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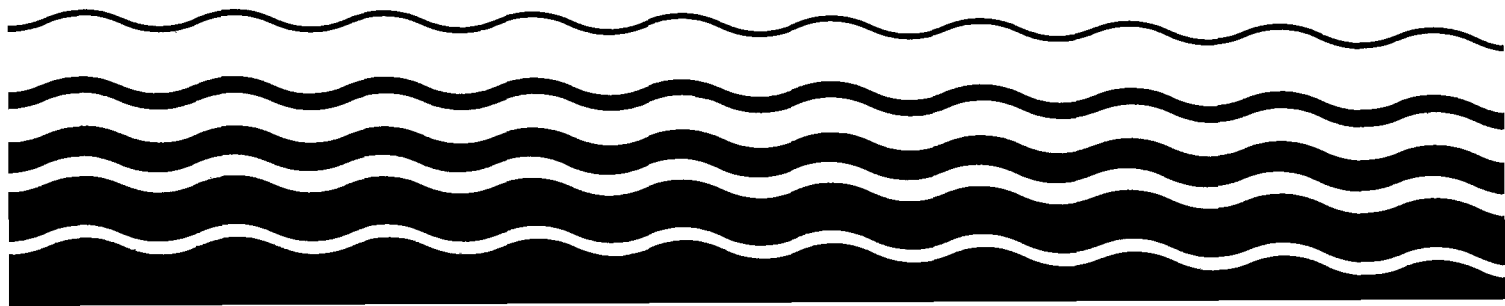
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# **AQUATIC FATE PROCESS DATA FOR ORGANIC PRIORITY POLLUTANTS**

## **Final Report**



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AQUATIC FATE PROCESS DATA FOR ORGANIC PRIORITY POLLUTANTS

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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.

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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.

## Pesticides

1. Acrolein
2. Aldrin
3. Chlordane (cis and trans isomers)
4. DDD
5. DDE
6. DDT
7. Dieldrin
8. Endosulfan ( $\alpha$  and  $\beta$  isomers)
9. Endosulfan sulfate
10. Endrin
11. Endrin aldehyde
12. Heptachlor
13. Heptachlor epoxide
14.  $\alpha$ -Hexachlorocyclohexane
15.  $\beta$ -Hexachlorocyclohexane
16.  $\delta$ -Hexachlorocyclohexane
17.  $\gamma$ -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 (ethylidene 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 (vinylidene chloride)
42. 1,2-trans-Dichloroethene
43. Trichloroethene
44. Tetrachloroethene (perchloroethylene)
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

#### 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

### 1.3. REFERENCES

- Callahan, M. A., M. W. Slimak, N. W. Gabel, I. P. May, C. F. Fowler, J. R. Freed, P. Jennings, R. L. Durfee, F. C. Whitmore, B. Maestri, W. R. Mabey, B. R. Holt, and C. Gould, 1979. Water-Related Environmental Fate of 129 Priority Pollutants. U.S. EPA, Washington, D.C. Vol. I, EPA-440/4-79-029a; Vol. II, EPA-440/4-790029b.
- Keith, L. H., and W. A. Telliard. 1979. Priority Pollutants. I. A Perspective View. Environ. Sci. Technol. 13(4):416-423.

## 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 studies (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 studies, 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.



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

particulates in the environment is not kinetically controlled (i.e., sorption equilibrium is attained instantaneously).

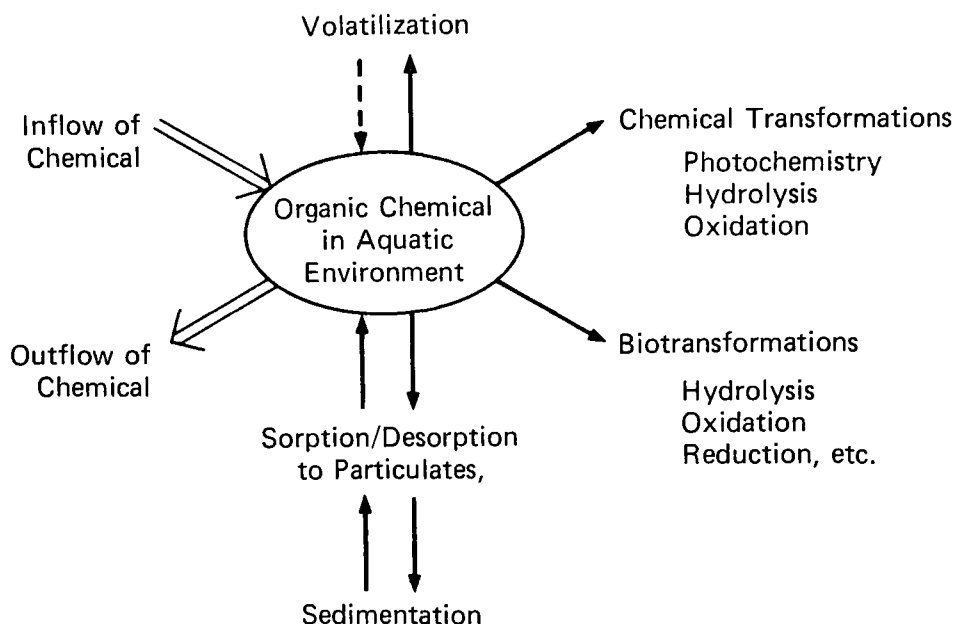


FIGURE 2.1 TRANSPORT AND TRANSFORMATION PROCESSES IN AQUATIC ENVIRONMENTS

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

$$R_T = \sum R_i = \sum k_i' [E_i] [C] \quad (2.1)$$

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

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  $E_i$ ;  $R_i$  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

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

or

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

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

$$t_{1/2} = \ln 2 / k_T \quad (2.4)$$

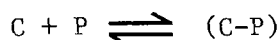
Influence of Sorption. In addition to losses of chemicals due to these transformation and volatilization processes, sorption to particulates can also reduce the concentrations of chemicals in aquatic systems. These particulates may be either suspended sediments or biotic in origin, and may eventually 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  $K_p$

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

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



and the partition coefficient can be rewritten as

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

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

$$[C_T] = [C-P] + [C_w] \quad (2.7)$$

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)

---

\* By convention,  $K_p$  is unitless when  $C_s$  is in units that are equivalent to  $C_w$  (i.e.,  $C_s$  is in  $\mu\text{g}$  chemical per g particulate and  $C_w$  is in  $\mu\text{g}$  chemical per g water). In this discussion,  $[C_w]$  will be defined in these weight units and  $[C]$  will be defined in molecular units ( $\text{moles liter}^{-1}$ ); since 1 g water is approximately 1 ml, it follows that  $[C] = 10^3 [C_w] [\text{MW}]^{-1}$  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:

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

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

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

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

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

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

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

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  $R_O$ , 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),

$$R_I = R_L = R_T + R_D + R_O \quad (2.12)$$

or

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

The steady-state concentration of chemical is then

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

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  $t_{1/2} = \ln 2 / k_T$ . The half-life is simply the time at which one-half of the initial 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

<u>% Chemical Remaining</u>	<u>Number of Half-Lives Elapsed</u>
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 incomplete 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 conducted 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

$$k_T = \sum k_i \quad (2.3)$$

and the half-life is then

$$t_{1/2} = \frac{\ln 2}{\sum k_i} \quad (2.15)$$

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



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<sup>-1</sup> 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 volatilization 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 ( $-\text{CO}_2\text{R}$ ), carboxylic acid amides ( $-\text{CONH}_2$ ), alkyl halides ( $\text{R-X}$ ), phosphoric acid esters ( $(\text{RO})_3\text{PO}$ ), 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 often unreliable because of the complex chemistry of photoexcited states. When absorption spectral data are available, a maximum rate constant (i.e., 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

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<sup>\*</sup> (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,  $\Delta H_{\text{vap}}$ , of a chemical is not available, it may be estimated from Trouton's rule

$$\Delta H_{\text{vap}} = 21T_{\text{BP}} \quad (2.16)$$

where the boiling point,  $T_{\text{BP}}$ , is given in degrees Kelvin ( $= ^\circ\text{C} + 273$ ); Trouton's Rule is discussed in most physical chemistry textbooks. A value of  $\Delta H_{\text{vap}}$  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.

