3.4 Ionization Constants

The pH values found in most aquatic systems range from approximately
pH 4 to 9, with extreme values down to pH 2 and up to pH 11. If a chemical
is ionized under environmental conditions, the physical properties as well
as the chemical reactivity will change with pH (for instance, the solubility
of an ionic form of an organic chemical will likely be greater than for the
neutral species). The ionization of a neutral organic chemical HA possess-
ing acidic properties can be written as

$$HA \rightleftharpoons H^+ + A^-$$

and the ionization constant K_A defined as

$$K_A = \frac{[H^+][A^-]}{[HA]} \qquad (2.17)$$

The constant K_A is often expressed logarithmically as the pK_A, where

$$pK_A = -\log K_A \qquad (2.18)$$

For basic compounds, the equilibrium between the neutral basic species,
B, and water is written as

$$B + H_2O \rightleftharpoons BH^+ + OH^-$$

and the ionization constant K_B is defined as

$$K_B = \frac{[BH^+][OH^-]}{[B]} \qquad (2.19)$$

where the water concentration (55.5 M) is taken as constant and included
in the K_B value. The negative logarithm of K_B is defined as the pK_B.

For some chemicals, several pK_A or pK_B values may exist for different moieties or stages of ionization. Although no such chemicals are among the organic priority pollutants, data on multifunctional ionization constants may be required for other chemicals. Note that K_A and K_B are also temperature-dependent; the temperature dependence of K_A or K_B is generally not available for organic compounds. In this report K_A or K_B is given for 25°C unless otherwise noted.

Data for pK_A or pK_B are reported as available. Where ionization or ionic forms do not occur in the aquatic environment, the code pK-NER (for pK not environmentally relevant) is entered for the data value. When several forms (ionic or netural) of the chemical may exist in the environment, process data are given for each form if data are available. Additional comments on such data are included in footnotes on the data sheets.

2.3.5 Partitioning Constants

Chemicals in aquatic environments may be sorbed to sediments, biota, or suspended particulates. If not degraded, the sorbed chemical may be transported on the particulates or enter the food chain and may later be desorbed from the particulates back into solution in the water column. The importance of sorption of a chemical in determining the concentration and half-life of a chemical in aquatic systems is discussed in Section 2.1; other aspects of the sorption/solubility phenomena and calculation of partitioning constants from empirical correlations are detailed in Section 4. The follow-ing discussion briefly defines each partition constant (including water solubility) and the units of data presented in this report. The sources of data and the codes used on the data sheets are also explained.

Water Solubility, S_w (ppm, or mg liter^{-1}). Water solubility data are required for calculating Henry's constant (see Section 2.3.6) and for calculating other partition coefficients using the correlation equations discussed in Section 4.

Octanol/Water Partition Coefficient, K_{ow} (unitless). This constant has been used in medical and environmental science as a measure of the hydrophobicity/hydrophilicity of chemicals (Hansch and Leo, 1979; Kenaga and Goring, 1978). The K_{ow} values in this report were used to calculate

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S_w, K_{oc}, and K_B data as discussed in Section 4.2. The calculation of K_{ow} itself from structural features of the molecule is discussed in Section 4.3.

Sediment Partition Coefficient, Normalized for Organic Carbon Fraction, K_{oc} (unitless). The product of K_{oc} and the environmental parameter value for the fraction of organic carbon in sediment, f_{oc}, gives the coefficient for partitioning onto that particular sediment, K_p. This K_p is only for sorption due to the hydrophobicity/hydrophilicity of a chemical and does not include ionic or other phenomena that may additionally contribute to sorption of a chemical to sediments.

Microorganisms/Water Partition Coefficient, K_B $[(\mu g/g)(mg/liter^{-1})]$. This value is used to evaluate the partitioning of a chemical between microorganisms and water in the water column. Since there are many complicating factors in the partitioning into biota, this value of K_B should be used with caution. The values of K_B listed in this report were calculated from the correlation equation discussed in Section 4.

As discussed in Section 4, values of K_{ow}, S_w, K_{oc}, and K_B are also useful for calculating their complementary partitioning coefficients either for direct use in assessments or for verifying the accuracy of a literature or laboratory-measured value. Many of the K_{ow} data in this report were calculated using the octanol/water partition coefficient calculation computer program developed at SRI using the procedures and data base of Hansch and Leo (1979) (see Section 4). Values of K_B and K_{oc} were generally calculated from values of K_{ow} using the correlation equations described in Section 4. S_w data were calculated from K_{ow} values using the correlation equations given in Section 4 when literature data were either unavailable or considered unreliable. Values of K_B, K_{oc}, and S_w calculated from K_{ow} values are coded in the form C-KB f Kow, C-Koc f Kow, and C-Sw f Kow respectively.

When literature data were available for K_{oc} or S_w, these values were compared with the values calculated from K_{ow}, and the best value was chosen based on a critical review of the original literature and an evaluation of the strengths and weaknesses of the data base used for the K_{ow} calculation. Some comparisons of data are discussed in Section 4. In a few cases, the calculated K_{ow} values were clearly inaccurate (by over an order of magnitude),

and therefore K_{ow} values were "back-calculated" from the K_{ow}-S_w correlation equations given in Section 5; such cases are discussed in footnotes to the data sheets in Section 3.

2.3.6 Volatilization Constants

Volatilization is an important loss process for some chemicals in aquatic systems, and current research is rapidly increasing the understanding of the process and improving methods for predicting volatilization rates for use in environmental assessments. The theory and procedures for calculating the rate constants and half-lives for volatilization of chemicals from aquatic systems are discussed in detail in Section 5. This section describes the use of the data on the data sheets in Section 3 and discusses the source of the data.

Vapor Pressure, P_v (torr). The vapor pressure of an organic chemical is, in itself, a qualitative or relative measure of the volatility of the chemical in its pure state and can be used to calculate the Henry's constant used in volatilization rate constant calculations. Most vapor pressure data in this report were taken directly from Callahan et al. (1979). It is not clear in that report if the vapor pressures for solids that were extrapolated to 20°C from literature vapor pressure data obtained above the melting point have been corrected for the phase change (see Section 5.3.) If the correction was not made, the calculated vapor pressure and H_c will be too high.

Henry's Constant, H_c (atm m^3 mole^{-1}). The calculation and use of Henry's constants for calculating volatilization rate constants and half-lives are discussed in Section 5. Most H_c values in this report were calculated from vapor pressure and water solubility data, which are also listed on the data sheets. In some cases where P_v and S_w were available only at slightly different temperatures (i.e., differences less than 10°C), H_c was calculated without any correction for temperature. If a better value for H_c is required, the user may interpolate or extrapolate the P_v or S_w data as necessary to recalculate another H_c value; this recalculation was not done for this report to minimize confusion and maintain the integrity of the individual S_w or P_v values as referenced. The values of H_c calculated

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in such a manner are coded as C-VP25°/S30° on the data sheets, indicating a value calculated from vapor pressure data at 25°C and water solubility data at 30°C. The H_c values calculated from P_v and S_w data at the same temperature are coded C-VP/S-30°, for example, indicating that both values were given for 30°C.

Reaeration Rate Ratio, k_v^C/k_v^0 (unitless). This value is ratio of the first-order rate constant for loss of chemical from aqueous solution divided by the rate constant for oxygen uptake by the same solution. It may be measured in the laboratory (Smith and Bomberger, 1980) or obtained by calculation procedures (see Section 5). The use of this ratio is applicable only to high volatility chemicals or to chemicals with Henry's constants (H_c) greater than 3 500 torr M^{-1} (or 4.6 x 10^{-3} m^3 atm mole^{-1}). For chemicals with smaller H_c values, the use of k_v^C/k_v^0 will overestimate the importance of volatilization.

Most of the k_v^C/k_v^0 data in this report were calculated using the equation

$$\frac{k_v^C}{k_v^0} = \left(\frac{D_e^C}{D_e^0}\right)^{0.7}$$

which is developed and discussed in Section 5 (equation 5.39). The source code for such values is C-DC.7, indicating a calculated value using diffusion coefficients with an exponent of 0.7. When the Henry's constant is so low that the use of rate ratio will overestimate the volatilization rate, as discussed in Section 5, the code NAV is entered for the value indicating that the reaeration rate ratio is not applicable for volatilization cal-culations. In general, NAV is entered for chemicals with H_c < 2 x 10^{-3} atm m^3 mol^{-1}.

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2.3.7 Photolysis Data

Photolysis of chemicals in aquatic systems occurs when sunlight of irradiating wavelengths above 290 nm is absorbed by the chemical. Stratospheric ozone filters out the lower, more energetic wavelengths of sunlight. Photolysis of a chemical may be considered to result from two types of processes. One process, in which the chemical absorbs light and then undergoes reaction, is referred to as direct photolysis. The rate of direct photolysis of a chemical in a dilute solution in pure water, R_p, is given by the equation

$$R_p = b\phi\Sigma\epsilon_\lambda I_\lambda [C] \qquad (2.20)$$

where b is a constant to provide appropriate units, ϕ is the reaction quant... yield, and ϵ_λ and I_λ are light absorption coefficients and light fluxes, respectively, at wavelength intervals, λ. Details on calculations of direct photolysis rates in aquatic systems have been described by Zepp and Cline (1977), Zepp (1979), and Mabey et al. (1980).

For direct photolysis of a chemical, the first-order photolysis rate constant, k_p, is then given by

$$k_p = b\phi\Sigma\epsilon_\lambda I_\lambda \qquad (2.21)$$

In sunlit aquatic environments, the rate constant k_p will vary because the distribution and intensity (or photon flux) of sunlight vary with time of day, season, and latitude. Thus a photolysis rate constant must be referenced to a specific time period (e.g., averaged over a 24-hour day, averaged over several hours at midday, instantaneous rate constant at noon), specific season, and latitude.

Photochemical transformations of a chemical in natural waters may also occur due to processes involving an initial light absorption by natural substances present in the water, which then causes reaction of the chemical. Since the chemical itself does not absorb the incident light, these processes have generally been referred to as indirect photolyses.

One type of indirect photolysis is a photosensitized process in which the excited state energy of the natural substances (probably humic or fulvic materials) is transferred to the chemical, which then undergoes reaction.

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At present there are a few examples of such reactions occurring in natural waters, and these reactions are the subject of current research (Zepp et al., 1980; Spanggord et al., 1980).

Other types of indirect photolyses are oxidation processes in which irradiation of natural materials produces free radical or singlet oxygen intermediates, which then react with a chemical to produce transformation products. Because the free radical or singlet oxygen intermediates react with the chemical in its ground state, it is usually convenient to consider such reactions as oxidation processes (see Section 2.3.8). In the evaluation of literature information or laboratory experiments, it is important to recognize that these oxidation processes, as well as direct photolysis or sensitized photolyses, may lead to oxidation and thereby complicate identification of the particular process for use in a generalized environmental assessment.

The rate of loss of a chemical due to an indirect process may be written in the general form

$$R_p' = k_p' [C] \qquad (2.22)$$

where k_p' is a first-order rate constant for the particular photoreaction. For a photosensitized process, k_p' would be a composite of terms, including the quantum yield for energy transfer from the natural substance excited state species to the chemical, the concentration of natural substance and the sunlight intensity. For the free radical or singlet oxygen reactions discussed in Section 2.3.8, the rate constant k_p' nominally would be equal to $k_{OX}[OX]$. As in direct photolysis, the value of k_p' must be referenced to a particular time period because the irradiating sunlight intensity and distribution responsible for these reactions will vary with time of day, season, and latitude.

Present knowledge of environmental photochemistry allows prediction of only the direct photolysis rate constant using equation (2.21). Although indirect photolyses can be faster than direct photolyses for some chemicals, incomplete knowledge of photosensitized reactions in the environment does not permit reliable predictions of k_p' values based on process data and

environmental parameters. Where literature information shows that indirect photolyses of a chemical in natural waters do occur, this information and the rate constant data are listed as a footnote on the data sheets in Section 3. Such data may be used at the option of the user. Process data for calculating the rate constants for direct photolysis of chemicals in aquatic environments are described below.

Absorption Spectrum Coefficients, ϵ_λ (in $M^{-1} cm^{-1}$). The absorption coefficients of the chemical are determined from the uv-visible spectrum of the chemical and are used with sunlight photon flux data, I_λ, to calculate the direct photolysis rate constant, k_p. The value of k_p may be calculated by computer (Zepp and Cline, 1977) or by manual calculation (Mabey et al., 1980). The ϵ_λ values are given at the wavelengths required for the k_p calculation computer program of Zepp and Cline (1977).

The absorption spectrum coefficients, ϵ_λ, for organic chemicals in this report are given as follows on the data sheets in Section 3:

(1) If the chemical has no significant absorptions above 290 nm, the code PNES (photolysis not environmental significant) is entered on the data sheet along with the source of this conclusion.

(2) If no spectra are available, the space is left blank. Chemicals in this category are known or suspected to have significant absorptions above 290 nm by analogy to similar chemicals structures and will require laboratory measurements to obtain data.

(3) When ϵ_λ data are available, DATA-ATT is entered in the value space to signify data attached, and the data are given in a footnote. If a published absorption spectrum is available but not suitable for accurate calculation of ϵ_λ values, SPEC-ATT is entered in the value space to signify that the spectrum is attached, and the spectrum is located by a footnote. Although some of these spectra were obtained in nonaqueous solvents, they are useful for a qualitative assessment of the possible importance of photolysis.

Reaction Quantum Yield, ϕ, (unitless). The reaction quantum yield is the efficiency with which light absorbed by a chemical results in transformation of the chemical and is defined as the ratio of the number of moles of chemical transformed to the number of einsteins (a light flux quantity) absorbed by the chemical. The reaction quantum yield is used

with ε_λ data and light flux data (an environmental parameter) to calculate the rate constant for direct photolysis, k_p. Values of ϕ are given on the data sheets along with the source of the value; when PNES is entered for the absorption spectrum coefficients, PNER is entered for the ϕ value, indicating that the reaction quantum yield is not environmentally relevant.

Photolysis Rate Constant, k_p (hr^{-1}). Some literature data are available for photolysis experiments conducted in sunlight, but without any measurements of ε_λ or ϕ. The rate constants for these experiments are entered as k_p values and with appropriate information (such as season, latitude) as may be available or surmised from the literature reference. In most cases, additional comments are also provided as footnotes.

Where data are available for ε_λ and ϕ, a value of k_p is calculated for a particular stated time interval to assist the reader who does not have access to I_λ data for calculating k_p. The source of such calculated values is usually the computer program SOLAR of Zepp and Cline (1977), and is designated CC-SOLAR, meaning computer calculated using the SOLAR program.

2.3.8 Oxidation Rate Constants

Chemical oxidation of organic chemicals in aquatic environments may occur due to several different oxidants, among which are singlet oxygen ($^1O_2$), alkyl peroxyl radical ($RO_2\cdot$), alkoxy radical ($RO\cdot$), or hydroxyl radical ($\cdot OH$). As discussed in Section 2.3.7, the source of these oxidants is primarily photochemical, but since the oxidants react with chemicals in their ground state, and oxidation therefore does not involve the photo-chemistry of the chemical itself, oxidations are reasonably considered as discrete processes apart from photochemistry.

Each oxidant has a unique reactivity toward organic moieties, and the relative as well as absolute concentrations of these oxidants will probably vary with environmental parameters such as concentrations , origin of humic-fulvic materials, and sunlight intensity. Therefore, the application of an "average oxidant concentration" concept to predict a total oxidation rate is not recommended.

Literature information has reported data on oxidation of organic

chemicals by oxy radicals such as $RO_2 \cdot$ and $^1O_2$. The laboratory study conducted by Mill et al. (1980) using natural waters indicates that $RO_2 \cdot$ radical concentrations of $\sim 1 \times 10^{-9}$ M may be present in the surface waters of sunlit water bodies. Oxidation reactions initiated by $RO_2 \cdot$ include the following:

$$RO_2 \cdot + -\overset{|}{\underset{|}{C}}-H \longrightarrow RO_2H + -\overset{|}{\underset{|}{C}} \cdot$$

$$RO_2 \cdot + \overset{\diagdown}{\underset{\diagup}{C}}=C\overset{\diagup}{\underset{\diagdown}{}} \longrightarrow RO_2-\overset{|}{\underset{|}{C}}-\overset{|}{\underset{|}{C}} \cdot$$

$$RO_2 \cdot + ArOH \longrightarrow RO_2H + ArO \cdot$$

$$RO_2 \cdot + ArNH_2 \longrightarrow RO_2H + Ar\overset{\bullet}{N}H$$
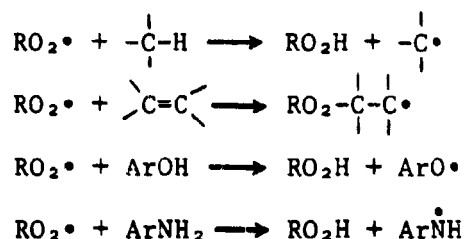
Of these reactions, the last two are quite rapid in aquatic environments ($t_{\frac{1}{2}} <$ several days), whereas the others are slower and usually will not be important for most chemicals.

Zepp et al. (1978) have shown that $^1O_2$ can be formed at $\approx 1 \times 10^{-12}$ M concentrations in sunlit natural waters. The most important reactions for $^1O_2$ with organic chemicals are those involving reaction with olefinic moieties (Ranby and Rabek, 1978).

$$^1O_2 + \overset{\diagdown}{\underset{\diagup}{C}}=C\overset{\diagup CH_2^-}{\underset{\diagdown}{}} \longrightarrow -\overset{|}{\underset{|}{C}}-C=CH \quad \overset{|}{\underset{OOH}{}}$$

$$\longrightarrow \overset{\diagdown}{\underset{\diagup}{C}}-C\overset{\diagup CH_2^-}{\underset{\diagdown}{}} \longrightarrow Products \quad \underset{O-O}{|\ |}$$
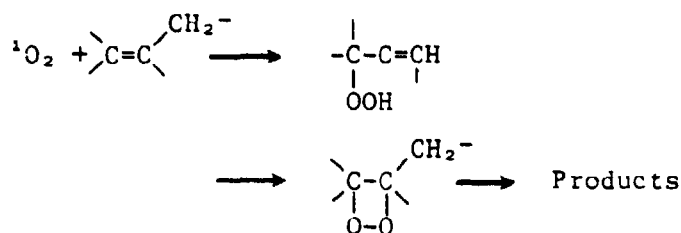
Some rate constants for $^1O_2$ and $RO_2 \cdot$ are listed in a review by Mill (1980).

The rate of loss of organic chemicals R_{OX} by oxidation is

$$R_{OX} = k_{RO_2 \cdot}[RO_2 \cdot][C] + k_{^1O_2}[^1O_2]C + k_{OX}[OX][C] \qquad (2.23)$$

where k_{OX} and [OX] are the rate constants and concentration values for other unspecified oxidants. Only data for second-order rate constants $k_{RO_2 \cdot}$ and $k_{^1O_2}$ have been estimated for this report. When two rate constants are given on the data sheets, the second-order rate constants should be multiplied by their respective oxidant concentrations to determine which of the first-order rate constant values is larger, and that rate constant should be used for an assessment.

Apart from a direct measurement of a rate constant at a specific temperature (which is rare), most rate constants in this report were obtained either from extrapolation of a rate constant for the organic chemical measured at another temperature or from a correlation of structure with reactivity as discussed below.

Rate Constant for Oxidation by Peroxyl Radical, $RO_2\bullet$, k_{OX} $(M^{-1} hr^{-1})$
Because many chemicals in the priority pollutant list have several kinds of reactive centers for oxidation by $RO_2\bullet$, the overall rate constant k_{RO_2} was obtained by first calculating the individual rate constants for each reactive site and then summing these rate constants. For example, acrolein has two reactive sites: (1) addition to the double bond and (2) H-atom transfer from the carbonyl

$$RO_2\bullet + CH_2=CHCHO \xrightarrow{k_1} RO_2\overset{\backslash}{C}-\overset{\bullet}{\underset{|}{C}}-CHO \qquad (2.24)$$

$$RO_2\bullet + CH_2=CHCHO \xrightarrow{k_2} CH_2=CH\overset{\bullet}{C}O + RO_2H \qquad (2.25)$$
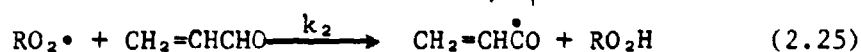
$$k_{RO_2} = k_1 + k_2$$

For aldrin, there are two kinds of double bonds and three kinds of CH bonds. Each rate constant was estimated, but since only the addition to the unsubstituted bond was very fast, the other reactions were ignored. When there were more than one -CH bond of a given kind, the rate constant was multiplied by the number of similar -CH bonds to give the correct total rate constant for oxidation of that CH bond.

Two kinds of procedures were used to calculate individual k_{OX} values for $RO_2\bullet$ reactions. In the first, when a structure was analogous to another chemical structure with a measured rate constant at a similar temperature, the measured rate constant was used directly (Hendry et al., 1974). (The -CHO bond in acrolein is an example.) The second procedure, used most often, is based on structure-reactivity relations established by Howard and coworkers for H-atom transfer (Korchek et al., 1972) and addition to double bonds (Howard, 1972), as shown here.

For the hydrogen atom transfer reaction

$$\log k_{RO_2} = 18.96-0.2 [D(R-H)] \qquad (2.26)$$

where D(R-H) is the bond dissociation energy of the CH bond.

For the RO_2 addition to double bonds

$$\log k_{RO_2} = [16.54-0.2D(xCR_2-H)]/0.75 \qquad (2.27)$$

where $D(XCR_2-H)$ is the bond dissociation energy of a species that gives
the radical formed by RO_2 addition and where RO_2 is assumed to have the same
effect as Me on $D(C-H)$. Thus for oxidation of vinyl chloride

$$RO_2\cdot + {}_{/}^{\backslash}C=C_{\backslash}^{/}Cl \longrightarrow RO_2\overset{|}{\underset{|}{C}}-\overset{/}{\underset{|}{C}}\cdot\,Cl$$
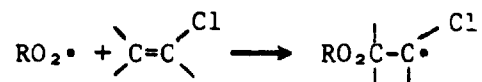
the closest analog would be $MeCH_2\overset{\bullet}{C}HCl$, and the value of $D(MeCH_2CHCl-H)$
would be used in equation (2.27). Bond dissociation energies were taken
from Furuyama et al. (1969).

Rate Constant for Oxidation by Singlet Oxygen, ${}^1O_2$, k_{ox} $(M^{-1}\ hr^{-1})$.
Only a few of the chemicals discussed in this report are reactive toward ${}^1O_2$;
these include some polycyclic aromatic and a few olefinic double bond or
diene systems. When no reactive center was recognized, chemicals were
assigned $k_{{}^1O_2} < 3600$ or $< 360\ M^{-1}\ h^{-1}$. All reactive chemicals were assigned
rate constants by analogy with similar structures having shown rate constants
for reaction with singlet oxygen. For cyclic olefins, the values of Matsuuro
et al. (1973) were used. For alicyclic olefins and other structures, the
rate data summarized by Gollnick (1978) were used.

Since all oxidation rate constants given in Section 3 were calculated
by the above methods, the data source code C-OX (calculated-oxidation) is
entered for all values.

2.3.9 Hydrolysis Rate Constants

Hydrolysis refers to reaction of a chemical with water, usually
resulting in the introduction of a hydroxyl function into a molecule and
loss of a leaving group -X

$$R-X + H_2O \longrightarrow ROH + HX$$

The hydrolyses of some classes of compounds are catalyzed by acid or base,
and therefore the hydrolysis rates of these chemicals in the environment
can be pH dependent. The subject of hydrolysis in aquatic systems has

been reviewed in detail by Mill et al. (1980), and an extensive compilation of hydrolysis data was published in a review by Mabey and Mill (1978).

The rate of hydrolysis of a compound at a specific pH value is given by the equation

$$R_H = k_h[C] = (k_A[H^+] + k_N + k_B[OH^-])[C] \qquad (2.28)$$

where k_h is the first-order rate constant for hydrolysis at the pH, k_A and k_B are second-order rate constants for acid- and base-promoted hydrolyses, and k_N is the first-order rate constant for the pH-independent, neutral hydrolysis process. Using the autoprotolysis equilibrium expression

$$[H^+][OH^-] = K_w, \qquad (2.29)$$

equation (2.28) can be rewritten as

$$k_h = k_A[H^+] + k_N + \frac{k_B K_w}{[H^+]} \qquad (2.30)$$

Equation (2.30) shows that k_h will be dependent on the pH of the aquatic system and on the relative values of k_A, k_B, and k_N. There is at present no reliable information to show that hydrolysis rates in aquatic environments will be catalyzed by species other than $[H^+]$ or $[OH^-]$.

The hydrolysis rate constants k_A, k_B, and k_N used to calculate k_h as a function of pH are described below along with the source codes for calculating or estimating the values of the rate constants.

Acid-Promoted Rate Constant, k_A (M^{-1} hr^{-1}). This rate constant is for the acid-promoted hydrolysis of a chemical. In regions where only k_A contributes to hydrolysis (i.e., $k_A[H^+] \gg k_N + k_B[OH^-]$), k_h will decrease by a factor of 10 for each 1-unit increase in pH.

Base-Promoted Hydrolysis Rate Constant, k_B (M^{-1} hr^{-1}). This rate constant is for the base, (OH^-), promoted hydrolysis of a chemical. In regions where only k_B contributes to hydrolysis, k_h will increase by a factor of 10 for each 1-unit increase in pH.

Neutral-Hydrolysis Rate Constant, k_N (hr^{-1}). This rate constant is for the pH-independent hydrolysis of a chemical.

Data or sources pertaining to the hydrolysis of the organic chemicals have been entered in the data sheets in several ways. When a chemical structure had no hydrolyzable functional groups, NHFG is entered. When chemical hydrolysis occurs only at extreme pH values or temperatures or with catalysts not available in aquatic environments, HNES is entered (hydrolysis not environmentally significant). The terms NACM (or NBCM) are used to indicate that no acid (or base) catalyzed mechanism involving H^+ (or OH^-) species is known. For all such cases, zero is entered for the value of the process data to clearly eliminate the particular process from further consideration. For alkyl halides, Mabey and Mill (1978) have shown that the acid- and base-catalyzed terms in equation (2.28) are not important compared with the neutral hydrolysis term, and therefore HPHI (hydrolysis pH-independent) is entered. Since k_A and k_B are not zero, but are insignificant for environmental assessment purposes, a hyphen has been entered for the process data value. Other data for hydrolysis are referenced, or the rationale is explained in footnotes to the data sheet.

2.3.10 Biotransformation Rate Constants

Biotransformations are undoubtedly important processes for degradation of chemicals in aquatic environments, resulting in hydrolysis, oxidation, and reduction of the chemical structure to ultimately produce carbon dioxide and water. The complex factors influencing the biotransformation of a chemical include pH, temperature, dissolved oxygen, available nutrients, the presence of other organic chemicals (synthetic or naturally occurring) that may serve as cometabolites or alternative energy sources, and the populations and types of organisms capable of transforming the chemical. For most assessments, the initial biotransformation step is of prime importance (i.e., removal of the specific chemical from the environment). However, the biotransformation process is still too complex to reliably predict a biotransformation rate constant using theoretical approaches such as those available for chemical and physical processes.

Maki et al. (1980) recently reviewed some of the aspects of the measurement of biotransformation rates and the use of such data. The rates of biotransformation are complex functions of chemical concentration and

microbial biomass. However, at the concentrations of a chemical in the environment (<1 ppm), the rates may be expected to follow second-order kinetics, being first order in chemical and first order in biomass. Furthermore, the microorganism growth due to consumption of the chemical may not be significant; therefore, the rates of biotransformation are pseudo-first order as a function of the chemical concentration.

The biotransformation data given in Section 3 were estimated for the approach described by Baughman et al. (1980), in which the rate of biotransformation of a chemical, R_B, is given by the expression

$$R_B = k_b [B] [C] \tag{2.31}$$

where k_b is a second-order rate constant for biotransformation of a chemical by bacteria of population [B] in the solution phase of the water column. When k_b is given in ml cell^{-1} hr^{-1}, the units of [B] are in cell ml^{-1}. Because data for k_b were not available for most chemicals covered by this report, the water column/bacteria rate constants were estimated solely for use in aquatic fate modeling by EPA. These data were estimated based on relative rates of biodegradation of the chemicals as reported in literature, based on structural analogies, and using the judgment of SRI staff with expertise in biotransformation studies. Chemicals were placed in one of five reactivity categories. Each category has a nominal rate constant that differs by a 30-fold factor from adjoining categories. The categories and rate constants are listed in Table 2.2.

The user of the biotransformation data is reminded that these data have been estimated and that appropriate caution should be exercised in the use of the data (see 3.1). For some chemicals where hydrolysis or volatilization is fast, and biotransformation will therefore not be important in aquatic systems, a hyphen is entered for the data value on the data sheets in Section 3, and the data source indicates that hydrolysis is fast (HF) or that volatilization is fast (VF), and therefore no biotransformation data (NBD) are estimated.

Table 2.2

ESTIMATED RATE CONSTANTS (ml cell^{-1} hr^{-1}) FOR BIOTRANSFORMATION
OF CHEMICALS BY BACTERIA IN WATER BODY SOLUTION PHASE

Category I 3 x 10^{-6}	Category II 1 x 10^{-7}	Category III 3 x 10^{-9}	Category IV 1 x 10^{-10}	Category V 3 x 10^{-12}
Phenol	4-Cl-phenyl phenyl ether	Acrolein	DDD	Chlordane
	Benzene	Aldrin	Endrin	DDE
	Toluene	Isophorone	Endosulfan sulfate	DDT
	2-Cl phenol	Endosulfan	Hexa-Cl-cyclohexane	Dieldrin
	2,4-Di-Cl phenol	Endrin aldehyde	Lindane	Heptachlor epoxide
	4-Nitro phenol	2-Cl-naphthalene	TCDD	Toxaphene
	2,4-Dimethyl phenol	Bis(2-Cl-ethyl)ether	Tetra-Cl-methane	.1s(2-Cl-ethoxy) methane
	4-Nitro phenol	4-Br-phenyl phenyl ether	1,2-Di-Cl-ethane	Hexa-Cl-benzene
	2,4-Dimethyl phenol	Cl-benzene	Tri-Cl-ethene	Benzo(b)fluoranthene
	Diethyl phthalate	Ethyl benzene	Tetra-Cl-ethene	Benzo(k)-fluoranthene
	Naphthalene	Nitrobenzene	1,2-Di-Cl-propane	Benzo[ghi]perylene
		2,4,6-Tri-Cl phenol	1,3-Di-Cl-propane	Benzo[a]pyrene
		Penta-Cl phenol	Hexa-Cl-ethane	Dibenzo[a]anthracene
		2-Nitro phenol	Hexa-Cl-butadiene	Indeno[1,2,3-cd]pyrene
		2,4-Dinitro phenol	Hexa-Cl-cyclo pentadiene	Dimethyl nitrosamine
		E-Cl-m-cresol	Br-di-Cl-methane	3,3'-Di-Cl-benzidine
		4,6-Dinitro-o-cresol	Di-Br-Cl-methane	Di-n-propyl nitrosamine
		Butyl benzyl phthalate	Tri-Br-methane	1,1,2-Tri-Cl-ethane
		Acenaphthene	Bis(2-Cl-isopropyl)ethyl	1,1,2,2-Tetra-Cl-ethane
		Acenaphthylene	2-Cl-ethyl vinyl ether	
		Anthracene	1,2-Di-Cl-benzene	
		Acrylonitrile	1,3-Di-Cl-benzene	(Category IV cont.)
		Fluorene	1,4-Di-Cl-benzene	
			1,2,4-Tri-Cl-benzene	Diphenyl nitrosamine
			2,6-Dinitrotoluene	Benzidine
			Benzo[a]anthracene	1,2-Diphenylhydrazine
			Chrysene	
			Fluoranthene	
			Pyrene	

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2.4 REFERENCES

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SECTION 3

PROCESS DATA FOR TRANSFORMATION AND TRANSPORT OF
CHEMICALS IN AQUEOUS SOLUTION

3.1 ORGANIZATION OF DATA SHEETS AND SOURCES OF DATA

Process data for organic priority pollutant chemicals are given
for the following properties or processes:

- Physical properties and transport processes

    Molecular weight

    Melting point

    Boiling point

    Ionization constant

    Partition constants

    Volatilization constants

- Transformation processes

    Photolysis data

    Oxidation rate constants

    H·drolysis rat. constants

    Biotransformation rate constant.

For each property or process, the property, rate constant, or parti-
tioning constant is de ned in Sections 2.3.2 through 2.3.10. These
section also give the units of the values reported and discuss the sig-
nificance and use of each value in terms of the particular process and
how it is used in calculating rate or equilibrium constants for environ-
mental assessments. The sources of the individual process data are also
discussed in these sections. The units for each value are also listed on
the data sheets for the individual chemicals.

The data in this report were estimated for the use of EPA-OWRS in
modeling the aquatic fate of the organic priority pollutants. For most
chemicals in this report the process data are useful for a general,

nonsite-specific evaluation of the persistence of the chemical. In modeling such situations, any uncertainties in the data are likely to be equalled or surpassed by the unknowns or variabilities in the environmental parameters. The process data also are generally useful for identifying processes that will be most important under general or specific aquatic conditions. When such processes are identified, the user of the data should review the sources and reliability of the data to determine what limitations, uncertainties, or weaknesses exist and therefore whether the data need improvement in the context of a particular use. This report represents information available as of mid-1980; the user is encouraged to seek more recent data to augment this information.

Data for the processes that occur in aquatic environments have been obtained by several methods. Some methods for calculating data based on structure reactivity relationships or empirical correlations were developed for use in environmental assessments. Other methods were developed in other basic and applied research activities in physical and life sciences. Data presented in this report were obtained by three methods; review of the literature, calculation, and estimation, as discussed below.

Environmental literature and other chemical and biological literature were the sources of most data. In many cases data were taken directly from the 1979 EPA report "Water-Related Environmental Fate of 129 Priority Pollutants" by Callahan et al. For some chemicals, the original paper cited in the Callahan report was critically reviewed to determine the source or reliability of the data. Other data were obtained from recent literature, from colleagues in the environmental research field, or from research under way at SRI.

Other data in this report were obtained from calculations based cn empirical correlations or on structure reactivity relationships. The rate constants for oxidation of chemicals by singlet oxygen and alkylperoxyl radical were calculated using structure reactivity relationships developed, in part, at SRI (see Section 2.3.9; Mill, 1979). Most of the partitioning data (K_{ow}, K_{oc}, S_w, and K_b) were obtained using the K_{ow} calculations and correlation equations described in Section 4. Data for volatilization rate constant calculations were calculated using the theory

and methods described in Section 5.

When reliable data suitable for use in aquatic fate assessments were
not available, the data were estimated. Estimated data should be clearly
differentiated from calculated data in that the latter has a defined
mathematical basis, whereas estimations, although based on the expertise
and judgment of a person experienced in research on a particular process,
have not been documented by experimental work. Estimated data are preceded
by the notation (E) on the data sheets. These data should be used only
to establish what processes may be important for a chemical in an aquatic
environment. If process data preceded by (E) are found to be important,
the value should be measured in laboratory studies or calculated using
structure reactivity correlations, if available. If process data preceded
by (E) are found to be unimportant, the value may be calculated or measured
if a more reliable and complete data base is desired.

For some processes or properties, conflicting data required that SRI
staff choose a "best" value for inclusion in this report. The choice of
the value was made based on the experience and judgment of the SRI staff
member. Whenever available, the reliability of the data is given as a standard
deviation; when no statistics were available, the value is given to the
appropriate number of significant figures as judged appropriate by the
author responsible for the evaluation.

The basis for the choice of any datum has not been detailed in this
report since such efforts would require extensive discussion. Users of
the data are, of course, encouraged to compare these data with other
values in current literature to determine the reliability of the data or
the range of values that have been reported. The persons responsible for
evaluations of the several kinds of process data are as follows:

> Partitioning constants: T. Podoll, J. Gates, and J. Jaber
> Volatilization constants: J. Smith, D. Haynes, and H. Jaber
> Photolysis data: W. Mabey
> Oxidation rate constants: T. Mill
> Hydrolysis rate constants: W. Mabey
> Biotransformation rate constants: T.-W. Chou

In the preparation of the data sheets, an effort has been made to enter information for each process on every chemical. The value and data source spaces have been left blank only when nothing is known about the process/property for a particular chemical. In these cases, data should be obtained from laboratory studies because sufficient information is not available for any theoretical or empirical estimates.

When no specific data are available, but evidence clearly shows that no reaction can occur in aquatic environments, this information has been indicated (i.e., no hydrolyzable functional groups and therefore no hydrolysis will occur).

The sources of data on the following data sheets are described in one of three ways:

(1) References are given by authors and year of referenced paper. Citation of a reference means that this publication was critically reviewed and that data were taken directly from the reference. References are given at the end of the section.

(2) A code is given in many cases to describe the basis for calculating or estimating the data. Thus CC-Kow entered as a source for K_{ow} values indicates that the octanol-water partition coefficient, K_{ow}, was computer calculated using the computer program described in Section 4. Similarly, C-Koc f Kow signifies that K_{oc} was calculated from K_{ow} value using a K_{oc}-K_{ow} correlation equation (see Section 4). An alphabetical list of the codes is given on the following pages. Where possible, each code refers to a section where the particular source is discussed more completely.

Data from the CRC Handbook or from the two-volume report "Water-Related Environmental Fate of 129 Priority Pollutants" by Callahan et al. (1979) have also been listed in code (CRC and WREF, respectively). Data cited by WREF were taken directly from the EPA report; the original paper was not reviewed.

(3) A footnote is used to describe a source of data that is not common enough to justify a code. The footnotes are noted in brackets and listed at the bottom of the second page of the data sheets.

As a convenience to the user, the chemicals are listed by formula and data sheet number following the List of Source Codes.

LIST OF SOURCE CODES

CC-Kow

Value of K_{ow} was obtained by computer calculation, using FRAGMENT calculation procedure (See Section 4.3).

CC-SOLAR

Direct photolysis rate constant was calculated using the SOLAR computer program (Zepp and Cline, 1977).

C-CT/CRC

Vapor pressure value was calculated from data in critical tables. Weast, R. C., ed., 1973. **Handbook of Chemistry and Physics**, 54th ed. CRC Press, Cleveland, Ohio. D-162.

C-DC.7

Reaeration rate ratio was calculated from D_ℓ^c/D_ℓ^o to 0.7 power (See Section 5.)

C-kB

Base catalyzed rate constant k_B was calculated from information in Callahan et al. (1979).

C-KBASE

Acid-catalyzed rate constant was calculated from k_B; assumption is made that acid and base catalyzed hydrolysis rate constants are equal at pH 5.0 (Mabey and Mill, 1978). As a result,

$$10^{-5} \, k_A = 10^{-9} \, k_B$$

or

$$k_A = 10^{-4} \, k_B$$

The value of k_A is probably good within a factor of 10.

C-KB f Kow

The value of K_B was calculated from the K_B-K_{ow} correlation of Baughman and Paris (1981) discussed in Section 4.2.3.

$$\log K_B = 0.907 \log K_{ow} - 0.21$$

C-Koc f Kow   The value of K_{oc} was calculated from the K_{ow} value
                using the equation $K_{oc} = 0.48K_{ow}$. Subsequent to the
                writing of Section 4, where several $K_{oc}-K_{ow}$ correlations
                are discussed, Hassett et al. (1980) have reported the
                following correlation equation for sorption of poly-
                nuclear aromatic chemicals onto whole sediments (i.e.,
                unfractionated sediments):

$$\log K_{oc} = \log K_{ow} - 0.317$$

                Another similar correlation equation for sorption of
                some 40 chemicals to whole sediments has been found by
                Karickhoff (1980):

$$\log K_{oc} = 0.987 \log K_{ow} - 0.336$$

                The equation used to calculate K_{oc} values in this
                report is the nonlogarithmic form of the equation of
                Hasset et al. (1980) (see Section 4).