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 possessing acidic properties can be written as



and the ionization constant  $K_A$  defined as

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

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

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

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



and the ionization constant  $K_B$  is defined as

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

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 following 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<sup>-1</sup>). 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

$S_w$ ,  $K_{oc}$ , 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,  $K_B$   $[(\mu\text{g/g})(\text{mg/liter})^{-1}]$ . 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<sup>3</sup> mole<sup>-1</sup>). 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



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 3500 torr  $M^{-1}$  (or  $4.6 \times 10^{-3} \text{ m}^3 \text{ atm mole}^{-1}$ ). 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 calculations. In general, NAV is entered for chemicals with  $H_c < 2 \times 10^{-3} \text{ atm m}^3 \text{ mol}^{-1}$ .

### 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

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

where  $b$  is a constant to provide appropriate units,  $\phi$  is the reaction quantum yield, and  $\epsilon_\lambda$  and  $I_\lambda$  are light absorption coefficients and light fluxes, respectively, at wavelength intervals,  $\lambda$ . 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

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

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.

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; Spanggard 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

$$R'_p = k'_p [C] \quad (2.22)$$

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,  $\epsilon_{\lambda}$  (in  $M^{-1} \text{ cm}^{-1}$ ). The absorption coefficients of the chemical are determined from the uv-visible spectrum of the chemical and are used with sunlight photon flux data,  $I_{\lambda}$ , 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  $\epsilon_{\lambda}$  values are given at the wavelengths required for the  $k_p$  calculation computer program of Zepp and Cline (1977).

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

Photolysis Rate Constant,  $k_p$  ( $\text{hr}^{-1}$ ). Some literature data are available for photolysis experiments conducted in sunlight, but without any measurements of  $\epsilon_{\lambda}$  or  $\phi$ . 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  $\epsilon_{\lambda}$  and  $\phi$ , a value of  $k_p$  is calculated for a particular stated time interval to assist the reader who does not have access to  $I_{\lambda}$  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.

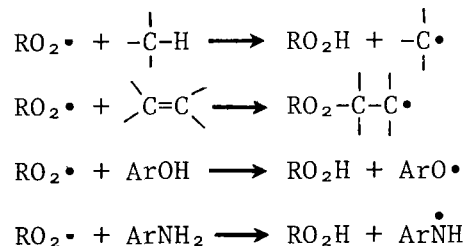
### 2.3.8 Oxidation Rate Constants

Chemical oxidation of organic chemicals in aquatic environments may occur due to several different oxidants, among which are singlet oxygen ( $^1\text{O}_2$ ), alkyl peroxy radical ( $\text{RO}_2\cdot$ ), alkoxy radical ( $\text{RO}\cdot$ ), or hydroxyl radical ( $\cdot\text{OH}$ ). 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 photochemistry 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.

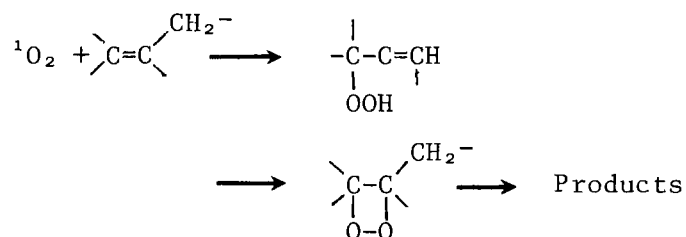
Literature information has reported data on oxidation of organic

chemicals by oxy radicals such as  $\text{RO}_2^\bullet$  and  $^1\text{O}_2$ . The laboratory study conducted by Mill et al. (1980) using natural waters indicates that  $\text{RO}_2^\bullet$  radical concentrations of  $\sim 1 \times 10^{-9}$  M may be present in the surface waters of sunlit water bodies. Oxidation reactions initiated by  $\text{RO}_2^\bullet$  include the following:



Of these reactions, the last two are quite rapid in aquatic environments ( $t_{1/2} < \text{several days}$ ), whereas the others are slower and usually will not be important for most chemicals.

Zepp et al. (1978) have shown that  $^1\text{O}_2$  can be formed at  $\approx 1 \times 10^{-12}$  M concentrations in sunlit natural waters. The most important reactions for  $^1\text{O}_2$  with organic chemicals are those involving reaction with olefinic moieties (Ranby and Rabek, 1978).



Some rate constants for  $^1\text{O}_2$  and  $\text{RO}_2^\bullet$  are listed in a review by Mill (1980).

The rate of loss of organic chemicals  $\text{R}_{\text{OX}}$  by oxidation is

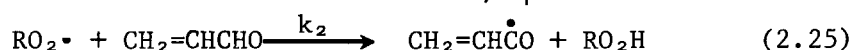
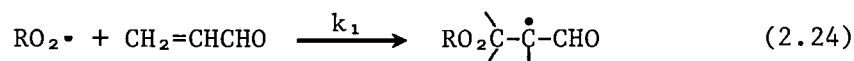
$$\text{R}_{\text{OX}} = k_{\text{RO}_2^\bullet} [\text{RO}_2^\bullet] [\text{C}] + k_{^1\text{O}_2} [^1\text{O}_2] \text{C} + k_{\text{OX}} [\text{OX}] [\text{C}] \quad (2.23)$$

where  $k_{\text{OX}}$  and  $[\text{OX}]$  are the rate constants and concentration values for other unspecified oxidants. Only data for second-order rate constants  $k_{\text{RO}_2^\bullet}$  and  $k_{^1\text{O}_2}$  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,  $RO_2\cdot$ ,  $k_{ox}$  ( $M^{-1} hr^{-1}$ )

Because many chemicals in the priority pollutant list have several kinds of reactive centers for oxidation by  $RO_2\cdot$ , 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



$$k_{RO_2} = k_1 + k_2$$

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  $RO_2\cdot$  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

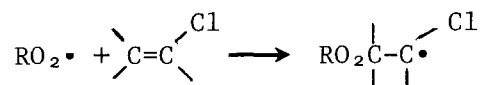
$$\log k_{RO_2} = 18.96 - 0.2 [D(R-H)] \quad (2.26)$$

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

For the RO<sub>2</sub> addition to double bonds

$$\log k_{\text{RO}_2} = [16.54 - 0.2D(\text{xCR}_2\text{-H})]/0.75 \quad (2.27)$$

where D(XCR<sub>2</sub>-H) is the bond dissociation energy of a species that gives the radical formed by RO<sub>2</sub> addition and where RO<sub>2</sub> is assumed to have the same effect as Me on D(C-H). Thus for oxidation of vinyl chloride



the closest analog would be MeCH<sub>2</sub>CHCl<sup>•</sup>, and the value of D(MeCH<sub>2</sub>CHCl-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, <sup>1</sup>O<sub>2</sub>, k<sub>ox</sub> (M<sup>-1</sup> hr<sup>-1</sup>).  
Only a few of the chemicals discussed in this report are reactive toward <sup>1</sup>O<sub>2</sub>; these include some polycyclic aromatic and a few olefinic double bond or diene systems. When no reactive center was recognized, chemicals were assigned k<sub><sup>1</sup>O<sub>2</sub></sub> < 3600 or < 360 M<sup>-1</sup> h<sup>-1</sup>. 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



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

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

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

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

equation (2.28) can be rewritten as

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

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,  $k_A$  ( $M^{-1} \text{ hr}^{-1}$ ). 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,  $k_B$  ( $M^{-1} \text{ hr}^{-1}$ ). 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,  $k_N$  ( $\text{hr}^{-1}$ ). 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

$$R_B = k_b [B] [C] \quad (2.31)$$

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  $\text{ml cell}^{-1} \text{ hr}^{-1}$ , the units of [B] are in  $\text{cell ml}^{-1}$ . 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 ( $\text{ml cell}^{-1} \text{hr}^{-1}$ ) FOR BIOTRANSFORMATION  
OF CHEMICALS BY BACTERIA IN WATER BODY SOLUTION PHASE

Category I $3 \times 10^{-6}$	Category II $1 \times 10^{-7}$	Category III $3 \times 10^{-9}$	Category IV $1 \times 10^{-10}$	Category V $3 \times 10^{-12}$
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	Bis(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	Benzo[ah]anthracene
		2-Nitro phenol	Hexa-Cl-butadiene	Indeno[1,2,3-cd]pyrene
		2,4-Dinitro phenol	Hexa-Cl-cyclo pentadiene	Dimethyl nitrosamine
		p-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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## 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

Hydrolysis rate constants

Biotransformation rate constant.

For each property or process, the property, rate constant, or partitioning constant is defined in Sections 2.3.2 through 2.3.10. These sections also give the units of the values reported and discuss the significance and use of each value in terms of the particular process and how it is used in calculating rate or equilibrium constants for environmental 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 on 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  $K_{ow}$  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.<sup>B</sup> (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 polynuclear 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 Hassett et al. (1980) (see Section 4).

C-OX      Oxidation rate constants are calculated, using functional group reactivity toward peroxy 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 calculation 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	<p>Rate constant was estimated by analogy to chloroform. 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 <math>k_B [\text{OH}] = k_N</math> when <math>[\text{OH}^-] = 10^{-8}</math>.</p> <p>If the assumption is made that the same expression holds for all trihalomethanes, then <math>k_N = 10^{-8} k_B</math>.</p>
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 available 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- <u>trans</u> -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	$\alpha$ -Hexachlorocyclohexane
$C_6H_6Cl_6$	15	$\beta$ -Hexachlorocyclohexane
$C_6H_6Cl_6$	16	$\delta$ -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- <u>o</u> -cresol
$C_7H_7Cl_1O_1$	83	<u>p</u> -Chloro- <u>m</u> -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	$\alpha,\beta$ -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

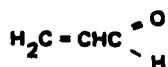
FORMULA	NUMBER	CHEMICAL NAME
$C_{19}H_{20}O_4$	90	Butyl benzyl phthalate
$C_{20}H_{12}$	95	Benzo[b]fluoranthene
$C_{20}H_{12}$	96	Benzo[k]fluoranthene
$C_{20}H_{12}$	98	Benzo[a]pyrene
$C_{22}H_{12}$	97	Benzo[ghi]perylene
$C_{22}H_{12}$	103	Indeno[1,2,3-cd]pyrene
$C_{22}H_{14}$	100	Benzo[a,h]anthracene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

### References for 3.1

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- Mabey, W. R., and T. Mill. 1978. Critical Review of Hydrolysis of Organic Compounds in Water Under Environmental Conditions. J. Phys. Chem. Ref. Data 7:383-415.
- UV Atlas. 1971. UV Atlas of Organic Compounds. Vol. I-V. Plenum Press, New York.
- Yalkowsky, S. H., and S. C. Valvani. 1980. Solubility and Partitioning. I: Solubility of Nonelectrolytes in Water. J. Pharm. Sci. 69(8): 912-922.
- Zepp, R. G., and D. M. Cline. 1977. Rate of Direct Photolysis in Aquatic Environment. Environ. Sci. Technol. 11(4):359-366.
- Zepp, R. G., G. L. Baughman, and P. F. Schlotzhauer. 1980. Photosensitization of Pesticide Reactions by Humic Substances. Abstract, 180th Meeting of American Chemical Society, San Francisco, August 25-29. PEST 6.

## SECTION 3.2. PESTICIDES

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



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)	$2.1 \times 10^5$ (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, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	0.44	C-KB f Kow

Volatilization constants: [1-1]

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

# 1. ACROLEIN

## TRANSFORMATION DATA

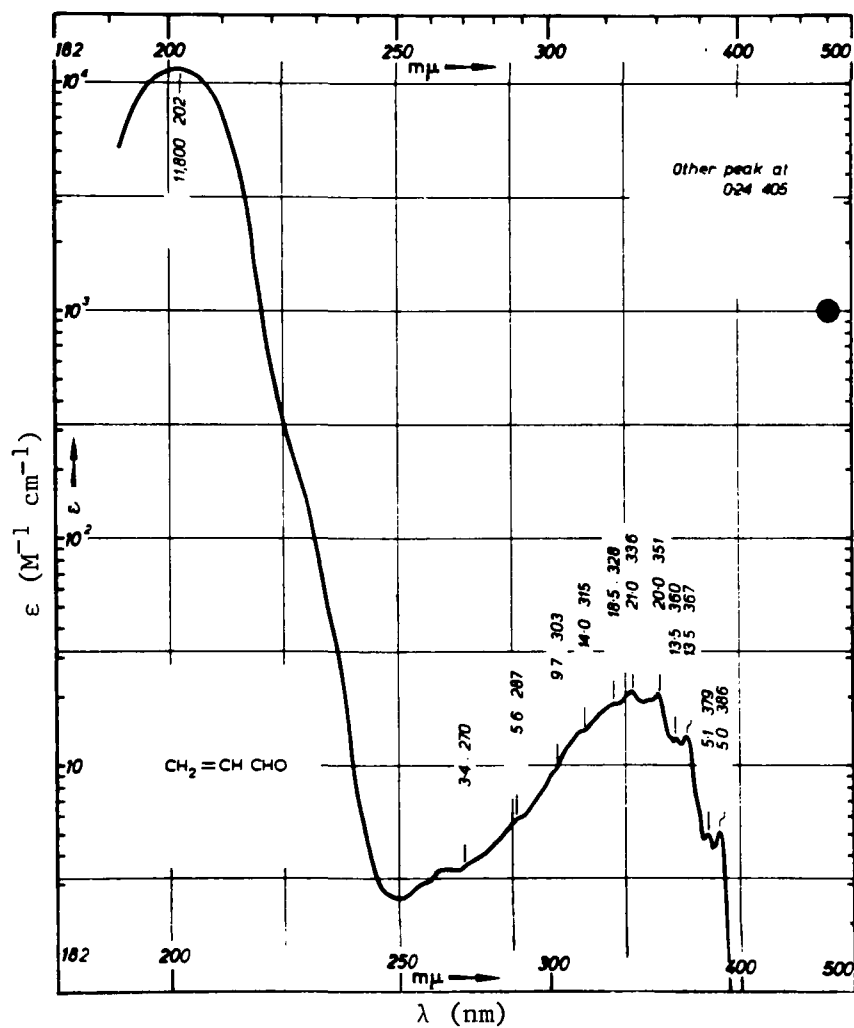
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [1-2]	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	_____	_____
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	[1-2]	_____
Oxidation constants at 25°C: [1-1]		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$1 \times 10^7$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$3.4 \times 10^3$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

E: Estimated value; see List of Source Codes.