C-OX   Oxidation rate constants are calculated, using functional
                group reactivity toward peroxyl radical (RO_2) and singlet
                oxygen ($^1O_2$) (see Section 2.3.8).

CRC   Weast, R.D., ed., 1975. Handbook of Chemistry and
                Physics, 56th ed. CRC Press, Cleveland, Ohio.

C-Sw f Kow   The value of S_w was calculated from the K_{ow} value using
                the equation of Yalkowsky and Valvani (1980); the cal-
                culation of S_w values is discussed in Section 4.2.3.

C-VP--°/S--°   Henry's constant, H_c, was calculated from vapor pressure
                and water solubilities at the temperatures given (°C),
                respectively. When the temperatures were the same,
                only one temperature is given (see Section 2.3.6).

DATA-ATT   UV-visible absorption coefficients are listed in
                footnotes (data attached).

E-AC-H   Rate constant was estimated by analogy to chlcroform. Mabey and Mill (1978) have calculated that the rate of the base catalyzed process for chloroform is equal to the neutral hydrolysis process at pH 6, or k_B [OH] = k_N when [OH$^-$] = $10^{-\varepsilon}$.

If the assumption is made that the same expression holds for all trihalomethanes, then $k_N = 10^{-8}\ k_B$.

E-APAH   This estimated value is the average of reaction quantum yields for several polycyclic aromatic hydrocarbons measured by Zepp and Schlotzhauer (1980).

E-KB   Estimate of biotransformation rate constant, k_b is based on relative rates of transformation reported in literature or on structure-reactivity analogies as judged by reviewer.

E-H   Estimate of hydrolysis rate constant is based on analogy to reactivity of other similar chemicals and judgment of reviewer.

E-P   This estimate of photolysis rate constant for environmental significance of photolysis is based on analogy to reactivity of other chemicals and judgment of reviewer.

HF-NBD   Hydrolysis is too fast for biotransformation studies to be conducted. No biotransformation data are therefore available.

HNES   Hydrolysis is not environmentally significant. Chemical hydrolysis occurs only at extreme pHs or temperatures or with catalysts not avilable in aquatic environments.

HPHI   Hydrolysis is pH-independent; this assignment is based on finding of Mabey and Mill (1978) that alkyl halides are, in general, hydrolyzed by the neutral hydrolysis process in the pH region from pH 3 to approximately 10, and without any evidence of base or acid catalyzed mechanisms.

NACM   No acid catalyzed mechanism.

NAV   Reaeration rate ratio is not applicable for calculating
                   the rate constant for volatilization (see 2.3.6).

NHFG   No hydrolyzable functional groups in molecule.

pK-NER pK_A or pK_B is not environmentally relevant for fate of
                   chemical.

PNER   Photolysis is not environmentally relevant.

PNES   Photolysis is not environmentally significant.

SPEC-ATT   UV-visible absorption spectrum is shown in footnotes
                   (spectrum attached).

UV-ATLAS   UV-visible spectrum is found in UV Atlas (Perkampus,
                   et al., 1966).

VF-NBD   Volatilization is too fast for biotransformation studies
                   to be conducted, and no biological data are available.

WREF   Water-related environmental fate of 129 priority
                   pollutants by Callahan et al. (1979). U.S. Environmental
                   Protection Agency, Office of Water Planning and Standards.
                   EPA-440/4-79-029.

FORMULA INDEX TO DATA SHEET

FORMULA	DATA SHEET NUMBER	CHEMICAL NAME
C_1Cl_4	32	Tetrachloromethane
$C_1Cl_2F_2$	53	Dichlorodifluoromethane
$C_1Cl_3F_1$	54	Trichlorofluoromethane
$C_1H_1Br_1Cl_2$	50	Bromodichloromethane
$C_1H_1Br_2Cl_1$	51	Dibromochloromethane
$C_1H_1Br_3$	52	Tribromomethane
$C_1H_1Cl_3$	31	Trichloromethane
$C_1H_2Cl_2$	30	Dichloromethane
$C_1H_3Br_1$	49	Bromomethane
$C_1H_3Cl_1$	29	Chloromethane
C_2Cl_4	44	Tetrachloroethene
C_2Cl_6	39	Hexachloroethane
$C_2H_1Cl_3$	43	Trichloroethene
$C_2H_2Cl_2$	42	1,2-trans-Dichloroethene
$C_2H_2Cl_2$	41	1,1-Dichloroethene
$C_2H_2Cl_4$	38	1,1,2,2-Tetrachloroethane
$C_2H_3Cl_1$	40	Chloroethene
$C_2H_3Cl_3$	36	1,1,1-Trichloroethane
$C_2H_3Cl_3$	37	1,1,2-Trichloroethane
$C_2H_4Cl_2$	34	1,1-Dichloroethane
$C_2H_4Cl_2$	35	1,2-Dichloroethane
$C_2H_4Cl_2O_1$	55	Bis(2-chloromethyl)ether
$C_2H_5Cl_1$	33	Chloroethane
$C_2H_6N_2O_1$	107	Dimethylnitrosamine
$C_3H_3N_1$	113	Acrylonitrile
$C_3H_4Cl_2$	46	1,3-Dichloropropene
$C_3H_4O_1$	1	Acrolein
$C_3H_6Cl_2$	45	1,2-Dichloropropane
C_4Cl_6	47	Hexachlorobutadiene
$C_4H_7Cl_1O_1$	58	2-Chloroethyl vinyl ether
$C_4H_8Cl_2O_1$	56	Bis(2-chloroethyl)ether

FORMULA	NUMBER	CHEMICAL NAME
C_5Cl_6	48	Hexachlorocyclopentadiene
$C_5H_{10}Cl_2O_2$	61	Bis(2-chloroethoxy)methane
C_6Cl_6	68	Hexachlorobenzene
$C_6H_1Cl_5O_1$	78	Pentachlorophenol
$C_6H_3Cl_3$	67	1,2,4-Trichlorobenzene
$C_6H_3Cl_3O_1$	77	2,4,6-Trichlorophenol
$C_6H_4Cl_2$	64	1,2-Dichlorobenzene
$C_6H_4Cl_2$	65	1,3-Dichlorobenzene
$C_6H_4Cl_2$	66	1,4-Dichlorobenzene
$C_6H_4Cl_2O_1$	76	2,4-Dichlorophenol
$C_6H_4N_2O_5$	81	2,4-Dinitrophenol
$C_6H_5Cl_1$	63	Chlorobenzene
$C_6H_5Cl_1O_1$	75	2-Chlorophenol
$C_6H_5N_1O_2$	70	Nitrobenzene
$C_6H_5N_1O_3$	79	2-Nitrophenol
$C_6H_5N_1O_3$	80	4-Nitrophenol
C_6H_6	62	Benzene
$C_6H_6Cl_6$	14	α-Hexachlorocyclohexane
$C_6H_6Cl_6$	15	β-Hexachlorocyclohexane
$C_6H_6Cl_6$	16	δ-Hexachlorocyclohexane
$C_6H_6Cl_6$	17	Lindane
$C_6H_6O_1$	74	Phenol
$C_6H_{12}Cl_2O_1$	57	Bis(2-chloroisopropyl)ether
$C_6H_{14}N_2O_1$	109	Di-n-propylnitrosamine
$C_7H_6N_2O_4$	72	2,4-Dinitrotoluene
$C_7H_6N_2O_4$	73	2,6-Dinitrotoluene
$C_7H_6O_5$	84	4,6-Dinitro-o-cresol
$C_7H_7Cl_1O_1$	83	p-Chloro-m-cresol
C_7H_8	71	Toluene
C_8H_{10}	69	Ethylbenzene
$C_8H_{10}O_1$	82	2,4-Dimethylphenol
$C_9H_6Cl_6O_3S_1$	8	α,β-Endosulfan
$C_9H_6Cl_6O_4S_1$	9	Endosulfan sulfate
$C_9H_{14}O_1$	18	Isophorone
$C_{10}H_5Cl_7$	12	Heptachlor

FORMULA	NUMBER	CHEMICAL NAME
$C_{10}H_5Cl_7O_1$	13	Heptachlor epoxide
$C_{10}H_6Cl_8$	3	Chlordane
$C_{10}H_7Cl_1$	28	2-Chloronaphthalene
$C_{10}H_8$	104	Naphthalene
$C_{10}H_{10}Cl_8$	20	Toxaphene
$C_{10}H_{10}O_4$	85	Dimethyl phthalate
$C_{12}H_4Cl_4O_2$	19	TCDD
$C_{12}H_8$	92	Acenaphthylene
$C_{12}H_8Cl_6$	2	Aldrin
$C_{12}H_8Cl_6O_1$	7	Dieldrin
$C_{12}H_8Cl_6O_1$	10	Endrin
$C_{12}H_8Cl_6O_1$	11	Endrin aldehyde
$C_{12}H_xCl_y$	21-27	PCBs; $x + y = 10$ and $2 \leq y \leq 10$
$C_{12}H_9Br_1O_1$	60	4-Bromophenyl phenyl ether
$C_{12}H_9Cl_1O_1$	59	4-Chlorophenyl phenyl ether
$C_{12}H_{10}$	91	Acenaphthene
$C_{12}H_{10}Cl_2N_2$	111	3,3'-Dichlorobenzidine
$C_{12}H_{10}N_2O_1$	108	Diphenylnitrosamine
$C_{12}H_{12}N_2$	112	1,2-Diphenylhydrazine
$C_{12}H_{12}N_2$	110	Benzidine
$C_{12}H_{14}O_4$	86	Diethyl phthalate
$C_{13}H_{10}$	102	Fluorene
$C_{14}H_8Cl_4$	5	DDE
$C_{14}H_9Cl_5$	6	DDT
$C_{14}H_{10}$	105	Phenanthrene
$C_{14}H_{10}$	93	Anthracene
$C_{14}H_{10}Cl_4$	4	DDD
$C_{16}H_{10}$	101	Fluroanthene
$C_{16}H_{10}$	106	Pyrene
$C_{16}H_{22}O_4$	87	Di-n-butyl phthalate
$C_{18}H_{12}$	99	Chrysene
$C_{18}H_{12}$	94	Benzo[a]anthracene

FORMULA	NUMBER	CHEMICAL NAME
$C_{19}H_{20}O_4$	90	Butyl benzyl phthalate
$C_{20}H_{12}$	95	Benzo[b]fluoranthene
$C_{20}H_{12}$	96	Benzo[k]fluoranthene
$C_{20}H_{12}$	98	Benzo[a]pyrene
$C_{22}H_{12}$	97	Benzo[ghi]perylene
$C_{22}H_{12}$	103	Indeno[1,2,3-cd]pyrene
$C_{22}H_{14}$	100	Benzo[a,h]anthracene
$C_{24}H_{38}O_4$	89	Bis(2-ethylhexyl)phthalate
$C_{24}H_{38}O_4$	88	Di-n-octyl phthalate

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SECTION 3.2. PESTICIDES

1. Acrolein
2. Aldrin
3. Chlordane (cis and trans isomers)
4. DDD
5. DDE
6. DDT
7. Dieldrin
8. Endosulfan (α and β isomers)
9. Endosulfan sulfate
10. Endrin
11. Endrin aldehyde
12. Heptachlor
13. Heptachlor epoxide
14. α-Hexachlorocyclohexane
15. β-Hexachlorocyclohexane
16. δ-Hexachlorocyclohexane
17. γ-Hexachlorocyclohexane (lindane)
18. Isophorone
19. TCDD
20. Toxaphene

$H_2C=CHC{\overset{O}{\underset{H}{<}}}$

1. ACROLEIN

CAS No. 107-02-8

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	56.06	
Melting point, °C	-87.7	WREF
Boiling point, °C	52.5	WREF
Ionization constant	pK-NER	

Partition constants: [1-1]

Water solubility, S_w (ppm)	2.1×10^5 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	1.02	CC-Kow
Sediment-water, K_{oc} (unitless)	0.49	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	0.44	C-KB f Kow

Volatilization constants: [1-1]

Henry's constant, H_c (atm m^3 mol^{-1})	5.66×10^{-5}	C-VP/S-20°
Vapor pressure, P_v (torr)	220 (20°C)	WREF
Reaeration rate ratio, k_v^C/k_v^O	NAV	

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1. ACROLEIN

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [1-2]	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude	[1-2]	
Oxidation constants at 25°C: [1-1]		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	1×10^7	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	3.4×10^3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	NHFG
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 3×10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

[1-1] The values of K_{ow}, K_{oc}, K_B, k_v^c/k_v^o, P_v and oxidation rate constants are calculated or given for the unhydrated acrolein species; hydration of acrolein may be extensive in aquatic environments, and the above properties will therefore be different than listed.

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1. ACROLEIN

[1-2]   UV spectrum of acrolein in hexane solvent is shown below
(UV Atlas, 1966). Acrolein undergoes rapid hydration
(t$_{1/2}$ < 1 day) to β-hydroxypropionaldehyde.   This hydration
destroys the chromophores that absorb light above 290 nm
and therefore the UV-spectrum of acrolein in water may be
insignificant above 290 nm (WREF).

λ (nm)
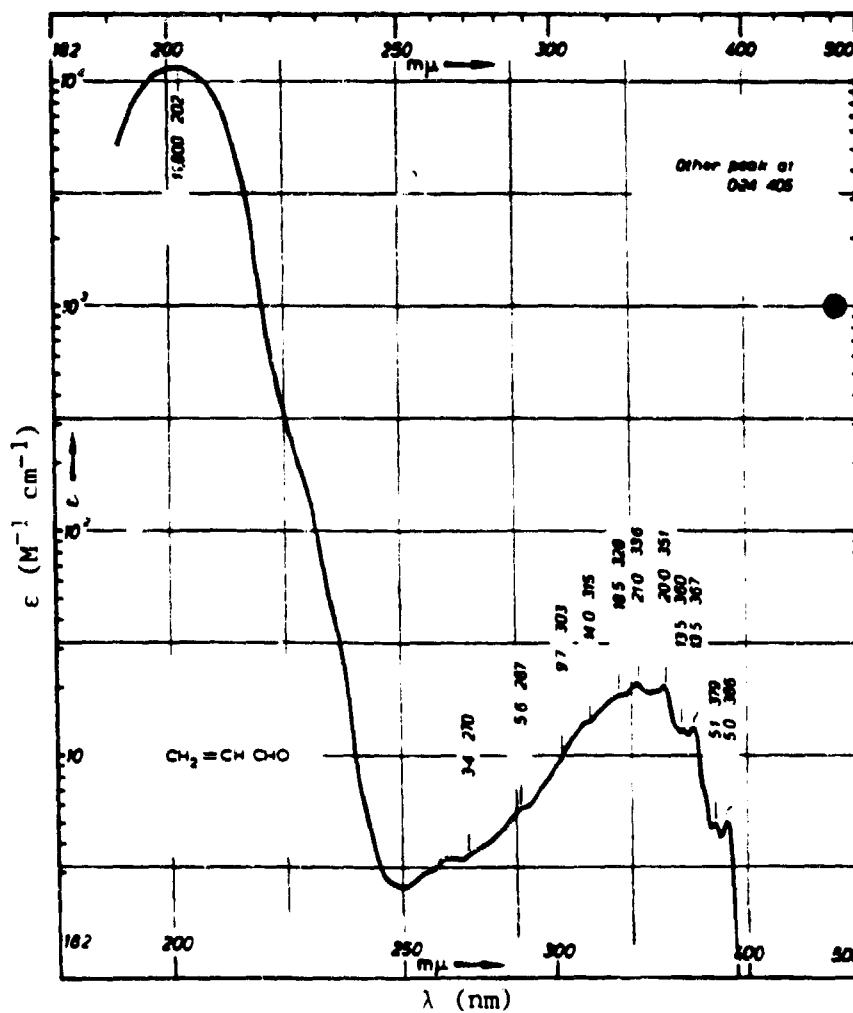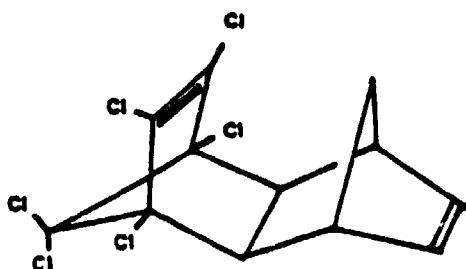
2. __ALDRIN__

CAS No. __309002__

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	365	
Melting point, °C	104-105	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.180 (25°C) [2-1]	WREF
Octanol-water, K_{ow} (unitless)	2.0×10^5	CC-Kow
Sediment-water, K_{oc} (unitless)	9.6×10^4	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	2.8×10^4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol^{-1})	1.6×10^{-5}	C-VP/S-25°
Vapor pressure, P_v (torr)	6×10^{-6} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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2. ALDRIN

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	5×10^3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b ($ml\ cell^{-1}\ hr^{-1}$)	(E) 3×10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

[2-1] Several water solubility values, ranging from 0.017-0.18 ppm, have been reported (WREF.)
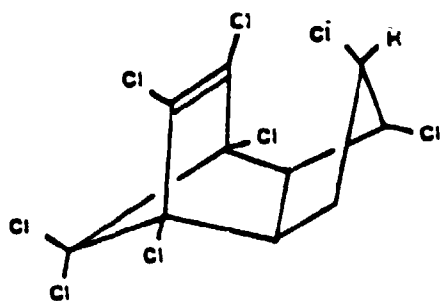
trans isomer [3-2]

3. CHLORDANE

CAS No. [3-1]

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	409.8	
Melting point, °C	[3-3]	WREF
Boiling point, °C	175 (2mm)	WREF [3-4]
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.056 (25°C) [3-5]	WREF
Octanol-water, K_{ow} (unitless)	3×10^5	CC-Kow
Sediment-water, K_{oc} (unitless)	1.4×10^5	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1} \right)$	4.0×10^4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	9.4×10^{-5}	C-VP/S-25°
Vapor pressure, P_v (torr)	1×10^{-5} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

3. CHLORDANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	$\sim$30	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}\ hr^{-1}$)	(E)3 x 10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

[3-1] Chemical Abstracts numbers are 5103-71-9 for trans isomer, 5103-74-2 for cis isomer.

3. CHLORDANE

[3-2]
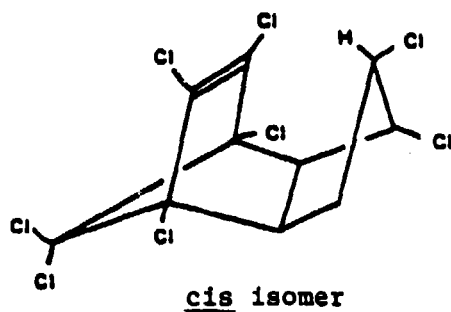
cis isomer

[3-3] Melting point 103.0 - 105.0 for trans isomer and 107.0 - 108.8 for cis isomer.

[3-4] Boiling point reported for a mixture of the isomers.

[3-5] Two solubility values, 0.056 ppm and 1.85 ppm were given in WREF. Solubility data are for a mixture of the isomers.
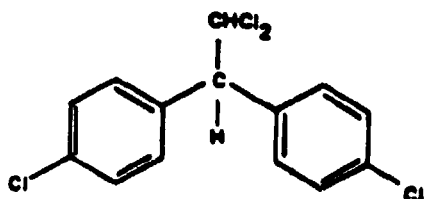
4. **DDD**

CAS No. 72548

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	320	
Melting point, °C	112	WREF
Boiling point, °C		
Ionization constant	pK–NER	

Partition constants:

Water solubility, S_w (ppm)	[4-1]	WREF
Octanol-water, K_{ow} (unitless)	1.6×10^6	CC–Kow
Sediment-water, K_{oc} (unitless)	7.7×10^5	C–Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	1.8×10^5	C–KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.2×10^{-8}	C–VP30°/S25°
Vapor pressure, P_v (torr)	[4-2]	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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4. DDD

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	$<5 \times 10^{-7}$	[4-3]
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<1600	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	5.0 (27°C)	WREF [4-4]
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	4×10^{-7} (27°C)	WREF [4-5]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[4-1]   Two water solubility values have been reported for the pp' isomer at 25°C: 0.02 ppm and 0.09 ppm. A value of 0.10 ppm has been reported for the op' isomer (WREF).

[4-2]   Vapor pressures at 30°C have been reported as 10.2 x 10^{-7} torr for the pp' isom. and 18.9 x 10^{-7} torr for the op' isomer.

4. DDD

[4-3] Several papers report that the direct photolysis of DDD is slower than that of DDT (WREF). Since the half-life of DDT is greater than 150 years, the photolysis rate constant of DDD should be much slower than 5×10^{-7} hr^{-1}.

[4-4] The hydrolysis half-life of DDD has been calculated using structure-reactivity relationships and literature data (WREF). The base promoted hydrolysis at 27°C was calculated to be 5.0 M^{-1} hr^{-1}.

[4-5] A half-life has been reported (WREF) of 190 years for DDD at pH 5 and 27°C. This corresponds to a rate constant of 4.2×10^{-7} hr^{-1}, which is assumed to be due to the neutral rate process, k_N.
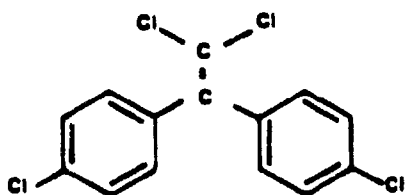
5. **DDE**

CAS No. 72559

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	318	
Melting point, °C	82	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.04 (20°C)	WREF [5-1]
Octanol-water, K_{ow} (unitless)	9.1×10^6	CC-Kow
Sediment-water, K_{oc} (unitless)	4.4×10^6	C-Koc f Kow
Microorganisms-water, $K_B \left((ug/g)(mg/\ell)^{-1} \right)$	8.9×10^5	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	6.8×10^{-5}	C-VP/S-20°
Vapor pressure, P_v (torr)	[5-2]	WREF
Reaeration rate ratio, k_v^c / k_v^o	NAV	

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5. DDE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at ___313___ nm	0.3	WREF
Direct photolysis rate constant, k_p (hr^{-1}) ___at___ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	1.2×10^5	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	$<6.6 \times 10^{-7}$ (27°C)	[5-3]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

[5-1] Several water solubility values have been reported for the pp' isomer at various temperatures (WREF). Water solubilities have been reported ranging from 0.014 ppm to 0.12 for the pp' isomer and 0.140 ppm for the op' isomer (WREF).

[5-2] Vapor pressures reported are 6.5×10^{-6} torr for pp' isomer and 6.2×10^{-6} torr for op' isomer at 20°C (WREF).

5. DDE

[5-3] A hydrolysis half-life for DDE of more than 120 years at pH 7 and 25°C has been reported (WREF). This corresponds to a rate constant of 6.6×10^{-7} hr^{-1}; it is assumed that at this pH only the neutral process is occurring.

6.   __DDT__

               CAS No.   __[6-1]__

pp' isomer [6-2]

PHYSICAL AND TRANSPORT DATA

Property or Process	Value		Data Source
Molecular weight	354.5		
Melting point, °C	108.5-109.0 [6-3]		WREF
Boiling point, °C	185		WREF [6-4]
Ionization constant	pK-NER		

Partition constants:

Water solubility, S_w (ppm)	5.5×10^{-3}	(25°C)	WREF [6-5]
Octanol-water, K_{ow} (unitless)	8.1×10^{6}		CC-Kow [6-6]
Sediment-water, K_{oc} (unitless)	3.9×10^{6}		C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	8.0×10^{6}		C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	1.58×10^{-5}		C-VP/S-25° [6-7]
Vapor pressure, P_v (torr)	1.9×10^{-7}	(25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV		

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6. DDT

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	$<5 \times 10^{-7}$	WREF [6-8]
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	3600	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	36 (27°C)	WREF [6-9]
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	6.8×10^{-6} (27°C)	WREF [6-10]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

[6-1]   Chemical Abstracts numbers are 502-93 for pp' isomer and 789-02-6 for op' isomer. Constants are calculated for the pp' isomer only.

6. DDT

[6-2]
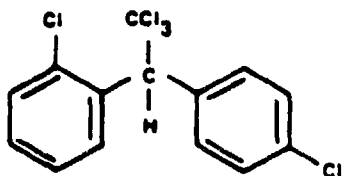
op' isomer

[6-3] The melting point given above is for the pp' isomer; the melting point of the op' isomer is 74-74.5°C.

[6-4] No boiling point is reported for the op' isomer (WREF).

[6-5] Several values for the water solubility of both isomers have been reported: a range of 1.2×10^{-3} - 2.5×10^{-2} ppm for the pp' isomer and 2.6×10^{-2} and 8.5×10^{-2} ppm for the op' isomer. See WREF for all values reported. The water solubility has also been calculated using the octanol-water partition coefficient to be 9.2×10^{-3} ppm.

[6-6] See WREF for other calculated and measured Kow values.

[6-7] Calculation of Henry's Law constant was based on data from the pp' isomer at 25°C, i.e., solubility - 5.5×10^{-3} pp' and vapor pressure - 1.9×10^{-7} pp'.

[6-8] A photolysis half-life of greater than 150 years has been reported for DDT (WREF). This corresponds to a rate constant of 5×10^{-7} hr^{-1}.

[6-9] The base-promoted hydrolysis rate constant for DDT has been measured (WREF) to be $k_B = 9.9 \times 10^{-3}$ M^{-1} sec^{-1}, which corresponds to a base-catalyzed process of 36 M^{-1} hr^{-1}.

[6-10] A hydrolysis rate constant of 6.8×10^{-6} hr^{-1} has been reported for DDT at pH 3-5 and 27°C (WREF). It is assumed that at these pHs, only a neutral process is occurring.
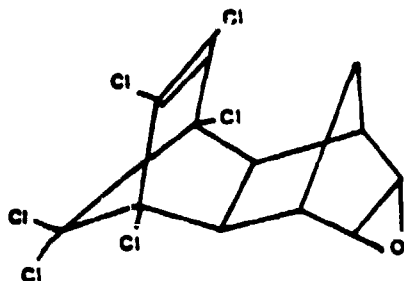
7. DIELDRIN

CAS No. 60-57-1

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	381	
Melting point, °C	175-176	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.195 (25°C)	WREF [7-1]
Octanol-water, K_{ow} (unitless)	3.5×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	1.7×10^3	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	710	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	4.57×10^{-10}	C-VP20°/S25°
Vapor pressure, P_v (torr)	1.78×10^{-7} (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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7. DIELDRIN

TRANSFORMATION DATA

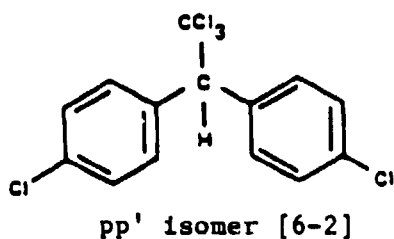| Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at 40° latitude	4.8×10^{-4}	[7-2]
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	30	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}\ hr^{-1}$)	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

[7-1] Several values, ranging from 0.186 ppm to 0.200 ppm, have been reported for the water solubility.

[7-2] The half-life for direct photolysis of dieldrin has been reported to be 2.1 to 1.8 months in sunlight (WREF). If the average half-life is used, a rate constant of 4.8×10^{-4} hr^{-1} is obtained.
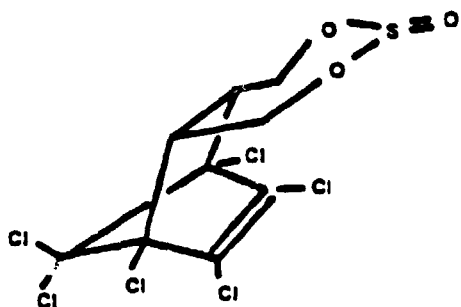
8. α-ENDOSULFAN

CAS No. 115-29-7

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	406.9	
Melting point, °C	108-110	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.530 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	0.02	CC-Kow
Sediment-water, K_{oc} (unitless)	9.6×10^{-3}	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1}\right)$	0.012	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	1.0×10^{-5}	C-VP/S-25°
Vapor pressure, P_v (torr)	1×10^{-5} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

8. α-ENDOSULFAN

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	>3.6 x 10^4	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	8.3 x 10^3 (20°C)	[8-1]
For acid-promoted process, k_A (M^{-1} hr^{-1})		
For neutral process, k_N (hr^{-1})	1.6 x 10^{-4} (20°C)	[8-2]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3 x 10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

[8-1] The hydrolysis rate constants for α-endosulfan have been measured at two pHs (WREF): pH 7 is 2.0 x 10^{-2} days^{-1} and pH 5.5 is 4.6 x 10^{-3} days^{-1}. Based on the assumption that only the base promoted process is responsible for hydrolysis at pH 7, k_h = k_B[OH] or 2.0 x 10^{-2} days^{-1} = k_B[10^{-7}]; k_B then equals 2.0 x 10^5 days^{-1}, or 8.3 x 10^{+3} hr^{-1}.

8. α-ENDOSULFAN

[8-2]   The neutral rate constant for α-endosulfan can be calculated
using the base-promoted rate constant and the overall rate
constant at pH 5.5, $k_h = k_B[OH] + k_N$ or $k_N = k_h - k_B[OH]$.
The assumption is that at pH 5.5 there is no acid-promoted
contribution to the overall hydrolysis rate process.
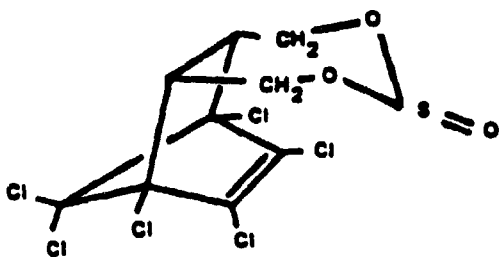
8. **β- ENDOSULFAN**

CAS No. 115-29-7

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	406.9	
Melting point, °C	207-209	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.280 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	0.02	CC-Kow
Sediment-water, K_{oc} (unitless)	9.6×10^{-3}	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	0.012	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	1.91×10^{-5}	C-VP/S-25°
Vapor pressure, P_v (torr)	1×10^{-5} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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8. β-ENDOSULFAN

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	>3.6 x 10^4	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	8.3 x 10^3 (20°C)	[8-3]
For acid-promoted process, k_A (M^{-1} hr^{-1})		
For neutral process, k_N (hr^{-1})	1.3 x 10^{-4} (20°C)	[8-4]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3 x 10^{-9}	E-KB

E: _Estimated value_; see List of Source Codes.

[8-3] See [8-1] for a discussion on calculation of k_B. The rate
constants at pH 7 and pH 5.5 are 1.9 x 10^{-2} days and
3.7 x 10^{-3} days, respectively.

[8-4] See [8-2] for calculation of k_N from k_B and pH 5.5 hydrolysis
rate constant.
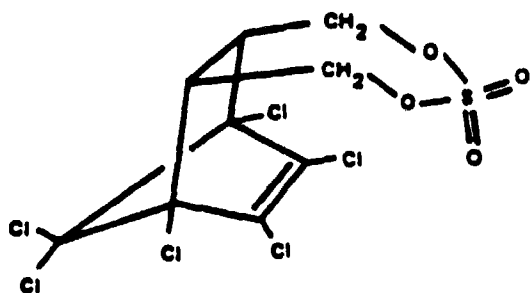
9. ENDOSULFAN SULFATE

CAS No. 1031-07-8

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	422.9	
Melting point, °C	198-201	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.22 [9-1]	WREF
Octanol-water, K_{ow} (unitless)	0.05	CC-Kow
Sediment-water, K_{oc} (unitless)	0 024	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	0.029	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	2.6×10^{-5}	C-VP/S-25° [9-2]
Vapor pressure, P_v (torr)	1×10^{-5} (25°C)	[9-2]
Reaeration rate ratio, k_v^c/k_v^o	NAV	

9. ENDOSULFAN SULFATE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	20	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	8.3×10^3 (20°C)	[9-3]
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$		
For neutral process, k_N (hr^{-1})	1.3×10^{-4} (20°C)	[9-4]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}\ hr^{-1}$)	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[9-1] No temperature was reported with the water solubility.

[9-2] Vapor pressure value was assigned by analogy to endosulfan. Henry's constant was calculated using vapor pressure value for endosulfan.

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9. ENDOSULFAN SULFATE

[9-3] See [8-1]. The assumption is made that rate constants for
β-endosulfan are the same for endosulfan sulfate.

[9-4] See [8-2] for the calculation of k_N.
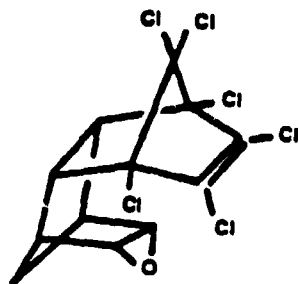
10. ENDRIN

CAS No. 72-20-8

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	381	
Melting point, °C	235	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.25 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	3.5×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	1.7×10^3	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	710	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	4.0×10^{-7}	C-VP/S-25°
Vapor pressure, P_v (torr)	2×10^{-7} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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10. ENDRIN

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	20	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

11. ENDRIN ALDEHYDE

CAS No. 7421-93-4

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	381	
Melting point, °C	145-149	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	50 (25°C)	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	1.4×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	670	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	310	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2×10^{-9}	C-VP/S-25° [11-1]
Vapor pressure, P_v (torr)	2.0×10^{-7} (25°C)	[11-1]
Reaeration rate ratio, k_v^c/k_v^o	NAV	

11. ENDRIN ALDEHYDE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	3100	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 3×10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

[11-1] Vapor pressure was assigned by analogy to endrin; this is the value used in the calculation of Henry's constant.
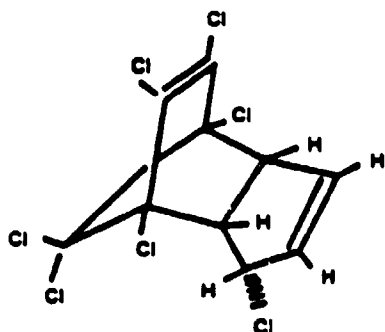
12.   HEPTACHLOR

CAS No.   76-44-8

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	373.5	
Melting point, °C	95-96	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.18 (25°C) [12-1]	WREF
Octanol-water, K_{ow} (unitless)	2.6×10^4	CC-Kow
Sediment-water, K_{oc} (unitless)	1.2×10^4	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	4.4×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	4.0×10^{-3}	C-VP/S-25°
Vapor pressure, P_v (torr)	3.0×10^{-4} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.355	C-DC.7

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12. HEPTACHLOR

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	3×10^{10}	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	2500	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	—	[12-2]
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	—	[12-2]
For neutral process, k_N (hr^{-1})	3.00×10^{-2} (30°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, k_b ($ml\ cell^{-1}\ hr^{-1}$)	—	HF-NBD

E: Estimated value; see List of Source Codes.

[12-1] Another solubility value has been reported as 0.056 ppm at 25-29°C (WREF).

[12-2] Hydrolysis rate is likely to be pH independent by analogy to allyl chloride (Mabey and Mill, 1978).

13. HEPTACHLOR EPOXIDE

CAS No. 1024-57-3

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	389.2	
Melting point, °C	157-160	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.350 (25°C)	WREF [13-1]
Octanol-water, K_{ow} (unitless)	450	CC-Kow
Sediment-water, K_{oc} (unitless)	2.2×10^2	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	1.1×10^2	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m² mol⁻¹)	3.9×10^{-4}	C-VP/S-25° [13-2]
Vapor pressure, P_v (torr)	3×10^{-4} (25°C)	[13-2]
Reaeration rate ratio, k_v^C/k_v^O	NAV	

13. HEPTACHLOR EPOXIDE

CAS No. 1024-57-3

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	389.2	
Melting point, °C	157-160	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.350 (25°C)	WREF [13-1]
Octanol-water, K_{ow} (unitless)	450	CC-Kow
Sediment-water, K_{oc} (unitless)	2.2×10^2	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	1.1×10^2	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	3.9×10^{-4}	C-VP/S-25° [13-2]
Vapor pressure, P_v (torr)	3×10^{-4} (25°C)	[13-2]
Reaeration rate ratio, k_v^c/k_v^o	NAV	

13. HEPTACHLOR EPOXIDE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	20	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 3×10^{-12}	E-KB

E: _Estimated value_; see List of Source Codes.

[13-1] Several water solubility values, ranging from 0.20 to 0.35 ppm, were reported (WREF).

[13-2] Vapor pressure value is assigned by analogy to heptachlor. This vapor pressure is used in the calculation of Henry's constant.

14. α-HEXACHLOROCYCLOHEXANE

CAS No. 319-84-6
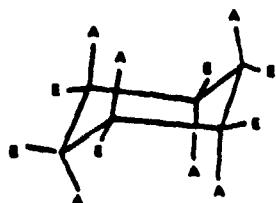
Orientation of Cl atoms on ring	Isomer
AAEEEE	α
EEEEEE	β
AAAEEE	γ(lindane)
AEEEEE	δ
AEEAEE	ε

PHYSICAL AND TRANSPORT DATA

Property o. Process	Value	Data Source
Molecular weight	291	
Melting point, °C	157-158	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	1.63 (25°C)	WREF [14-1]
Octanol-water, K_{ow} (unitless)	7.8×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	3.8×10^3	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	1.5×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	6.0×10^{-6}	C-VP20°/S25°
Vapor pressure, P_v (torr)	2.5×10^{-5} (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	–

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14. α-HEXACHLOROCYCLOHEXANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}\ hr^{-1}$)	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[14-1] Several water solubility values, ranging from 1.21 ppm to 2.03 ppm, have been reported (WREF).

15. β-HEXACHLOROCYCLOHEXANE

CAS No.   319-85-7

See α-Chlorocyclohexane for structure

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	291	
Melting point, °C	309	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.24 (25°C)	WREF [15-1]
Octanol-water, K_{ow} (unitless)	7.8×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	3.8×10^3	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/ml^{-1}) \right)$	1.5×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	4.5×10^{-7}	C-VP20°/S25°
Vapor pressure, P_v (torr)	2.8×10^{-7} (20°C)	WREF
R·aeration rate ratio, k_v^c/k_v^o	NAV	

15. β-HEXACHLOROCYCLOHEXANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
bsorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[15-1]   Several water solubility values, ranging from 0.13 ppm to 0.70 ppm, have been reported (WREF).

16.   δ-HEXACHLOROCYCLOHEXANE

CAS No.   319-86-8

See α-Chlorocyclohexane for structure

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	291	
Melting point, °C	138-139	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	31.4 (25°C)	WREF [16-1]
Octanol-water, K_{ow} (unitless)	1.4×10^4	Pomona
Sediment-water, K_{oc} (unitless)	6.6×10^3	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	3.5×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	2.07×10^{-7}	C-VP20°/S25°
Vapor pressure, P_v (torr)	1.7×10^{-5} (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

16. δ-HEXACHLOROCYCLOHEXANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}\ hr^{-1}$)	(E) 1×10^{-10}	E-KB

E: <u>Estimated value</u>; see List of Source Codes.

[16-1] Several water solubility values, ranging from 8.64 ppm to 31.4 ppm, have been reported (WREF).
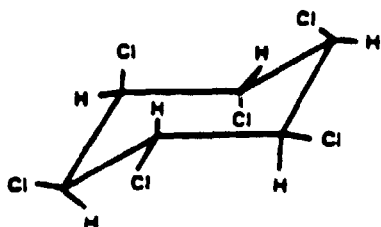
17. LINDANE

CAS No. 58-89-9

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	291	
Melting point, °C	112.9	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	7.8 (25°C)	WREF [17-1]
Octanol-water, K_{ow} (unitless)	7.8×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	3.8×10^3	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	1.5×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	7.8×10^{-6}	C-VP/S-25°
Vapor pressure, P_v (torr)	1.6×10^{-4} (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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17. LINDANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\ddagger$, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[17-1] Several solubility values, ranging from 0.04 ppm to 12 ppm, have been reported (WREF).
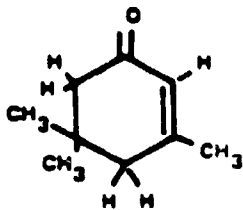
18. ISOPHORONE

CAS No. 78591

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	138.2	
Melting point, °C	-8	WREF
Boiling point, °C	15	WREF
Ionization constant	pK-NFR	

Partition constants:

Water solubility, S_w (ppm)	1.2×10^4 [18-1]	WREF
Octanol-water, K_{ow} (unitless)	180	CC-Kow
Sediment-water, K_{oc} (unitless)	87	C-Koc f Kow
Microorganisms-water, $K_B \left((ug/g)(mg/\ell)^{-1} \right)$	48	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	5.75×10^{-6}	C-VP20°/S-[18-1]
Vapor pressure, P_v (torr)	0.38 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

18. ISOPHORONE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [18-2]	
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	$<1 \times 10^7$	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	225	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	0	NHFG
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 3×10^{-9}	E-KB

E: _Estimated value_; see List of Source Codes.