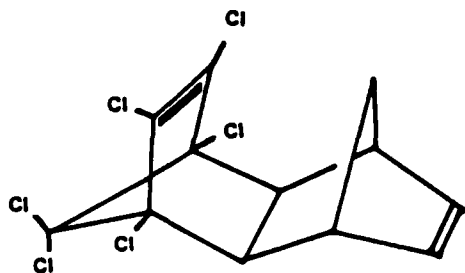
[1-1] The values of  $K_{\text{ow}}$ ,  $K_{\text{oc}}$ ,  $K_B$ ,  $k_v^c/k_v^o$ ,  $P_v$  and oxidation rate constants are calculated or given for the unhydrated acrolein species; hydration of acrolein may be extensive in aquatic environments, and the above properties will therefore be different than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

## 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  $\beta$ -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).







2. ALDRIN

CAS No. 309002

PHYSICAL AND TRANSPORT DATA

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

Partition constants:

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

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	<u><math>1.6 \times 10^{-5}</math></u>	<u>C-VP/S-25°</u>
Vapor pressure, $P_v$ (torr)	<u><math>6 \times 10^{-6}</math> (25°C)</u>	<u>WREF</u>
Reaeration rate ratio, $k_v^C/k_v^O$	<u>NAV</u>	

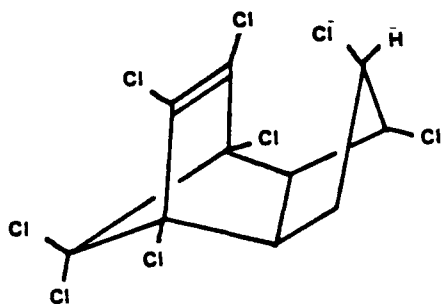
2. ALDRIN

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>E-P</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	_____
Direct photolysis rate constant, $k_p$ (hr <sup>-1</sup> ) _____ at _____ latitude	<u>PNER</u>	_____
Oxidation constants at 25°C:		
For <sup>1</sup> O <sub>2</sub> (singlet oxygen), $k_{OX}$ (M <sup>-1</sup> hr <sup>-1</sup> )	<u>&lt;3600</u>	<u>C-OX</u>
For RO <sub>2</sub> (peroxy radical), $k_{OX}$ (M <sup>-1</sup> hr <sup>-1</sup> )	<u>5 x 10<sup>3</sup></u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ (M <sup>-1</sup> hr <sup>-1</sup> )	<u>0</u>	<u>HNES</u>
For acid-promoted process, $k_A$ (M <sup>-1</sup> hr <sup>-1</sup> )	<u>0</u>	<u>HNES</u>
For neutral process, $k_N$ (hr <sup>-1</sup> )	<u>0</u>	<u>HNES</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ (ml cell <sup>-1</sup> hr <sup>-1</sup> )	<u>(E) 3 x 10<sup>-9</sup></u>	<u>E-KB</u>

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)	$3 \times 10^5$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.4 \times 10^5$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$4.0 \times 10^4$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$9.4 \times 10^{-5}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$1 \times 10^{-5}$ (25°C)	WREF
Reaeration rate ratio, $k_v^C/k_v^O$	NAV	

### 3. CHLORDANE

#### TRANSFORMATION DATA

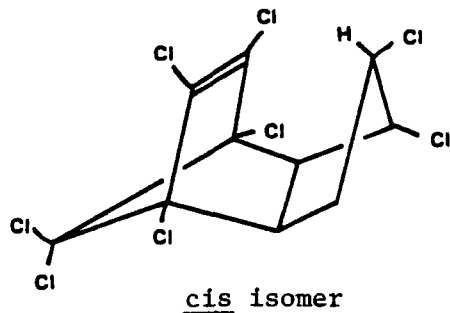
<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>E-P</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;3600</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>~30</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E)3 x 10<sup>-12</sup></u>	<u>E-KB</u>

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

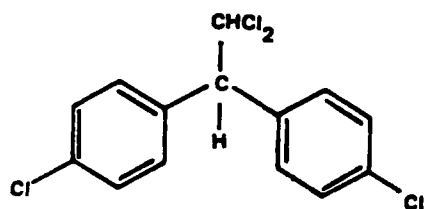
[3-2]



[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)	$1.6 \times 10^6$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$7.7 \times 10^5$	C-Koc f Kow
Microorganisms-water, $K_B ((\mu g/g)(mg/l)^{-1})$	$1.8 \times 10^5$	C-KB f Kow

## Volatilization constants:

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

4. DDD

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	$<5 \times 10^{-7}$	[4-3]
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<3600$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<1600$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	5.0 (27°C)	WREF [4-4]
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$4 \times 10^{-7}$ (27°C)	WREF [4-5]
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	E-KB

E: Estimated value; see List of Source Codes.

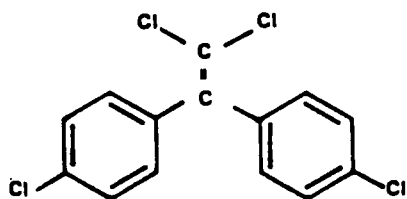
[4-1] Two water solubility values have been reported for the pp' isomer at 25°C: 0.02 ppm and 0.09 ppm. A value of 0.10 ppm has been reported for the op' isomer (WREF).

[4-2] Vapor pressures at 30°C have been reported as  $10.2 \times 10^{-7}$  torr for the pp' isomer and  $18.9 \times 10^{-7}$  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  $5 \times 10^{-7} \text{ hr}^{-1}$ .
- [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  $5.0 \text{ M}^{-1} \text{ hr}^{-1}$ .
- [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  $4.2 \times 10^{-7} \text{ hr}^{-1}$ , 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)	$9.1 \times 10^6$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$4.4 \times 10^6$	C-Koc f Kow
Microorganisms-water, $K_B ((\mu\text{g/g})(\text{mg/l})^{-1})$	$8.9 \times 10^5$	C-KB f Kow

## Volatilization constants:

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

5. DDE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at <u>313</u> nm	<u>0.3</u>	<u>WREF</u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;3600</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>1.2 \times 10^5</math></u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u><math>&lt;6.6 \times 10^{-7}</math> (27°C)</u>	<u>[5-3]</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>3 \times 10^{-12}</math></u>	<u>E-KB</u>

E: Estimated value; see List of Source Codes.

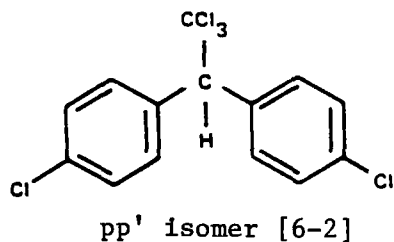
[5-1] Several water solubility values have been reported for the pp' isomer at various temperatures (WREF). Water solubilities have been reported ranging from 0.014 ppm to 0.12 for the pp' isomer and 0.140 ppm for the op' isomer (WREF).

[5-2] Vapor pressures reported are  $6.5 \times 10^{-6}$  torr for pp' isomer and  $6.2 \times 10^{-6}$  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  $6.6 \times 10^{-7} \text{ hr}^{-1}$ ; it is assumed that at this pH only the neutral process is occurring.

6. DDT  
 CAS No. [6-1]



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

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$1.58 \times 10^{-5}$	C-VP/S-25° [6-7]
Vapor pressure, $P_v$ (torr)	$1.9 \times 10^{-7}$ (25°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

6. DDT

## TRANSFORMATION DATA

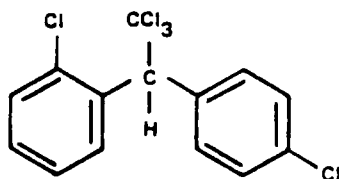
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	$<5 \times 10^{-7}$	WREF [6-8]
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<3600$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	3600	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	36 (27°C)	WREF [6-9]
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$6.8 \times 10^{-6}$ (27°C)	WREF [6-10]
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	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.