[18-1] No temperature is reported for water solubility. This
        value was used in the calculation of Henry's constant.

18. ISOPHORONE

[18-2] UV spectrum of isophorone in ethanol solvent is shown below (UV Atlas, 1966).

λ (nm)
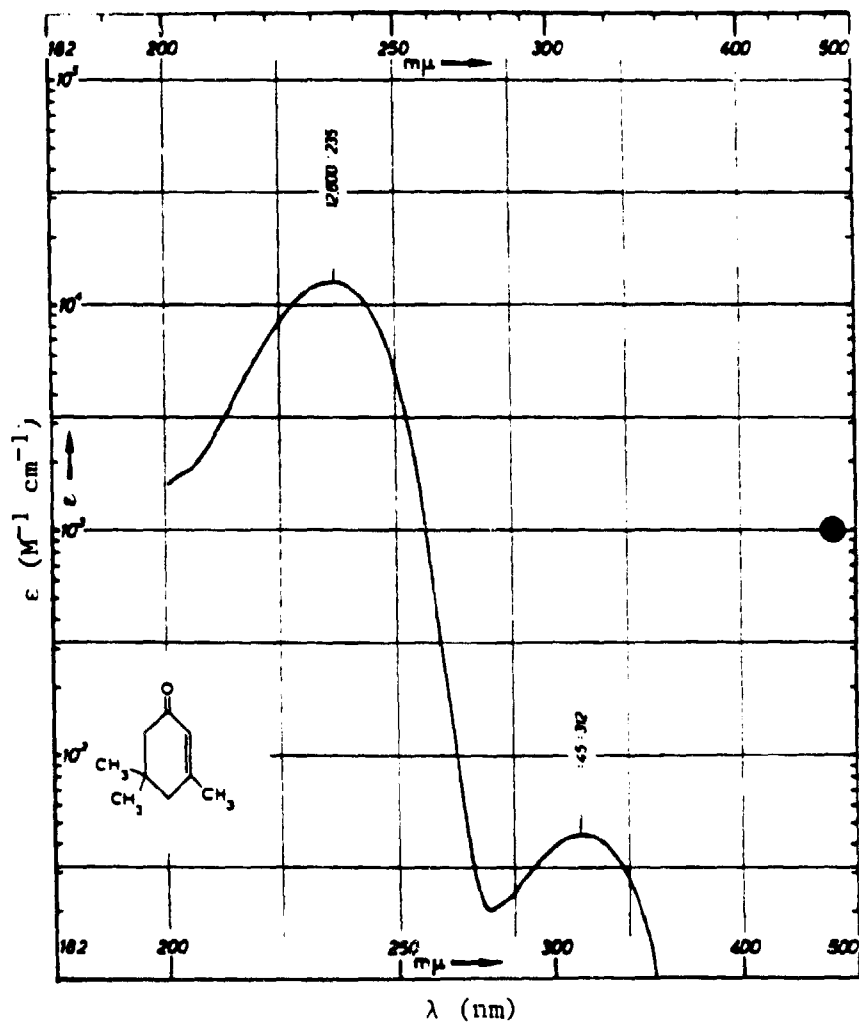
19. TCDD

CAS No. 1746-01-6
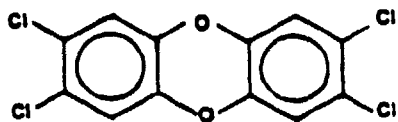
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	322	
Melting point, °C	303-305	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	2×10^{-4}	WREF [19-1]
Octanol-water, K_{ow} (unitless)	6.9×10^{6}	CC-Kow
Sediment-water, K_{oc} (unitless)	3.3×10^{6}	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	6.9×10^{5}	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.1×10^{-3}	C-VP/S [19-2]
Vapor pressure, P_v (torr)	1×10^{-6}	[19-3]
Reaeration rate ratio, k_v^c/k_v^o	0.373	C-DC.7

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19.   TCDD

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<360	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}\ hr^{-1}$)	(E) 1 x 10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[19-1] No temperature is reported for the water solubility.

[19-2] Vapor pressure and the water solubility given above are used in the calculation of Henry's constant.

[19-3] Vapor pressure calculated from structure using methods described by Lyman et al. (1982). Calculation conducted by R. T. Podoll, SRI International.

20. TOXAPHENE

CAS No. 8001-35-2

TOXAPHENE (AVERAGE FORMULA $C_{10}H_{10}Cl_8$)

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	414	[20-1]
Melting point, °C		
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.50 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	2.00×10^3	WREF
Sediment-water, K_{oc} (unitless)	964	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	429	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	0.21	C-VP/S-25°
Vapor pressure, P_v (torr)	0.2-0.4 (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.330	C-DC.7

20. TOXAPHENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

[20-1] Toxaphene is a chlorinated camphene mixture containing 67-69% chlorine. Value reported here is an average molecular weight for the mixture.

References for 3.2

Lyman, W. J., W. F. Rechl and D. H. Rosenblatt. 1982. Handbook of
    Chemical Property Estimation Methods. McGraw-Hill, New York.

Mabey, W. R., and T. Mill. 1978. Critical Review of Hydrolysis of
    Organic Compounds in Water Under Environmental Conditions. J. Phys.
    Chem. Ref. Data 7:383.

Pomona College Medicinal Data Base, June 1982.

UV Atlas. 1971. UV Atlas of Organic Compounds. Vol. I-V. Plenum
    Press, New York.

SECTION 3.3. PCBS AND 2-CHLORONAPHTHALENE[*]

21. Aroclor 1016
22. Aroclor 1221
23. Aroclor 1232
24. Aroclor 1242
25. Aroclor 1248
26. Aroclor 1254
27. Aroclor 1260
28. 2-Chloronaphthalene

[*] See footnotes for Aroclor 1016 (data sheet number 21) for comments
on data for PCB mixtures that constitute Aroclors

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21. AROCLOR 1016

CAS No. —
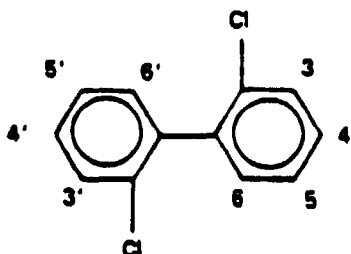
Numbering sequence for polychlorinated biphenyl

PHYSICAL AND TRANSPORT DATA [21-1]

Property or Process	Value	Data Source
Molecular weight	257.9	
Melting point, °C		
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.42 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	3.8×10^5	WREF
Sediment-water, K_{oc} (unitless)	1.8×10^5	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	5.0×10^4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	3.3×10^{-4}	C-VP/S-25°C
Vapor pressure, P_v (torr)	4×10^{-4} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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21.   AROCLOR 1016

TRANSFORMATION DATA [21-2]

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E)3 x 10^{-9}~3 x 10^{-12}	E-KB [21-2]

E: Estimated value; see List of Source Codes.

[21-1] These process data are given for the specific mixtures of PCBs
called Aroclors as listed in WREF. The data are "average"
values for each property, and the properties of individual PCBs
will vary depending on the number and position of chlorines on
the biphenyl ring.

[21-2] As discussed in [21-1] above, Aroclors are mixtures of PCBs.
PCBs are not hydrolyzable under environmental conditions. In
general, the more highly chlorinated isomers are less suscep-
tible to biological or abiotic oxidation processes.

22. AROCLOR 1221

CAS No. 11-042-82

PHYSICAL AND TRANSPORT DATA (see [21-1])

Property or Process	Value	Data Source
Molecular weight	200.7	
Melting point, °C		
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Property or Process	Value	Data Source
Water solubility, S_w (ppm)	40.0 (25°C)	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	1.2×10^4	WREF
Sediment-water, K_{oc} (unitless)	5.8×10^3	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	2.2×10^3	C-KB f Kow

Volatilization constants:

Property or Process	Value	Data Source
Henry's constant, H_c (atm m^3 mol^{-1})	1.7×10^{-4}	C-VP/S-25°
Vapor pressure, P_v (torr)	6.7×10^{-3} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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22. AROCLOR 1221

TRANSFORMATION DATA (see [21-2])

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C.		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	$<<360$	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) $3 \times 10^{-9} \sim 3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

23. <u>AROCLOR 1232</u>

CAS No. <u>111-411-65</u>

PHYSICAL AND TRANSPORT DATA (see [21-1])

Property or Process	Value	Data Source
Molecular weight	232.2	
Melting point, °C		
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	407 (25°C)	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	1.6×10^3	WREF
Sediment-water, K_{oc} (unitless)	771	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	351	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	1.13×10^{-5}	C-VP/S-25°
Vapor pressure, P_v (torr)	4.06×10^{-3} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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23. AROCLOR 1232

TRANSFORMATION DATA (see [21-2])

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b ($ml\ cell^{-1}\ hr^{-1}$)	(E) $3 \times 10^{-9} \sim 3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

24.   AROCLOR 1242

CAS No. 534-692-19

PHYSICAL AND TRANSPORT DATA (see [21-1])

Property or Process	Value	Data Source
Molecular weight	266.5	—
Melting point, °C	,	
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.23 (25°C)	WREF [24-2]
Octanol-water, K_{ow} (unitless)	1.3×10^4	WREF
Sediment-water, K_{oc} (unitless)	6.3×10^3	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	2.3×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	1.98×10^{-3}	C-VP/S-25°
Vapor pressure, P_v (torr)	1.3×10^{-3} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.382	C-DC.7

24. AROCLOR 1242

TRANSFORMATION DATA (see [21-2])

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	$<<360$	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b ($ml\ cell^{-1}\ hr^{-1}$)	(E) $3 \times 10^{-9} \sim 3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

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25. AROCLOR 1248

CAS No. 126-722-96

PHYSICAL AND TRANSPORT DATA (see [21-1])

Property or Process	Value	Data Source
Molecular weight	299.5	
Melting point, °C		
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.054 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	5.75×10^5	WREF
Sediment-water, K_{oc} (unitless)	2.77×10^5	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	7.29×10^4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	3.6×10^{-3}	C-VP/S-25°
Vapor pressure, P_v (torr)	4.94×10^{-4} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.370	C-DC.7

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25. AROCLOR 1248

TRANSFORMATION DATA (see [21-2])

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) $3 \times 10^{-9} \sim 3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

124

26. AROCLOR 1254

CAS No. 110-976-91

PHYSICAL AND TRANSPORT DATA (see [21-1])

Property or Process	Value	Data Source
Molecular weight	328.4	
Melting point, °C		
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.031 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	1.1×10^6	WREF
Sediment-water, K_{oc} (unitless)	5.3×10^5	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	1.3×10^5	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	2.6×10^{-3}	WREF
Vapor pressure, P_v (torr)	7.71×10^{-5} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.359	C-DC.7

26. AROCLOR 1254

TRANSFORMATION DATA (see [21-2])

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) $3 \times 10^{-9} \sim 3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

27. __AROCLOR 1260__

CAS No. __110-968-25__

PHYSICAL AND TRANSPORT DATA (see [21-1])

Property or Process	Value	Data Source
Molecular weight	375.7	
Melting point, °C		
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	2.7×10^{-3} (25°C)	WREF
Octanol-water, K_{ow} (unitless)	1.4×10^{7}	WREF
Sediment-water, K_{oc} (unitless)	6.7×10^{6}	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1} \right)$	1.3×10^{6}	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	0.74	C-VP/S-25°
Vapor pressure, P_v (torr)	4.05×10^{-5} (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.346	C-DC.7

27. AROCLOR 1260

TRANSFORMATION DATA (see [21-1])

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) $3 \times 10^{-9} \sim 3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

28. 2-CHLORONAPHTHALENE

CAS No. 91-58-7

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	162.62	
Melting point, °C	61	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	6.74 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	1.0×10^4	WREF
Sediment-water, K_{oc} (unitless)	4.8×10^3	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1} \right)$	1.8×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	5.4×10^{-4}	C-VP20°/S25°
Vapor pressure, P_V (torr)	0.017 (20°C)	WREF
Reaeration rate ratio, k_V^c/k_V^o	NAV	

28. 2-CHLORONAPHTHALENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) 3×10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

SECTION 3.4. HALOGENATED ALIPHATIC CHEMICALS

29. Chloromethane (methyl chloride)
30. Dichloromethane (methylene chloride)
31. Trichloromethane (chloroform)
32. Tetrachloromethane (carbon tetrachloride)
33. Chloroethane (ethyl chloride)
34. 1,1-Dichloroethane (ethylidine chloride)
35. 1,2-Dichloroethane (ethylene dichloride)
36. 1,1,1-Trichloroethane (methyl chloroform)
37. 1,1,2-Trichloroethane
38. 1,1,2,2-Tetrachloroethane
39. Hexachloroethane
40. Chloroethene (vinyl chloride)
41. 1,1-Dichloroethane (vinylidine chloride)
42. 1,2-trans-Dichloroethene
43. Trichloroethene
44. Tetrachloroethene (perchloroetnylene)
45. 1,2-Dichloropropane
46. 1,3-Dichloropropene
47. Hexachlorobutadiene
48. Hexachlorocyclopentadiene
49. Bromomethane (methyl bromide)
50. Bromodichloromethane
51. Dibromochloromethane
52. Tribromomethane (bromoform)
53. Dichlorodifluoromethane
54. Trichlorofluoromethane
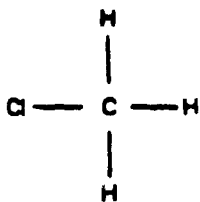
29. CHLOROMETHANE

CAS No. 74-87-3

$$Cl - \underset{\underset{H}{\overset{\overset{H}{|}}{|}}}{\overset{}{C}} - H$$

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	50.49	
Melting point, °C	-97.73	CRC
Boiling point, °C	-24.2	CRC
Ionization constant	pK-NER	

Partition constants:

Property or Process	Value	Data Source
Water solubility, S_w (ppm)	6.45×10^3 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	8.9	CC-Kow
Sediment-water, K_{oc} (unitless)	4.3	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	3.2	C-KB f Kow

Volatilization constants:

Property or Process	Value	Data Source
Henry's constant, H_c (atm m^3 mol^{-1})	0.04	C-VP/S-20°
Vapor pressure, P_v (torr)	3.76×10^3 (20°C)	WRIF
Reaeration rate ratio, k_v^c/k_v^o	0.52	C-DC 7

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29. CHLOROMETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	0.05	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	—	HPHI
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NACM
For neutral process, k_N (hr^{-1})	6.8×10^{-5} (25°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	—	VF-NBD

E: Estimated value; see List of Source Codes.

30. DICHLOROMETHANE

CAS No. 75-09-2

```
        Cl
        |
Cl ——— C ——— H
        |
        H
```
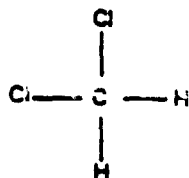
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	84.94	
Melting point, °C	-95	WREF
Boiling point, °C	39.75	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	2.0×10^4 (20°C)	WREF [30-1]
Octanol-water, K_{ow} (unitless)	18.2	CC-Kow
Sediment-water, K_{oc} (unitless)	8.8	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	6.0	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.03×10^{-3}	C-VP20°/S25°
Vapor pressure, P_v (torr)	362.4 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.650	C-DC.7

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30. DICHLOROMETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	0.2	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$		HPHI
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	NACM
For neutral process, k_N (hr^{-1})	1.15×10^{-7} (25°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}\ hr^{-1}$)	—	VF-NBD

E: *Estimated value*; see List of Source Codes.

[30-1] Several values, ranging from $(1.32 - 2.00) \times 10^4$ ppm, have been reported (WREF).
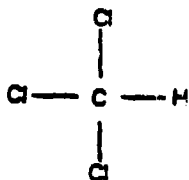
31. TRICHLOROMETHANE

CAS No. 67-66-3

$$Cl - \overset{\displaystyle Cl}{\underset{\displaystyle Cl}{\overset{|}{\underset{|}{C}}}} - H$$

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	119.38	
Melting point, °C	-63.5	WREF
Boiling point, °C	61.7	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	8.2×10^3 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	91	CC-Kow
Sediment-water, K_{oc} (unitless)	44	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1} \right)$	26	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.88×10^{-3}	C-VP/S-20°
Vapor pressure, P_v (torr)	150.5 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.583	C-DC.7

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31. TRICHLOROMETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	0.7	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0.23 (25°C)	Mabey & Mill, 1978
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NACM
For neutral process, k_N (hr^{-1})	2.5 x 10^{-9} (25°C)	Mabey & Mill, 1978
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	—	VF-NBD

E: Estimated value; see List of Source Codes.
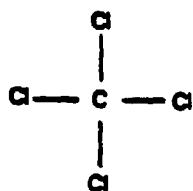
32. TETRACHLOROMETHANE

CAS No. 56-23-5

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	153.82	
Melting point, °C	-22.99	CRC
Boiling point, °C	76.54	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	785 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	912	CC-Kow
Sediment-water, K_{oc} (unitless)	439	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	211	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	0.023	C-VP/S-20°
Vapor pressure, P_v (torr)	90 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.536	C-DC.7

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32. TETRACHLOROMETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	–	HPHI
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NACM
For neutral process, k_N (hr^{-1})	[32-1]	
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) 1 x 10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[32-1] The kinetics of hydrolysis of CCl_4 has been reported as being second order in CCl_4 concentration, although no explanation for this behavior is available. At 1 ppm concentrations, the calculated half-life is 7000 years at pH 7 and 25°C (Mabey and Mill, 1978).

33. CHLOROETHANE

CAS No. 75-00-3

H—C—C—Cl (structure diagram of chloroethane)
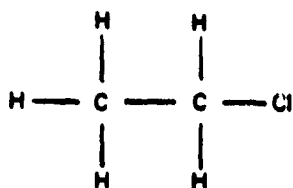
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	64.52	
Melting point, °C	-136.4	WREF
Boiling point, °C	12.27	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	5.74×10^3 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	30.9	CC-Kow
Sediment-water, K_{oc} (unitless)	14.9	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	9.8	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	0.148	C-VP/S-20°
Vapor pressure, P_v (torr)	1.0×10^3 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.645	C-DC.7

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33. CHLOROETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1} hr^{-1}$)	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1} hr^{-1}$)	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1} hr^{-1}$)	–	HPHI
For acid-promoted process, k_A ($M^{-1} hr^{-1}$)	0	NACM
For neutral process, k_N (hr^{-1})	7.2×10^{-4} (25°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	–	VF-NBD

E: __Estimated value__; see List of Source Codes.

34. 1,1-DICHLOROETHANE

CAS No. 75-34-3

H—C—C—H structure (1,1-dichloroethane)
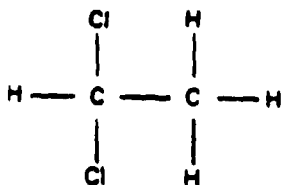
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	98.96	
Melting point, °C	-96.98	WREF
Boiling point, °C	57.28	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	5.5×10^3 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	63	CC-Kow
Sediment-water, K_{oc} (unitless)	30	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	19	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	4.26×10^{-3}	C-VP/S-20°
Vapor pressure, P_v (torr)	180 (20°C)	Verschueren, 1977
Reaeration rate ratio, k_v^c/k_v^o	0.580	C-DC.7

34. 1,1-DICHLOROETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)		
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	NACM
For neutral process, k_N (hr^{-1})	1.15×10^{-7} (25°C)	[34-1]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}\ hr^{-1}$)	—	VF-NBD

E: Estimated value; see List of Source Codes.

[34-1] Hydrolysis neutral rate constant has been assigned by analogy to dichloromethane.

35. 1,2- ICHLOROETHANE

CAS No. 107-06-2

```
   Cl        Q
   |         |
H——C————C——H
   |         |
   H         H
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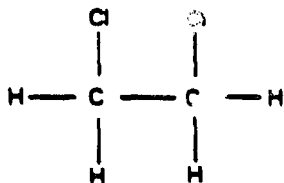
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	98.98	
Melting point, °C	-35.36	WREF
Boiling point, °C	83.47	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	8.69×10^3	WREF
Octanol-water, K_{ow} (unitless)	30	CC-Kow
Sediment-water, K_{oc} (unitless)	14	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1} \right)$	9	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	9.14×10^{-4}	C-VP/S-20°
Vapor pressure, P_v (torr)	61 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

35. 1,2-DICHLOROETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$		
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	NACM
For neutral process, k_N (hr^{-1})	1.8×10^{-9} (25°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

36. 1,1,1-TRICHLOROETHANE

CAS No. 71-55-6

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	133.41	
Melting point, °C	-30.41	W^{---}
Boiling point, °C	74.1	W^{---}
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	720 (25°C)	Dilling, 1977
Octanol-water, K_{ow} (unitless)	320	CC-Kow
Sediment-water, K_{oc} (unitless)	152	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	81	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	0.03	C-VP/S-25°
Vapor pressure, P_v (torr)	123 (25°C)	Dilling, 1977
Reaeration rate ratio, k_v^c/k_v^o	0.533	C-DC.7

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36. 1,1,1-TRICHLOROETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})		
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NACM
For neutral process, k_N (hr^{-1})	1.7×10^{-4} (25°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	—	VF-NBD

E: Estimated value; see List of Source Codes.

37. 1,1,2-TRICHLOROETHANE

CAS No. 79-00-5
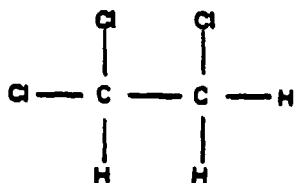
Cl—C—C—H

(structural diagram)

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	133.41	
Melting point, °C	-36.5	WREF
Boiling point, °C	113.77	CRC
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	4.5×10^3 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	117	CC-Kow
Sediment-water, K_{oc} (unitless)	56	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	33	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	7.42×10^{-4}	C-VP/S-20°
Vapor pressure, P_v (torr)	19 (20°C)	WREF
Reaeration rate ratio, k_v^C/k_v^O	NAV	

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TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$		
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	NACM
For neutral process, k_N (hr^{-1})	1.2×10^{-7} (25°C)	E-H [37-1]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-12}	E-RB

E: <u>Estimated value</u>; see List of Source Codes.

[37-1]   Neutral hydrolysis rate constant was assigned by analogy to dichloromethane.

38. 1,1,2,2-TETRACHLOROETHANE

CAS No. 79-34-5

H — C — C — H

(structure: two central carbon atoms each bonded to two Cl; CH on each end)
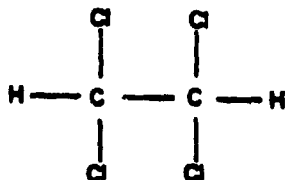
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	167.85	
Melting point, °C	-36	WREF
Boiling point, °C	146.2	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	2.9×10^3 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	245	Pomona
Sediment-water, K_{oc} (unitless)	118	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	91	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	3.8×10^{-4}	C-VP/S-20°
Vapor pressure, P_v (torr)	5 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

38. 1,1,2,2-TETRACHLOROETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	2	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})		
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NACM
For neutral process, k_N (hr^{-1})	1.2×10^{-7} (25°C)	E-H [38-1]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

[38-1] Hydrolysis neutral rate constant is assigned by analogy to dichloromethane.

39. HEXACHLOROETHANE

CAS No. 67-72-1

$$
\begin{array}{c}
\text{Cl} \quad\quad \text{Cl} \\
| \quad\quad\quad | \\
\text{Cl} - \text{C} - \text{C} - \text{Cl} \\
| \quad\quad\quad | \\
\text{Cl} \quad\quad \text{Cl}
\end{array}
$$
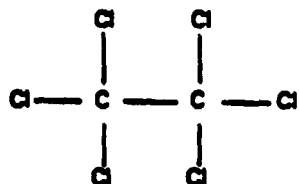
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	236.74	
Melting point, °C	186.8-187.4	CRC [39-1]
Boiling point, °C	186 (777mm)	WREF [39-1]
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	50 (22°C)	WREF
Octanol-water, K_{ow} (unitless)	4.2×10^4	CC-Kow
Sediment-water, K_{oc} (unitless)	2.0×10^4	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	6.75×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	2.49×10^{-3}	C-VP20°/S22°
Vapor pressure, P_v (torr)	0.4 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.443	C-DC.7

39. HEXACHLOROETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	0	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	0	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	NACM
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[39-1] Hexachloroethane sublimes on heating.
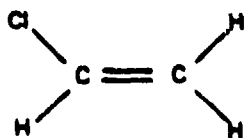
40. CHLOROETHENE

CAS No. 75-01-4

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	62.5	
Melting point, °C	-153.8	WREF
Boiling point, °C	-13.37	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	2.7×10^3 (25°C)	Dilling, 1977
Octanol-water, K_{ow} (unitless)	17	CC-Kow
Sediment-water, K_{oc} (unitless)	8.2	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	5.7	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	8.14×10^{-2}	C-VP/S-25°
Vapor pressure, P_v (torr)	2.66×10^3 (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.675	C-DC.7

40.   CHLOROETHENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	$<10^8$	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	—	VF-NBD

E: Estimated value; see List of Source Codes.

41. 1,1-DICHLOROETHENE

CAS No. 75-35-4

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	96.94	
Melting point, °C	-122.1	WREF
Boiling point, °C	37	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	400 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	135	Pomona
Sediment-water, K_{oc} (unitless)	65	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	53	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	0.190	C-VP25°/S20°
Vapor pressure, P_v (torr)	591 (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.601	C-DC.7

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41.   1,1-DICHLOROETHENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	_____
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	_____
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	$<10^8$	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	—	VF-NBD

E: _Estimated value_; see List of Source Codes.

42. **1,2-TRANS-DICHLOROETHENE**
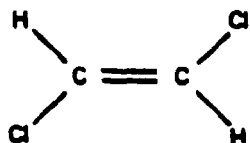
C^S No. 540-59-0

H C=C Cl structure diagram (H, Cl / C=C \ Cl, H)

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	96.94	
Melting point, °C	-50	WREF
Boiling point, °C	47.5 [42-1]	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	600 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	123	Pomona
Sediment-water, K_{oc} (unitless)	59	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1} \right)$	48	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	0.067	C-VP/S-20°
Vapor pressure, P_v (torr)	326 (20°C)	Dilling, 1977
Reaeration rate ratio, k_v^c/k_v^o	0.601	C-DC.7

42. 1,2-TRANS-DICHLOROETHENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	$<10^5$	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	—	VF-NBD

E: Estimated value; see List of Source Codes.

[42-1] No pressure is reported for the boiling point.
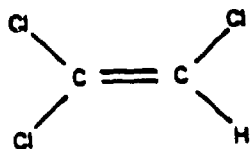
43. <u>TRICHLOROETHENE</u>

                                         CAS No. <u>79-01-6</u>

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	131.39	
Melting point, °C	-73	WREF
Boiling point, °C	87	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	1.1×10^3 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	263	Pomona
Sediment-water, K_{oc} (unitless)	126	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	97	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	9.1×10^{-3}	C-VP/S-20°C
Vapor pressure, P_v (torr)	57.9 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.548	C-DC.7

43.   TRICHLOROETHENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	$<10^3$	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 1×10^{-10}	E-KB

E: _Estimated value_; see List of Source Codes.

44. TETRACHLOROETHENE

CAS No. 127-18-4

C = C structure with Cl atoms

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	165.83	
Melting point, °C	-22.7	WREF
Boiling point, °C	121	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	200 (20°C)	WREF (44-1)
Octanol-water, K_{ow} (unitless)	759	Pomona
Sediment-water, K_{oc} (unitless)	364	C-Koc f K
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	25	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	0.0153	C-VP/S-20°
Vapor pressure, P_v (torr)	14 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.509	C-DC.7

44.   TETRACHLOROETHENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	$\ll 100$	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b ($ml\ cell^{-1}\ hr^{-1}$)	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[44-1]   A range of solubility values, from 150 ppm to 200 ppm, has been reported (WREF).

45. 1,2-DICHLOROPROPANE

CAS No. 78-87-5

```
      H    Cl    H
      |    |     |
Cl —  C —  C  —  C — H
      |    |     |
      H    H     H
```
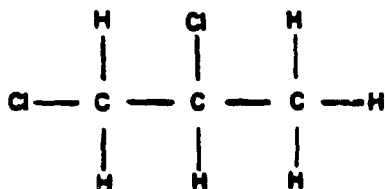
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	112.99	
Melting point, °C	-100	WREF
Boiling point, °C	96.8	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	2.7×10^3 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	105	CC-Kow
Sediment-water, K_{oc} (unitless)	51	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1} \right)$	30	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.31×10^{-3}	C-VP/S-20°
Vapor pressure, P_v (torr)	42 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.530	C-DC.7

45. 1,2-DICHLOROPROPANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	∿1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$		
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	NACM
For neutral process, k_N (hr^{-1})	7.2×10^{-4} (25°C)	[45-1]
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[45-1] Hydrolysis neutral rate constant is assigned by analogy to chloroethane.
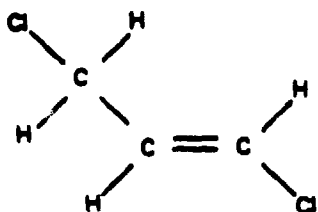
46. 1,3-DICHLOROPROPENE

CAS No. 542-75-6

(TRANS ISOMER) [46-1]

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	110.98	
Melting point, °C		
Boiling point, °C	104.3, 112	WREF [46-2]
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	2.7×10^3 2.8×10^3 (25°C)	WREF [46-3]
Octanol-water, K_{ow} (unitless)	100	Pomona
Sediment-water, K_{oc} (unitless)	48	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	40	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mo^{-1})	1.33×10^{-3}	C-VP20°/S25°[46-33]
Vapor pressure, P_v (torr)	25 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

46. 1,3-DICHLOROPROPENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	$<10^8$	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	44	C-OX [46-4]
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$		HPHI
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	0	NACM
For neutral process, k_N (hr^{-1})	4.2×10^{-4} (25°C)	[46-5]
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1×10^{-10}	E-KB

E: Estimated value: see List of Source Codes.

[46-1]
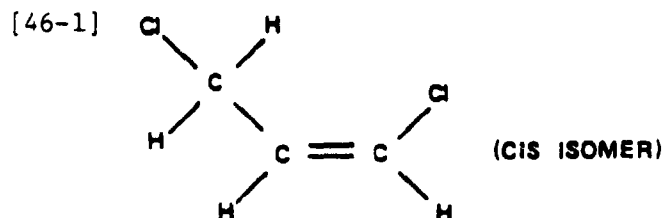
(CIS ISOMER)

46. 1,3-DICHLOROPROPENE

[46-2]   Boiling points of 104.3°C for the cis isomer and 112°C for the trans isomer were reported.

[46-3]   Water solubilities of 2700 ppm for the cis isomer and 2800 ppm for the trans isomer were reported. The solubility of the cis isomer is used in the calculation of Henry's constant.

[46-4]   44 M^{-1} hr^{-1} is the minimum oxidation rate constant for oxidation by peroxy radical.

[46-5]   The hydrolysis rate constant for 1,3-dichloropropene which is reported in WREF does not reflect the hydrolytic reactivity characteristic of allylic halides. For example, allyl chloride has a rate constant of 4.16 x 10^{-4} hr^{-1} at 25°C and is pH independent (Mabey and Mill, 1978). Because of its similar structure compared with allyl chloride, a hydrolysis rate constant of 4.2 x 10^{-4} hr^{-1} has been assigned to 1,3-dichloropropene.
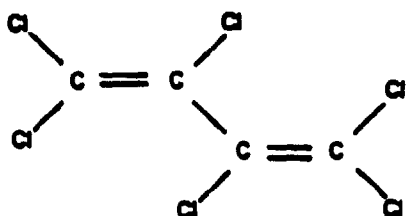
47. HEXACHLORO-1,3-BUTADIENE

CAS No. 87-68-3

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	260.76	
Melting point, °C	-21	WREF
Boiling point, °C	215	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	2.0 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	6.0×10^4	Pomona
Sediment-water, K_{oc} (unitless)	2.9×10^4	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	1.3×10^4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	0.0256	C-VP/S-20°
Vapor pressure, P_v (torr)	0.15 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.415	C-DC.7

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47. HEXACHLOROBUTADIENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	$<10^3$	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 1 x 10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

48. HEXACHLOROCYCLOPENTADIENE

CAS No. 77-47-4

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	272.77	
Melting point, °C	-9.9	WREF
Boiling point, °C	239 (753mm)	CRC
Ionization constant	pK-NER	

Partition constants:

	Value	Data Source
Water solubility, S_w (ppm)	1.8 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	1.0×10^4	CC-Kow
Sediment-water, K_{oc} (unitless)	4.8×10^3	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	1.8×10^3	C-KB f Kow

Volatilization constants:

	Value	Data Source
Henry's constant, H_c (atm m^3 mol^{-1})	0.016	C-VP/S-25°
Vapor pressure, P_v (torr)	0.081 (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.413	C-DC.7

48. HEXACHLOROCYCLOPENTADIENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [48-1]	Zepp, 1980
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude	3.9	WREF
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	$<10^3$	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	12	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	—	HPHI
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NACM
For neutral process, k_N (hr^{-1})	2.0×10^{-3} (25°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

48. HEXACHLOROCYCLOPENTADIENE

[48-1] Table of absorption coefficients and the corresponding wavelengths is given below (Zepp, 1980).

WAVELENGTH (nm)	EPSILON $(M^{-1} cm^{-1})$
297.50	0.1120E+04
300.00	0.1140E+04
302.50	0.1150E+04
305.00	0.1240E+04
307.50	0.1300E+04
310.00	0.1360E+04
312.50	0.1420E+04
315.00	0.1460E+04
317.50	0.1500E+04
320.00	0.1510E+04
323.10	0.1520E+04
330.00	0.1410E+04
340.00	0.1170E+04
350.00	0.8000E+03
360.00	0.4480E+03
370.00	0.2120E+03
380.00	0.8200E+02
390.00	0.2000E+02
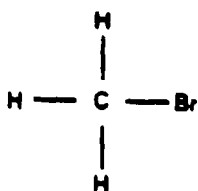
49. BROMOMETHANE

CAS No. 74-83-9

```
        H
        |
  H ——— C ——— Br
        |
        H
```

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	94.94	
Melting point, °C	-93.6	CRC
Boiling point, °C	3.56	CRC
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	900 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	12.3	CC-Kow
Sediment-water, K_{oc} (unitless)	5.9	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	4.2	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	0.197	C-VP/S-20°
Vapor pressure, P_v (torr)	1.42×10^3 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.737	C-DC.7

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49. BROMOMETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	0.1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	—	HPHI
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NACM
For neutral process, k_N (hr^{-1})	1.44×10^{-3} (25°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	—	VF-NBD

E: Estimated value; see List of Source Codes.
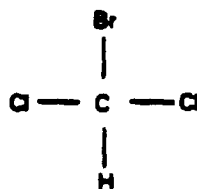
50. BROMODICHLOROMETHANE

CAS No. 75-27-4

Br
|
Cl — C — Cl
|
H

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	163.83	
Melting point, °C	-57.1	WREF
Boiling point, °C	90	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	4.5×10^3	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	126	CC-Kow
Sediment-water, K_{oc} (unitless)	61	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	35	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.41×10^{-3}	C-VP20°/S22°
Vapor pressure, P_v (torr)	50 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.655	C-DC.7

50. BROMODICHLOROMETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	0.2	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	5.76	WREF
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	NACM
For neutral process, k_N (hr^{-1})	5.76×10^{-8} (25°C)	E-AC-H
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}\ hr^{-1}$)	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[50-1] Solubility value was obtained from unpublished work done at SRI International.

51. DIBROMOCHLOROMETHANE

CAS No. 124-48-1

```
        Br
        |
Cl ——  C  —— Br
        |
        H
```
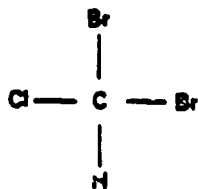
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	208.29	
Melting point, °C	<-20	WREF
Boiling point, °C	119-120 (748mm)	CRC
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	4.0×10^3	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	174	CC-Kow
Sediment-water, K_{oc} (unitless)	84	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	47	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	9.9×10^{-4}	C-VP20°/S22° [51-2]
Vapor pressure, P_v (torr)	76 (20°C)	[51-2]
Reaeration rate ratio, k_v^c/k_v^o	NAV	

51. DIBROMOCHLOROMETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	0.5	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	2.88 (25°C)	WREF
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	NACM
For neutral process, k_N (hr^{-1})	2.88×10^{-8} (25°C)	E-AC-H
Biotransformation rate constant.		
For bacterial transformation in water, k_b (ml $cell^{-1}\ hr^{-1}$)	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[51-1] Water solubility data obtained from unpublished results at SRI International.

[51-2] Vapor pressure value at 20°C is obtained from the value at 10.5°C and the Clausius Clapeyron equation.
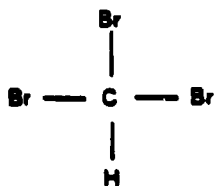
52. TRIBROMOMETHANE

CAS No. 75-25-2

Br
|
Br —— C —— Br
|
H

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	252.75	
Melting point, °C	8.3	WREF
Boiling point, °C	149.5	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	3.01×10^3 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	240	CC-Kow
Sediment-water, K_{oc} (unitless)	116	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	63	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	5.6×10^{-4}	C-VP/S-20'
Vapor pressure, P_v (torr)	5 (20°C)	Jordan, 1954
Reaeration rate ratio, k_v^c/k_v^o	NAV	

52. TRIBROMOMETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	0.5	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	1.15 (25°C)	WREF [52-1]
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	2.5×10^{-9} (25°C)	[52-2]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[52-1] This hydrolysis rate constant at pH 7 and 25°C reported in WREF is assumed to be due to the base promoted process.

[52-2] The neutral hydrolysis rate constant, K_N, has been assigned by analogy to trichloromethane.
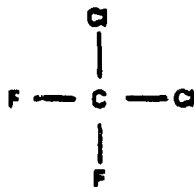
53. DICHLORODIFLUOROMETHANE

CAS No. 75-71-8

```
        Cl
        |
        |
 F ──── C ──── Cl
        |
        |
        F
```

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	120.91	
Melting point, °C	-158	WREF
Boiling point, °C	-29.8	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	280 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	120	CC-Kow
Sediment-water, K_{oc} (unitless)	58	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	33	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.98	C-VP/S-25°
Vapor pressure, P_v (torr)	4.87×10^3 (25°C)	Jordan, 1954
Reaeration rate ratio, k_v^c/k_v^o	0.615	C-DC.7

53. DICHLORODIFLUOROMETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	0	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	0	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	—	VF-NBD

E: Estimated value; see List of Source Codes.

54. TRICHLOROFLUOROMETHANE

CAS No. 75-69-4

$$F - \underset{\underset{Cl}{|}}{\overset{\overset{Cl}{|}}{C}} - Cl$$

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	137.4	
Melting point, °C	-111	WREF
Boiling point, °C	23.8	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	1.1×10^3 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	331	CC-Kow
Sediment-water, K_{oc} (unitless)	159	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	84	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	0.11	C-VP/S-20°
Vapor pressure, P_v (torr)	667.4 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.571	C-DC.7

54. TRICHLOROFLUOROMETHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	0	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	0	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	—	VF-NBD

E: Estimated value; see List of Source Codes.

References for 3.4

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Pomona College Medicinal Data Base, June 1982.

SECTION 3.5. HALOGENATED ETHERS

55. Bis(chloromethyl)ether
56. Bis(2-chloroethyl)ether
57. Bis(2-chloroisopropyl)ether
58. 2-Chloroethyl vinyl ether
59. 4-Chlorophenyl phenyl ether
60. 4-Bromophenyl phenyl ether
61. Bis(2-chloroethoxy)methane

55. BIS(CHLOROMETHYL)ETHER

CAS No. 542-88-1

$$Cl - \underset{\underset{H}{|}}{\overset{\overset{H}{|}}{C}} - O - \underset{\underset{H}{|}}{\overset{\overset{H}{|}}{C}} - Cl$$
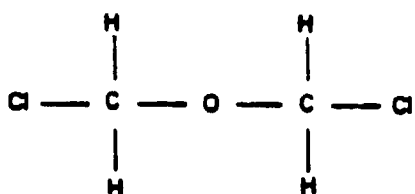
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	115	
Melting point, °C	-41.5	WREF
Boiling point, °C	104	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	2.2×10^4 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	2.4	CC-Kow
Sediment-water, K_{oc} (unitless)	1.2	C-Koc f :ow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	1.0	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.3×10^{-4}	C-VP22°/S25°
Vapor pressure, P_v (torr)	30 (22°C)	WREF
Reaeration rate ratio, k_v^C/k_v^O	NAV	

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55.   BIS(CHLOROMETHYL)ETHER

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNEk	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	$\prec<360$	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	$-$	HPHI
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	$-$	HPHI
For neutral process, k_N (hr^{-1})	65 (20°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	$-$	HF-NBD

E: Estimated value; see List of Source Codes.

56.   BIS(2-CHLOROETHYL)ETHER

CAS No.   111-44-4
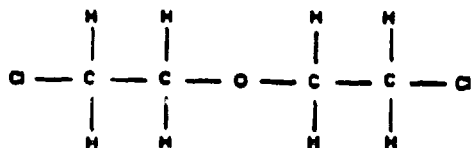
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	143	
Melting point, °C	-24.5	CRC
Boiling point, °C	178	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	1.02×10^4 [56-1]	WREF
Octanol-water, K_{ow} (unitless)	29	CC-Kow
Sediment-water, K_{oc} (unitless)	13.9	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	9.2	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	1.3×10^{-5}	C-VP20°/S-[56-1]
Vapor pressure, P_v (torr)	0.71 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

56. BIS(2-CHLOROETHYL)ETHER

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	24	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	—	HPHI
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	—	HPHI
For neutral process, k_N (hr^{-1})	4×10^{-6} (25°C)	[56-2]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

[56-1] No temperature reported for the water solubility; data generated at room temperature. This value is used in the calculation of Henry's constant.

56. BIS(2-CHLOROETHYL)ETHER

[56·2] A hydrolysis rate constant of 1.5×10^{-5} min^{-1} has been reported for bis(2-chloroethyl)ether in aqueous dioxane at 100°C (WREF). This rate constant corresponds to a half-life of 32 days. Allowing for a factor of two decrease in rate constant f⁻r each 10°C decrement, the half-life is calculated as 22 years (or 256 times slower) at 20°C. This rate constant is much slower than expected based on a simple analogy to ethyl chloride where a half-life of 38 days is predicted at pH 7 and 25°C (Mabey & Mill, 1978).

The relatively slow hydrolysis rate of bis(2-chloroethyl) ether compared with ethyl chloride is due to the effect on the adjacent carbon of the $-OCH_2CH_2Cl$ group. Data have been obtained which show that aqueous solvolysis of 2-methoxy-ethyl iodide at 60°C is 6.4×10^{-3} times the rate of ethyl iodide under the same reaction conditions (Streitwieser, 1962). Assuming that this 6.4×10^{-3} factor holds for the chloroaliphatic compounds as well as for the iodo compounds, the 38 day half-life of ethyl chloride can be used to obtain a half-life of 16 years for bis(2-chloro-ethyl)ether. This estimate of the half-life is in fair agreement with the 22 year half-life calculated from the aqueous dioxane solvent data cited in WREF. For this assessment, an estimated half-life of 20 years is used to obtain a neutral rate process, k_N, of 4×10^{-6} hr^{-1}. The hydrolysis of bis(2-chloromethyl)ether should be independent of pH by analogy to other aliphatic halocarbons.

57. BIS(2-CHLOROISOPROPYL)ETHER

CAS No. 108-60-1

PHYSICAL AND TRANSPORT DATA
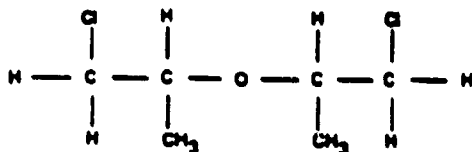
Property or Process	Value	Data Source
Molecular weight	171.1	
Melting point, °C	-97	WREF
Boiling point, °C	189	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	1.7×10^3 [57-1]	WREF
Octanol-water, K_{ow} (unitless)	126	CC-Kow
Sediment-water, K_{oc} (unitless)	61	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	35	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	1.1×10^{-4}	C-VP20°/S-[57-1]
Vapor pressure, P_v (torr)	0.85 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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57.   BIS(2-CHLOROISOPROPYL)ETHER

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	2	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	—	HPHI
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	—	HPHI
For neutral process, k_N (hr^{-1})	4×10^{-6} (25°)	[57-2]
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[57-1]   Experimental water solubility data was generated at room temperature; no specific temperature was reported.
This value was used in the calculation of Henry's constant.

57. BIS(2-CHLOROISOPROPYL)ETHER

[57-2] Rate constant assigned by analogy to bis(2-chloroethyl)ether
        (see footnote [56-3])

58. 2-CHLOROETHYL VINYL ETHER

CAS No. 110-75-8

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	106.6	
Melting point, °C		
Boiling point, °C	108	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	1.5×10^4 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	13.8	CC-Kow
Sediment-water, K_{oc} (unitless)	6.6	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	4.7	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.50×10^{-7}	C-VP20°/S25°
Vapor pressure, P_v (torr)	26.75 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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58. 2-CHLOROETHYL VINYL ETHER

TRANSFORMATION DATA

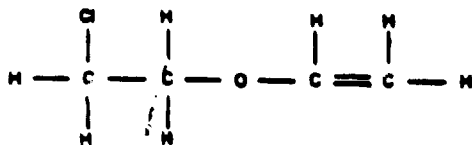| Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	1×10^{10}	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	34	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	—	HPHI
For acid-promoted process, k_A (M^{-1} hr^{-1})	—	HPHI
For neutral process, k_N (hr^{-1})	4×10^{-6} (25°C)	[58-1]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[58-1] The chloride group in 2-chloroethyl vinyl ether will be hydrolyzed at a rate similar to that of bis(2-chloroethyl)ether. The assigned hydrolysis rate constant, k_N, is 4×10^{-6} hr^{-1} as for bis(2-chloroethyl)ether. No data are available to assess the possible effect of the vinyl ether functional group on the rate of hydrolysis. Hydrolysis of the chloride group is expected to be independent of pH by analogy to other halogenated aliphatics.

59. 4-CHLOROPHENYL PHENYL ETHER

CAS No. 7005-72-3
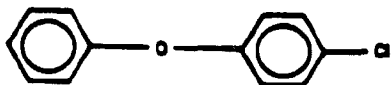
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	204.66	
Melting point, °C	-8	WREF
Boiling point, °C	293	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	3.3 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	1.2×10^5	CC-Kow
Sediment-water, K_{oc} (unitless)	5.8×10^4	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1} \right)$	1.8×10^4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	2.19×10^{-4}	C-VP/S-25°
Vapor pressure, P_v (torr)	2.7×10^{-3}	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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59. 4-CHLOROPHENYL PHENYL ETHER

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 1 x 10^{-7}	E-KB

E: Estimated value; see List of Source Codes.

60.   **4-BROMOPHENYL PHENYL ETHER**

<div align="right">CAS No.   101-55-3</div>
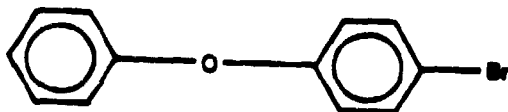
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	249.11	
Melting point, °C	18.72	WREF
Boiling point, °C	310.14	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	4.8 (25°C)	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	8.7×10^4	CC-Kow
Sediment-water, K_{oc} (unitless)	4.2×10^4	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	1.3×10^4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	1.0×10^{-4}	C-VP20°/S25°
Vapor pressure, P_v (torr)	1.5×10^{-3} (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

60. 4-BROMOPHENYL PHENYL ETHER

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3 x 10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

61. BIS(2-CHLOROETHOXY)METHANE

CAS No. 111-91-1

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	173.1	
Melting point, °C		
Boiling point, °C	218.1	WREF
Ionization constant	pK-NER	

Partition constants:

Property or Process	Value	Data Source
Water solubility, S_w (ppm)	8.1×10^4 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	10.7	CC-Kow
Sediment-water, K_{oc} (unitless)	5.2	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	3.7	C-KB f Kow

Volatilization constants:

Property or Process	Value	Data Source
Henry's constant, H_c (atm m^3 mol^{-1})	2.8×10^{-7}	C-VP20°/S25°
Vapor pressure, P_v (torr)	<0.1 (20°C)	WREF
Reaeration rate ratio, k_v^C/k_v^O	NAV	

61.   BIS(2-CHLOROETHOXY)METHANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	52	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	—	HPHI
For acid-promoted process, k_A (M^{-1} hr^{-1})	—	HPHI
For neutral process, k_N (hr^{-1})	4×10^{-6} (25°C)	[61-1]
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

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61. BIS(2-CHLOROETHOXY)METHANE

[61-1] A neutral hydrolysis rate constant, k_N, of 4×10^{-8} hr^{-1}
for the loss of chloride from the ethane group is assigned
to 2-chloroethoxy methane by analogy to bis(2-chloroethyl)ether.
Hydrolysis with loss of chloride is independent of pH by
analogy to other alkyl halides (Mabey & Mill, 1978).

The carbon-oxygen bonds of the acetal linkage are also
suspectible to hydrolysis. The acid-catalyzed hydrolysis
rate constant, k_A, for this process has been measured at
2.53×10^{-6} M^{-1} sec^{-1} (WREF). At pH 3, this rate constant
corresponds to a half-life of 8.7 years. Since the acid-
promoted hydrolysis will decrease by a factor of ten for
each pH unit increase, hydrolysis of the compound at
the chlorinated position will dominate over the acetal
hydrolysis at environmental pHs.

References for 3.5

Mabey, W. R., and T. Mill. 1978. Critical Review of Hydrolysis of Organic Compounds in Water Under Environmental Conditions. J. Phys. Chem. Ref. Data 7:383.

Streitwieser, A., Jr. 1962. Solvolytic Displacement Reactions. McGraw-Hill, New York.

SECTION 3.6. MONOCYCLIC AROMATIC CHEMICALS

62. Benzene
63. Chlorobenzene
64. 1,2-Dichlorobenzene (o-dichlorobenzene)
65. 1,3-Dichlorobenzene (m-dichlorobenzene)
66. 1,4-Dichlorobenzene (p-dichlorobenzene)
67. 1,2,4-Trichlorobenzene
68. Hexachlorobenzene
69. Ethylbenzene
70. Nitrobenzene
71. Toluene
72. 2,4-Dinitrotoluene
73. 2,6-Dinitrotoluene
74. Phenol
75. 2-Chlorophenol
76. 2,4-Dichlorophenol
77. 2,4,6-Trichlorophenol
78. Pentachlorophenol
79. 2-Nitrophenol
80. 4-Nitrophenol
81. 2,4-Dinitrophenol
82. 2,4-Dimethyl phenol
83. p-Chloro-m-cresol
84. 4,6-Dinitro-o-cresol

62. BENZENE

CAS No. 71-43-2

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	78.12	
Melting point, °C	5.5	WREF
Boiling point, °C	80.1	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	1.78×10^3 (25°C)	WREF [62-1]
Octanol-water, K_{ow} (unitless)	135	CC-Kow
Sediment-water, K_{oc} (unitless)	65	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	37	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	5.5×10^{-3}	C-VP/S-25°
Vapor pressure, P_v (torr)	95.2 (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.574	C-DC.7

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62. BENZENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	NHFG
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1×10^{-7}	E-KB

E: Estimated value; see List of Source Codes.

[62-1] Several water solubilities, ranging from 820 ppm to 1800 ppm, have been reported.

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63. CHLOROBENZENE

CAS No. 108-90-7
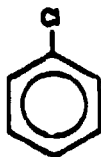
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	112.56	
Melting point, °C	-45	WREF
Boiling point, °C	132	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	488 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	690	CC-Kow
Sediment-water, K_{oc} (unitless)	330	C-Koc f Kow
Microorganisms-water, K_B $\left((\text{ug/g})(\text{mg/}\ell)^{-1}\right)$	164	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	$3.5\epsilon \times 10^{-3}$	C-VP20°/S25°
Vapor pressure, P_v (torr)	11.7 (20°C)	WREF [63-1]
Reaeration rate ratio, k_v^c/k_v^o	0.528	C-DC.7

63. CHLOROBENZENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b ($ml\ cell^{-1}\ hr^{-1}$)	(E) 3×10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

[63-1] Two values for vapor pressure - 11.7 torr and 8.8 torr - have
        been reported. The 11.7 torr value was obtained from the
        table of vapor pressures, critical temperatures and critical
        pressures in CRC Handbook, while the 8.8 torr value is
        reported in Verschueren, 1977.

64. 1,2-DICHLOROBENZENE

CAS No. 95-50-1
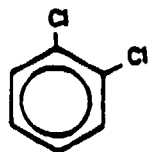
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	147.01	
Melting point, °C	-17.0	WREF
Boiling point, °C	180.5	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	100 (20°C)	Verschueren, 1977
Octanol-water, K_{ow} (unitless)	3.6×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	1.7×10^3	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	730	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	1.93×10^{-3}	C-VP/S-20°
Vapor pressure, P_v (torr)	1.0 (20°C)	Verschueren, 1977
Reaeration rate ratio, k_v^c/k_v^o	0.495	C-DC.7

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1×10^{-10}	E-KB

E: _Estimated value_; see List of Source Codes.

65. 1,3-DICHLOROBENZENE

CAS No. 541-73-1
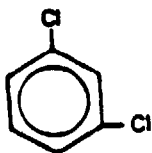
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	147.01	
Melting point, °C	-24 7	WREF
Boiling point, °C	173	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	123 (25°C)	Verschueren, 1977
Octanol-water, K_{ow} (unitless)	3.6×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	1.7×10^3	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	730	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	3.61×10^{-3}	C-VP/S-25°
Vapor pressure, P_v (torr)	2.28 (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.495	C-DC.7

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 1 x 10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

66. 1,4-DICHLOROBENZENE

CAS No. 106-46-7
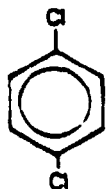
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	147.01	
Melting point, °C	53.1	WREF
Boiling point, °C	174	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	79 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	3.6×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	1.7×10^3	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	730	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	3.1×10^{-3}	C-VP/S-25°
Vapor pressure, P_v (torr)	1.18 (25°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.495	C-DC.7

66. 1,4-DICHLOROBENZENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, φ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 1 x 10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

67. 1,2,4-TRICHLOROBENZENE

CAS No. 120-82-1

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	181.45	
Melting point, °C	16.95	WREF
Boiling point, °C	213.5	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	30 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	1.9×10^4	CC-Kow
Sediment-water, K_{oc} (unitless)	9.2×10^3	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	3.3×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.3×10^{-3}	C-VP/S-25°
Vapor pressure, P_v (torr)	0.29 (25°C)	Dreisbach, 1955
Reaeration rate ratio, k_v^c/k_v^o	0.465	C-DC.7

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67.   1,2,4-TRICHLOROBENZENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [67-1]	Zepp, 1980
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at ____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1 x 10^{-10}	E-KB

E: <u>Estimated value</u>; see List of Source Codes.

67. 1,2,4-TRICHLOROBENZENE

[67-1] The absorption coefficients and the corresponding wavelengths are as follows (Zepp, 1980):

WAVELENGTH (nm)	EPSILON (M^{-1} cm^{-1})
297.50	0.4000E+01
300.00	0.1400E+01
302.50	0.6100E+00
305.00	0.3600E+00
307.50	0.2600E+00
310.00	0.2200E+00
312.50	0.2000E+00
315.00	0.1800E+00
317.50	0.1600E+00
320.00	0.1500E+00
323.10	0.1000E+00
330.00	0.5300E-01
340.00	0.1300E-01

68. HEXACHLOROBENZENE

CAS No. 118-74-1
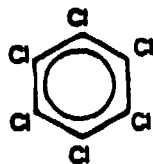
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	284.79	
Melting point, °C	230	WREF
Boiling point, °C	322 [68-1]	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	6×10^{-3} (25°C)	WREF
Octanol-water, K_{ow} (unitless)	2.6×10^6	CC-Kow
Sediment-water, K_{oc} (unitless)	1.2×10^6	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	2.9×10^5	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	6.8×10^{-4}	C-VP20°/S25°
Vapor pressure, P_v (torr)	1.09×10^{-5} (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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68. HEXACHLOROBENZENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		

Direct photolysis rate
  constant, k_p (hr^{-1})
    _____ at _____ latitude		

Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

[68-1] No pressure is reported with the boiling point.

69. ETHYLBENZENE

CAS No. 100-41-4

CH_3CH_2

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	106.16	
Melting point, °C	-94.9	WREF
Boiling point, °C	136.2	CRC
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	152 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	2.2×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	1.1×10^3	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	470	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	6.6×10^{-3}	C-VP/S-20°
Vapor pressure, P_v (torr)	7 (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.489	C-DC.7

69. ETHYLBENZENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	720	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) 3×10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

70. NITROBENZENE

CAS No. 98-95-3

NO_2
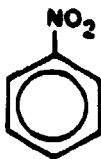
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	123.11	
Melting point, °C	5.6	WREF
Boiling point, °C	211	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	1.9×10^3 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	74	CC-Kow
Sediment-water, K_{oc} (unitless)	36	C-Koc f Kow
Microorganisms-water K_B $\left((\mu g/g)(mg/\ell)^{-1} \right)$	22	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	1.31×10^{-5}	C-VP/S-20°
Vapor pressure, P_v (torr)	0.15 (20°C)	WREF
Reaeration rate ratio, k_v^C/k_v^O	NAV	

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70. NITROBENZENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [70-1]	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b ($ml\ cell^{-1}\ hr^{-1}$)	(E) 3×10^{-9}	E-KD

E: Estimated value; see List of Source Codes.

70. NITROBENZENE

[70-1] UV spectrum in light petroleum solvent (b.p. 100-120°C) is shown below (UV Atlas, 1966).

λ (nm)
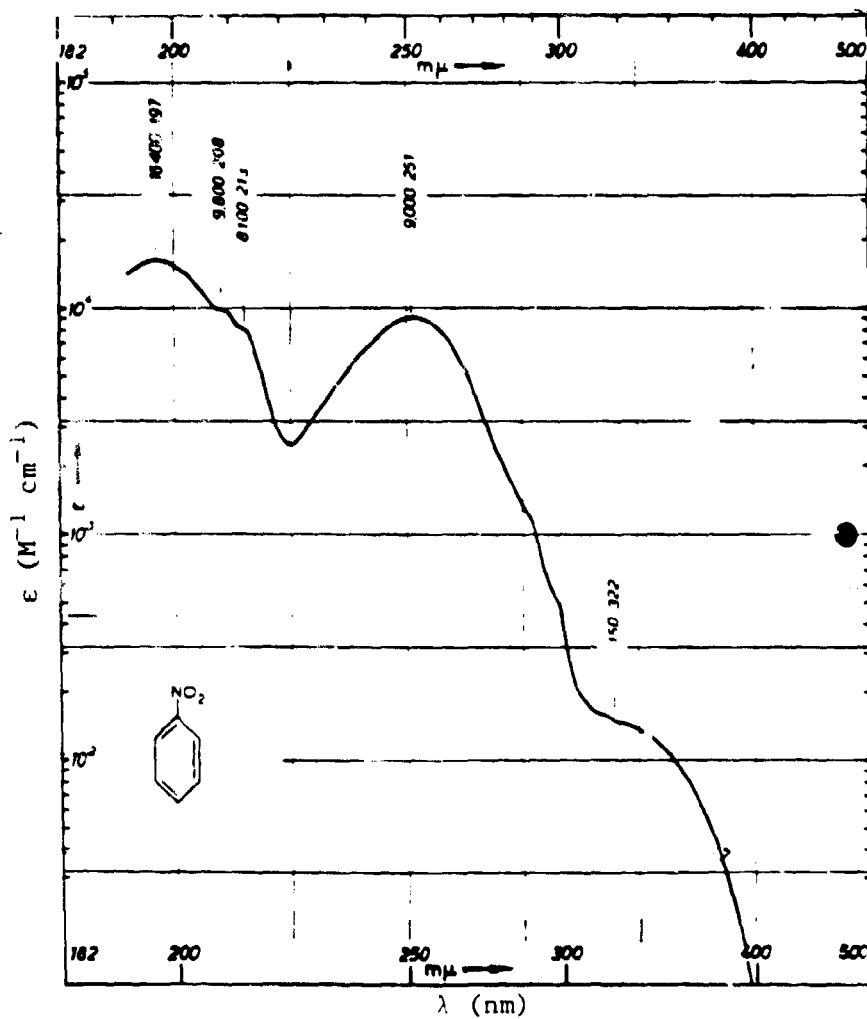
71. TOLUENE

CAS No. 108-88-3

CH_3

(toluene structure)

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	92.13	
Melting point, °C	-95	WREF
Boiling point, °C	110.6	CRC
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	534.8 (25°C)	Verschueren, 1977
Octanol-water, K_{ow} (unitless)	620	CC-Kow
Sediment-water, K_{oc} (unitless)	300	C-Koc f Kow
Microorganisms- K_B $((\mu g/g)(mg/\ell)^{-1})$	148	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	6.66×10^{-3}	C-VP20°/S25°
Vapor pressure, P_v (torr)	28.7 (20°C)	Verschueren, 1977
Reaeration rate ratio, k_v^c/k_v^o	0.526	C-DC.7

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71. TOLUENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	144	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	NHFG
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 1 x 10$^-$	E-KB

E: <u>Estimated value</u>; see List of Source Codes.

72. 2,4-DINITROTOLUENE

CAS No. 121-14-2
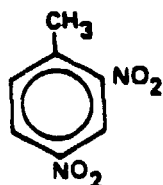
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	182.14	
Melting point, °C	70	WREF
Boiling point, °C	300	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	270 (22°C)	WREF
Octanol-water, K_{ow} (unitless)	95	Pomona
Sediment-water, K_{oc} (unitless)	45	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	39	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	4.5×10^{-6}	C-VP20°/S22°
Vapor pressure, P_v (torr)	5.1×10^{-3} (20°C)	Maksimov, 1968
Reaeration rate ratio, k_v^c/k_v^o	NAV	

72. 2,4-DINITROTOLUENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT	[72-1]
Reaction quantum yield, ϕ, at $\underline{\quad 313 \quad}$ nm	7.5×10^{-4}	[72-1]
Direct photolysis rate constant, k_p (hr^{-1})		
$\underline{summer}$ at $\underline{\quad 40° \quad}$ latitude	1.6×10^{-2}	[72-1]
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	144	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	1×10^{-7}	[72-1]

E: Estimated value; see List of Source Codes.

72. 2,4-DINITROTOLUENE

[72-1] Photolysis and biotransformation data are reported in Spanggord et al. (1980). The measured sunlight photolysis half-life of 2,4 DNT in pure water is approximately 42 hours; however, the sunlight photolysis half-lives in three natural waters ranged from 3 hrs to 10 hrs, showing that humic substances can promote the photolysis.

It also should be noted that an acclimated system capable of biotransforming 2,4 DNT was obtained in only one natural water sample, and k_b was measured using that mixed culture system.

The absorption coefficients for 2,4 DNT reported in Spanggord et al. (1980) are listed below.

WAVELENGTH (nm)	EPSILON (M^{-1} cm^{-1})
297.50	0.4104E+04
300.00	0.3747E+04
302.50	0.3390E+04
305.00	0.3033E+04
307.50	0.2677E+04
310.00	0.2320E+04
312.50	0.1963E+04
315.00	0.1784E+04
317.50	0.1606E+04
320.00	0.1338E+04
323.10	0.1249E+04
330.00	0.1071E+04
340.00	0.7140E+03
350.00	0.5350E+03
360.00	0.3570E+03
370.00	0.2680E+03
380.00	0.1780E+03
390.00	0.8900E+02
400.00	0.3600E+02
410.00	0.0000E+00

73. 2,6-DINITROTOLUENE

CAS No. 606-20-2
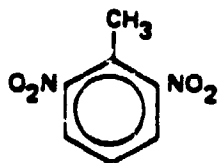
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	182.14	
Melting point, °C	65	WREF
Boiling point, °C	285	WREF [73-1]
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	180 (20°C)	[73-2]
Octanol-water, K_{ow} (unitless)	190	CC-Kow
Sediment-water, K_{oc} (unitless)	92	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	51	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	7.9×10^{-6}	C-VP/S-20° [73-3]
Vapor pressure, P_v (torr)	0.018 (20°C)	Maksimov, 1968
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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73. 2,6-DINITROTOLUENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	144	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[73-1] No pressure value is reported for the boiling point.

[73-2] The water solubility value has been estimated from the water solubility of 2,4-dinitrotoluene.

73. 2,6-DINITROTOLUENE

[73-3] The Henry's Law constant was obtained by extrapolating the data beyond the melting point and adjusting by

$$\exp\left[\frac{\Delta H_f}{R} \left(\frac{1}{T_M} - \frac{1}{T}\right)\right]$$

where T_M is the melting point in °C and T is the temperature at which H_c is being estimated.

74.　PHENOL
CAS No.　108-95-2

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data source
Molecular weight	94.11	
Melting point, °C	43	CRC
Boiling point, °C	181.75	WREF
Ionization constant	9.89 (20°C)	CRC

Partition constants:

Water solubility, S_w (ppm)	9.3×10^4 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	30	CC-Kow
Sediment-water, K_{oc} (unitless)	14.2	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	9.4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	4.54×10^{-7}	C-VP/S-25°
Vapor pressure, P_v (torr)	0.341 (25°C)	Biddiscombe & Martin, 1958
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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74. PHENOL

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<7 x 10^5	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	1 x 10^7	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3 x 10^{-6}	E-KB

E: Estimated value; see List of Source Codes.

75. 2-CHLOROPHENOL

CAS No. 95-57-8
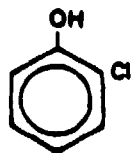
PHYSICAL AND TRANSPORT DATA

Property or Process [75-1]	Value	Data Source
Molecular weight	128.56	
Melting point, °C	9	CRC
Boiling point, °C	175.6	WREF
Ionization constant	8.85 (25°C)	CRC

Partition constants:

Water solubility, S_w (ppm)	2.85×10^4 (20°C)	WREF
Octanol-water, K_{ow} (unitless)	151	CC-Kow
Sediment-water, K_{oc} (unitless)	73	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1}\right)$	41	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	1.03×10^{-5}	C-VP/S-20°
Vapor pressure, P_v (torr)	1.77 (20°C)	C-CT/CRC
Reaeration rate ratio, k_v^C/k_v^O	NAV	

75.   2-CHLOROPHENOL

TRANSFORMATION DATA

Property or Process [75-1]	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm.	PNER	
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	$<7 \times 10^5$	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	1×10^7	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1×10^{-7}	E-KB

E: Estimated value; see List of Source Codes.

[75-1]   All data are calculated for the neutral form unless otherwise stated.

76. 2,4-DICHLOROPHENOL

CAS No. 120-83-2
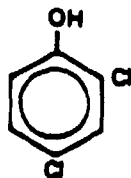
PHYSICAL AND TRANSPORT DATA

Property or Process [76-1]	Value	Data Source
Molecular weight	163.0	
Melting point, °C	45	WREF
Boiling point, °C	210	WREF
Ionization constant	7.85 [76-2]	WREF

Partition constants:

Water solubility, S_w (ppm)	4.6×10^3 (20°C)	Verschueren 1977
Octanol-water, K_{ow} (unitless)	790	CC-Kow
Sediment-water, K_{oc} (unitless)	380	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	186	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.8×10^{-6}	C-VP/S-20° [76-3]
Vapor pressure, P_v (torr)	0.059 (20°C)	C-CT/CRC
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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76. 2,4-DICHLOROPHENOL

TRANSFORMATION DATA

Property or Process [76-1]	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude	[76-4]	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	$<7 \times 10^5$	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	1×10^7	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b ($ml\ cell^{-1}\ hr^{-1}$)	(E) 1×10^{-7}	E-KB

E: **Estimated value**; see List of Source Codes.

[76-1] All data are calculated for the neutral form unless otherwise stated.

[76-2] No temperature is reported for the ionization constant.

76. 2,4-DICHLOROPHENOL

[76-3] The Henry's Law constant was obtained by extrapolating the data beyond the melting point and adjusting by

$$\exp\left[\frac{\Delta H_f}{R} \left(\frac{1}{T_M} - \frac{1}{T} \right) \right]$$

where T_M is the melting point in °C and T is the temperature at which H_c is being estimated.

[76-4] Conflicting literature information has bee reported for the photolysis of 2,4-dichlorophenol (WREF). One paper reports that, after 10 days exposure to s light, no starting chemical could be detected in solution; the other reference indicated that at wavelengths greater than 280nm, irradiation induced negligible photolysis.
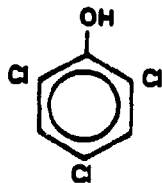
77. 2,4,6-TRICHLOROPHENOL

CAS No. 88-06-2

PHYSICAL AND TRANSPORT DATA

Property or Process [77-1]	Value	Data Source
Molecular weight	197.5	
Melting point, °C	68	WREF
Boiling point, °C	244.5	WREF
Ionization constant	5.99 [77-2]	Verschueren, 1977

Partition constants:

Water solubility, S_w (ppm)	800 (25°C)	Verschueren, 1977
Octanol-water, K_{ow} (unitless)	4.1×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	2.0×10^3	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	824	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	4×10^{-6}	C-VP/S-25° [77-3]
Vapor pressure, P_v (torr)	0.012 (25°C)	C-CT/CRC
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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77.   2,4,6-TRICHLOROPHENOL

TRANSFORMATION DATA

Property or Process [77-1]	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	$<7 \times 10^4$	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	1×10^6	C-OX
Hydrolysis rate constant :		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) 3×10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

[77-1] All data are calculated for the neutral form unless otherwise stated.
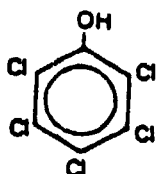
[77-2] No temperature is reported for the ionization constant.

77. 2,4,6-TRICHLOROPHENOL

[77-3] The Henry's Law constant was obtained by extrapolating the data beyond the melting point and adjusting by

$$\exp\left[\frac{\Delta H_f}{R} \left(\frac{1}{T_M} - \frac{1}{T}\right)\right]$$

where T_M is the melting point in °C and T is the temperature at which H_c is being estimated.

78. PENTACHLOROPHENOL

CAS No. 87-86-5

PHYSICAL AND TRANSPORT DATA

Property or Process [78-1]	Value	Data Source
Molecular weight	266.4	
Melting point, °C	190	WREF
Boiling point, °C	310	WREF
Ionization constant	4.74 [78-2]	WREF

Partition constants:

Water solubility, S_w (ppm)	14 (20°C)	Verschueren, 1977
Octanol-water, K_{ow} (unitless)	1.1×10^5	CC-Kow
Sediment-water, K_{oc} (unitless)	5.3×10^4	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	1.6×10^4	(-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.8×10^{-6}	C-VP/S-20°
Vapor pressure, P_v (torr)	1.1×10^{-4} (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

78. PENTACHLOROPHENOL

TRANSFORMATION DATA

Property or Process [78-1]	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	$<7 \times 10^3$	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	1×10^5	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b ($ml\ cell^{-1}\ hr^{-1}$)	(E) 3×10^{-9}	E-KB

E: <u>Estimated value</u>; see List of Source Codes.

[78-1] All data are calculated for the neutral form unless otherwise stated.

[78-2] No temperature was reported for the ionization constant.

79. 2-NITROPHENOL

CAS No. 88-75-5
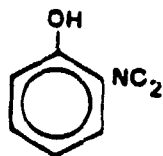
OH
NC₂ (structure)

PHYSICAL AND TRANSPORT DATA

Property or Process [79-1]	Value	Data Source
Molecular weight	139.1	
Melting point, °C	45.3	WREF
Boiling point, °C	216	WREF
Ionization constant	8.28 (25°C)	CRC

Partition constants:

Water solubility, S_w (ppm)	2.1×10^3 (20°C)	Verschueren, 1977
Octanol-water, K_{ow} (unitless)	56	CC-Kow
Sediment-water, K_{oc} (unitless)	27	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	17	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	7.56×10^{-6}	C-VP-/S20° [79-2]
Vapor pressure, P_v (torr)	0.151 (20°C)	C-CT/CRC [79-3]
Reaeration rate ratio, k_v^c/k_v^o	NAV	

79. 2-NITROPHENOL

TRANSFORMATION DATA

Property or Process [79-1]	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [79-4]	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	<2 x 10^5	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	2 x 10^6	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 3 x 10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

[79-1] All data are calculated for the neutral form unless otherwise stated.

[79-2] The Henry's Law constant was obtained by extrapolating the
        data beyond the melting point and adjusting by

$$\exp\left[\frac{\Delta H_f}{R}\left(\frac{1}{T_M}-\frac{1}{T}\right)\right]$$

where T_M is the melting point in °C and T is the temperature
at which H_c is being estimated.

[79-3] No temperature is reported for the vapor pressure.

[79-4] UV spectrum of 2-nitrophenol in water is shown below
        (UV Atlas, 1966).

λ (nm)
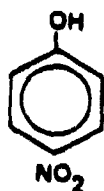
80. 4-NITROPHENOL

CAS No. 100-07-7

OH

NO$_2$

PHYSICAL AND TRANSPORT DATA

Property or Process [80-1]	Value	Data Source
Molecular weight	139.1	
Melting point, °C	114.9	WREF
Boiling point, °C	279	WREF
Ionization constant	7.15 (25°C)	CRC

Partition constants:

Water solubility, S_w (ppm)	1.6×10^4 (25°C)	Verschueren, 1977
Octanol-water, K_{ow} (unitless)	~3	CC-Kow
Sediment-water, K_{oc} (unitless)	45	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1}\right)$	27	C-KB f Koc

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.5×10^{-5}	C-VP146°/S25°
Vapor pressure, P_v (torr)	2.2 (146°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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TRANSFORMATION DATA

Property or Process [80-1]	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [80-2]	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	[80-3]	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	$<2 \times 10^5$	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	2×10^6	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1×10^{-7}	E-KB

E: Estimated value; see List of Source Codes.

[80-1] All data are calculated for the neutral form unless otherwise stated.
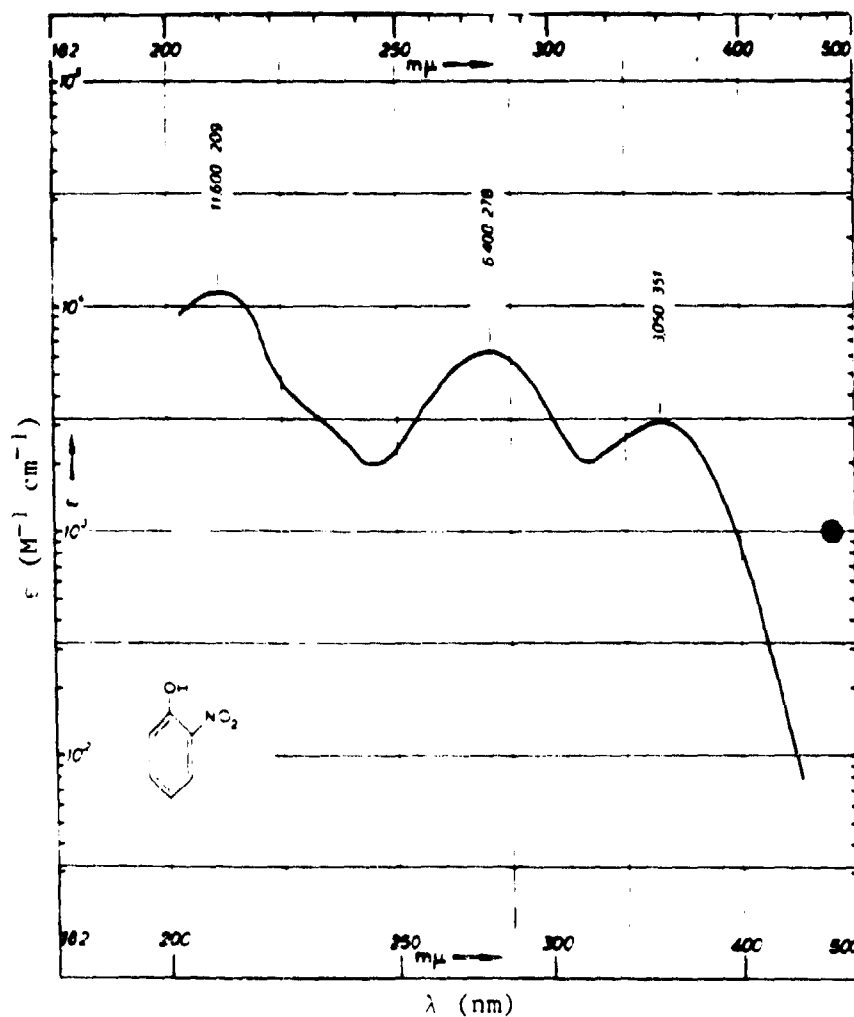
80. 4-NITROPHENOL

[80-2] UV spectrum of 4-nitrophenol in water is given below (UV Atlas, 1966).

λ (nm)
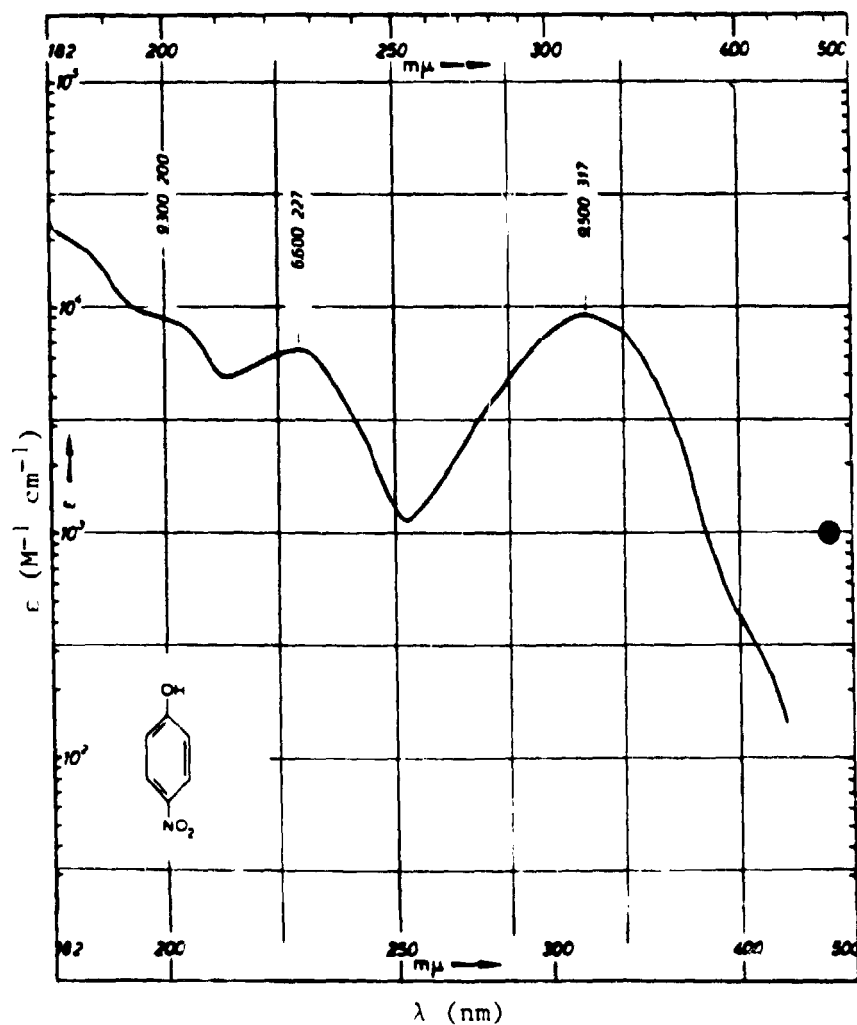
[80-3] 4-Nitrophenol at concentrations of 200 ppm in aqueous solutions has been reported to be degraded after 1-2 months in sunlight. Given the high concentration of chemical and uncertain pH of the solution, this information should be considered only as a qualitative observation that 4-nitrophenol can be photolyzed in sunlight.

81. 2,4-DINITROPHENOL

CAS No. 51-28-5

PHYSICAL AND TRANSPORT DATA