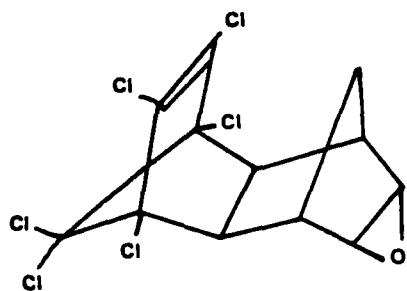
## 6. DDT

[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  $1.2 \times 10^{-3}$  -  $2.5 \times 10^{-2}$  ppm for the pp' isomer and  $2.6 \times 10^{-2}$  and  $8.5 \times 10^{-2}$  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  $9.2 \times 10^{-3}$  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 -  $5.5 \times 10^{-3}$  pp' and vapor pressure -  $1.9 \times 10^{-7}$  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  $5 \times 10^{-7}$  hr<sup>-1</sup>.
- [6-9] The base-promoted hydrolysis rate constant for DDT has been measured (WREF) to be  $k_B = 9.9 \times 10^{-3}$  M<sup>-1</sup> sec<sup>-1</sup>, which corresponds to a base-catalyzed process of 36 M<sup>-1</sup> hr<sup>-1</sup>.
- [6-10] A hydrolysis rate constant of  $6.8 \times 10^{-6}$  hr<sup>-1</sup> 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)	$3.5 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.7 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	710	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$4.57 \times 10^{-10}$	C-VP20°/S25°
Vapor pressure, $P_v$ (torr)	$1.78 \times 10^{-7}$ (20°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

## 7. DIELDRIN

### TRANSFORMATION DATA

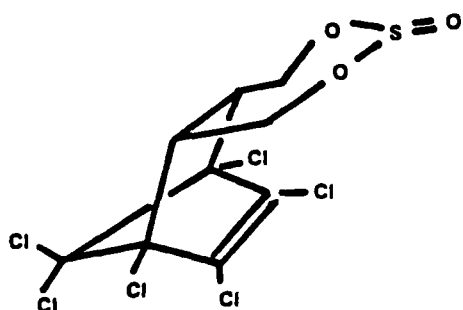
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at $40^\circ$ latitude	$4.8 \times 10^{-4}$	[7-2]
Oxidation constants at $25^\circ\text{C}$ :		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	30	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	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  $4.8 \times 10^{-4} \text{ hr}^{-1}$  is obtained.





8.  $\alpha$ -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)	$9.6 \times 10^{-3}$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	0.012	C-KB f Kow

Volatilization constants:

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

8.  $\alpha$ -ENDOSULFAN

## TRANSFORMATION DATA

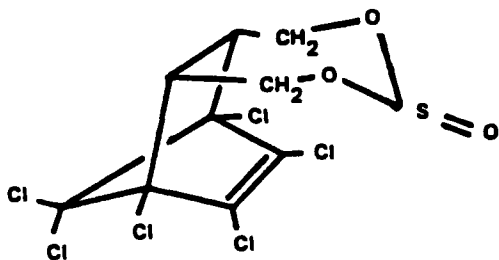
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$>3.6 \times 10^4$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$8.3 \times 10^3$ (20°C)	[8-1]
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )		
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$1.6 \times 10^{-4}$ (20°C)	[8-2]
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

E: Estimated value; see List of Source Codes.

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

## 8. $\alpha$ -ENDOSULFAN

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



8.  $\beta$ - 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)	$9.6 \times 10^{-3}$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	0.012	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$1.91 \times 10^{-5}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$1 \times 10^{-5}$ (25°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

8.  $\beta$ -ENDOSULFAN

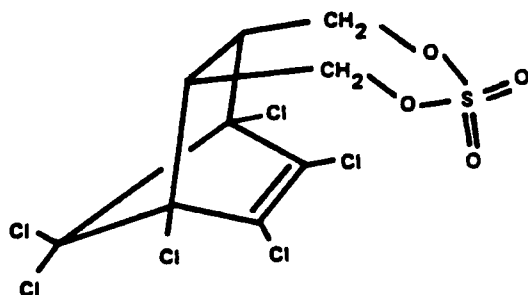
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;3600</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&gt;3.6 x 10<sup>4</sup></u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>8.3 x 10<sup>3</sup> (20°C)</u>	<u>[8-3]</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )		
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>1.3 x 10<sup>-4</sup> (20°C)</u>	<u>[8-4]</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) 3 x 10<sup>-9</sup></u>	<u>E-KB</u>

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  $1.9 \times 10^{-2}$  days and  $3.7 \times 10^{-3}$  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, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	0.029	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$2.6 \times 10^{-5}$	C-VP/S-25° [9-2]
Vapor pressure, $P_v$ (torr)	$1 \times 10^{-5}$ (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, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	20	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$8.3 \times 10^3$ (20°C)	[9-3]
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )		
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$1.3 \times 10^{-4}$ (20°C)	[9-4]
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	E-KB

E: Estimated value; see List of Source Codes.

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

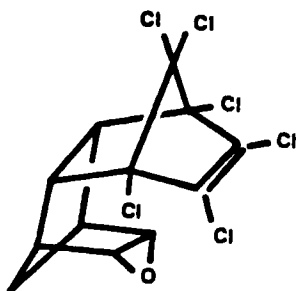
[9-2] Vapor pressure value was assigned by analogy to endosulfan.  
Henry's constant was calculated using vapor pressure value for endosulfan.

## 9. ENDOSULFAN SULFATE

[9-3] See [8-1]. The assumption is made that rate constants for  $\beta$ -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)	$3.5 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.7 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	710	C-KB f Kow

Volatilization constants:

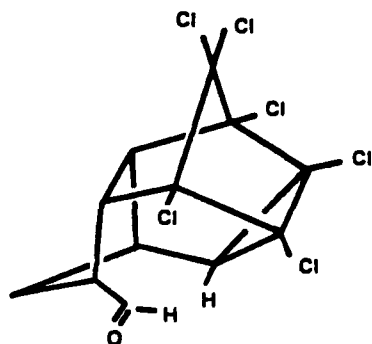
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$4.0 \times 10^{-7}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$2 \times 10^{-7}$ (25°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

10. ENDRIN

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	20	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0.	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	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)	$1.4 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	670	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	310	C-KB f Kow

## Volatilization constants:

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

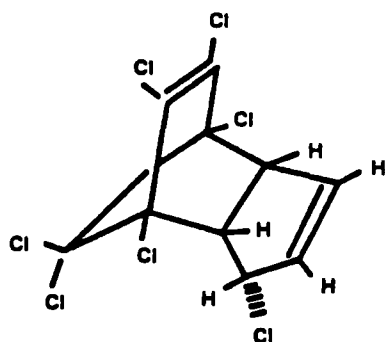
11. ENDRIN ALDEHYDE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	3100	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	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)	$2.6 \times 10^4$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.2 \times 10^4$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$4.4 \times 10^3$	C-KB f Kow

Volatilization constants:

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

12. HEPTACHLOR

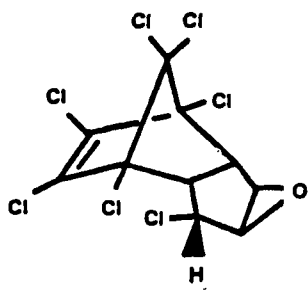
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$3 \times 10^{10}$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	2500	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	—	[12-2]
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	—	[12-2]
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$3.00 \times 10^{-2}$ (30°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	—	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	<u>389.2</u>	
Melting point, °C	<u>157-160</u>	<u>WREF</u>
Boiling point, °C		
Ionization constant	<u>pK-NER</u>	

Partition constants:

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

Volatilization constants:

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

### 13. HEPTACHLOR EPOXIDE

#### TRANSFORMATION DATA

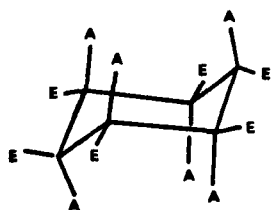
<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	20	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	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.  $\alpha$ -HEXACHLOROCYCLOHEXANECAS No. 319-84-6