Property or Process [81-1]	Value	Data Source
Molecular weight	184.1	
Melting point, °C	114	WREF
Boiling point, °C		
Ionization constant	3.96 (15°C)	CRC

Partition constants:

Water solubility, S_w (ppm)	5.6×10^3 (18°C)	Verschueren, 1977
Octanol-water, K_{ow} (unitless)	34.7	Pomona
Sediment-water, K_{oc} (unitless)	16.6	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	15.4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	6.45×10^{-10}	C-VP/S-18°
Vapor pressure, P_v (torr)	1.49×10^{-5} (18°C)	Hoyer & Peperle, 1953
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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81.   2,4-DINITROPHENOL

TRANSFORMATION DATA

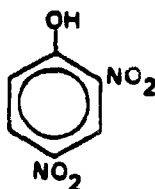| Property or Process [81-1]	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	3×10^4	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	5×10^5	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	HNES
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}\ hr^{-1}$)	(E) 3×10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

82. 2,4-DIMETHYLPHENOL

CAS No. 105-67-9

OH
CH₃
CH₃
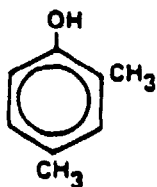
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	122.2	
Melting point, °C	27-28	CRC
Boiling point, °C	210.9	WREF
Ionization constant	10.60 [82-1]	WREF

Partition constants:

Water solubility, S_w (ppm)	590 (25°C)	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	200	Pomona
Sediment-water, K_{oc} (unitless)	96	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	75	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	1.7×10^{-5}	C-VP20°/S25°
Vapor pressure, P_v (torr)	0.062 (20°C)	WREF [82-2]
Reaeration rate ratio, k_v^C/k_v^O	NAV	

82. 2,4-DIMETHYLPHENOL

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<4 x 10^6	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	1.1 x 10^8	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) 1 x 10^{-7}	E-KB

E: Estimated value; see List of Source Codes.

[82-1] No temperature is reported for the ionization constant.

[82-2] This value of the vapor pressure is for the supercooled liquid.
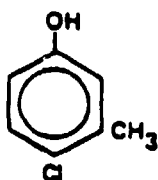
83. p-CHLORO-m-CRESOL

CAS No. 59-50-7

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	142.6	
Melting point, °C	66	WREF
Boiling point, °C	235	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	3.85×10^3 (20°C)	Verschueren, 1977
Octanol-water, K_{ow} (unitless)	1259	Pomona
Sediment-water, K_{oc} (unitless)	604	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	400	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.5×10^{-6}	C-VP/S-20°
Vapor pressure, P_v (torr)	0.05 (20°C)	[83-1]
Reaeration rate ratio, k_v^C/k_v^O	NAV	

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83. p-CHLORO-m-CRESOL

TRANSFORMATION DATA

Property or Process	Value	Dat Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	$<7 \times 10^5$	C-OX
For RO$_2$ (peroxy radical), k_{OX} (M^{-1} hr^{-1})	1×10^7	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-9}	E-KB

E: __Estimated value__; see List of Source Codes.

[83-1] Vapor pressure value is assigned by analogy; no data are available.
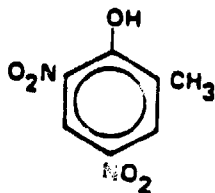
84. **4,6-DINITRO-o-CRESOL**

CAS No. **534-52-1**

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	198.1	
Melting point, °C	85.8	WREF
Boiling point, °C		
Ionization constant	4.35 [84-1]	WREF

Partition constants:

Water solubility, S_w (ppm)	290 (25°C)	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	500	CC-Kow
Sediment-water, K_{oc} (unitless)	240	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1} \right)$	122	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	4×10^{-5}	C-VP20°/S25°
Vapor pressure, P_v (torr)	5×10^{-2} (20°C)	[84-2]
Reaeration rate ratio, k_v^c/k_v^o	NAV	

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		

Direct photolysis rate
  constant, k_p (hr^{-1})
    _____ at _____ latitude		

Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	3×10^4	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	5×10^5	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-9}	E-KB

E: _Estimated value_; see List of Source Codes.

[84-1] No temperature is reported with the ionization constant.

[84-2] Vapor pressure value assigned by analogy; no data were available.

References for 3.6

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Pomona College Medicinal Data Base, June 1982.

SECTION 3.7. PHTHALATE ESTERS

85. Dimethyl phthalate
86 D'ethyl phthalate
87. Di-n-butyl phthalate
88. D -n-octyl phthalate
89. Bis(2-ethylhexyl)phthalate
90. Butyl benzyl phthalate

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85. DIMETHYL PHTHALATE

CAS No. 131-11-3

$$\text{(benzene ring)} \begin{array}{c} -\overset{\overset{\textstyle O}{\|}}{C} - O - CH_3 \\ -\underset{\underset{\textstyle O}{\|}}{C} - O - CH_3 \end{array}$$
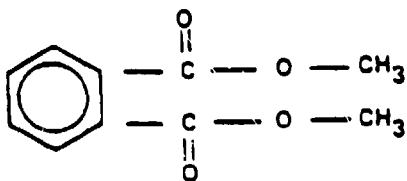
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	194.2	
Melting point, °C	0	WREF
Boiling point, °C	282	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	5.00×10^3 (20°C)	Verschueren, 1977
Octanol-water, K_{ow} (unitless)	36.3	Pomona
Sediment-water, K_{oc} (unitless)	17.4	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	16.0	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	2.15×10^{-6}	C-VP/S-20°
Vapor pressure, P_v (torr)	4.19×10^{-3} (20°C)	C-CT/CRC
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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85. DIMETHYL PHTHALATE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [85-1]	Zepp, 1980
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	0.05	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	248 (30°C)	WREF
For acid-promoted process, k_A (M^{-1} hr^{-1})	0.025 (30°C)	C-KBASE
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	5.2×10^{-6}	Wolfe et al., 1980

E: Estimated value; see List of Source Codes.

85. DIMETHYL PHTHALATE

[85-1] Table of absorption coefficients and the corresponding
        wavelengths for dimethyl phthalate is given below (Zepp, 1980).

WAVELENGTH (nm)	EPSILON $(M^{-1} cm^{-1})$
297.50	0.8000E+01
300.00	0.2800E+01
302.50	0.1000E+01
305.00	0.3700E+00
307.50	0.1600E+00
310.00	0.3000E-01
312.50	0.6000E-01
315.00	0.4000E-01
317.50	0.4000E-01
320.00	0.3000E-01
323.10	0.3000E-01
330.00	0.2000E-01
340.00	0.1000E-01
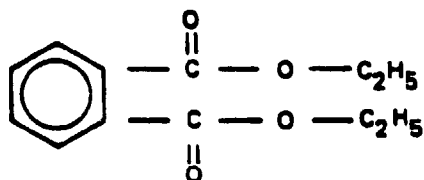
86. DIETHYL PHTHALATE

CAS No. 84-66-2

(chemical structure diagram)

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	222.?	
Melting point, °C	-40.5	WREF
Boiling point, °C	298	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	896 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	295	Pomona
Sediment-water, K_{oc} (unitless)	142	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	107	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	1.2×10^{-6}	C-VP/S-25°
Vapor pressure, P_v (torr)	3.5×10^{-3} (25°C)	C-CT/CRC
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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86. DIETHYL PHTHALATE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	1.4	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	43.2 (30°C)	WREF
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	4.32×10^{-3} (30°C)	C-KBASE
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml \ cell^{-1} \ hr^{-1})$	(E) 1×10^{-7}	E-KB

E: Estimated value; see List of Source Codes.

87. DI-n-BUTYL PHTHALATE

CAS No. 84-74-2

(structural diagram of di-n-butyl phthalate)

$$- \overset{O}{\underset{\parallel}{C}} - O - C_4H_9$$
$$- \underset{\parallel}{\overset{}{C}} - O - C_4H_9$$
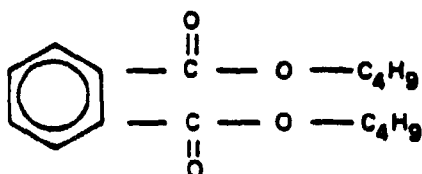
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	278.3	
Melting point, °C	-35	WREF
Boiling point, °C	340	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	13 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	3.6×10^5	CC-Kow
Sediment-water, K_{oc} (unitless)	1.7×10^5	C-Koc f Kow
Microorganisms-water, K_B $\left((ug/g)(mg/\ell)^{-1}\right)$	4.7×10^4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	2.8×10^{-7}	C-VP/S-25°
Vapor pressure, P_v (torr)	1.0×10^{-5} (25°C)	Jaber, 1982
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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87.   DI-n-BUTYL PHTHALATE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	

Direct photolysis rate
   constant, k_p (hr^{-1})
   _____ at _____ latitude
	PNER	

Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	1.4	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	79.2 (30°C)	WREF
For acid-promoted process, k_A (M^{-1} hr^{-1})	7.92×10^{-3} (30°C)	C-KBASE
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	$(1.9-4.4) \times 10^{-8}$	Steen et al., 1979

E: Estimated value; see List of Source Codes.
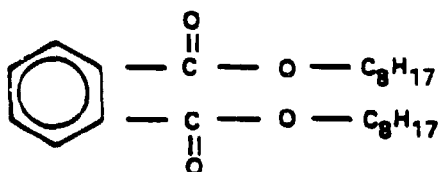
88. DI-n-OCTYL PHTHALATE

CAS No. 117-84-0

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	391	
Melting point, °C	-25	WREF
Boiling point, °C	220 (4mm)	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	3.0 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	7.4×10^9	CC-Kow
Sediment-water, K_{oc} (unitless)	3.6×10^9	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	3.9×10^8	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	1.7×10^{-5}	C-VP/S-25°
Vapor pressure, P_v (torr)	1.4×10^{-4} (25°C)	[88-1]
Reaeration rate ratio, k_v^c/k_v^o	NAV	

88. DI-n-OCTYL PHTHALATE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	1.4	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	79.2 (30°C)	[88-2]
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	7.92×10^{-3} (30°C)	[88-2]
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	3.1×10^{-10}	Wolfe et al., 1980

E: Estimated value; see List of Source Codes.

[88-1] Vapor pressure value assigned by analogy. This value is used in the calculation of Henry's constant.

[88-2] Hydrolysis rate constant is assigned by analogy to di-n-butyl phthalate.

89.   BIS(2-ETHYLHEXYL)PHTHALATE

CAS No.   117-81-7
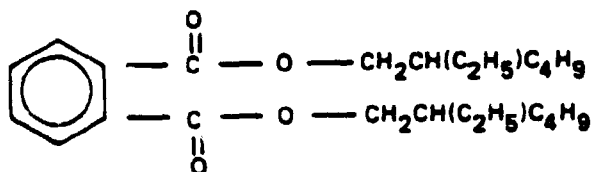
$$\bigcirc \begin{array}{l} - \overset{\overset{O}{\|}}{C} - O - CH_2CH(C_2H_5)C_4H_9 \\ - \underset{\underset{O}{\|}}{C} - O - CH_2CH(C_2H_5)C_4H_9 \end{array}$$

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	391	
Melting point, °C	-50	WREF
Boiling point, °C	386.9 (5mm)	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.4 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	4.1×10^9	CC-Kow
Sediment-water, K_{oc} (unitless)	2.0×10^9	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	2.3×10^8	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	3×10^{-7}	C-VP20°/S25°
Vapor pressure, P_v (torr)	2×10^{-7} (20°C)	C-CT/CRC
Reaeration rate ratio, k_v^c/k_v^o	NAV	

89. BIS(2-ETHYLHEXYL)PHTHALATE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	7.2	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0.4 (30°C)	WREF
For acid-promoted process, k_A (M^{-1} hr^{-1})	4.0×10^{-5} (30°C)	C-KBASE
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	4.2×10^{-12}	Wolfe et al., 1980

E: Estimated value; see List of Source Codes.

90. BUTYL BENZYL PHTHALATE

CAS No. 85-68-7
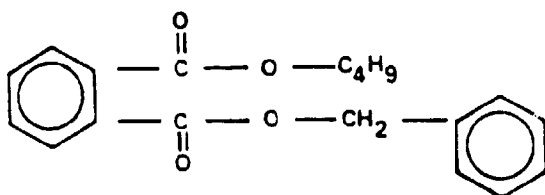
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	312	
Melting point, °C	-35	WREF
Boiling point, °C	377	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	2.9	WREF [90-1]
Octanol-water, K_{ow} (unitless)	3.6×10^5	CC-Kow
Sediment-water, K_{oc} (unitless)	1.7×10^5	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	4.7×10^4	C-kB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	8.3×10^{-6}	C-VP/S [90-2]
Vapor pressure, P_v (torr)	6×10^{-5}	[90-3]
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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90.   BUTYL BENZYL PHTHALATE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<80	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	79.2 (30°C)	[90-4]
For acid-promoted process, k_A (M^{-1} hr^{-1})	7.92×10^{-3} (30°C)	[90-4]
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-9}	E-KB

E: _Estimated value_; see List of Source Codes.

[90-1]   No temperature is reported with the water solubility.

[90-2]   Henry's constant calculated using solubility and vapor pressure values at unknown temperatures.

90. BUTYL BENZYL PHTHALATE

[90-3] The vapor pressure was calculated using Trouton's Rule. No specific temperature is given.

[90-4] Hydrolysis rate constant is assigned by analogy to di-n-butyl phthalate.

References for 3.7

Steen, W. C., D. F. Paris and G. L. Baughman. 1979. 177th National
    Meeting of American Chemical Society, Honololo, Hawaii. April.
    (ENVR 43)

Verschueren, K. 1977. Handbook of Environmental Data on Organic Chemicals.
    Van Norstrand/Reinhold Press, New York. 659 pp.

Wolfe, N. L., D. F. Paris, W. C. Steen, and G. L. Baughman. 1980. Correla-
    tion of Microbial Degradation Rates with Chemical Structure. Environ-
    mental Sci. Technol. 14:1143-4.

Zepp, R. G. 1980. Private communication.

SECTION 3.8 POLYCYCLIC AROMATIC HYDROCARBONS

91. Acenaphthene
92. Acenaphthylene
93. Anthracene
94. Benzo(a)anthracene
95. Benzo(b)fluoranthene
96. Benzo(k)fluoranthene
97. Benzo(ghi)perylene
98. Benzo(a)pyrene
99. Chrysene
100. Dibenzo(a,h)anthracene
101. Fluoranthene
102. Fluorene
103. Indeno(1,2,3-cd)pyrene
104. Naphthalene
105. Phenanthrene
106. Pyrene

91. ACENAPHTHENE

CAS No. 83-32-9
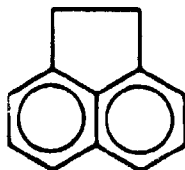
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	154.2	
Melting point, °C	96	WREF
Boiling point, °C	279	CRC
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	3.42 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	9.6×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	4.6×10^3	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	1.8×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	9.1×10^{-5}	C-VP/S-25°
Vapor pressure, P_v (torr)	1.55×10^{-3} (25°C)	Hoyer & Peperle, 1958
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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91. ACENAPHTHENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [91-1]	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm	(E)5 x 10^{-3}	E-APAH
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	< 3600	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	8 x 10^3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	0	NHFG
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 3 x 10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

91. ACENAPHTHENE

[91-1] UV spectrum of acenaphthene in heptane solvent is shown below (UV Atlas, 1966).

λ (nm)
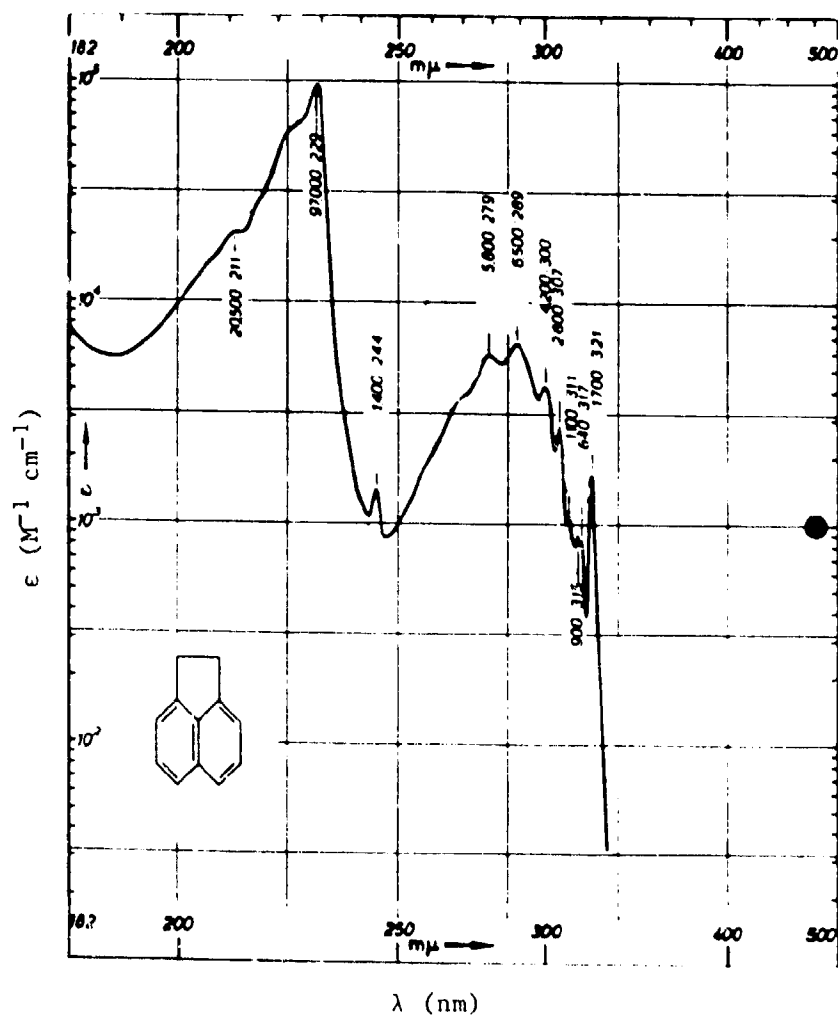
92. ACENAPHTHYLENE

CAS No. 208-96-8

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	152.2	
Melting point, °C	92	WREF
Boiling point, °C	265-275	CRC [92-1]
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	3.93 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	5.3×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	2.5×10^3	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	1.0×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	1.45×10^{-3}	C-VP20°/S25°
Vapor pressure, P_v (torr)	0.029 (20°C)	WREF
Reaeration rate ratio, k_v^C/k_v^O	NAV	

92. ACENAPHTHYLENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [92-2]	UV ATLAS
Reaction quantum yield, ϕ, at _____ nm	(E)5×10^{-3}	E-APAH
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	$\sim 4 \times 10^7$	C-OX
For RO$_2$ (peroxy radical), k_{OX} (M^{-1} hr^{-1})	5×10^3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
.or neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

[92-1] No pressure is reported for the boiling point.

92. ACENAPHTHYLENE

[92-2] UV spectrum of acenaphthylene in hexane solvent is shown below (UV Atlas, 1966).

λ (nm)
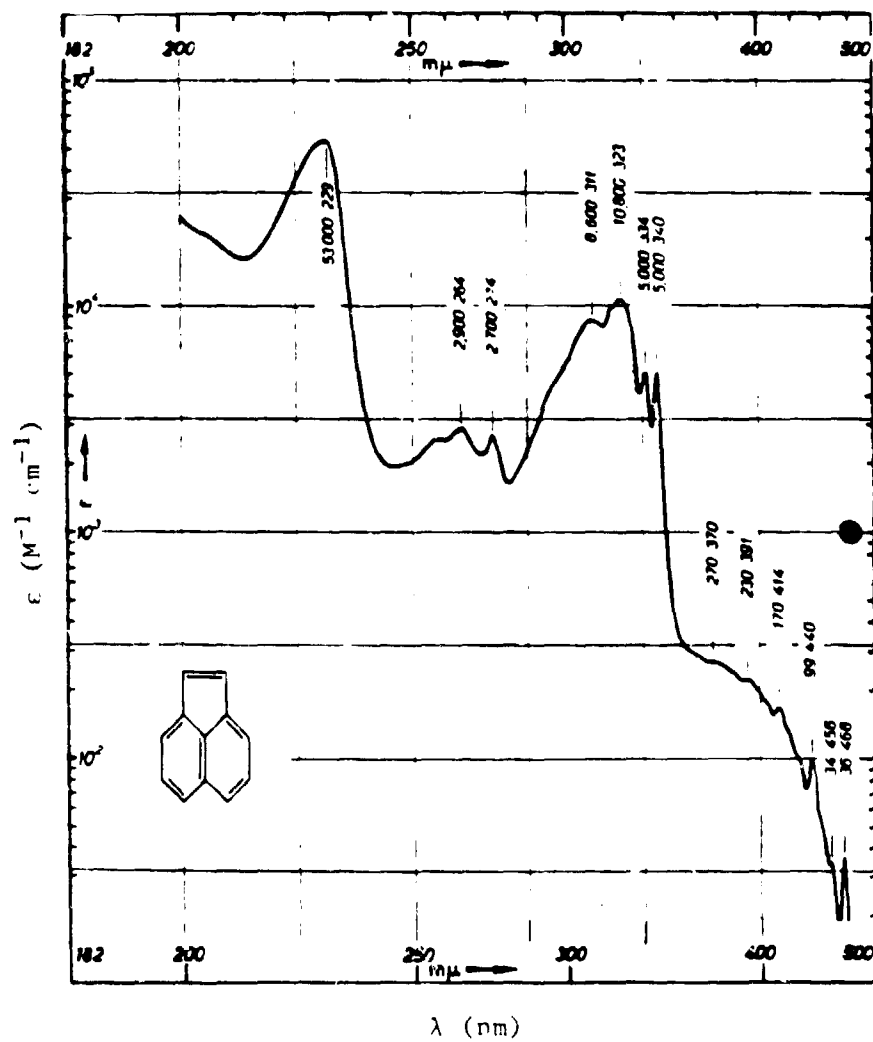
93. ANTHRACENE

CAS No. 120-12-7
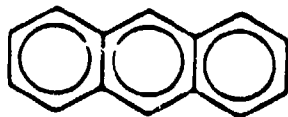
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	178.2	
Melting point, °C	216	WREF
Boiling point, °C	226.5 (53mm)	CRC [93-1]
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.045 (25°C)	May et al, 1978
Octanol-water, K_{ow} (unitless)	2.8×10^4	CC-Kow
Sediment-water, K_{oc} (unitless)	1.4×10^4	C-Koc f Kow
Microorganisms-water, $K_B \left((ug/g)(mg/\ell)^{-1} \right)$	4.7×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	8.6×10^{-5}	C-VP/S-25°
Vapor pressure, P_v (torr)	1.7×10^{-5} (25°C)	Jaber, 1982
Reaeration rate ratio, k_v^C/k_v^O	NAV	

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93. ANTHRACENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [93-2]	Zepp, 1980
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
winter at 35° latitude	0.15	WREF
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	5×10^8	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	2.2×10^5	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	NHFG
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-9}	E-KB

E: Estimated value; see List of Source Codes.

[93-1] Compound sublimes at 226.5°C and 53 mm pressure.

93. ANTHRACENE

[93-2] Table of absorption coefficients and the corresponding wavelengths for anthracene is given below (Zepp, 1980).

WAVELENGTH (nm)	EPSILON $(M^{-1}\ cm^{-1})$
279.50	0.6700E+03
300.00	0.7200E+03
302.50	0.8500E+03
305.00	0.3000E+03
307.50	0.5000E+03
310.00	0.6700E+03
312.50	0.7900E+03
315.00	0.1100E+04
317.50	0.1100E+04
320.00	0.1700E+04
323.10	0.2300E+04
330.00	0.2030E+04
340.00	0.3300E+04
350.00	0.3430E+04
360.00	0.4430E+04
370.00	0.2840E+04
380.00	0.2640E+04
390.00	0.7500E+02

94. BENZO[a]ANTHRACENE

CAS No. 56-55-3
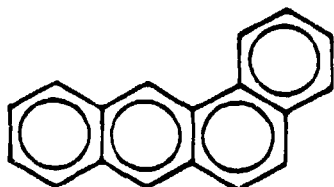
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	228.3	
Melting point, °C	155-157	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	5.7×10^{-3} (20°C)	Smith et al, 1978
Octanol-water, K_{ow} (unitless)	4.1×10^5	CC-Kow
Sediment-water, K_{oc} (unitless)	2.0×10^5	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	5.3×10^4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	1×10^{-6}	C-VP/S-20°
Vapor pressure, P_v (torr)	2.2×10^{-8} (20°C)	Hoyer & Peperle, 1958
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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94. BENZO[a]ANTHRACENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [94-1]	Smith et al, 1978
Reaction quantum yield, ϕ, at ___313___ nm	3.3×10^{-3}	Smith et al, 1978
Direct photolysis rate constant, k_p (hr^{-1}) midday ___summer___ at ___40°___ latitude	1.39	Smith et al, 1978
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	5×10^{8}	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	2×10^{4}	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

94. BENZO[a]ANTHRACENE

[94-1] Absorption coefficients and the corresponding wavelengths for benzo[a]anthracene obtained from work done at SRI are listed below.

WAVELENGTH (nm)	EPSILON $(M^{-1} cm^{-1})$
297.50	0.7930E+04
300.00	0.7070E+04
302.50	0.5880E+04
305.00	0.3790E+04
307.50	0.3200E+04
310.00	0.3480E+04
312.50	0.3900E+04
315.00	0.4200E+04
317.50	0.4170E+04
320.00	0.4120E+04
323.10	0.4800E+04
330.00	0.5450E+04
340.00	0.5390E+04
350.00	0.4850E+04
360.00	0.3350E+04
370.00	0.1560E+04
380.00	0.6620E+03
390.00	0.4170E+03
400.00	0.1720E+02
410.00	0.1810E+02
420.00	0.1810E+02
430.00	0.1360E+02
440.00	0.3360E+02
450.00	0.1540E+02
460.00	0.1180E+02
470.00	0.3630E+02
480.00	0.8200E+01
490.00	0.1800E+01
500.00	0.0000E+00
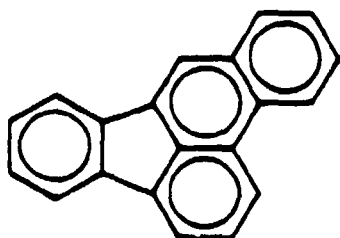
95. BENZO[b]FLUORANTHENE

 CAS No. 205-99-2

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	252.3	
Melting point, °C	167-168	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.014 (25°C)	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	1.15×10^6	CC-Kow
Sediment-water, K_{oc} (unitless)	5.5×10^5	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	1.4×10^5	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	1.22×10^{-5}	C-VP20°/S25°
Vapor pressure, P_v (torr)	5×10^{-7} (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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95. BENZO[b]FLUORANTHENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	4×10^7	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	5×10^3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	NHFG
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

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96. BENZO[k]FLUORANTHENE

CAS No. 207-08-9
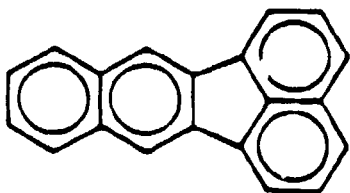
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	252.3	
Melting point, °C	217	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	4.3×10^{-3} (25°C)	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	1.15×10^6	CC-Kow
Sediment-water, K_{oc} (unitless)	5.5×10^5	C-Koc f Kow
Microorganisms-water, K_B $\left((ug/g)(mg/\ell)^{-1}\right)$	1.4×10^5	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	3.87×10^{-5}	C-VP20°/S25°
Vapor pressure, P_v (torr)	5×10^{-7} (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	0.374	C-DC.7

96. BENZO[k]FLUORANTHENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	4×10^7	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	5×10^3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

97. BENZO[ghi]PERYLENE

CAS No. 191-24-2
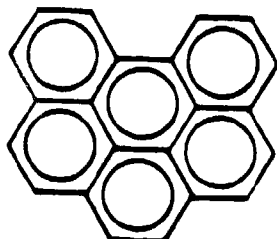
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	276	
Melting point, °C	222	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	2.6×10^{-4} (25°C)	WREF
Octanol-water, K_{ow} (unitless)	3.2×10^{6}	CC-Kow
Sediment-water, K_{oc} (unitless)	1.6×10^{5}	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1} \right)$	3.5×10^{5}	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	1.44×10^{-7}	C-VP/S-25°
Vapor pressure, P_v (torr)	1.03×10^{-10} (25°C)	Murray et al, 1974
Reaeration rate ratio, k_v^c/k_v^o	NAV	

97. BENZO[ghi]PERYLENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<36	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E)3 x 10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

98. BENZO[a]PYRENE

CAS No. 50-32-8

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	252	
Melting point, °C .	179	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	3.8×10^{-3} (25°C)	WREF
Octanol-water, K_{ow} (unitless)	1.15×10^{6}	CC-Kow
Sediment-water, K_{oc} (unitless)	5.5×10^{6}	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	1.4×10^{5}	C-KB f Kow

Volatilization constants:

Henry's constant, h_c (atm m^3 mol^{-1})	4.9×10^{-7}	C-VP/S-25°
Vapor pressure, P_v (torr)	5.6×10^{-9} (25°C)	Murray et al, 1974
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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98. BENZO[a]PYRENE

TRANSFORMATION DATA

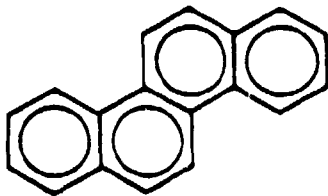| Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [98-1]	Smith et al, 1978
Reaction quantum yield, ϕ, at ___313___ nm	8.9×10^{-4}	Smith et al, 1978
Direct photolysis rate constant, k_p (hr^{-1}) winter, at ___40°___ latitude midday	0.58 [98-2]	Smith et al, 1978
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	___ $\times 10^8$	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	2×10^4	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFC
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

98. BENZO[a]PYRENE

[98-1] Absorption coefficients and the corresponding wavelengths
for benzo[a]pyrene were obtained from work done at SRI
(Smith et al, 1978).

WAVELENGTH (nm)	EPSILON $(M^{-1} \ cm^{-1})$
297.50	0.4660E+05
300.00	0.2770E+05
302.50	0.1390E+05
305.00	0.6670E+04
307.50	0.4840E+04
310.00	0.3970E+04
312.50	0.3890E+04
315.00	0.3650E+04
317.50	0.3730E+04
320.00	0.3570E+04
323.10	0.3650E+04
330.00	0.5400E+04
340.00	0.8330E+04
350.00	0.1230E+05
360.00	0.1810E+05
370.00	0.1968E+05
380.00	0.2191E+05
390.00	0.1516E+05
400.00	0.2100E+04
410.00	0.1100E+04
420.00	0.0000E+00

[98-2] Photolysis rate constant calculated using SOLAR (see Section
2.3.7).

99. CHRYSENE

CAS No. 218-01-9

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	228.3	
Melting point, °C	256	WREF
Boiling point, °C	448	CRC [99-1]
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	1.8×10^{-3} (25°C)	May, 1978
Octanol-water, K_{ow} (unitless)	4.1×10^5	CC-Kow
Sediment-water, K_{oc} (unitless)	2.0×10^5	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	5.3×10^4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	1.05×10^{-6}	C-VP/S-25°
Vapor pressure, P_v (torr)	6.3×10^{-9} (25°C)	Hoyer & Peperle, 1958
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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TRANSFORMATION DATA

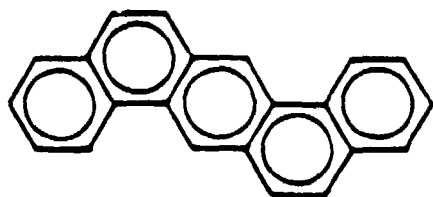| Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [99-2]	Zepp, 1980
Reaction quantum yield, ϕ, at _____ nm	2.8×10^{-3}	Zepp & Schlotzhauer,1979
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	$>1 \times 10^6$	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	1×10^3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) 1×10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[99-1] No pressure is reported for the boiling point.

99. CHRYSENE

[99-2] Table of absorption coefficients and the corresponding wavelengths of chrysene is given below (Zepp, 1980).

WAVELENGTH (nm)	EPSILON $(M^{-1}\ cm^{-1})$
297.50	0.6160E+04
300.00	0.6080E+04
302.50	0.6900E+04
305.00	0.7720E+04
307.50	0.6960E+04
310.00	0.5160E+04
312.50	0.4760E+04
315.00	0.5810E+04
317.50	0.7100E+04
320.00	0.7000E+04
323.10	0.3600E+04
330.00	0.8740E+03
340.00	0.3230E+03
350.00	0.1960E+03
360.00	0.1940E+03
370.00	0.2400E+02
380.00	0.1300E+02

100. DIBENZO[a,h]ANTHRACENE

CAS No. 53-70-3

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	278.4	
Melting point, °C	27U	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	5×10^{-4} (25°C)	WREF
Octanol-water, K_{ow} (unitless)	6.9×10^6	CC-Kow
Sediment-water, K_{oc} (unitless)	3.3×10^6	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	6.9×10^5	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	7.3×10^{-8}	C-VP20°/S25°
Vapor pressure, P_v (torr)	1×10^{-10} (20°C)	WREF
Reaeration rate ratio, k_v^C/k_v^O	NAV	

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100. DIBENZO[a,h]ANTHRACENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [100-1]	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} ($M^{-1}\ hr^{-1}$)	5×10^8	C-OX
For RO_2 (peroxy radical), k_{OX} ($M^{-1}\ hr^{-1}$)	1.5×10^4	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B ($M^{-1}\ hr^{-1}$)	0	NHFG
For acid-promoted process, k_A ($M^{-1}\ hr^{-1}$)	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b ($ml\ cell^{-1}\ hr^{-1}$)	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

100. DIBENZO[a,h]ANTHRACENE

[100-1] UV spectrum of dibenzo[a,h]anthracene in heptane solvent is shown below (UV Atlas, 1966).

λ (nm)
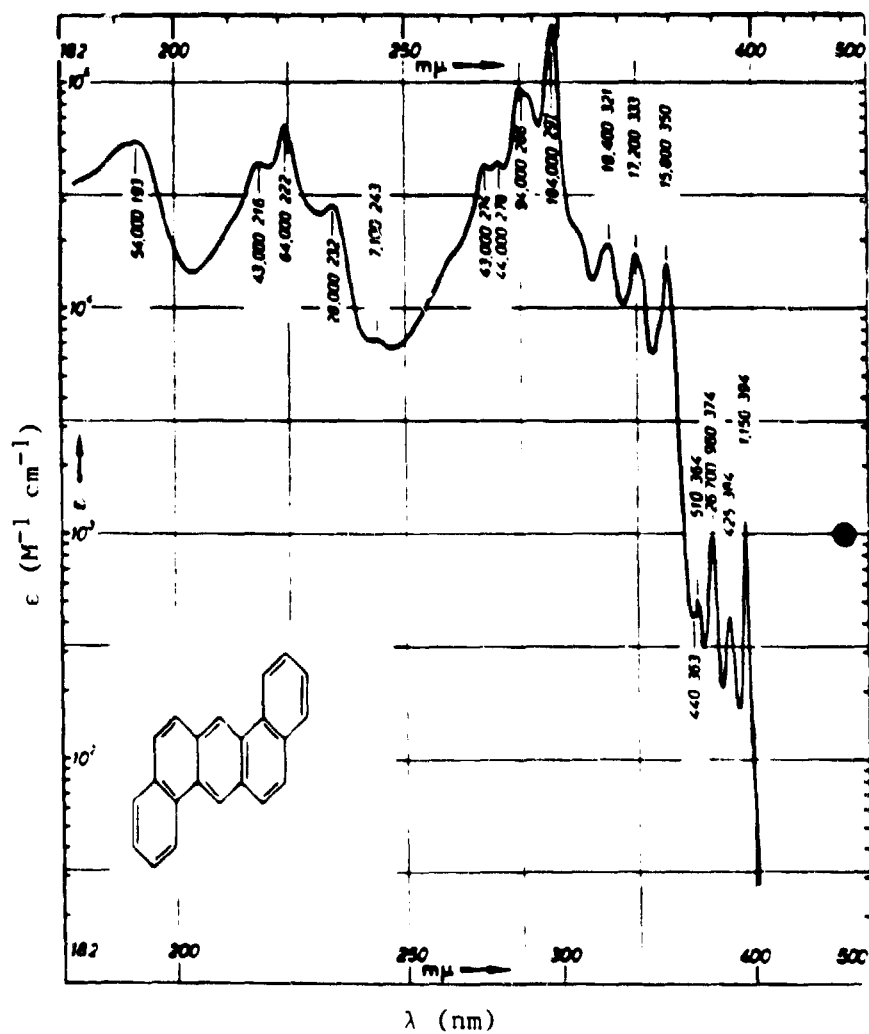
101. FLUORANTHENE

CAS No. 206-44-0
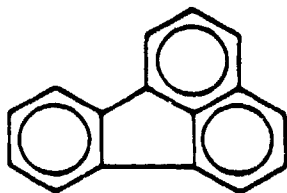
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	202.3	
Melting point, °C	111	WREF
Boiling point, °C	217 (30mm)	CRC
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.26 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	7.9×10^4	CC-Kow
Sediment-water, K_{oc} (unitless)	3.8×10^4	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	1.2×10^4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	6.5×10^{-6}	C-VP/S-25°
Vapor pressure, P_v (torr)	5.0×10^{-6} (25°C)	Hoyer & Peperle, 1958
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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101. FLUORANTHENE

TRANSFORMATION DATA

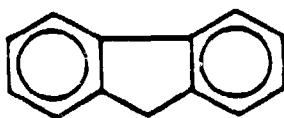| Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [101-1]	UV-ATLAS
Reaction quantum yield, ϕ, at ___313___ nm	1.2×10^{-4} [101-2]	Zepp & Schlotzhauer, 1979
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	<360	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	NHFG
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 1×10^{-10}	E-KB

E: **Estimated value**; see List of Source Codes.

101. FLUORANTHENE

[101-1] UV spectrum of fluoranthene in methanol solvent is
shown below (UV Atlas, 1966).

λ (nm)
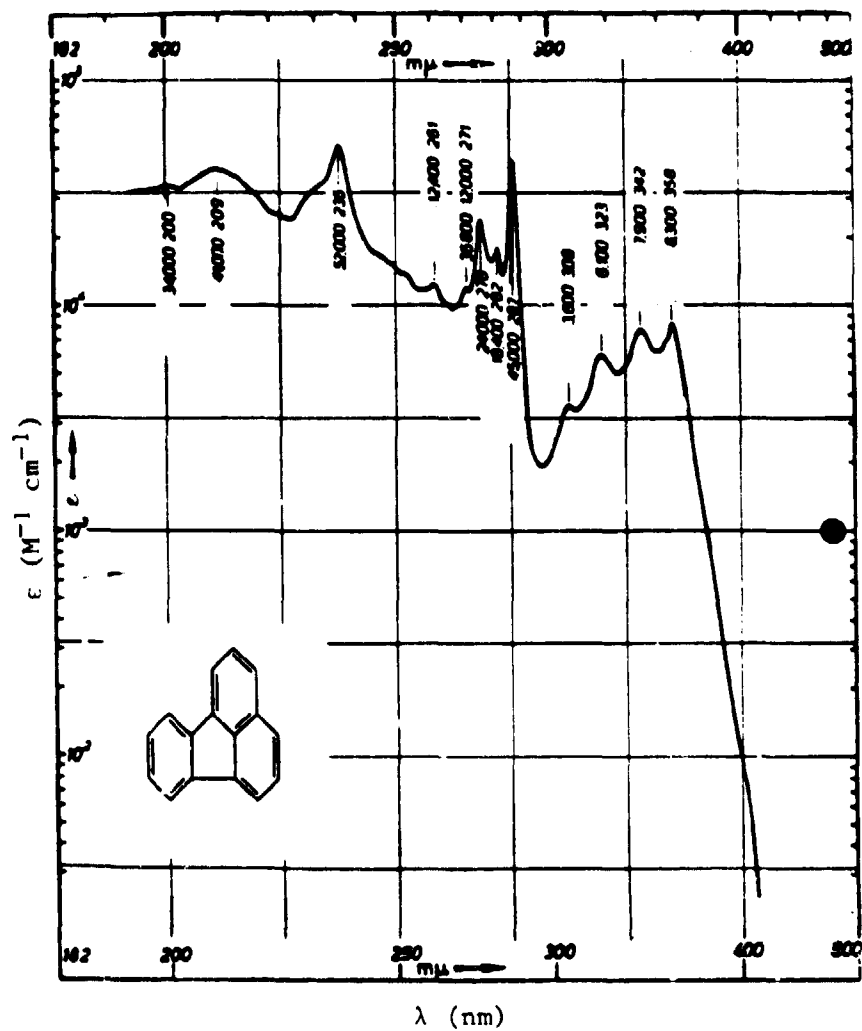
[101-2] At 366 nm, the quantum yield is 2×10^{-6}.

102. FLUORENE

CAS No. 86-73-7

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	116.2	
Melting point, °C	116-117	WREF
Boiling point, °C	293-295	CRC
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	1.69 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	1.5×10^4	Pomona
Sediment-water, K_{oc} (unitless)	7.3×10^3	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	3.8×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	6.4×10^{-5}	C-VP/S-25°
Vapor pressure, P_v (torr)	7.1×10^{-4}	Irwin, 1982
Reaeration rate ratio, k_v^C/k_v^O	NAV	

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102. FLUORENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [102-1]	UV-ATLAS
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	3×10^3	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-9}	E-KB

E: _Estimated value_; see List of Source Codes.

102. FLUORENE

[102-1] UV spectrum of fluorene in heptane solvent is shown
below (UV Atlas, 1966).

λ (nm)
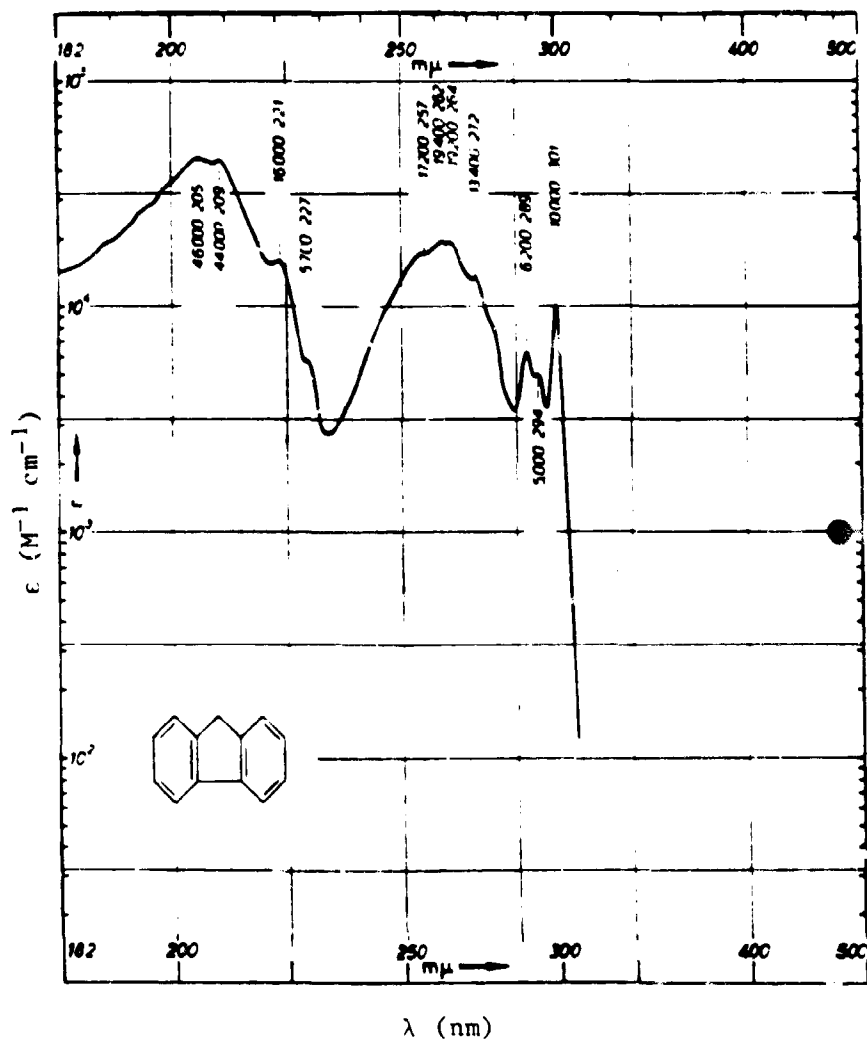
103. INDENO[1,2,3-cd]PYRENE

CAS No. 193-39-5
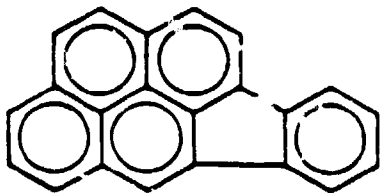
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	276.3	
Melting point, °C	164	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility S_w (ppm)	5.3×10^{-4} (25°C)	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	3.2×10^{6}	CC-Kow
Sediment-water, K_{oc} (unitless)	1.6×10^{6}	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	3.5×10^{5}	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	6.95×10^{-8}	C-VP20°/S25°
Vapor pressure, P_v (torr)	1.0×10^{-10} (20°C)	WREF
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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103. INDENO[1,2,3-cd]PYRENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	5×10^8	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	2×10^4	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml $cell^{-1}$ hr^{-1})	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

104. NAPHTHALENE

CAS No. 91-20-3
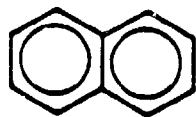
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	128.2	
Melting point, °C	80	WREF
Boiling point, °C	218	CRC
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	31.7 (25°C)	May et al, 1978
Octanol-water, K_{ow} (unitless)	1.95×10^3	CC-Kow
Sediment-water, K_{oc} (unitless)	940	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	420	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	4.6×10^{-4}	C-VP/S-25°
Vapor pressure, P_v (torr)	0.087 (25°C)	C-CT/CRC
Reaeration rate ratio, k_v^c/k_v^o	NAV	

104. NAPHTHALENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [104-1]	Zepp, 1980
Reaction quantum yield, ϕ, at ___313___ nm	1.5×10^{-2}	Zepp & Schlotzhauer, 1979
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<360	C-OX
For RO_2 (peroxy radical), $k_{O\lambda}$ $(M^{-1}\ hr^{-1})$	<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	NHFG
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E)1×10^{-7}	E-KB

E: Estimated value; see List of Source Codes.

104. NAPHTHALENE

[104-1] Table of absorption coefficients and the corresponding
wavelengths for naphthalene is given below (Zepp, 1980).

WAVELENGTH (nm)	EPSILON $(M^{-1} \, cm^{-1})$
297.50	0.3160E+03
302.50	0.2400E+03
305.00	0.2140E+03
307.50	0.1660E+03
310.00	0.1990E+03
312.50	0.1120E+03
315.00	0.7200E+02
317.50	0.2800E+02
320.00	0.2400E+02
323.10	0.1200E+02
330.00	0.2000E+01

105. PHENANTHRENE

CAS No. 85-0108
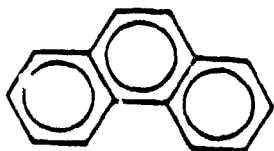
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	178.2	
Melting point, °C	101	WREF
Boiling point, °C	210-215 (12mm)	CRC
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	1.00 (25°C)	May et al, 1978
Octanol-water, K_{ow} (unitless)	2.8×10^4	CC-Kow
Sediment-water, K_{oc} (unitless)	1.4×10^4	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	4.7×10^3	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	2.26×10^{-4}	C-VP/S-25°
Vapor pressure, P_v (torr)	9.6×10^{-4} (25°C)	C-CT/CRC
Reaeration rate ratio, k_v^C/k_v^O	NAV	

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105. PHENANTHRENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [105-1]	Zepp, 1980
Reaction quantum yield, ϕ, at ___313___ nm	0.01	Zepp & Schlotzhauer, 1979
Direct photolysis rate constant, k_p (hr^{-1}) ___ at ___ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<360	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<36	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	1.6×10^{-7}	Paris et al., 1980

E: Estimated value; see List of Source Codes.

105. PHENANTHRENE

[105-1]   Table of absorption coefficients and the corresponding
          wavelengths for phenanthrene is given below (Zepp, 1980).

WAVELENGTH (nm)	EPSILON (M^{-1} cm^{-1})
297.50	0.1590E+04
300.00	0.5090E+03
302.50	0.2860E+03
305.00	0.2050E+03
307.50	0.2000E+03
310.00	0.1860E+03
312.50	0.2010E+03
315.00	0.2390E+03
317.50	0.1780E+03
320.00	0.1780E+03
323.10	0.2600E+03
330.00	0.2040E+03
340.00	0.1640E+03
350.00	0.8220E+02
360.00	0.1290E+02

106. PYRENE

CAS No. 129-00-0
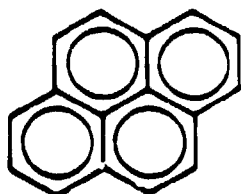
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	202.3	
Melting point, °C	150	WREF
Boiling point, °C	393	CRC
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	0.13 (25°C)	May et al, 1978
Octanol-water, K_{ow} (unitless)	8.0×10^4	CC-Kow
Sediment-water, K_{oc} (unitless)	3.8×10^4	C-Koc f Kow
Microorganisms-water $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	1.2×10^4	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	5.1×10^{-6}	C-VP/S-25°
Vapor pressure, P_v (torr)	2.5×10^{-6} (25°C)	Hoyer & Peperle 1958
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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106. PYRENE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [106-1]	Zepp, 1980
Reaction quantum yield, ϕ, at ___313___ nm	2.1×10^{-3} [106-2]	Zepp & Schlotzhauer, 1979
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	5×10^8	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	2.2×10^4	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	NHFG
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 1×10^{-10}	E-KB

_: __Estimated value__; see List of Source Codes.

106. PYRENE

[106-1] Table of absorption coefficients and the corresponding wavelengths for pyrene is given below (Zepp, 1980).

WAVELENGTH (nm)	EPSILON $(M^{-1} cm^{-1})$
297.50	0.3500E+04
300.00	0.3900E+04
302.50	0.6030E+04
305.00	0.7810E+04
307.50	0.7850E+04
310.00	0.7140E+04
312.50	0.8480E+04
315.00	0.1170E+05
317.50	0.1800E+05
320.00	0.1960E+05
323.10	0.1250E+05
330.00	0.1810E+05
340.00	0.1060E+05
350.00	0.5370E+03
360.00	0.2850E+03
370.00	0.1400E+03
380.00	0.1500E+02

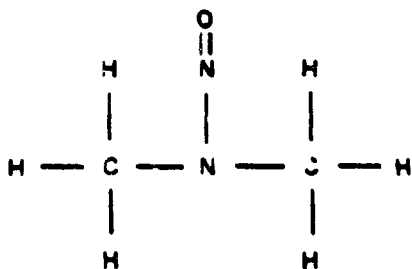[106-2] At 366 nm, the quantum yield is 2.1×10^{-3}.

References for 3.8

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May, W. E., S. P. Wasik, and D. H. Freeman. 1978. Determination of the Solubility Behavior of Some Polycyclic Aromatic Hydrocarbons in Water. Anal. Chem. 50(7):997-1000.

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UV Atlas. 1971. UV Atlas of Organic Compounds. Vol. I-V. Plenum Press, New York.

Zepp, R. C., and P. F. Schlotzhauer. 1979. Photoreactivity of Selected Aromatic Hydrocarbons in Water. In: Polynuclear Aromatic Hydrocarbons, P. W. Jones and P. Leber, editors. Ann Arbor Publishers, Inc., Ann Arbor, MI.

Zepp, R. G. 1980. Private communication.

SECTION 3.9. NITROSAMINES AND OTHER NITROGEN-CONTAINING CHEMICALS

107. Dimethyl nitrosamine
108. Diphenyl nitrosamine
109. Di-n-propyl nitrosamine
110. Benzidine
111. 3,3'-Dichlorobenzidine
112. 1,2-Diphenylhydrazine (hydrazobenzene)
113. Acrylonitrile

CAS No. 62-75-9

```
              O
              ||
    H         N         H
    |         |         |
H — C    —    N    —    C — H
    |                   |
    H                   H
```

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	74.1	
Melting point, °C		
Boiling point, °C	154	CRC
Ionization constant	pK-NE	

Partition constants:

Water solubility, S_w (ppm)	miscible	WREF
Octanol-water, K_{ow} (unitless)	0.21	CC-Kow
Sediment-water, K_{oc} (unitless)	0.10	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	0.11	C-KB f Kc

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	3.3×10^{-5}	C-VP/S-25° [107-1]
Vapor pressure, P_v (torr)	8.1 (25°C)	Chang (1976)
Reaeration rate ratio, k_v^c/k_v^o	NAV	

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107. DIMETHYL NITROSAMINE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude	[107-2]	WREF
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	<3600	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 3×10^{-12}	E-K?

E: Estimated value; see List of Source Codes.

[107-1] A water solubility value of 6.3×10^4 ppm, calculated from Kenaga and Goring's equation, is used in the calculation of Henry's constant (see Section 4).

[107-2] Although nitrosamines are reported to be unstable to sunlight, no environmentally relevant and reliable data are available to estimate photolysis rate constants.

108.   DIPHENYL NITROSAMINE

CAS No.   86-30-6
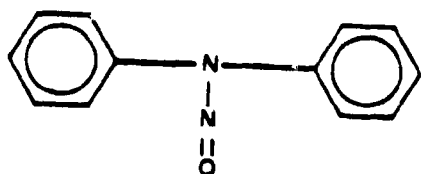
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	198.2	
Melting point, °C	67	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	40 (25°C)	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	1349	Pomona
Sediment-water, K_{oc} (unitless)	648	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	426	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	6.6×10^{-4}	C-VP/S-25° [108-1]
Vapor pressure, P_v (torr)	0.1 (25°C)	[108-1]
Reaeration rate ratio, k_v^c/k_v^o	NAV	

108. DIPHENYL NITROSAMINE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude	see [107-2]	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	<3600	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 1 x 10^{-10}	E-KB

E: Estimated value; see List of Source Codes.

[108-1] Vapor pressure value was assigned by analogy; no data were available. This value is used in the calculation of Henry's constant.

109. DI-n-PROPYL NITROSAMINE

CAS No. 621-64-7

$$CH_3\ CH_2\ CH_2 \underset{\underset{\displaystyle N}{\displaystyle |}}{\overset{\overset{\displaystyle O}{\displaystyle \|}}{}} N \underset{}{} CH_2\ CH_2\ CH_3$$
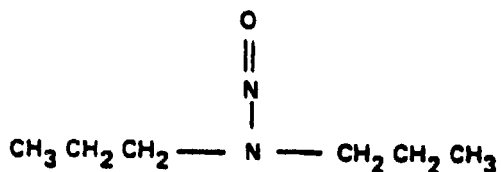
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	130.2	
Melting point, °C		
Boiling point, °C	205	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	9900 (25°C)	WREF
Octanol-water, K_{ow} (unitless)	31	CC-Kow
Sediment-water, K_{oc} (unitless)	15	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	9.8	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	6.3×10^{-6}	C-VP37°/S25° [109-1]
Vapor pressure, P_v (torr)	0.4 (37°C)	[109-1]
Reaeration rate ratio, k_v^c/k_v^o	NAV	

109. DI-n-PROPYL NITROSAMINE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	see [107-2]	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	<3600	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	<3600	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 3×10^{-12}	E-KB

E: __Estimated value__; see List of Source Codes.

[109-1] Vapor pressure was calculated using Trouton's rule; this value was used in the calculation of Henry's constant.

110. BENZIDINE

CAS No. 92-87-5
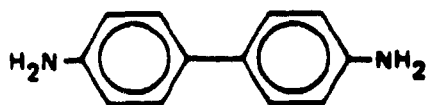
H₂N—⟨ ⟩—⟨ ⟩—NH₂

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	184.2	
Melting point, °C	129	WREF
Boiling point, °C	402	WREF
Ionization constant	4.66, 3.57 [110-1]	CRC

Partition constants:

Water solubility, S_w (ppm)	400 (12°C)	WREF
Octanol-water, K_{ow} (unitless)	21.9	Pomona
Sediment-water, K_{oc} (unitless)	10.5	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	10.1	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	3×10^{-7}	C-VP-/S12° [110-2]
Vapor pressure, P_v (torr)	5×10^{-4}	[110-2]
Reaeration rate ratio, k_v^c/k_v^o	NAV	

110. BENZIDINE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
_____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} $(M^{-1} hr^{-1})$	$<4 \times 10^7$	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1} hr^{-1})$	1.1×10^8	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1} hr^{-1})$	0	NHFG
For acid-promoted process, k_A $(M^{-1} hr^{-1})$	0	NHFG
For neutral process, k_N (hr^{-1})	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml \ cell^{-1} \ hr^{-1})$	$(E) 1 \times 10^{-10}$	E-KB

E: _Estimated value_; see List of Source Codes.

[110-1] The two ionization constants are pKa1 = 4.66 and pKa2 = 3.57 at 30°C.

[110-2] Vapor pressure was calculated using Trouton's rule; no temperature was specified. This value was used in the calculation of Henry's constant.

111. 3,3'-DICHLOROBENZIDINE

CAS No. 91-94-1
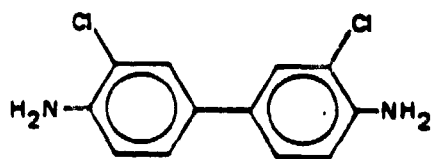
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	253.1	
Melting point, °C	132	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	4.0 (22°C)	WREF
Octanol-water, K_{ow} (unitless)	3.236×10^3	Pomona
Sediment-water, K_{oc} (unitless)	1553	C-Koc f Kow
Microorganisms-water, K_B $\left((\mu g/g)(mg/\ell)^{-1}\right)$	941	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	8×10^{-7}	C-VP/S-22° [111-1]
Vapor pressure, P_v (torr)	1×10^{-5} (22°C)	[111-1]
Reaeration rate ratio, k_v^c/k_v^o	NAV	

111. 3,3'-DICHLOROBENZIDINE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1})		
summer at 40° latitude	2.1×10^{-6}	REF
Oxidation constants at 25°C:		
For $^{1}O_2$ (singlet oxygen), k_{OX} $(M^{-1}\ hr^{-1})$	$<4 \times 10^{7}$	C-OX
For RO_2 (peroxy radical), k_{OX} $(M^{-1}\ hr^{-1})$	4×10^{7}	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B $(M^{-1}\ hr^{-1})$	0	HNES
For acid-promoted process, k_A $(M^{-1}\ hr^{-1})$	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b $(ml\ cell^{-1}\ hr^{-1})$	(E) 3×10^{-12}	E-KB

E: Estimated value; see List of Source Codes.

[111-1] Vapor pressure value was assigned by analogy; no data were available. This value was used in the calculation of Henry's constant.

112. 1,2-DIPHENYLHYDRAZINE

CAS No. 122-66-7
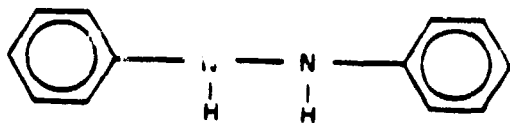
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	184.2	
Melting point, °C	131	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	1.84×10^3	C-Sw f Kow
Octanol-water, K_{ow} (unitless)	871	Pomona
Sediment-water, K_{oc} (unitless)	418	C-Koc f Kow
Microorganisms-water, $K_B \left((ug/g)(mg/\ell)^{-1} \right)$	286	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m³ mol⁻¹)	3.4×10^{-9} (25°C)	C-VP/S
Vapor pressure, P (torr)	2.6×10^{-5} (25°C)	Jaber, 1981
Reaeration rate ratio, k_v^c/k_v^o	NAV	

112.   1,2-DIPHENYLHYDRAZINE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, ϕ, at _____ nm		
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	$<4 \times 10^7$	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	1×10^9	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E)1×10^{-10}	E-KB

E: **Estimated value**; see List of Source Codes.

113. ACRYLONITRILE

CAS No. 107-13-1

$$H_2C = CH - C \equiv N$$
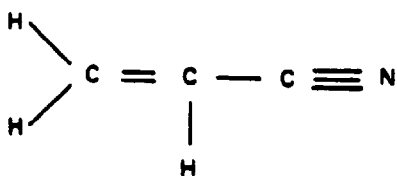
PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	53.1	
Melting point, °C	-83.5	CRC
Boiling point, °C	78.5	WREF
Ionization constant	pK-NER	

Partition constants:

Water solubility, S_w (ppm)	7.9×10^4 (25°C)	Klein et al, 1957
Octanol-water, K_{ow} (unitless)	1.78	Pomona
Sediment-water, K_{oc} (unitless)	0.85	C-Koc f Kow
Microorganisms-water, $K_B \left((\mu g/g)(mg/\ell)^{-1} \right)$	1.04	C-KB f Kow

Volatilization constants:

Henry's constant, H_c (atm m^3 mol^{-1})	8.8×10^{-5}	C-VP22.8°/S25°
Vapor pressure, P_v (torr)	100 (22.8°C)	WREF
Reaeration rate ratio, k_v^C/k_v^O	NAV	

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113. ACRYLONITRILE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, ϕ, at _____ nm	PNER	
Direct photolysis rate constant, k_p (hr^{-1}) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1O_2$ (singlet oxygen), k_{OX} (M^{-1} hr^{-1})	$<1 \times 10^8$	C-OX
For RO_2 (peroxy radical), k_{OX} (M^{-1} hr^{-1})	36	C-OX
Hydrolysis rate constants:		
For base-promoted process, k_B (M^{-1} hr^{-1})	0	HNES
For acid-promoted process, k_A (M^{-1} hr^{-1})	0	HNES
For neutral process, k_N (hr^{-1})	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, k_b (ml cell^{-1} hr^{-1})	(E) 3×10^{-9}	E-KB

E: _Estimated value_; see List of Source Codes.

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References for 3.9

Chang, E. T. 1976. Vapor Pressure of N-Nitrosodimethylamine. NTIS AD-A021 064/1ST Space and Missile Systems Organization, Zir Force Systems Command. Los Angeles, CA.

Jaber, H. M. 1981. Unpublished work at SRI.

Klein, E., J. W. Weaver, and B. G. Webre. 1957. Solubility of Acrylonitrile in Aqueous Bases and Alkali Salts. Chem. Eng. Data Ser. 2:72-75.

Pomona College Medicinal Data Base, June 1982.

Section 4

CALCULATION OF PARTITION COEFFICIENTS OF
ORGANIC CHEMICALS IN AQUATIC ENVIRONMENTS

4.1 BACKGROUND

The partitioning of a chemical between water and sediment and between water and biota will affect the concentration of the chemical in water and the rate of loss of the chemical from aquatic systems (See Section 2.1). Solubility data, on the other hand, are required for calculation of Henry's constants, which are needed to calculate volatilization rates of chemicals in aquatic systems (see Section 5.2.2).

This section discusses the relationships between water solubility, the partition coefficients for a chemical between sediment and biota, and the partition coefficient for a chemical between octanol and water. Moreover, the theoretical basis for such relationships is explained, and some of the published correlations for these data are discussed. This section also briefly discusses the calculation of the octanol-water partition coefficient data used to calculate many of the other partitioning constants. The data for the four partitioning constants (including water solubility) are given for 114 individual organic chemicals in Section 3.

As discussed in Section 2.2, the partioning of a chemical is given by the equation

$$K_p = C_p/C_w \qquad (4.1)$$

where C_p and C_w are the concentrations on a particulate material (sediment or biota) and in water, respectively, and K_p is the partitioning constant (or coefficient) whose units are determined by those of C_p and C_w (see Section 2.2). In practice, C_p is usually defined as the amount of chemical per dry weight of sediment (or organisms) to correct for the variability of the particulate water content. The partition coefficient between

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microorganism and water, K_B, given for individual organic chemicals in Section 3, is in units of micrograms of chemical per gram of microorganism divided by grams of chemical per liter of water. Because the amount of organic chemical sorbed to sediments has been found to depend on the amount of organic carbon in the sediment, it is useful to normalize a measured sediment partition coefficient (K_p) for organic carbon content:

$$K_{oc} = K_p/f_{oc} \qquad (4.2)$$

where f_{oc} is the fraction of organic carbon and K_{oc} is the normalized (for organic carbon content) partition coefficient. Karickhoff et al. (1979) have also shown that, because f_{oc} varies with sediment particle size, the distribution of sediment particle size will markedly affect measured K_{oc} values.

The octanol-water partion coefficient K_{ow} has commonly been used as a measure of the hydrophobicity of a chemical in medical and toxicological applications as well as in environmental chemistry (Hansch and Leo, 1979; Kenaga and Goring, 1978). A large number of K_{ow} values is therefore available as a result of the number of uses of such data. Most significantly, K_{ow} values can be calculated from molecular structure (see Section 4.4). The K_{ow} data in Section 3 are given to allow calculations of other properties (partitioning coefficients for biota as well as toxicological data) for use in environmental assessments of the organic priority pollutants.

4.2 CALCULATION METHODS

Several correlation equations have been proposed to calculate the water solubility (S_w), K_{oc}, and K_B from K_{ow} values and to calculate K_{oc} values from water solubility. The more widely used of these equations are discussed and analyzed in Section 4.3. Although we recognize that better equations are evolving as more experimental data are obtained, the following equations are recommended for use in environmental fate assessments.

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4.2.1 Correlation Equations

In the following equations, all partition coefficients (K_{oc}, K_{ow} and K_B) are unitless, and water solubility (S_w) is in units of parts per million (ppm).* As discussed in Section 4.2.2, however, the solubility units of molarity (moles per liter) or mole fraction are preferred.

K_{oc} and K_{ow} are correlated by the following equation (Karickhoff, 1979):

$$\log K_{oc} = 1.00 \log K_{ow} - 0.21 \qquad (4.3)$$

Correlation of S_w and K_{ow} was reported by Yalkowsky and Valvani (1980). For organic pollutants that are liquid in their pure state at 25°C:

$$\log S_w = -1.08 \log K_{ow} + 3.70 + \log MW \qquad (4.4)$$

where MW is the molecular weight of the pollutant (g mole^{-1}). For organic pollutants that are solid in their pure state at 25°C:

$$\log S_w = -1.08 \log K_{ow} + 3.70 + \log MW - \left(\frac{\Delta S_F}{1360}\right) (mp-25) \qquad (4.5)$$

where mp is the melting point of the pollutant (°C) and ΔS_f is the entropy of fusion of the pollutant (cal mol^{-1} deg^{-1}). If ΔS_f is not known, it may be approximated by (Yalkowsky and Valvani, 1980):

$$\Delta S_f \approx 13.6 + 2.5 \ (n - 5) \qquad (4.6)$$

where n is the number flexible atoms (i.e., atoms not involved in double bonds, triple bonds, or part of a ring structure) in the pollutant molecule, other than hydrogen. If n is less than 5, (n - 5) is set equal to zero.

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*The original equations in the literature are different if they were reported in different solubility units. Refer to Section 4.2.2 for the appropriate solubility units conversion factors.

Correlation of K_{oc} and S_w is provided by (Kenaga and Goring, 1978):

$$\log K_{oc} = -0.55 \log S_w + 3.64 \qquad (4.7)$$

K_B can be correlated with K_{ow} by

$$K_B = 0.16 \; K_{ow} \qquad (4.8)$$

4.2.2 Units and Conversion Factors

Three commonly used units of aqueous solubility are defined below:

(1) Mole fraction, x, the unitless ratio of the number of moles of solute to the total number of moles of solute plus water. In symbols, for a binary solution of n moles of solute in n_w moles of water

$$x = n/(n + n_w)$$
$$\sim n/n_w \text{ for } n_w \gg n \qquad (4.9)$$

(2) Molarity, S, expressed in moles of solute per liter of solution (M):

$$S(M) = n(mol)/\text{liter of solution} \qquad (4.10)$$

(3) Weight fraction, expressed in milligrams of solute per liter of water, or parts per million, ppm

$$S_w \text{ (ppm)} = \frac{n \text{ (mol) MW (g mol}^{-1}) \; 1000 \text{ (mg g}^{-1})}{\text{liter of water}} \qquad (4.11)$$

where MW is the molecular weight of the solute.

For solutions with $S < 1$ M, one liter of aqueous solution contains approximately 55.5 moles of water. Thus

$$x = \frac{S}{55.5 + S} \sim \frac{S}{55.5} \text{ for } S < 1 \text{ M} \qquad (4.12)$$

or

$$S = \frac{55.5 \, x}{(1 - x)} \sim 55.5 \, x \text{ for } x < 10^{-2} \tag{4.13}$$

To convert from molarity to ppm is straightforward by substituting Equation (4.10) into equation (4.11)

$$ppm \sim S(MW)(1000) \text{ for } S < 1 \, M \tag{4.14}$$

Thus to convert from mole fractions to ppm follows from equations (4.11) and (4.13)

$$ppm = \frac{55.5 \, x}{(1 - x)} (MW)(1000)$$

$$\sim 55.5(x)(MW)(1000) \text{ for } x < 10^{-2} \tag{4.15}$$

These conversion factors are summarized in Table 4.1.

Table 4.1

CONVERSION FACTORS FOR COMPOSITION UNITS

FROM \ TO	ppm	x (mole fraction)	M (Molarity)
ppm	---	$\dfrac{1.80 \times 10^{-5}}{MW}$	$\dfrac{10^{-3}}{MW}$
(mole fraction)	$5.55 \times 10^{4} (MW)$	---	55.5
M (Molarity)	$(MW)(10^{3})$	$\dfrac{1}{55.5}$	---

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FIGURE 4.2   LATTICE MODEL OF A HIGHER MOLE FRACTION OF SOLUTE (S) PARTITIONING BETWEEN OCTANOL (O) AND WATER (W) PHASES

Because the environment of each solute molecule is the same, $K_{ow} = C_o/C_w = 2$ as in Figure 4.1.

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FIGURE 4.1   LATTICE MODEL OF A SOLUTE (S) PAR̄...NG BETWEEN OCTANOL (O), ...̄ER (W) PHASES

$K_{ow} = 2$

and solute) in both phases occupies a particular site on a three-dimensional
lattice, with uniform spacing between sites, then the fraction of sites
in each phase occupied by the chemical is the mole fraction x. A two-
dimensional cross section of this lattice is shown in Figures 4.1 and
4.2.

The tendency for a solute molecule to leave either phase is propor-
tional to the solute mole fraction in that phase and to the forces acting
on the solute in that phase. The forces acting on a solute molecule will
depend on which molecules occupy neighboring sites on the lattice.
Figures 4.1 and 4.2 show that, over the mole fraction range of $x_w = 1/28$
to $x_w = 1/14$, solute molecules in the water phase are surrounded by water
molecules. Thus, the forces acting on the solute in the water phase are
independent of the solute mole fraction. Consequently, the tendency (f)
of a solute molecule to leave the water phase is directly proportional
to its mole fraction:

$$f = Hx \qquad (4.16)$$

where H is a constant representing the forces exerted on the solute by
the solvent. At higher solute mole fractions, where solute-solute inter-
actions become important (that is, where the solute is concentrated
enough that solute molecules occupy neighboring lattice sites), H becomes
a function [H(x)] of the solute mole fraction, and thus f is no longer
directly proportional to x:

$$f = H(x) \, x \qquad (4.17)$$

The partitioning of the chemical between the octanol and water phases
depends on this relative tendency of the chemical to leave each phase (f),
which is conveniently viewed as a force per unit area. In thermodynamics,
f is called the fugacity[*] and, as explained above, is proportional to the
relative amount of the solute in the phase, x, and the forces acting on
the solute within each phase; explicitly,

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[*]See, for example, G. L. Lewis and M. Randall, Thermodynamics, revised
by K. S. Pitzer and L. Brewer (McGraw-Hill, NY, 1961).

$$f_w = (f^R \gamma_w) x_w \qquad (4.18)$$

$$f_o = (f^R \gamma_o) x_o \qquad (4.19)$$

where subscripts w and o refer, respectively, to the water and octanol phases, and f^R and γ_i are, respectively, the reference fugacity and activity coefficient, which together represent the forces acting on the solute in the ith phase. At equilibrium

$$f_w = f_o \qquad (4.20)$$

so that

$$x_o/x_w = \frac{f^R \gamma_w}{f^R \gamma_o} = \frac{\gamma_w}{\gamma_o} \qquad (4.21)$$

In general, at constant pressure, f^R depends only on the temperature and γ_i depends on the composition as well as the temperature of the ith phase. In sufficiently dilute solutions, however, the forces acting on a solute molecule will be independent of x_i because, as explained above, the environment of a solute molecule will remain constant. Thus $(f^R \gamma_i)$ will be a function only of temperature

$$(f^R \gamma_i) = H_i \qquad (4.22)$$

where H_i is the Henry's constant for a very dilute solution of the solute in phase i. Thus

$$x_o/x_w = H_w/H_o \qquad (4.23)$$

is a function only of temperature. However, if x_o or x_w is large enough that γ_o or γ_w is not constant, then K_{ow} will also no longer be constant.

Because composition is commonly measured in moles liter^{-1}(M), it is convenient to define:

$$K_{ow} = C_o/C_w = r_{wo}(x_o/x_w) = r_{wo}(H_w/H_o) \tag{4.25}$$

where r_{wo} is a constant equal to the ratio of the molar volume of water

$$r_{wo} = v_w/v_o \quad (= 0.115) \tag{4.26}$$

to that of octanol. (In terms of the lattice mode, r_{wo} is equal to the ratio of the number of sites per unit volume of octanol to that of water.)

Numerous workers have correlated the partitioning of chemicals between sediment and water and between biota and water with octanol/water partition coefficients. Before discussing these specific correlations in detail, it is useful to understand the conditions that must be met for these correlations to be successful.

Partitioning of a solute between water and any other water immiscible phase p (i.e., biota, sediment) may be described by

$$K_{pw} = r_{wp}(H_w/H_p) \tag{4.27}$$

From equation (4.25) for partitioning between octanol and water

$$H_w = K_{ow} H_o/r_{wo} \tag{4.28}$$

thus

$$K_{pw} = (r_{wp}/r_{wo})(H_o/H_p)K_{ow} = r_{op}(H_o/H_p)K_{ow} \tag{4.29}$$

where r_{op} is the ratio of the molar volume of octanol to that of phase p. Thus, taking the logarithm of both sides of equation (4.29)

$$\log K_{pw} = \log K_{ow} + \log (r_{op} H_o / H_p) \qquad (4.30)$$

Thus, for the second term on the right-hand side of equation (4.30) to remain constant for a set of chemicals partitioning between water-octanol and water-phase p, phase p must be chemically similar to octanol and both K_{ow} and K_{pw} must be measured at low enough solute concentrations that solute-solute interactions are absent.

The success of K_{ow}-K_{oc} correlations (to be discussed in detail below), for example, may thus be understood. First, by normalizing adsorption for organic carbon content, we ensure the chemical similarity of phase p (that is, the organic content) and octanol. Second, the partitioning of the chemical between the water and sediment phases is usually measured at very low surface coverage (in the linear region of the adsorption isotherm) where adsorbate-adsorbate interactions are minimal.

Octanol/water partition coefficients have been used not only to correlate other partitioning data, but also to predict aqueous solubilities. The assumptions implicit in these predictions become apparent on close examination of the octanol/water partition experiment.

If it is assumed that the ratio of the number of solute molecules in each phase remains constant up to the limit of solubility, then

$$K_{ow} = (C_o / C_w)_{dilute} = (C_o / C_w)_{saturated} \qquad (4.31)$$

From equation (4.21), this means that the ratio of activity coefficients γ_w / γ_o remains constant up to saturation. As explained above, however, the ratio γ_x / γ_o will depend on solute concentration,[*] particularly if C_w (saturated) is large enough that solute-solute interactions become

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[*]Because of the chemical similarity of a neutral organic solute with n-octanol, it is expected that γ_o will not vary significantly with C_o.

important. Furthermore, if we assume that the solubility of the chemical in pure water equals its solubility in the octanol-saturated water phase of the partition measurement, then

$$K_{ow} = S_o / S_w \qquad (4.32)$$

where S_o and S_w are solubilities in moles liter^{-1}(M) in pure octanol and pure water, respectively.

To correlate aqueous solubility with K_{ow}, many authors have proposed an equation of the form:

$$\log S_w = -(1/a) \log K_{ow} + c \qquad (4.33)$$

where a and c are constants. Equation (4.33) may be derived by modifying equation (4.32) to account for deviations of real systems from model behavior:

$$K_{ow} = (S_o / S_w)^a \qquad (4.34)$$

This equation is clearly identical to equation (4.32) for a = 1. Taking the logarithm of both sides of equation (4.34) and rearranging terms:

$$\log S_w = - (1/a) \log K_{ow} + (1/a) \log S_o \qquad (4.35)$$

If S_o is assumed constant for a set of solutes in octanol, equation (4.35) becomes

$$\log S_w = - (1/a) \log K_{ow} + c \qquad (4.36)$$

and the correlation coefficients a and c may be calculated from a plot of known values of $\log S_w$ versus known values of $\log K_{ow}$ for the given

set of solutes. Clearly, if the assumptions implicit in equation (4.32) are reasonable, the calculated value of a should be close to one.

The variability of S_o for a set of solutes is difficult to quantify except by comparing liquid and solid solutes. If two solutes are identical except that one is a liquid and the other is a solid in its pure state at temperature T, the solid will be less soluble than the liquid because of the additional energy required to remove solute molecules from the solid phase. Thus, if we assume that all liquid solutes have the same solubilities in n-octanol, and we use this pure liquid solute as the reference state, calculated solid solubilities must be corrected for the energy necessary to transform the solid to the liquid state. This energy is called the enthalpy of fusion, and from simple thermodynamic arguments, we can modify equation (4.35) for solid solutes:

$$\log S_w = - (1/a) \log K_{ow} + c - (1/a) \frac{\Delta H_f}{2.303 \, RT_f} \frac{T_{f-} T}{T} \qquad (4.37)$$

where ΔH_f is the enthalpy of fusion, R is the gas constant, and T_f is the melting temperature of the solute. At the melting point,

$$\Delta H_f = T_f \, \Delta S_f \qquad (4.38)$$

Therefore at 25°C, equation (4.38) becomes

$$\log S_w = - (1/a) \log K_{ow} + c - \frac{\Delta S_f}{a(1360)} (mp-25) \qquad (4.39)$$

where mp is the melting point (in °C) and ΔS_f is the entropy of fusion (in cal deg^{-1} $mole^{-1}$). This correction is zero for solutes that are liquid at 25°C, but substantial for solutes with high melting points. Assuming that the theory is approximately correct and the correlation coefficient a is approximately equal to one, Table 4.2 and Figure 4.3 illustrate the magnitude of this correction as a function of melting point for a hypothetical solute with an uncorrected solubility of 100 ppm and a typical entropy of fusion of 13.6 entropy units (cal deg^{-1} mol^{-1}).

Table 4.2

EFFECT OF MELTING POINT CORRECTION
ON WATER SOLUBILITY VALUES

Solubility (uncorrected) (ppm)	Melting Point (^{c}C)	Solubility[*] (corrected) (ppm)
100	25	100
100	50	56
100	100	18
100	200	2
100	300	0.2

---

[*] $\log S_w$ (corrected) $= \log S_w$ (uncorrected) $- 0.01$ (mp-25) at 25°C, where $\Delta S_f = 13.6$ and $a = 1$ are assumed in equation (4.39) and S_w is the water solubility in ppm.

$$f = S_w \text{ (corrected)}/S_w \text{ (uncorrected)}$$

$$f = 10^{-(0.01)(mp - 25)}$$
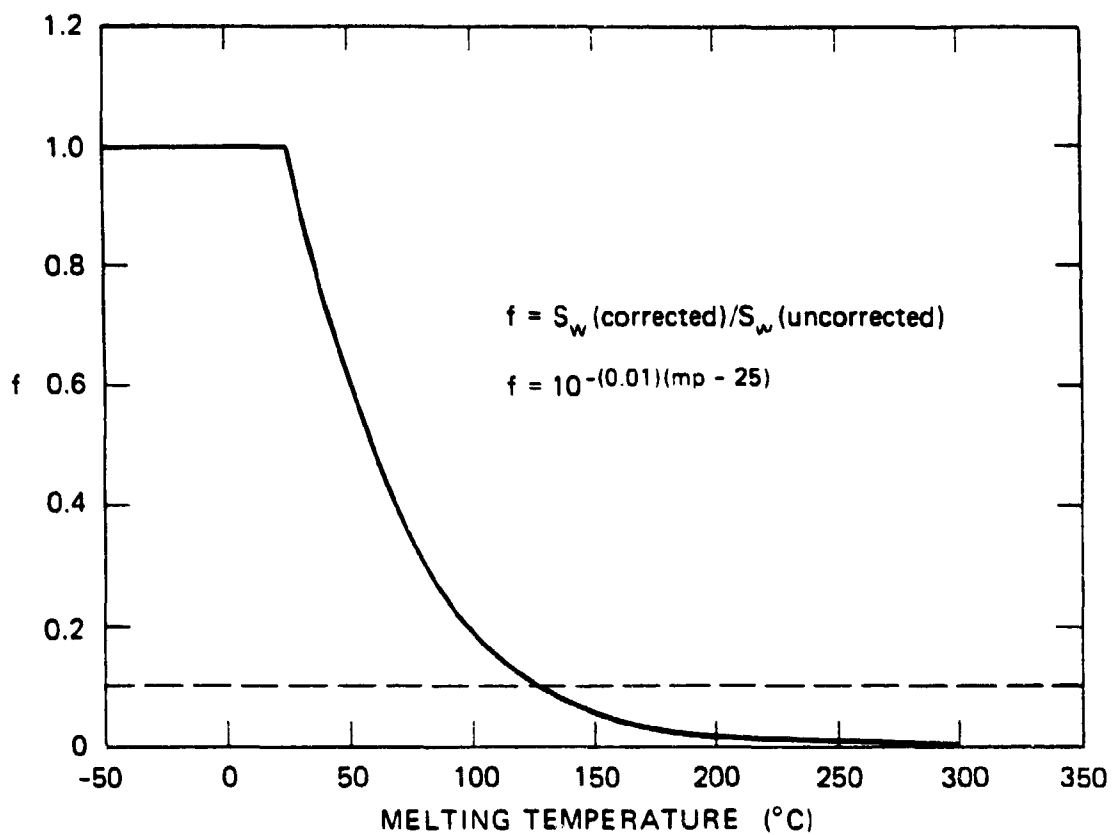
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FIGURE 4.3 ENTHALPY OF FUSION CORRECTION FACTOR FOR AQUEOUS SOLUBILITY AT 25°C AS A FUNCTION OF MELTING TEMPERATURE

4.3.2 Comparison of Reported Correlations

Table 4.3 lists a representative sample of recently published correlations among K_{ow}, K_{oc}, S_w. This section examines these correlations in detail.

$\underline{K_{oc}-K_{ow}}$. As discussed earlier, the sorption constant K_{oc} is the amount of chemical adsorbed per unit weight of organic carbon in the sediment divided by the equilibrium concentration of the chemical in the water phase. This constant is useful because, once K_{oc} has been determined for a chemical, the sorption partition coefficient may be calculated if the fraction organic content (f_{oc}) is known:

$$K_p = K_{oc}(f_{oc}) = C_s/C_w \qquad (4.40)$$