<u>Orientation of Cl atoms on ring</u>	<u>Isomer</u>
AAEEEE	$\alpha$
EEEEEE	$\beta$
AAAEEE	$\gamma$ (lindane)
AEEEEE	$\delta$
AEEAEE	$\epsilon$

## PHYSICAL AND TRANSPORT DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
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)	$7.8 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$3.8 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$1.5 \times 10^3$	C-KB f Kow

## Volatilization constants:

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

14.  $\alpha$ -HEXACHLOROCYCLOHEXANE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	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.  $\beta$ -HEXACHLOROCYCLOHEXANECAS No. 319-85-7See  $\alpha$ -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)	$7.8 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$3.8 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$1.5 \times 10^3$	C-KB f Kow

## Volatilization constants:

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

15.  $\beta$ -HEXACHLOROCYCLOHEXANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>E-P</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;3600</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>6</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-10}</math></u>	<u>E-KB</u>

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.  $\delta$ -HEXACHLOROCYCLOHEXANE

CAS No. 319-86-8

See  $\alpha$ -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)	$1.4 \times 10^4$	Pomona
Sediment-water, $K_{oc}$ (unitless)	$6.6 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$3.5 \times 10^3$	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$2.07 \times 10^{-7}$	C-VP20°/S25°
Vapor pressure, $P_v$ (torr)	$1.7 \times 10^{-5}$ (20°C)	WREF
Reaeration rate ratio, $k_v^C/k_v^O$	NAV	

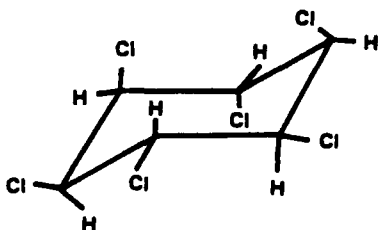
16.  $\delta$ -HEXACHLOROCYCLOHEXANE

TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	E-KB

E: Estimated value; 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)	$7.8 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$3.8 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$1.5 \times 10^3$	C-KB f Kow

Volatilization constants:

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

## 17. LINDANE

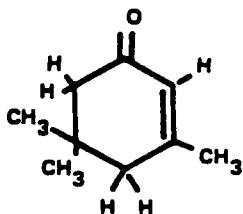
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	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	215	WREF
Ionization constant	pK-NER	

Partition constants:

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

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$5.75 \times 10^{-6}$	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

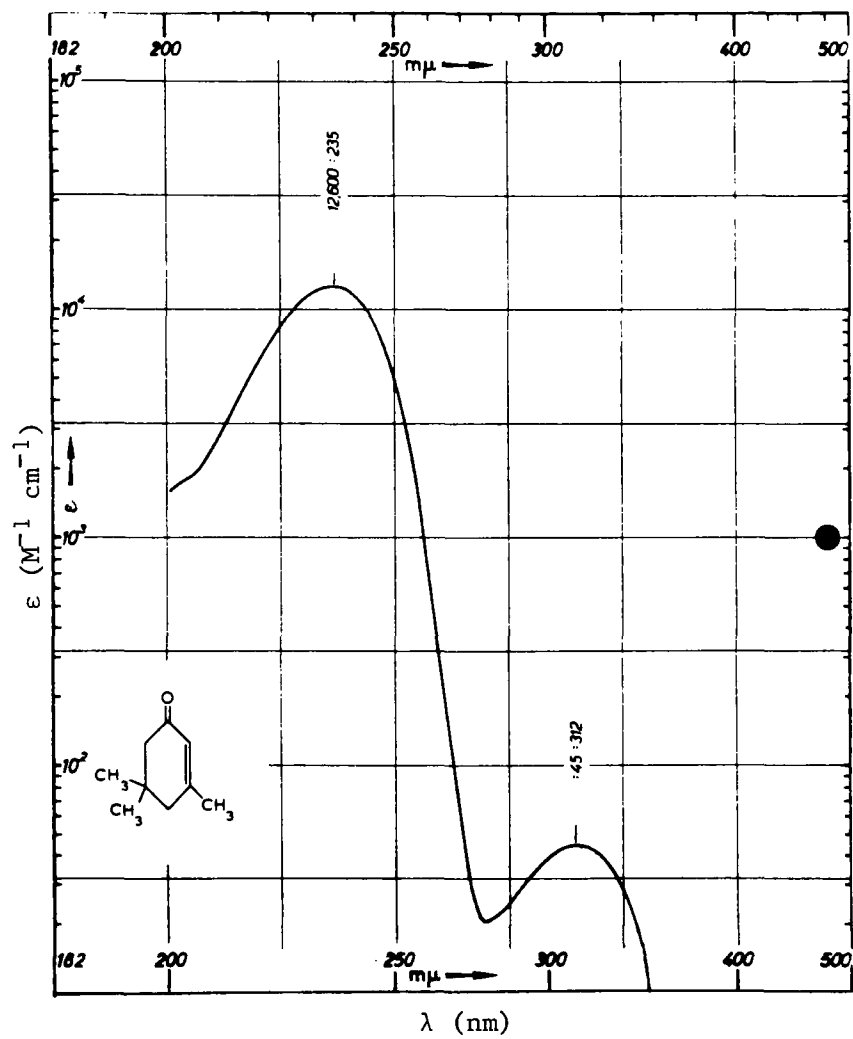
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [18-2]	
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<1 \times 10^7$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	225	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	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.

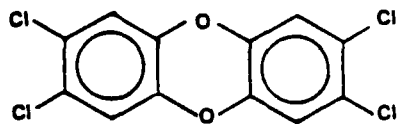
## 18. ISOPHORONE

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



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

## Volatilization constants:

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

19. TCDD

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	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



## 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)	$2.00 \times 10^3$	WREF
Sediment-water, $K_{oc}$ (unitless)	964	C-Koc f Kow
Microorganisms-water, $K_B ((\mu\text{g/g})(\text{mg/l})^{-1})$	429	C-KB f Kow

## Volatilization constants:

Henry's constant, $H^c$ (atm m <sup>3</sup> mol <sup>-1</sup> )	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, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	3	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	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. Reehl 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.

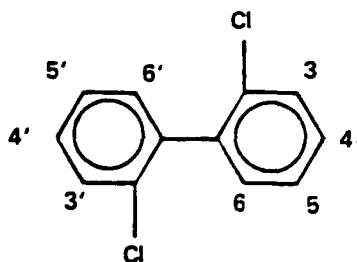
UV Atlas. 1971. UV Atlas of Organic Compounds. Vol. I-V. Plenum Press, New York.



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

21. AROCLOR 1016CAS 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)	$3.8 \times 10^5$	WREF
Sediment-water, $K_{oc}$ (unitless)	$1.8 \times 10^5$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$5.0 \times 10^4$	C-KB f Kow

## Volatilization constants:

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

21. AROCLOR 1016

## TRANSFORMATION DATA [21-2]

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	$(E) 3 \times 10^{-9} \sim 3 \times 10^{-12}$	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 susceptible to biological or abiotic oxidation processes.