where

K_p = Sorption partition coefficient

K_{oc} = Sorption partition coefficient normalized for organic carbon content

f_{oc} = Fraction of organic content in the sediment (0 < OC <1)

C_s = Concentration of the adsorbed chemical

C_w = Equilibrium solution concentration.

Furthermore, it is useful to be able to predict K_{oc} values from the more easily measured K_{ow} values. The theoretical basis for expecting good $K_{oc}-K_{ow}$ correlations has been discussed above. Two recent $K_{oc}-K_{ow}$ correlations that have appeared in the literature are listed in Table 4.3. The significantly different correlation equations of Kenaga and Goring (1978) and Karickhoff et al. (1979) probably reflect the different data bases used to correlate K_{oc} with K_{ow}.

Table 4.3

REPORTED CORRELATIONS OF K_{ow}, K_{oc} AND S_w

Correlation	Eq.	Data Base*	Authors	Equation
$K_{oc} - K_{ow}$	(4.41)	Pollutants: Aromatic hydrocarbons (8), Carboxylic acids and esters (5), Phosphorus containing insecticides (5), Ureas and uracils (7), Symmetrical triazines (6), Miscellaneous (14); Adsorbents: Variety of soils	Kenaga and Goring (1978)	$\log K_{oc} = 0.544 \log K_{ow} + 1.377$
$K_{oc} - K_{ow}$	(4.3)	Pollutants: Polycyclic aromatics (8), Chlorinated hydrocarbons (2)	Karickhoff et al. (1979)	$\log K_{oc} = 1.00 \log K_{ow} - 0.21$
$S_w - K_{ow}$	(4.42)	Pollutants: Substituted benzenes and halobenzenes (12), Halogenated biphenyls and diphenyl oxides (11), Aromatic hydrocarbons (9), Phosphorus containing insecticides (16), Carboxylic acids and esters (9), Ureas and uracils (7), Miscellaneous (24)	Kenaga and Goring (1978)	$\log S_w = -0.922 \log K_{ow} + 4.184$, S_w in ppm
$S_w - K_{ow}$	(4.43)	Simple aliphatics and aromatics in the following groups (n = 114): Alcohols, Halogens, Amines, Carboxylic acids and esters, Aldehydes and ketones, Ethers, Nitro compounds	Yalkowsky (1980)	$\log x_s = -1.08 \log K_{ow} - 1.04 - \left\| \dfrac{\Delta S_f}{1360} (mp - 25) \right\|$

x_s is the mole fraction solubility at 25°C

ΔS_f is the entropy of fusion in cal deg^{-1} mol^{-1}

mp is the melting point in °C (if mp $\leq$ 25 then the term in brackets is zero)

*Number in parentheses refer to the number of pollutants in the data base.

Table 4.3 (continued)

REPORTED CORRELATIONS OF K_{ow}, K_{oc} AND S_w

Correlation	Equation	Eq.	Data Base	Authors
$K_{oc} - S_w$	$\log K_{oc} = -0.55 \log S_w + 3.64$ in ppm	(4.7)	Similar to data base for equation (4.41)	Kenaga and Goring (1978)
$K_{oc} - S_w^*$	$\log K_{om} = -0.56 \log S_w + 0.70$ $\log K_{oc} = -0.56 \log S_w + 0.93$	(4.44) (4.45)	Pollutants Polychlorinated biphenyls (3) Pesticides (4) Halogenated ethanes and propanes (6) Tetrachloroethene 1,2-Dichlorobenzene Adsorbents Willamette silt loam Miscellaneous other soils	Chiou et al. (1979)
$K_{oc} - S_w$	$\log K_{oc} = -0.54 \log x_s + 0.44$ x_s in the mole fraction solubility	(4.46)	Similar to data base for equation (4.3)	Karickhoff (1979)

*K_{om} is the sorption partition coefficient normalized for organic matter reported by
Chiou et al. (1979). Assuming $K_a = 1.7 K_{om}$, equation (4.45) is derived.

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The theoretical equation of Table 4.4,

$$\log K_{oc} = 1.00 \log K_{ow} + \text{constant} \qquad (4.47)$$

follows from assuming that the second term on the right-hand side of equation (4.30) is constant; the data base required for a good fit with equation (4.47) follows from the assumptions used in the derivation of equation (4.30). It is clear from Table 4.4 that the data base and correlation equation of Karickhoff et al. (1979) closely conform with the theoretical model; however, the data base and correlation equation of Kenaga and Goring (1978) do not.

The advantages and disadvantages of using these alternative equations are not as well defined, however. Although the equation of Karickhoff et al. (1979) conforms to a simple model and accurately predicts sorption coefficients from K_{ow} data for a limited class of organic chemicals, it has not been widely tested and may be highly inaccurate for a more universal set of pollutants and soil/sediments. The equation of Kenaga and Goring (1978), however, is strictly empirical and only roughly predicts K_{cc} values from K_{ow} data, but it is applicable to a more universal set of pollutant/adsorbent systems because of the data base used. When more precise K_{oc} and K_{ow} data are available, it will be of interest to assess the predictive value of both of these correlations for both the universal set and individual classes of pollutant/adsorbent systems. It may become apparent that several correlation equations may be required to adequately predict K_{oc} values from K_{ow} values for the variety of systems of interest.

S_w - K_{ow}. Several comparisons of the equations of Kenaga and Goring (1973) and Yalkowsky (1980) can be made. For reasons discussed earlier, the mole fraction units of solubility used by Yalkowsky are to be preferred to the ppm units used by Kenaga and Goring. In fact, to compare equation (4.42) of Kenaga and Goring with equation (4.43) of Yalkowsky, we must assume an average molecular weight for the chemicals in the data

Table 4.4

DATA BASES FOR $K_{oc}-K_{ow}$ CORRELATIONS

	Kenaga and Goring (1978)	Karickhoff et al. (1979)	Theoretical
$\log K_{oc} =$	$0.54 \log K_{ow} + 1.38$	$1.00 \log K_{ow} - 0.21$	$1.00 \log K_{ow} + \text{constant}$
K_{ow}	Measured and calculated values compiled from literature	Measured by Karickhoff et al.	Measured for very dilute solution
K_{oc}	Calculated average values for each chemical from adsorption coefficients for widely differing soils	Measured values for the silt (high organic content) fractions of two natural sediments	Uniform organic content of soil/sediment. Measured for adsorption from very dilute solutions
Chemicals	Very wide range of organic classes	Nonpolar or slightly polar organics	Nonpolar organics

base of Kenaga and Goring. Converting equation (4.42) from ppm to mole fractions units

$$\log x_s = -0.922 \log K_{ow} - 0.56 - \log MW \qquad (4.48)$$

where x_s is the mole fraction solubility and MW is the average molecular weight.

The variation of equation (4.48) with MW is shown in Figure 4.4 and compared with Yalkowsky's equation for liquid solutes. Two observations can be made about Figure 4.4. First, the molecular weight dependence of equation (4.48) is not very great for chemicals in the molecular weight range of 100-400. Second, because the average molecular weight of chemicals in the data base used to determine equation (4.48) is in the range of 100-400, it is clear that solubilities predicted by equation (4.48) will be approximately an order of magnitude lower than those predicted by equation (4.43).

A comparison of measured solubilities (in molarity units, M) with those predicted by the equations of Kenaga and Goring and of Yalkowsky is shown in Table 4.5 for a series of chlorinated methanes and ethanes. Note that all the chemicals listed in Table 4.5 (except hexachloroethane, which sublimes) are liquid at 25°C. Furthermore, is is clear from Table 4.5 that equation (4.43) of Yalkowsky predicts the aqueous solubility of chlorinated methanes and ethanes very accurately, whereas the corresponding prediction of equation (4.42) is an order of magnitude lower. Table 4.6, which compares calculated and measured solubilities for some low melting point aromatics, further supports these conclusions.

The cause of this discrepancy becomes clear when we examine the contrasting methods and data bases used by Kenaga and Goring and by Yalkowsky to develop their correlations. Kenaga and Goring empirically correlated K_{ow} with the solubility o. a set of chemicals, most of which are solid at 25°C. In other words, Kenaga and Goring implicitly used a solid solute reference state; consequently, their correlation equation cannot accurately predict the solubility of a chemical that is liquid at 25°C.
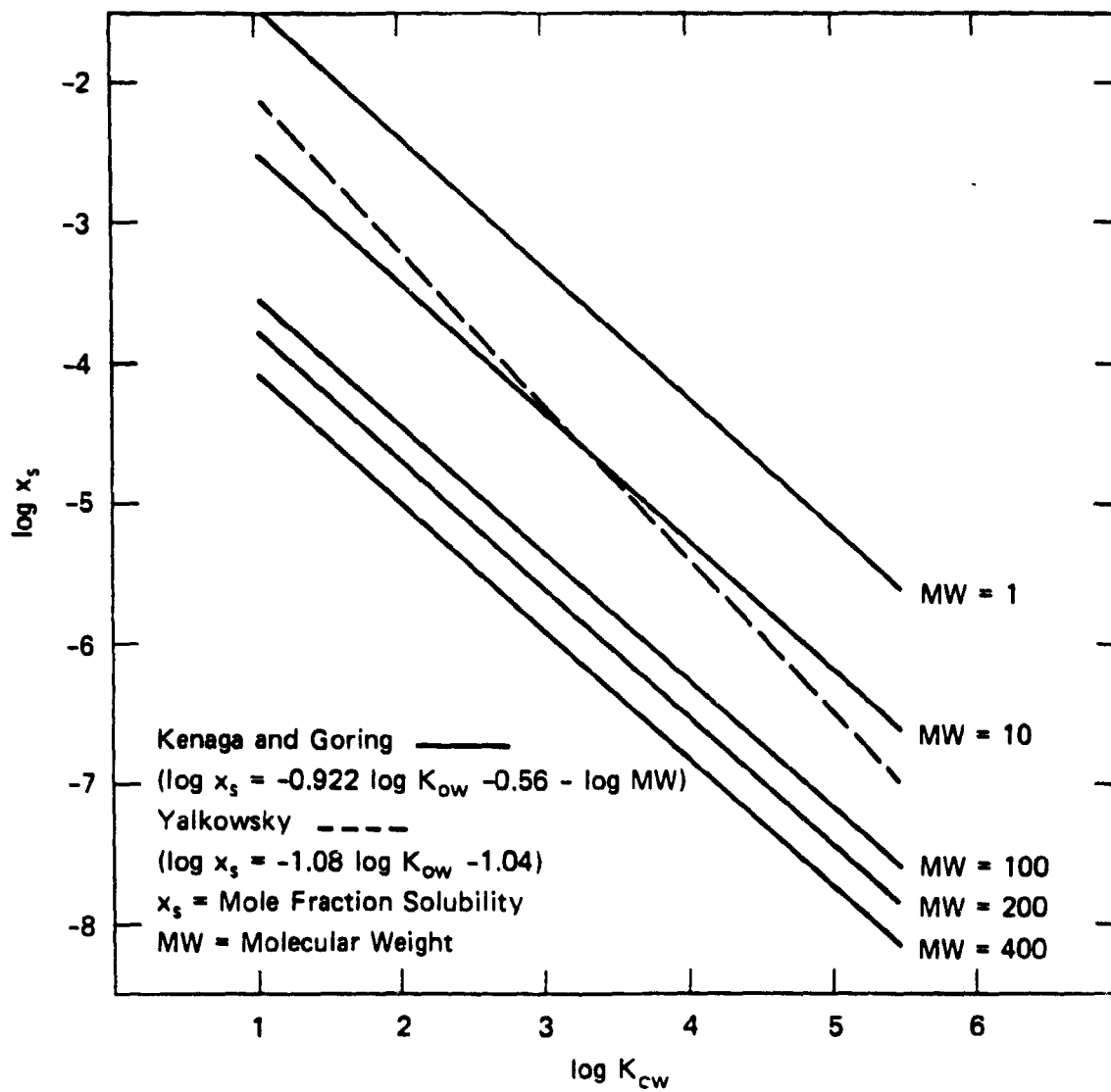
FIGURE 4 4   COMPARISON OF SOLUBILITY - K_{ow} EQUATIONS FOR LIQUID SOLUTES

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Table 4.5

CALCULATED VERSUS MEASURED SOLUBILITIES FOR CHLORINATED METHANES AND ETHANES

	$\log K_{ow}$	mp (°C)	$\log S_w$ (M) Kenaga and Goring	$\log S_w$ (M) Yalkowsky	$\log S_w$ (M) Measured[a]
Chloromethane	0.95	-98	-1.4	-0.32	-0.89
Dichloromethane	1.26	-95	-1.87	-0.66	-0.80
Chloroethane	1.49	-136	-2.03	-0.91	-1.05
1,1-Dichloroethane	1.80	-97	-2.45	-1.24	-1.25
Trichloromethane	1.96	-64	-2.67	-1.41	-1.16
1,1,2-Trichloroethane	2.07	-37	-2.84	-1.53	-1.47
1,1,1-Trichloroethane	2.50	-30	-3.25	-2.00	-2.27
1,1,2,2-Tetrachloroethane	2.66	-36	-3.48	-2.17	-1.76
Tetrachloromethane	2.76	-23	-3.70	-2.49	-2.29
Hexachloroethane	4.62	Sublimes	-5.45	-4.29	-3.68

[a] Sources for these measured values are given on the data sheet for each chemical (see Section 3).

Yalkowsky, on the other hand, explicitly used a liquid solute reference state. To calculate the solubilities of chemicals that are solid at $25^{\circ}C$, Yalkowsky included an entropy of melting correction term. Thus the equation of Yalkowsky, assuming accurate known values of the entropy of fusion (ΔS_f) and melting point (T_f), is equally valid for liquid and solid solutes.

As discussed earlier, if two solutes are identical except that one is a liquid and the other is a solid in its pure state at $25^{\circ}C$, then the solid will be less soluble than the liquid by a factor of

$$\exp\ [-2.303(\Delta S_f/1360)(mp-25)] \tag{4.49}$$

where ΔS_f is the entropy of fusion and mp is the melting point $(^{\circ}C)$. If ΔS_f is constant, then it is clear from equation (4.46) that solubility decreases as the melting point increases. Assuming $\Delta S_f = 13.6$ entropy units and converting mole fraction solubilities to molarity units, Figure 4.5 illustrates that equation (4.43) of Yalkowsky, in contrast with equation (4.42) of Kenaga and Goring, successfully predicts the decrease in solubility with increase in melting point for α-, β-, δ-, and γ-BHC.

Figure 4.5 also indicates that implicit in equation (4.42) of Kenaga and Goring is an empirical average of the solid solute correction term. Because the solubilities of liquid solutes predicted by equation (4.42) are approximately an order of magnitude lower than measured values, we can assume that this average correction term is approximately equal to 0.10, which is the dashed line in Figure 4.3. Thus, the predicted solubilities of equation (4.42) should approximate those of Yalkowsky and measured values for solutes with melting points in the 100° to $200^{\circ}C$ temperature range. Figure 4.6 illustrates, in fact, that for solutes with an approximate molecular weight of 150, an entropy of fusion of 13.6 and a melting point of $125^{\circ}C$, the correlation equations of Yalkowsky and of Kenaga and Goring are similar. Moreover, Table 4.7 illustrates

Table 4.6

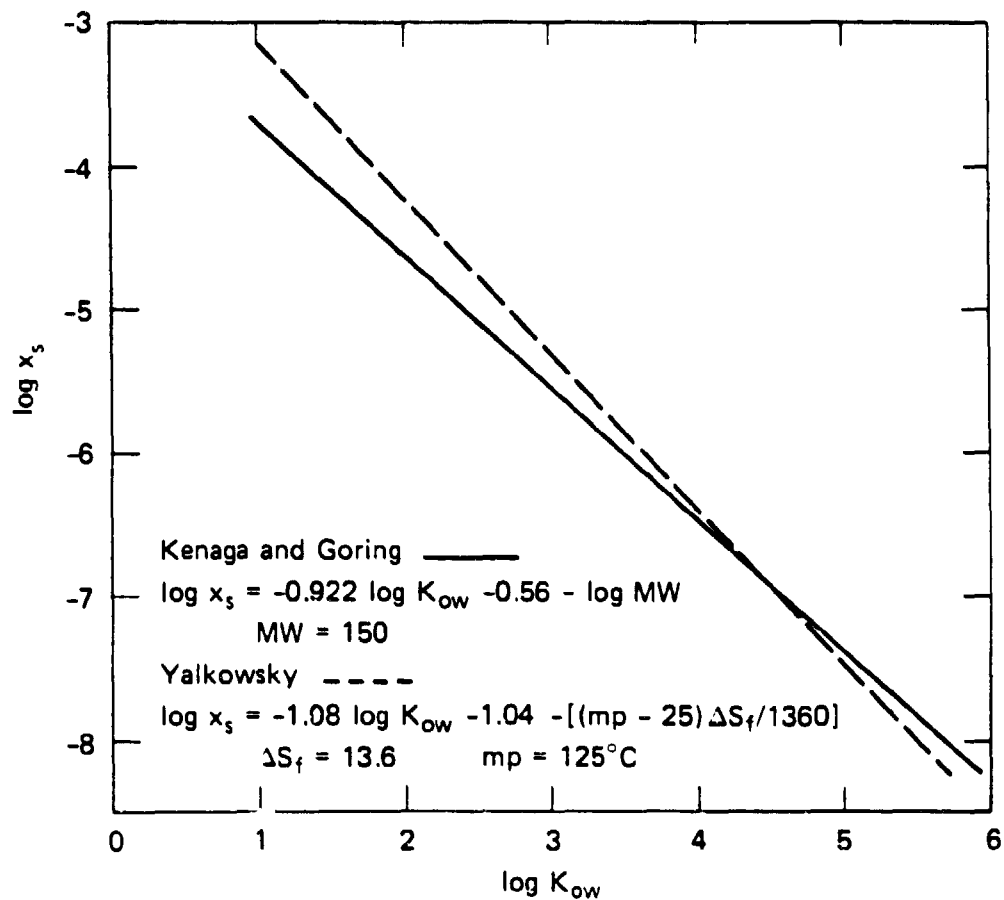CALCULATED VERSUS MEASURED SOLUBILITIES FOR LOW MELTING POINT AROMATICS

	log K_{ow}	mp (°C)	log S_w (M)		
			Kenaga and Goring	Yalkowsky	Measured[a]
Nitrobenzene	1.87	5.6	-2.63	-1.32	-1.82
Benzene	2.13	5.5	-2.63	-1.60	-1.64
Toluene	2.79	-95	-3.35	-2.31	-2.24
Chlorobenzene	2.84	-45	-3.48	-2.37	-2.37
Ethylbenzene	3.34	-94.9	-3.92	-2.90	-2.85
1,2-Dichlorobenzene	3.56	-17	-4.26	-3.14	-3.00

[a] Sources for measured values are given on data sheet for each chemical (see Section 3)
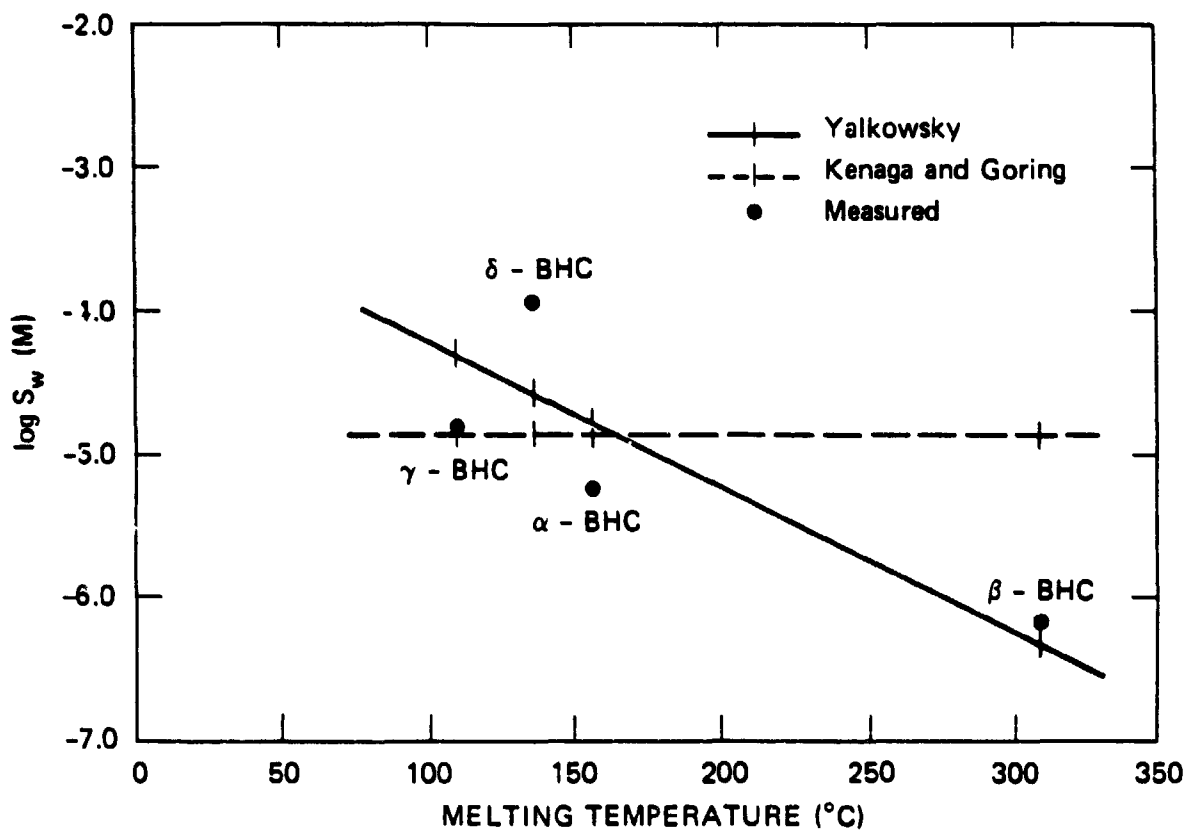
FIGURE 4.5 SOLUBILITIES OF HEXACHLOROCYCLOHEXANES (α-, β-, δ-, γ-BHC) AS A FUNCTION OF MELTING TEMPERATURE

FIGURE 4.6   COMPARISON OF SOLUBILITY - K_{ow} EQUATIONS FOR SOLID SOLUTES

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Table 4.7

CALCULATED VERSUS MEASURED SOLUBILITIES FOR SELECTED PESTICIDES

| | log K_{ow} | MP (°C) | log S_w (M) | | |
			Kenaga and Goring	Yalkowsky	Measured
Lindane	3.89	113	-4.85	-4.38	-4.40 to -5.15
Aldrin	5.30	104	-6.24	-5.80	-6.30 to -7.35
Chlordane	5.48	108	-6.46	-6.04	-5.30 to -6.85
DDD	6.20	112	-7.04	-6.85	-6.5 to -7.2
DDT	6.91	109	-7.74	-7.59	-6.6 to -8.5

a Sources of measured values are given on the data sheets for each chemical (see Section 3).

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that for selected pesticides with melting points around $110^{o}C$ the correlations of Yalkowsky and of Kenaga and Goring compare equally well with measured values.

Figure 4.5 also suggests that solubilities predicted from equation (4.42) of Kenaga and Goring will become progressively higher relative to measured values as the melting temperature increases above $200^{o}C$. Table 4.8 indicates that, indeed, measured solubilities of chemicals with melting points above $200^{o}C$ systematically fall below those predicted by Kenaga and Goring.

In summary, equation (4.42) of Kenaga and Goring should be restricted to chemicals with melting points in the 100° to $200^{o}C$ range, but equation (4.43) of Yalkowsky, because it includes a melting point correction factor is not limited by melting point restrictions.

K_{oc} - S_w. To compare equation (4.7) with equations (4.45) and (4.46), it is again necessary to assume an average molecular weight for the correlation equation of Kenaga and Goring. If an average molecular weight of 200 is assumed, converting equations (4.7) and (4.45) to mole fraction solubility units gives

$$\log K_{oc} = -0.55 \log x_s - 0.23 \qquad \text{(Kenaga and Goring, 1978)} \qquad (4.50)$$

$$\log K_{oc} = -0.56 \log x_s - 0.04 \qquad \text{(Chiou et al., 1979)} \qquad (4.51)$$

$$\log K_{oc} = -0.54 \log x_s + 0.44 \qquad \text{(Karickhoff et al., 1979)} \qquad (4.46)$$

Several observations can be made about these equations. First, the similarity of equations (4.50) and (4.51) is remarkable, considering the contrasting data bases used by Kenaga and Goring and by Chiou et al. to determine their correlation coefficients. In fact, equations (4.50), (4.51), and (4.46) may all be written in the form

$$K_{oc} = (\text{constant}) \; x_s^{-0.55(\pm 0.01)} \qquad (4.52)$$

Table 4.8

AQUEOUS SOLUBILITIES OF HIGH MELTING POINT CHEMICALS

Chemical Name	Melting Point (^{o}C)	Solubilities (ppm) Measured	Solubilities (ppm) Predicted by Equation (4.42)[a]
Benzo[k]fluoranthene	217	5.6×10^{-4}	0.04
Anthracene	219	0.045	1.2
Benzo[g,h,i]perylene	222	2.6×10^{-4}	0.015
Chrysene	258	1.8×10^{-3}	0.1
Dibenz[a,h]anthracene	270	5×10^{-4}	9×10^{-3}
TCDD	303	2×10^{-4}	7.5×10^{-3}
B-BHC	309	0.24	4.0

[a] Kenaga and Goring (1978)

It is not clear why the solubility coefficient of $-0.55(\pm 0.01)$ should appear in each of these correlations. If as expected from the above discussions [see equations (4.3), (4.42), and (4.43)],

$$\log K_{oc} = a \log K_{ow} + constant \qquad (4.53)$$

and

$$\log K_{ow} = - a \log x_s + constant \qquad (4.54)$$

where $a \sim 1$, then by substituting equation (4.54) into equation (4.53)

$$\log K_{oc} = - a^2 \log x_s + constant \qquad (4.55)$$

$$\sim - 1.0 \log x_s + constant$$

It is also apparent that none of these three equations accounts for the variation in solubility and hence variation in K_{oc} value with the melting point of the adsorbed chemical. The difference in adsorption behavior between solid and liquid solutes, in general, has been well documented in the literature (see, for example, Kipling, 1965). In fact, Roe (1975) has accounted for this difference in terms of the solid solute correction factor discussed earlier in this report. Karickhoff et al. (1979), in discussing their relatively poor correlation of K_{oc} with x_s (compared with their excellent correlation of K_{oc} with K_{ow}), mention that a correction term is probably needed in equation (4.40) to account for the enthalpy of fusion of the chemicals they studied.

$\underline{K_B - K_{ow}}$. The partitioning of organic chemicals has recently been reviewed by Baughman and Paris (1981), who noted the paucity of reliable data available for correlating K_B with other partitioning parameters. For the chemicals in Section 3, the following equation was used to calculate K_B

$$K_B = 0.16 K_{ow} \qquad (4.8)$$

which is the simplified version of the equation given by Baughman and Paris (1981),

$$\log K_B = 0.907 \log K_{ow} - 0.21 \qquad (4.56)$$

The reader is referred to the above review for an excellent exposition on the problems of reliably measuring K_B and the use of correlation equations to calculate K_B from S_w or from K_{oc} or K_{ow} data.

4.4 CALCULATION OF K_{ow} FROM STRUCTURAL PARAMETERS

The thermodynamics of partitioning of a chemical solution between octanol and water phases was discussed in 4.3.1, and the use of the octanol/water partition coefficient, K_{ow}, for calculating S_w, K_{oc} and K_B was described in Section 4.3.2. Although K_{ow} is the symbol used by many scientists for this partition coefficient, earlier literature and some current medical toxicology literature has commonly referred to the logarithm value of K_{ow} as "log P" (Hansch and Leo, 1979). For discussion in this section only, the log P nomenclature will be used instead of log K_{ow}, although the K_{ow} term will be used.

The K_{ow} data on the data sheets in Section 3 were calculated using a computer program developed at SRI; it uses the FRAGMENT method for calculating log P values (Hansch and Leo, 1979). The theory and procedures for these calculations are discussed in detail in that reference. Briefly, the method assumes that select groups of atoms in a molecule can be considered fragments, each of which contributes to the total log P value in an additive manner

$$\log P = \sum_{1}^{n} a_n f_n \qquad (4.57)$$

where a is the number of occurrences of fragment f of structural type n. Values of f have been empirically derived from the vast body of log P data available in the literature. Since the calculation of log P values

for complex molecules can be time-consuming and subject to numerous calculation errors. the FRAGMENT calculation method and the data base for fragment values have been incorporated into a computer program using the PROPHET computer network.[*] The log P data are generated by first entering the structure on a graphic tablet. The log P program then uses an ordered substructure search routine to obtain fragment values for fragments of the molecular structure. Fragments are used, rather than atoms, because atomic contributions to log P vary with certain structural environments. The program then adds the fragment values to obtain log P values. It also identifies where the log P calculation may be incomplete because of the absence of values for particular fragments or because polar interactions must be accommodated by manual calculations. The log P program is under continuing development and evaluation at SRI and other laboratories.

The manual calculation of log P values using the FRAGMENT method is already established as a valid method for obtaining these data (Hansch and Leo, 1979). The calculations are, of course, subject to errors arising from subtle structural differences that are not recognized or cannot be accounted for when obtaining empirical values for the molecular fragments. In fact, the primary source of error is the original data on which the fragment values are based. The lack of reliable data is also a dilemma for verification of calculated log P values.

As an indicator of the accuracy of the log P calculation program Table 4.9 compares the K_{ow} values recently published by Hassett et al. (1980) with the K_{ow} values calculated by the log P program. Although the chemicals are not among the organic priority pollutants, they do represent some of the best K_{ow} data currently available. The calculated and measured K_{ow} values agree within the factor of two for 8 of the 14

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[*]PROPHET is a NIH resource available to biological and chemical scientists on a time-share basis. Information on the log P/PROPHET system can be obtained from Dr. Howard L. Johnson at SRI.

Table 4.9

CORRELATION OF MEASURED AND CALCULATED VALUES OF K_{ow}

Compound	Measured K_{ow} ± S.D.[a]	Computer-Calculated K_{ow}	r[b]
Pyrene	124,000 ± 11,000	79,400	1.6
7,12-Dimethylbenz[a]anthracene	953,000 ± 59,000	871,000	1.1
Dibenz[a,h]anthracene	3,170,000 ± 883,000	5,890,000	0.54
3-Methylcholanthrene	2,632,000 ± 701,000	9,330,000	0.28
Dibenzothiophene	24,000 ± 2,200	33,900	0.71
Acridine	4,200 ± 940	2,570	1.6
13H-Dibenzo[a,i]carbazole	2,514,000 ± 761,000	692,000	3.6
Acetophenone	38.6 ± 1.2	38.9	0.99
1-Napthol	700 ± 62	417	1.7
Benzidine	46.0 ± 2.2	35.5	1.3
2-Aminoanthracene	13,400 ± 930	1,660	8.1
6-Aminochrysene	96,600 ± 4,200	24,000	4.0
Anthracene-9-carboxylic acid	1,300 ± 130	15,500	0.08

a Hassett et al. (1980).
b Ratio of measured K_{ow} to calculated K_{ow}.

compounds listed and agree within a factor of five for 12 of the 14 compounds. It is also significant to note that the last three compounds in Table 4.9 show the most disagreement between calculated and measured K_{ow} values, and these compounds are large molecules containing groups that may participate in H-bonding interactions.

In general, the accuracy of log P calculations by this method closely approaches the accuracy of experimental determinations performed over the last ten or twenty years because the fragment values were derived largely from those experimental data (by regression analysis) and incorporate the same experimental errors. It is not uncommon for measured log P values for a given compound in the literature to vary by 1 to 2 units; this corresponds to a factor of 10 to 100 in measured K_{ow} variation.

4.5 REFERENCES

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SECTION 5

CALCULATION OF THE RATES OF VOLATILIZATION
OF ORGANIC CHEMICALS FROM NATURAL WATER BODIES

5.1 INTRODUCTION

This section describes the procedures and theory used to calculate
the rates of volatilization of organic chemicals from aquatic systems.
The data needed for these calculations include the Henry's constant and
oxygen eaer tion rate ratio, which are used to calculate volatilization
data in many aquatic fate models, plus the vapor pressure. The calcula-
tion methods are outlined in Section 5.2. The results are summarized
under the respective organic chemical in Section 5.3. Since the rate
constants and half-lives for volatilization of chemicals depend on
environmental parameters as well as process data, the rate constants
have not been included in Section 5.3. Section 5.4 describes the theo-
retical basis of estimation methods and presents a plot of volatilization
half-lives as a function of Henry's constant for the organic priority
pollutants for two representative aquatic systems.

5.2 CALCULATION METHODS

5.2.1 Outline of the General Procedure

The general procedure to be used is based on the two-film theory
first proposed by Whitman (1923). The detailed theory will be described
in Section 5.4. In this section, onl the calculation procedure will be
described.

Volatilization of an organic chemical from water is a first-order
rate process. Therefore, the volatilization rate, R_v, is written as

$$R_v = - \frac{d[C_w]}{dt} = k_v \, [C_w] \tag{5.1}$$

where $[C_w]$ is the concentration of the chemical in moles liter^{-1} (M) in water and k_v is the volatilization rate constant in units of time^{-1} (usually hr^{-1} or day^{-1}). The full expression for estimating the volatilization rate constant of the chemical from a natural water body is

$$k_v^C = \frac{1}{L} \left[\frac{1}{k_\ell^0 \left(D_\ell^C / D_\ell^0 \right)^m} + \frac{RT}{H_c \, k_g^W \left(D_g^C / D_g^W \right)^n} \right]^{-1} \qquad (5.2)$$

where

    L = mixing depth of the water body (cm)

    k_ℓ^0 = liquid phase mass transport coefficient of oxygen in the water body (cm hr^{-1})

    D_ℓ = liquid phase diffusion coefficient of the chemical (C) or oxygen (O) in water (cm^2 sec^{-1})

    m = 0.5 to 1.0, depending on the liquid phase turbulence

    R = gas constant, 62.4 torr deg^{-1} M^{-1} or 8.205 x 10^{-5} m^3 atm deg^{-1} mol^{-1}

    T = temperature (K)

    H_c = Henry's constant (torr M^{-1} or m^3 atm mol^{-1})

    k_g^W = gas phase mass transport coefficient for water (cm hr^{-1})

    D_g = gas phase diffusion coefficient for the chemical (C) or water (W) in air (cm^2 sec^{-1})

    n = 0.5 to 1.0, depending on the gas phase turbulence

Equation (5.2) takes into account mass transport resistance in both the gas and liquid phases. The derivation of equation (5.2) is given in Section 5.4.1.

In the following subsections, we will show how to estimate each of the parameters in equation (5.2) and how to calculate k_v^C for various water bodies. The value of k_v^C obtained by using this procedure depends on the accuracy of the value of the Henry's constant and the choice of k_ℓ^0 and k_g^W for the specific water body.

5.2.2 Calculation of the Henry's Constant

Henry's law states that, for ideal gases and solutions, the partial pressure of chemical above a solution, P_i, is proportional to its concentration in the solution, $[C_w]$. Mathematically, it can be written

$$P_i = H_c [C_{wi}] \qquad (5.3)$$

Henry's constant, H_c, is the proportionality constant. In other words, the magnitude of H_c is a measure of the tendency of a chemical to partition between the gas and liquid phases at equilibrium.

Several different units for Henry's constant are reported in the literature. Units of torr M^{-1} can be converted to atm m^3 mole^{-1} by the following equation:

$$H_c \text{ (atm } m^3 \text{ mole}^{-1}) = \frac{H_c \text{ (torr } M^{-1})}{760 \times 1000} = 1.32 \times 10^{-6} \, H_c \text{ (torr } M^{-1}) \qquad (5.4)$$

Henry's constant is also reported as the ratio of concentrations in the gas and solution phase. This conversion factor depends on temperature and, at 20°C, is:

$$H \text{ (unitless)} = \frac{H_c \text{(torr } M^{-1})}{RT} = 5.47 \times 10^{-5} \, H_c \text{(torr } M^{-1}) \qquad (5.5)$$

If a measured value of Henry's constant H_c is not available, the following physical property data for a chemical must be obtained or measured before H_c can be calculated:

- Melting point (T_m, °C and K)
- Solubility in water at 20°C (S_w, g liter^{-1} and mole liter^{-1})
- Vapor pressure at 20°C (P_v, torr)
- Heat of fusion, ΔH_f, is required if the chemical is a solid at at 20°C and if the vapor pressure used to calculate H_c is for the liquid. If a measured value of ΔH_f is not available, an estimation method can be used.

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Mackay and Wolkoff (1973) showed that the value of H_c is equal to the vapor pressure of the chemical, P, divided by the solubility at S_w

$$H_c = P/S_w \qquad (5.6)$$

This equation is correct only if the vapor pressure and the solubility data are for the pure material at the same temperature and the same phase (solid or liquid). The equation is also true for gases. The major difficulty in calculating H_c is often the estimation of P and the lack of reliable solubility data for many chemicals with solubility below 1 ppm.

If the chemical is a liquid over the temperature range of interest, the vapor pressure data can be calculated using the Clausius-Clapeyron equation

$$P_{2\ell} = P_{1\ell}\left[\exp\frac{\Delta H_v}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right] \qquad (5.7)$$

$P_{2\ell}$ is the vapor pressure of the liquid at temperature T_2, which is the ambient temperature and $P_{1\ell}$ is the vapor pressure of the liquid at temperature T_1, which is a higher temperature for which vapor pressure data are available. Vapor pressure data are also often reported in the form