22. AROCLOR 1221CAS 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:

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

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$1.7 \times 10^{-4}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$6.7 \times 10^{-3}$ (25°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

## 22. AROCLOR 1221

## TRANSFORMATION DATA (see [21-2])

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9} \sim 3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

23. AROCLOR 1232CAS No. 111-411-65

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

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

## Partition constants:

Water solubility, $S_w$ (ppm)	<u>407 (25°C)</u>	<u>C-Sw f Kow</u>
Octanol-water, $K_{ow}$ (unitless)	<u><math>1.6 \times 10^3</math></u>	<u>WREF</u>
Sediment-water, $K_{oc}$ (unitless)	<u>771</u>	<u>C-Koc f Kow</u>
Microorganisms-water, $K_B ((\mu\text{g/g})(\text{mg/l})^{-1})$	<u>351</u>	<u>C-KB f Kow</u>

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	<u><math>1.13 \times 10^{-5}</math></u>	<u>C-VP/S-25°</u>
Vapor pressure, $P_v$ (torr)	<u><math>4.06 \times 10^{-3}</math> (25°C)</u>	<u>WREF</u>
Reaeration rate ratio, $k_v^c/k_v^o$	<u>NAV</u>	<u></u>

23. AROCLOR 1232

## TRANSFORMATION DATA (see [21-2])

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$\ll 360$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$\ll 1$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9} \sim 3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

24. AROCOR 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)	$1.3 \times 10^4$	WREF
Sediment-water, $K_{oc}$ (unitless)	$6.3 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$2.3 \times 10^3$	C-KB f Kow

Volatilization constants:

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



24. AROCLOL 1242

## TRANSFORMATION DATA (see [21-2])

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$ ~ $3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

25. AROCLOR 1248CAS 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)	$5.75 \times 10^5$	WREF
Sediment-water, $K_{oc}$ (unitless)	$2.77 \times 10^5$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$7.29 \times 10^4$	C-KB f Kow

## Volatilization constants:

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

## 25. AROCLOR 1248

## TRANSFORMATION DATA (see [21-2])

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<<360$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<<1$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$ ~ $3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

26. AROCLOR 1254CAS No. 110-976-91

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

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

## Partition constants:

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

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	<u><math>2.6 \times 10^{-3}</math></u>	<u>WREF</u>
Vapor pressure, $P_v$ (torr)	<u><math>7.71 \times 10^{-5}</math> (25°C)</u>	<u>WREF</u>
Reaeration rate ratio, $k_v^c/k_v^o$	<u>0.359</u>	<u>C-DC.7</u>

## 26. AROCLOR 1254

## TRANSFORMATION DATA (see [21-2])

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9} \sim 3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

27. AROCLOR 1260CAS 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)	$2.7 \times 10^{-3}$ (25°C)	WREF
Octanol-water, $K_{ow}$ (unitless)	$1.4 \times 10^7$	WREF
Sediment-water, $K_{oc}$ (unitless)	$6.7 \times 10^6$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$1.3 \times 10^6$	C-KB f Kow

## Volatilization constants:

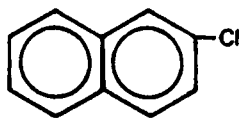
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	0.74	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$4.05 \times 10^{-5}$ (25°C)	WREF
Reaeration rate ratio, $k_v^C/k_v^O$	0.346	C-DC.7

27. AROCLOR 1260

## TRANSFORMATION DATA (see [21-1])

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9} \sim 3 \times 10^{-12}$	E-KF

E: Estimated value; see List of Source Codes.

28. 2-CHLORONAPHTHALENECAS 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)	$1.0 \times 10^4$	WREF
Sediment-water, $K_{oc}$ (unitless)	$4.8 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$1.8 \times 10^3$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$5.4 \times 10^{-4}$	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, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

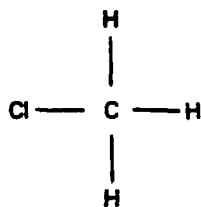
E: Estimated value; see List of Source Codes.

#### 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 (ethylidene 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 (vinylidene chloride)
42. 1,2-trans-Dichloroethene
43. Trichloroethene
44. Tetrachloroethene (perchloroethylene)
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



## 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:

Water solubility, $S_w$ (ppm)	$6.45 \times 10^3$ (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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	3.2	C-KB f Kow

## Volatilization constants:

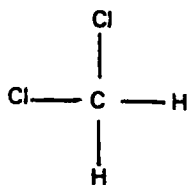
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	0.04	C-VP/S-20°
Vapor pressure, $P_v$ (torr)	$3.76 \times 10^3$ (20°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	0.752	C-DC.7

29. CHLOROMETHANE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>E-P</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0.05</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>—</u>	<u>HPHI</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NACM</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u><math>6.8 \times 10^{-5}</math> (25°C)</u>	<u>WREF</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>—</u>	<u>VF-NBD</u>

E: Estimated value; see List of Source Codes.

30. DICHLOROMETHANECAS No. 75-09-2

## 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)	$2.0 \times 10^4$ (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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	6.0	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$2.03 \times 10^{-3}$	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

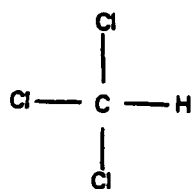
30. DICHLOROMETHANE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$\ll 360$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0.2	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )		HPII
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NACM
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$1.15 \times 10^{-7}$ (25°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	--	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

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

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$2.88 \times 10^{-3}$	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

31. TRICHLOROMETHANE

## TRANSFORMATION DATA

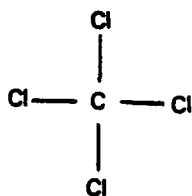
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>UV-ATLAS</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0.7</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0.23 (25°C)</u>	<u>Mabey &amp; Mill, 1978</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NACM</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u><math>2.5 \times 10^{-9}</math> (25°C)</u>	<u>Mabey &amp; Mill, 1978</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>—</u>	<u>VF-NBD</u>

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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	211	C-KB f Kow

## Volatilization constants:

Henry's constant, $H^c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	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

## TRANSFORMATION DATA

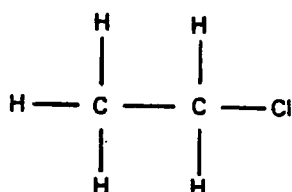
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$\ll 360$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$\ll 1$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	—	HPHI
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NACM
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	[32-1]	
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	E-KB

E: Estimated value; see List of Source Codes.

[32-1] The kinetics of hydrolysis of  $\text{CCl}_4$  has been reported as being second order in  $\text{CCl}_4$  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



## 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)	$5.74 \times 10^3$ (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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	9.8	C-KB f Kow

## Volatilization constants:

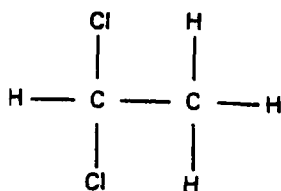
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	0.148	C-VP/S-20°
Vapor pressure, $P_v$ (torr)	$1.0 \times 10^3$ (20°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	0.645	C-DC.7

33. CHLOROETHANE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<<360$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<<1$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	—	HPII
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NACM
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$7.2 \times 10^{-4}$ (25°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	—	VF-NBD

E: Estimated value; see List of Source Codes.


34. 1,1-DICHLOROETHANE

CAS No. 75-34-3

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

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$4.26 \times 10^{-3}$	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

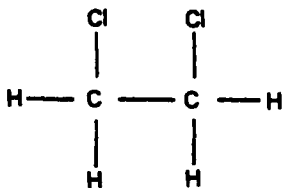
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )		
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NACM
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$1.15 \times 10^{-7}$ (25°C)	[34-1]
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	—	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-DICHLOROETHANE

CAS No. 107-06-2



## 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)	$8.69 \times 10^3$	WREF
Octanol-water, $K_{ow}$ (unitless)	30	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	14	C-Koc f Kow
Microorganisms-water, $K_B ((\mu\text{g/g})(\text{mg/l})^{-1})$	9	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$9.14 \times 10^{-4}$	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	<u>PNES</u>	<u>E-P</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;1</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>                    </u>	<u>                    </u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NACM</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u><math>1.8 \times 10^{-9}</math> (25°C)</u>	<u>WREF</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-10}</math></u>	<u>E-KB</u>

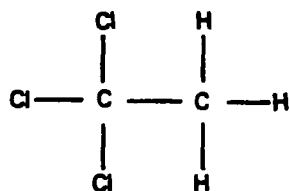
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E: Estimated value; see List of Source Codes.