$$\log_{10} P_{2\ell} = (- 0.2185\ A/T_2) + B \qquad (5.8)$$

where A and B are constants; data in the CRC handbook are given in this form. Since the vapor pressure versus temperature equation is given in various forms in the literature, the vapor pressure at 20°C should be calculated for each chemical using the equation available.

If the chemical is a solid at 20°C and the vapor pressure data were obtained above the melting point of the chemical, extrapolation of the vapor pressure data at 20°C will give the vapor pressure of the super-cooled liquid $(P_{2s\ell})$. Thus, equation (5.7) becomes

$$P_{2s\ell} = P_1 \left[\exp \frac{\Delta H_f}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \right] \qquad (5.9)$$

However, to calculate H_c, it is necessary to obtain the vapor pressure for the solid phase at the same temperature as the solubility data, because the vapor pressure P in equation (5.6) must be for the stable pure form of the chemical at the same temperature as the solubility data (e.g., ambient temperature). Prausnitz (1979) has shown that the extrapolated vapor pressure for the solid phase (P_{2s}) can be estimated from the extrapolated vapor pressure of the supercooled liquid phase $(P_{2s\ell})$ by

$$P_{2s} = P_{2s\ell} \left[\exp \frac{\Delta H_f}{R} \left(\frac{1}{T_m} - \frac{1}{T_2} \right) \right] \qquad (5.10)$$

where ΔH_f is the heat of fusion for the chemical (cal mol^{-1}), R is the gas constant (1.987 cal K^{-1} mol^{-1}), and T_m is the melting point in Kelvin.

If solubility data are not available, the solubility can be estimated using equation (4.4), in Section 4.2.1 of this report.

Therefore, the following expressions should be used to calculate the vapor pressure and Henry's constants. For chemicals that are liquids at the ambient temperature T_2:

$$P_{2\ell} = P_{1\ell} \left[\exp \frac{\Delta H_v}{1.987} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \right] \qquad (5.11)$$

or

$$\log_{10} P_{2\ell} = (- 0.2185 \, A/T_2) + B \qquad (5.8)$$

$$H_c = P_{2\ell}/S_W \qquad (5.12)$$

For solids, at 20°C, when a value for ΔH_f is available:

$$P_{2s} = P_{1\ell} \left[\exp \frac{\Delta H_v}{1.987} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \right] \left[\exp \frac{\Delta H_f}{1.987} \left(\frac{1}{T_m} - \frac{1}{T_2} \right) \right] \qquad (5.13)$$

$$H_c = P_{2s}/S_W \qquad (5.14)$$

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The value of T_2 is chosen as $20°C = 293$ K, or equal to the same temperature as reported for the solubility data.

Yalkowski and Valvani (1979) have suggested that ΔH_f be calculated from the melting temperature and entropy of fusion, ΔS_f, using equation (5.15)

$$\Delta H_f = T_m \Delta S_f \qquad (5.15)$$

where $\Delta S_f = 13.5$ entropy units and is nearly constant for rigid molecules. If the value of ΔH_f is not available, equation (5.16) is used to calculate P_{2s} for solids.

$$P_{2s} = P_{1\ell} \left[\exp \frac{\Delta H_v}{1.987} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \right] \left[\exp \frac{\Delta S_f}{1.987} \left(1 - \frac{T_m}{T_2} \right) \right] \qquad (5.16)$$

5.2.3 Calculation of Diffusion Coefficients

As shown in Section 5.4, the gas and liquid phase diffusion coefficients are used in Equation (5.2). The liquid phase diffusion coefficients D_ℓ should be estimated using the Haydeck and Lauoie modification of the Othmer and Thakar relation (Reid et al., 1977, p. 573)

$$D_\ell = \frac{13.26 \times 10^{-5}}{\eta_w^{1.4} \, V_b^{0.589}} \qquad (5.17)$$

where η_w is the viscosity of water (centipoise) and V_b is the molar volume at the normal boiling point ($cm^3 \, mol^{-1}$). The ratio of liquid diffusion constants for the chemical and oxygen in water, D_ℓ^C / D_ℓ^O, becomes

$$D_\ell^C / D_\ell^O = \left(V_b^O / V_b^C \right)^{0.589} \qquad (5.18)$$

The molar volume is estimated using the molar volume increments proposed by LeBas (Reid et al., 1977, p. 58) and the molar volume of oxygen, 25.6 $cm^3 \, mol^{-1}$, which was calculated from diffusion coefficient data (Reid et al., 1977, p. 58).

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The ratio of the gas phase diffusion coefficients D_g^C/D_g^W should be calculated using the Fuller, Schettler, and Giddings method (Reid et al., 1977, p. 554). The gas phase diffusion coefficients are

$$D_g = \frac{0.001\ T^{1.75}\ (1/M_1 + 1/M_2)^{1/2}}{P\left[(\Sigma v)_1^{1/3} + (\Sigma v)_2^{1/3}\right]^2} \qquad (5.19)$$

where M is the molecular weight and Σv is the atomic diffusion volume. The subscripts 1 and 2 refer to the chemical or water and to air, respectively. The value of Σv is 12.7 for water and can be calculated for other chemicals using the volume increments recommended in Reid et al. (1977, p. 554). The ratio, D_g^C/D_g^W, reduces to

$$D_g^C/D_g^W = 85\ \frac{(1/M_c + 0.0347)^{1/2}}{\left[(\Sigma v)_c^{1/3} + 2.72\right]^2} \qquad (5.20)$$

where M_c and $(\Sigma v)_c$ are the molecular weights and the diffusion volume of the chemical, respectively.

5.2.4 Other Parameters

The values entered into equation (5.2) for calculation of the volatilization rate constant, k_v^C, are summarized in Table 5.1. The rationales for these choices are given in the Section 5.4.2. The half-life of the chemical is

$$t_{\frac{1}{2}}\ (hr) = (\ln^2)\ k_v^C \qquad (5.21)$$

The rationales for the choices of k^O, m, k_g^W, and n are also discussed in Section 5.4.2.

5.2.5 Sample Calculation

As an example, the calculation of the volatilization rate constant for 2,6-dinitrotoluene (2,6-DNT) is shown in this section. The necessary physical properties are:

Table 5.1

SUMMARY OF CONSTANTS AND VALUES FOR SUBSTITUTION INTO EQUATION (5.2)

Constant/value	Rivers	Lakes
L (cm)	200	200
k_i^0 (cm hr^{-1})	8	1.8
m	0.7	1.0
T (K)	293	293
RT (torr M^{-1})	18,283	18,283
RT (m^3 atm mol^{-1})	2.40×10^{-2}	2.40×10^{-2}
k_g^W (cm hr^{-1})	2100	2100
n	0.7	0.7

Molecular weight: 182.14

Solubility: No data. Estimated to be equal to the solubility of 2,4-DNT, which is 180 mg liter^{-1} at 20°C or 9.88 x 10^{-4} M.

Melting Point: 65°C.

Sample Calculation of H_c for 2,6-DNT. The vapor pressure data used here are from Maksimov (1968), who reported 11 measurements between 150° and 260°C. Since all the data are above the melting point, extrapolation of the vapor pressure data to 20°C will give the vapor pressure of the supercooled liquid. The vapor pressure data for 2,6-DNT are not reported in a form that fits equation (5.5). However, Maksimov reports that ΔH_v = 13.55 kcal mol^{-1} and that the boiling point is 285°C (where the vapor pressure must equal 760 torr). The heat of fusion, ΔH_f, is not available, but the melting point, T_m, is 65°C. Therefore, equation (5.16) is used to calculate the vapor pressure of the solid phase of 2,6-DNT at 20°C.

$$P_{2s} = 760 \left[\exp \frac{13,550}{1.987} \left(\frac{1}{285 + 273} - \frac{1}{293} \right) \right] \left[\exp \frac{13.5}{1.987} \left(1 - \frac{65 + 273}{293} \right) \right]$$

$$= 4.2 \times 10^{-3} \text{ torr}$$

This value can be compared with the data of Pella (1977), who measured the vapor pressure of solid 2,6-DNT at 20°C and obtained 3.5 x 10^{-4} torr. The agreement is reasonable, considering the range of extrapolation of the vapor pressure data and that a value for ΔH_f is not available. Using Pella's vapor pressure data, Henry's constant is

$$H_c = P_{2s}/S_w$$
$$= 3.5 \times 10^{-4}/9.88 \times 10^{-4} = 0.35 \text{ torr M}^{-1} \tag{5.14}$$

To convert H_c in torr M^{-1} to atm m^3 mol^{-1},

$$H_c (\text{atm m}^3 \text{ mol}^{-1}) = \frac{1}{760} \left(\frac{\text{atm}}{\text{torr}} \right) \frac{1}{10^3} \left(\frac{\text{m}^3}{\text{liter}} \right) H_c (\text{torr M}^{-1})$$

$$= 1.32 \times 10^{-6} H_c (\text{torr M}^{-1})$$

For 2,6-DNT,

$$H_c = 0.35 \times 1.32 \times 10^{-6} = 4.6 \times 10^{-7} \text{ atm m}^3 \text{ mol}^{-1}$$

<u>Calculation of the Diffusion Constant Ratios for 2,6-DNT</u>. The
liquid phase diffusion constant for 2,6-DNT was calculated from equation
(5.18),

$$D_\ell^C / D_\ell^O = \left(V_b^O / V_b^C \right)^{0.589} \qquad (5.18)$$

The molar volumes, V_b, were calculated from the molar volume increments
proposed by LeBas (Reid et al., 1977, p. 58). For 2,6-DNT, there are
7 carbons, 6 hydrogens, 4 oxygens jointed to nitrogen, 2 nitrogens, and
1 six-membered ring. Therefore,

$$V_b^C = (7 \times 14.8) + (6 \times 3.7) + (4 \times 8.3) + (2 \times 15.6) - 15.0 = 175.2 \text{ cm}^3 \text{mol}^{-1}$$

The recommended value of V_b for O_2 is 25.6 cm^3 mol^{-1}. Then

$$D_\ell^C / D_\ell^O = \left(V_b^O / V_b^C \right)^{0.589} = (25.6/175.2)^{0.589} = 0.322 \text{ cm}^3 \text{mol}^{-1}$$

Similarly,

$$D_g^C / D_g^W = 85 \frac{\left(1/M_c + 0.0347 \right)^{1/2}}{\left[(\Sigma v)_c^{1/3} + 2.72 \right]^2}$$

The diffusion volume of 2,6-DNT, using the molecular increments of LaBas,
is

$$(\Sigma v)^{1/3} = [(7 \times 16.5) + (6 \times 1.98) + (4 \times 5.48) + (2 \times 5.69) - 20.2]^{1/3}$$

$$= 140.48^{1/3} = 5.20 \text{ cm}^3 \text{ mol}^{-1}$$

Then,

$$D_g^C / D_g^W = 85 \frac{(1/182 + 0.0347)^{1/2}}{[5.20 + 2.72]^2}$$

$$= 85 \times (0.200/62.7) = 0.271$$

To calculate k_v^C, the appropriate constants and values in Table 5.1 plus the constants calculated above are substituted into equation (5.2).

For lakes,

$$k_v^C = \frac{1}{200} \left[\frac{1}{1.8 \times (0.322)^{1.0}} + \frac{62.4 \times 293}{0.35 \times 2100 \times (0.271)^{0.7}} \right]^{-1}$$

$$= \frac{1}{200} (1.72 + 62.0)^{-1} = 7.84 \times 10^{-5} \text{ hr}^{-1}$$

$$t_{\frac{1}{2}} = (\ln 2)/7.84 \times 10^{-5} = 8.84 \times 10^3 \text{ hr} = 368 \text{ days}$$

For rivers,

$$k_v^C = \frac{1}{200} \left[\frac{1}{8 \times (0.322)^{0.7}} + \frac{62.4 \times 293}{0.35 \times 2100 \times (0.271)^{0.7}} \right]^{-1}$$

$$= \frac{1}{200} (0.276 + 62.0)^{-1} = 8.02 \times 10^{-5} \text{ hr}^{-1}$$

$$t_{\frac{1}{2}} = (\ln 2)/8.02 \times 10^{-5} = 8.64 \times 10^3 \text{ hr} = 360 \text{ days}$$

5.3 CALCULATION OF THE VOLATILIZATION RATES OF THE PRIORITY POLLUTANTS

The volatilization rate constants of the priority pollutants were estimated using the methods described in Section 5.2. The Henry's constant, H_c, is the critical parameter in these estimates. If a measured value of H_c was not available, the literature values of the vapor pressures and solubilities were used.

In many cases, the vapor pressure at 20°C was obtained from the report of Callahan et al. (1979); however, because it was not clear in that report how the vapor pressure for solids was calculated, we do not know if their vapor pressure data were extrapolated from data obtained above the melting point of the chemical or from the solid phase. In other cases, the vapor pressures reported were obtained from Verschueren (1977), but the source of those data is not cited in the reference. Therefore, we do not know the reliability of many of the values of H_c for solids. We mention this in detail because, if the reported vapor

pressure at 20°C was calculated from data obtained above melting point and not corrected for the phase change, using equation (5.13), H_c could be as much as an order of magnitude too high.

Values of D_ℓ^C/D_ℓ^O and D_g^C/D_g^W were calculated using equations (5.18) and (5.20). The values for D_ℓ^C/D_ℓ^O ranged from 0.21 to 0.66, and D_g^C/D_g^W ranged from 0.18 to 0.52. Figures 5.1 and 5.2 are plots of H_c versus the calculated half-lives, $t_{1/2}$, and k_v^C for the priority pollutants in example rivers (Figure 5.1) and lakes or ponds (Figure 5.2). The striking conclusion from these calculations is that the value of H_c determines k_v and $t_{1/2}$ for volatilization, while the size of the molecule, which affects the diffusion coefficients, causes only a range in $t_{1/2}$ or k_v^C of a factor of less than two for a given value of H_c. Also, volatilization may be a significant process ($t_{1/2} > 10$ days) in lakes and ponds if H_c is greater than about 50 torr M^{-1} ($= 6.6 \times 10^{-5}$ atm m^3 mol^{-1}), when liquid phase mass transport resistance controls about 80% of the volatilization rate for lakes or ponds and 14% for rivers.

<u>Aroclors</u>. The seven aroclors consist of various proportions of chlorinated biphenyls, which include components with chlorine substitution ranging from zero to nine. The diffusion coefficient ratios D_ℓ^C/D_ℓ^O and D_g^C/D_g^W for each component of the mixtures (e.g., the Cl_2 component) were first calculated. Overall diffusion coefficient ratios for each of the seven mixtures were then determined by

$$D_\ell^C/D_\ell^O = \sum_{i=1}^{9} f_i (D_\ell^C/D_\ell^O)_i$$

and

$$D_g^C/D_g^W = \sum_{i=1}^{9} f_i (D_g^C/D_g^W)_i$$

where f_i is the fraction of the ith component of the mixture and $(D^C/D^O)_i$ and $(D_g^C/D_g^W)_i$ are the diffusion coefficient ratios of the ith components. The Henry's constants for the aroclors were calculated from solubility and vapor pressure data of the complete mixture.
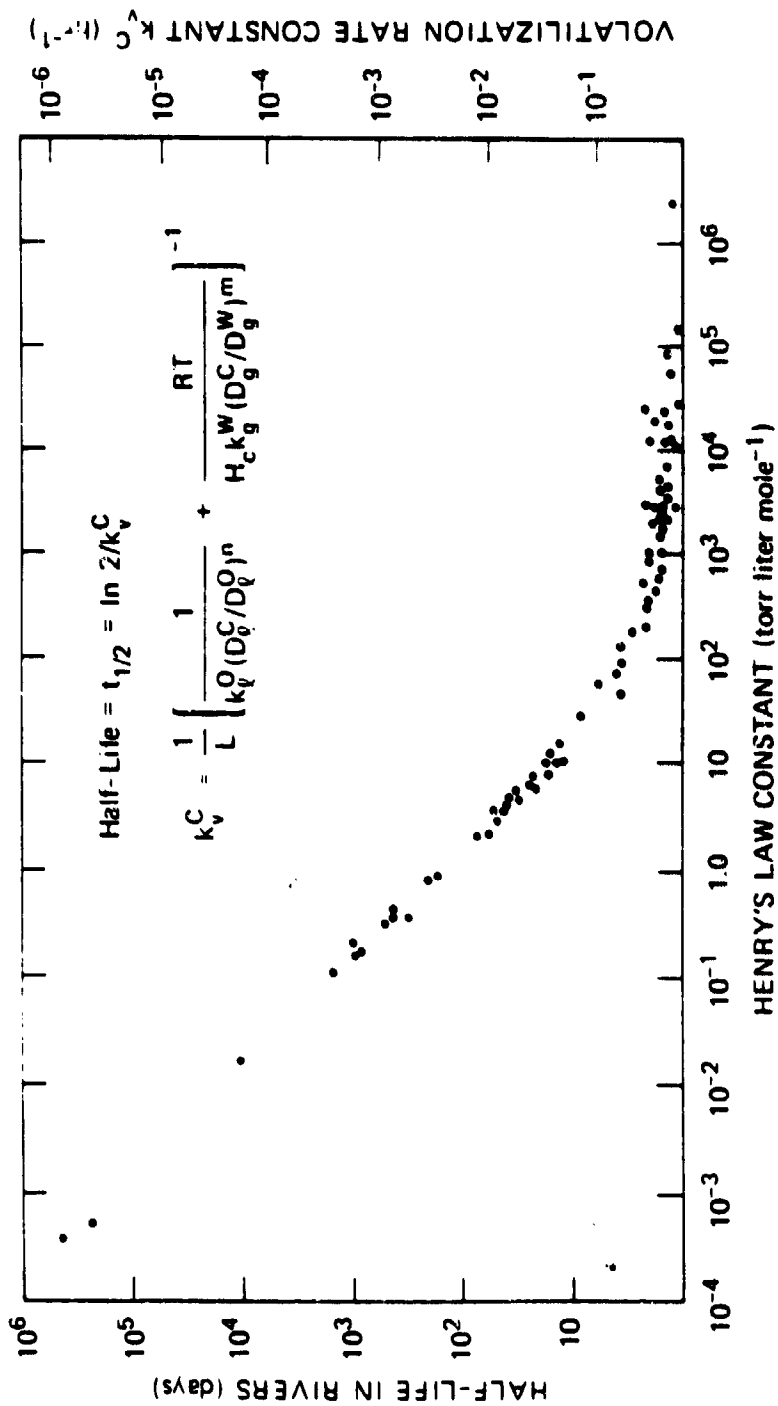
FIGURE 5.1 ESTIMATED HALF-LIVES VERSUS HENRY'S CONSTANT FOR THE PRIORITY POLLUTANTS IN RIVERS

(Values used: $L = 200$ cm, $k_\ell^O = 8.0$ cm hr^{-1}, $k_g^W = 2100$ cm hr^{-1}, $n = m = 0.7$)

VOLATILIZATION RATE CONSTANT k_v^C (hr^{-1})

Half-Life = $t_{1/2} = \ln 2/k_v^C$

$$k_v^C = \frac{1}{L}\left[\frac{1}{k_\ell^O(D_\ell^C/D_\ell^O)^n} + \frac{RT}{H_c k_g^W(D_g^C/D_g^W)^m}\right]^{-1}$$

HENRY'S LAW CONSTANT (torr liter mole^{-1})

HALF-LIFE IN RIVERS (days)

SA-6729-4B

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VOLATILIZATION RATE CONSTANT k_v^C (hr^{-1})

SA-6729-38

HENRY'S LAW CONSTANT (torr liter mole^{-1})

HALF-LIFE IN PONDS AND LAKES (days)

Half-Life = $t_{1/2}$ = ln $2/k_v^C$

$$k_v^C = \frac{1}{L}\left[\frac{1}{k_\ell^O(D_\ell^C/D_\ell^O)^n} + \frac{RT}{H_c k_g^W(D_g^C/D_g^W)^m}\right]^{-1}$$
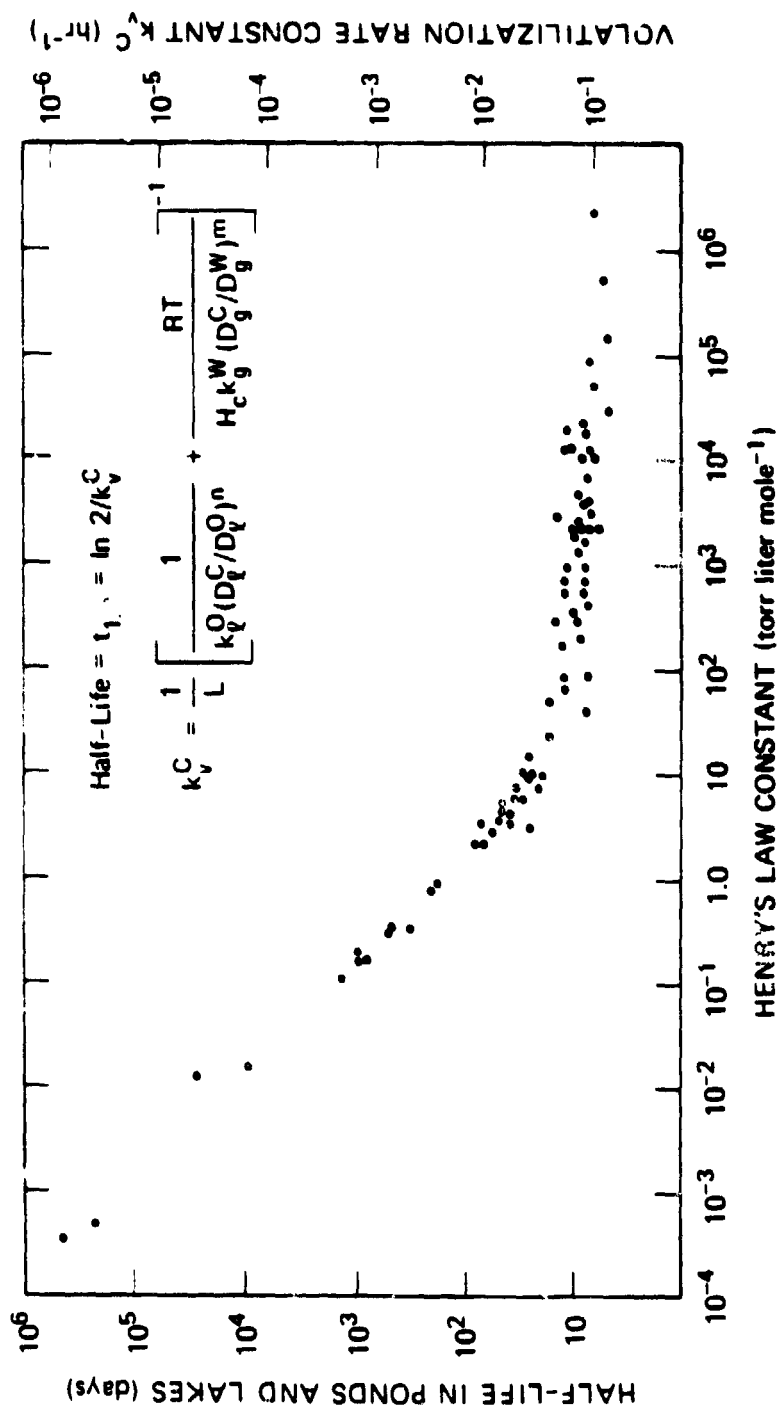
FIGURE 5.2 ESTIMATED HALF-LIVES VERSUS HENRY'S CONSTANT FOR THE PRIORITY POLLUTANTS IN LAKES OR PONDS

(Values used: L = 200 cm, k_ℓ^O = 1.8 cm hr^{-1}, k_g^W = 2160 cm hr^{-1}, n = 1; m = 0.7.)

Toxaphene. Toxaphene is mainly a mixture of polychlorinated camphenes. The average formula is $C_{10}H_{10}Cl_8$, which was used to calculate an "average" diffusion coefficient ratio. A Henry's constant was determined from solubility and vapor pressure data for the complete mixture.

Chlordane. The two major isomers of chlordane were considered in these calculations. Diffusion coefficient ratios were calculated for these isomers and were found to be equal because they have the same molecular formula and very similar structures. The Henry's constant for clordane was determined from solubility and vapor pressure data for the complete mixture.

5.4 THEORETICAL CONSIDERATIONS

In this section, we will derive equation (5.2) and discuss the selection of environmental parameters recommended in Table (5.1). The reader is referred to the references for the theoretical discussion of the calculation of vapor pressures (any general physical chemistry textbook plus Reid et al. 1977), Henry's constant (Mackay and Wolkoff, 1973), and the diffusion constants (Reid et al., 1977).

5.4.1 Two-Film Theory

The approach we have used is based on the two-film theory developed by Whitman (1923), which was recently described by Liss and Slater (1974), by Mackay and Leinonen (1975), and Smith and Bomberger (1980). The general expression for the volatilization rate of a chemical is

$$R_v = - \frac{d[C_w]}{dt} = k_v[C_w] \tag{5.1}$$

$$k_v = \frac{1}{L} \left[\frac{1}{k_\ell} + \frac{RT}{H_c k_g} \right]^{-1} \tag{5.22}$$

where

R_v = volatilization rate of a chemical, C (moles liter^{-1} hr^{-1})

C_w = concentration of C in water

k_v = volatilization rate constant (hr^{-1})

L = depth (cm)

k = liquid phase mass transport coefficient $(cm\ hr^{-1})$

H_c = Henry's law constant $(torr\ M^{-1})$

k_g = gas phase mass transport coefficient $(cm\ hr^{-1})$

The derivation of equation (5.22) is given in Liss and Slater (1974) and Mackay and Leinonen (1975). It is based on the assumption that the fluxes of a chemical through the liquid and gas phase boundary layers and the air-water interface are equal. The equation suggests that volatilization is inversely proportional to the solution depth and directly proportional to the turbulence in either or both the liquid and gas phases.

The volatilization rate of a chemical may depend on liquid phase or gas phase resistance or both, depending on the relative magnitude of k_ℓ and $H_c k_g$. Liss and Slater (1974) estimated values of k_ℓ for CO_2 $(20\ cm\ hr^{-1})$ and of k_g for water (1000 to 3000 $cm\ hr^{-1}$). These values were assumed to be typical and substituted into equation (5.22). Then, the ratio of the first term to to the sum of the two terms is set equal to the fraction of gas or liquid phase control, and the equation is solved for H_c. The calculation shows that mass transfer in the liquid phase controls about 95% of the volatilization rate constant when the value of H_c is greater than about 3500 torr M^{-1} (4.6×10^{-3} atm m^3 mol^{-1}). We have called chemicals that meet this requirement high volatility compounds. A similar calculation shows that if H_c is less than 10 torr M^{-1} (1.3×10^{-5} atm m^3 mol^{-1}), mass transfer in the gas phase is rate controlling. These are low volatility compounds. If H_c is between about 10 and 3500 torr M^{-1}, then both terms in equation (5.22) are significant. A similar procedure has been described by Dilling (1977).

If $H_c > 3500$ torr M^{-1}, R_v is determined by the value of k_ℓ and is limited by diffusion through the liquid phase boundary layer since

$$k_v = k_\ell / L \qquad (5.23)$$

For low volatility compounds, where $H_c < 10$ torr M^{-1}, only the second term in equation (5.22) is significant. Then

$$k_v = \frac{H_c k_g}{LRT}$$ (5.24)

and the volatilization rate is limited by gas phase mass transport resistance. For intermediate volatility compounds, where $3500 < H_c < 10$ torr M^{-1}, both terms in equation (5.22) are significant. The method we recommend for calculating k_v^C takes into account the fact that either or both terms in equation (5.22) may be important, depending on the magnitude of H_c.

In both the gas and liquid phase

$$k_\ell = D_\ell / \delta_\ell$$ (5.25)

$$k_g = D_g / \delta_g$$ (5.26)

where D is the diffusion coefficient and δ is the boundary layer thickness. These equations suggest that the liquid and gas phase mass transport coefficients of the chemical, k_ℓ^C and k_g^C, are proportional to the gas and liquid phase diffusion coefficients, D_ℓ^C and D_g^C, respectively. The diffusion constants depend on the temperature and viscosity of the fluid phase, but are independent of the turbulence. Therefore, numerous authors have proposed that the ratio of mass transport coefficients for two chemicals in the same solution should be independent of the turbulence level (Hill et al., 1976; Tsivoglou et al., 1965; Paris et al., 1978; Smith et al., 1977 a,b; Smith and Bomberger, 1978 and 1980; Smith et al., 1980).

$$k_\ell^A / k_\ell^B = f(D_\ell^A / D_\ell^B)$$ (5.27)

$$k_g^A / k_g^B = f(D_g^A / D_g^B)$$ (5.28)

In the liquid phase, oxygen is a convenient choice for a reference chemical since H_c for oxygen is 1.2×10^5 torr M^{-1} at 25°C and liquid phase mass transport controls the transport of oxygen from air to water.

If liquid phase mass transport resistance controls the volatilization rate, then equation (5.29) is correct for a wide range of chemicals and

$$k_v^C/k_v^O = k_\ell^C/k_\ell^O \cdot f(D_\ell^C/D_\ell^B) = \text{constant} \qquad (5.29)$$

laboratory conditions (see Smith et al. 1980 and references therein). Smith et al. (1980) have shown that

$$f(D_\ell^C/D_\ell^O) = (D_\ell^C/D_\ell^O)^m \qquad (5.30)$$

where m = 0.61 for their laboratory conditions. The exponent arises because the classical two-film theory is not the correct mathematical formulation of the mass transport theories. The theoretical reasons may be found elsewhere (Trebal, 1968; Smith and Bomberger, 1980; Smith et al., 1980).

Since the ratio k_v^C/k_v^O is a constant over a wide range of environmental conditions, equation (5.22) should be applicable over a wide range of environmental conditions, provided H_c is greater than about 3500 torr $M^{-1} = 4.6 \times 10^{-3}$ atm $m^3 mol^{-1}$

$$(k_v^C)_{env} = (k_v^C/k_v^O)_{lab} \ (k_v^O)_{env} \qquad (5.31)$$

where k_v^C is the volatilization rate constant for the chemical (hr^{-1}) and k_v^O is the oxygen reaeration rate constant (hr^{-1}) in the laboratory or the environment. The ratio k_v^C/k_v^O for benzene is independent of turbulence, salt concentration (seawater), temperature (4°-50°C), or the presence of a surface-active compound (Smith et al., 1980). Also the value of $(k_v^C/k_v^O)_{lab}$ can be predicted using

$$\left(\frac{k_v^C}{k_v^O}\right)_{lab} = \left(\frac{D_\ell^C}{D_\ell^O}\right)^{0.61} \qquad (5.32)$$

where D_ℓ is the liquid phase diffusion coefficient. This equation was also tested using laboratory measurements of k_v^C/k_v^O and estimates of D^C for 13 compounds (Smith et al., 1980).

For chemicals where gas phase mass transport resistance determines the volatilization rate, the ratio of the gas phase mass transport coefficients for two chemicals measured simultaneously will be constant. Thus, from equation (5.28)

$$k_g^A/k_g^B = f(D_g^A/D_g^B) = \text{a constant} \qquad (5.33)$$

which means that the ratio of mass transport coefficients should be independent of the gas phase turbulence. Then, for the chemical and for water evaporation

$$(k_g^C/k_g^W)_{env} = (k_g^C/k_g^W)_{lab} = f(D_g^C/D_g^W) = \text{a constant} \qquad (5.34)$$

If classical two-film theory were a valid description of the mass transport, equation (5.33) would become

$$k_g^C/k_g^W = f(D_g^C/D_g^W) = (D_g^C/D_g^W)^m = \text{a constant} \qquad (5.35)$$

where m = 1. However, for theoretical reasons beyond the scope of this discussion, m is probably less than 1 (see Tamir and Merchuk, 1978).

Rearranging equations (5.30) and (5.35) gives

$$k_{\ell}^C = k_{\ell}^O (D_{\ell}^C/D_{\ell}^O)^m \qquad (5.36)$$

$$k_g^C = k_g^W (D_g^C/D_g^W)^n \qquad (5.37)$$

If we know or can estimate k_{ℓ}^O, k_g^W, the diffusion constant ratios, and H_c, then k_v^C can be calculated by substituting equations (5.36) and (5.37) into equation (5.22).

$$k_v^C = \frac{1}{L} \left[\frac{1}{k_{\ell}^C} + \frac{RT}{H_c^C k_g^C} \right]^{-1} \qquad (5.22)$$

$$= \frac{1}{L} \left[\frac{1}{k_{\ell}^O (D_{\ell}^C/D_{\ell}^O)^m} + \frac{RT}{H_c k_g^W (D_g^C/D_g^W)^n} \right]^{-1} \qquad (5.2)$$

This equation was used to estimate the volatilization rate constants of the priority pollutants.

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5.4.2 Choice of Parameters in Table 5.1

The values of L and T for the environment are arbitrary and could be adjusted to fit specific situations. The value of k_v^C is not strongly dependent on temperature, especially if liquid phase mass transport resistance is significant (the chemical is a high or intermediate volatility chemical).

The values of k_ℓ^O were calculated from literature estimates of k_v^O, which are summarized in Table 5.2.

Table 5.2

OXYGEN REAERATION RATES IN REPRESENTATIVE WATER BODIES

	Literature values (day^{-1})	Values used in Smith et al.[a] k_v^O			Corresponding value of k_ℓ^O (cm hr^{-1})
		(day^{-1})	(hr^{-1})	l (cm)	
Pond	0.11 - 0.23[b]	0.19	0.008	200	1.6
River	0.2,[c] 0.1 - 9.3[d]	0.96	0.04	300	12
Lake	0.10 - 0.30[b]	0.24	0.01	500	5

[a]Smith et al. (1977).

[b]Metcalf and Eddy (1972).

[c]Grenney et al. (1976).

[d]Langbein and Durum (1967); taken from Table 2 for rivers such as the Allegheny, Kansas, Rio Grande, Tennessee, and Wabash. Values for other rivers as well as a method for calculating k_v^O in rivers are given in this reference.

One way to calculate an appropriate value of the gas phase mass transport coefficient for water, k_g^W, is to use the water evaporation rate or flux, N^W, since

$$N^W = k_g^W \left(\frac{P_s^W - P^W}{RT} \right) \qquad (5.38)$$

where P_s^W and P^W are the saturated and actual partial pressure of water vapor at temperature T. The field data that we have found for water evaporation rates from lakes are summarized in Table 5.3. We have not been able to locate equivalent data for streams or rivers. Assuming an average relative humidity of 50%, the average value of k_g^W for the fresh-water lakes would be 0.59 cm sec^{-1} = 2100 cm hr^{-1}. An alternative method is described in the next section (Section 5.4.3).

Table 5.3

WATER EVAPORATION RATES FOR LAKES

Location	Average Evaporation Rate (cm sec^{-1} x 10^6)	Reference
Lake Hefner, Oklahoma	4.8	Marciano and Harbeck (1952)
Lake Mead, Nevada and Arizona	6.8	Harbeck et al. (1958)
Pretty Lake, Indiana	3.8	Ficke (1972)
Average	5.1	

The values of the exponents m and n in equation (5.2) are based on laboratory work carried out at SRI International. Smith et al. (1980) found that, for the volatilization rates of 13 high volatility compounds measured in the laboratory, m = 0.62. The data for four chemicals suggest that n is about 0.8 or 0.9 under their laboratory conditions. Both m and n should vary from 0.5 to 1.0, depending on the turbulence; the values approach 1.0 as the turbulence level decreases. However, systematic studies to estimate the values of m and n in environmental situations have not been made. Therefore, the choices recommended in Table 5.1 are reasonable, but somewhat arbitrary.

5.4.3 Selection of Volatilization Rate Input Data for the EXAMS Model

The EXAMS model was described in Section 2.2. If no other volatilization rate data are available, FXAMS uses the Henry's constant to calculate the volatilization rate constant, using a modified version of equation (5.2). The value of Henry's constant is calculated by EXAMS using equation (5.7), the Clausius-Clapeyron equation. If the chemical is a solid, equation (5.13) should be used to calculate H_c, since EXAMS does not make the vapor pressure correction for the heat of fusion.

If a value for k_v^C/k_v^O (variable KVOG in EXAMS) is not entered, the environmental mass transport coefficients for k_ℓ^O (variable KO2 in EXAMS and k_g^W (variable WAT in EXAMS) are estimated from the inverse ratio of the square roots of the molecular weight of oxygen or water and the chemical. This assumption gives values that are within about $\pm 20\%$ of the experimental values, (Smith et al., 1980). In EXAMS, estimation procedure can be overidden by entering a value of k_v^C/k_v^O (variable KVOG). Therefore, for high volatility compounds, the measured value of k_v^C/k_v^O is reported in Section 3. If an experimental value is not available, the value calculated from equation (5.39) for streams and rivers is reported.

$$k_v^C/k_v^O = k_\ell^C/k_\ell^O = \text{KVOG} = (D_\ell^C/D_\ell^O)^{0.7} \qquad (5.39)$$

The calculation procedure for k_g^C cannot be overridden in the current version of EXAMS, so estimates of D_g^C/D_g^W have not been included in Section 3.

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In EXAMS, the value of k_g^C is calculated from the wind speed, which used to calculate k_g^W from

$$WAT(k_g^W) = 0.1857 + 11.36 \text{ WINDG} \qquad (5.40)$$

where WINDG is the wind speed 10 cm above the water surface. The default value of WINDG is 2 m $\sec^{-1}$, which gives a value of $k_g^W = 2290$ cm hr^{-1}, in good agreement with the value of 2100 cm hr^{-1} that was estimated from the field data for water evaporation summarized in Table 5.3.

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