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	WREF
Boiling point, °C	74.1	WREF
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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	81	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	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

36. 1,1,1-TRICHLOROETHANE

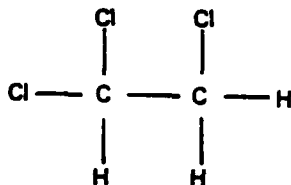
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$\ll 360$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )		
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NACM
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$1.7 \times 10^{-4}$ (25°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	—	VF-NBD

E: Estimated value; see List of Source Codes.

## 37. 1,1,2-TRICHLOROETHANE

CAS No. 79-00-5



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

## Volatilization constants:

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

## 37. 1,1,2-TRICHLOROETHANE

## TRANSFORMATION DATA

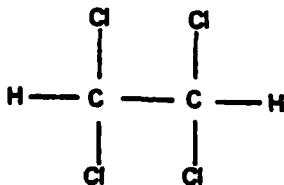
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	3	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )		
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NACM
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$1.2 \times 10^{-7}$ (25°C)	E-H [37-1]
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	E-KB

E: Estimated value; 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



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

## Volatilization constants:

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

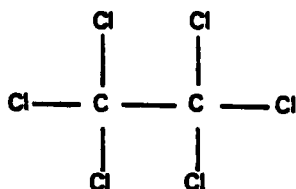
## 38. 1,1,2,2-TETRACHLOROETHANE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	2	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )		
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NACM
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$1.2 \times 10^{-7}$ (25°C)	E-H [38-1]
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

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

39. HEXACHLOROETHANECAS No. 67-72-1

## 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)	$4.2 \times 10^4$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$2.0 \times 10^4$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$6.75 \times 10^3$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$2.49 \times 10^{-3}$	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, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NACM
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	E-KB

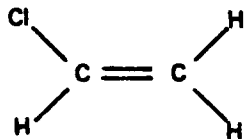
E: Estimated value; see List of Source Codes.

[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)	$2.7 \times 10^3$ (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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	5.7	C-KB f Kow

## Volatilization constants:

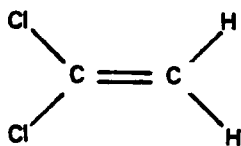
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$8.14 \times 10^{-2}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$2.66 \times 10^3$ (25°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	0.675	C-DC.7

## 40. CHLOROETHENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<10^8$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	3	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	—	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, $K_B ((\mu\text{g/g})(\text{mg/l})^{-1})$	53	C-KB f Kow

Volatilization constants:

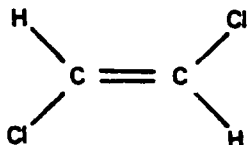
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	0.190	C-VP25°/S20°
Vapor pressure, $P_v$ (torr)	591 (25°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	0.601	C-DC.7

41. 1,1-DICHLOROETHENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<10^8$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	3	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	—	VF-NBD

E: Estimated value; see List of Source Codes.

42. 1,2-TRANS-DICHLOROETHENECAS No. 540-59-0

## 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, $K_B ((\mu\text{g/g})(\text{mg/l})^{-1})$	48	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	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

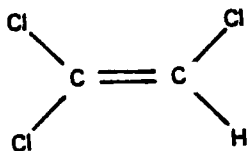
42. 1,2-TRANS-DICHLOROETHENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<10^5$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	—	VF-NBD

E: Estimated value; see List of Source Codes.

[42-1] No pressure is reported for the boiling point.



43. TRICHLOROETHENE

CAS No. 79-01-6

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)	$1.1 \times 10^3$ (20°C)	WREF
Octanol-water, $K_{ow}$ (unitless)	263	Pomona
Sediment-water, $K_{oc}$ (unitless)	126	C-Koc f Kow
Microorganisms-water, $K_B$ ( $(\mu\text{g/g})(\text{mg/l})^{-1}$ )	97	C-KB f Kow

Volatilization constants:

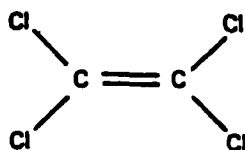
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$9.1 \times 10^{-3}$	C-VP/S-20°C
Vapor pressure, $P_v$ (torr)	57.9 (20°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	0.548	C-DC.7

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>UV-ATLAS</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>&lt;10^3</math></u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>6</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-10}</math></u>	<u>E-KB</u>

E: Estimated value; see List of Source Codes.





44. TETRACHLOROETHENE

CAS No. 127-18-4

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 Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	252	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	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

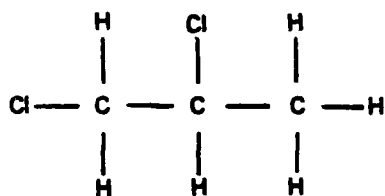
44. TETRACHLOROETHENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$\ll 100$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	6	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	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

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

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$2.31 \times 10^{-3}$	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

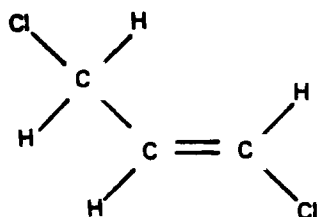
45. 1,2-DICHLOROPROPANE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>WREF</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>\sim 1</math></u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>                    </u>	<u>                    </u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NACM</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u><math>7.2 \times 10^{-4}</math> (25°C)</u>	<u>[45-1]</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-10}</math></u>	<u>E-KB</u>

E: Estimated value; see List of Source Codes.

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

46. 1,3-DICHLOROPROPENECAS No. 542-75-6

(TRANS ISOMER) [46-1]

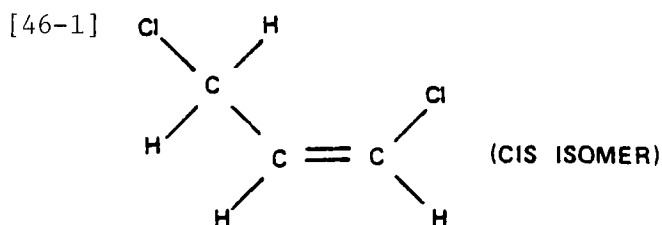
## PHYSICAL AND TRANSPORT DATA

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)	$2.7 \times 10^3$ $2.8 \times 10^3$ (25°C)	WREF [46-3]
Octanol-water, $K_{ow}$ (unitless)	100	Pomona
Sediment-water, $K_{oc}$ (unitless)	48	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	40	C-KB f Kow
Volatilization constants:		
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$1.33 \times 10^{-3}$	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

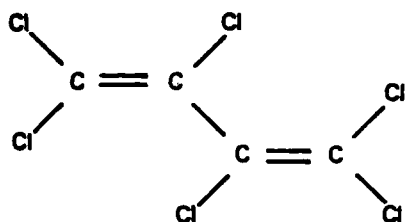
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>E-P</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>&lt;10^8</math></u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>44</u>	<u>C-OX [46-4]</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>                    </u>	<u>HPHI</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NACM</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u><math>4.2 \times 10^{-4}</math> (25°C)</u>	<u>[46-5]</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-10}</math></u>	<u>E-KB</u>

E: Estimated value; see List of Source Codes.

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]  $44 \text{ M}^{-1} \text{ hr}^{-1}$  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  $4.16 \times 10^{-4} \text{ hr}^{-1}$  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  $4.2 \times 10^{-4} \text{ hr}^{-1}$  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)	$6.0 \times 10^4$	Pomona
Sediment-water, $K_{oc}$ (unitless)	$2.9 \times 10^4$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$1.3 \times 10^4$	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	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

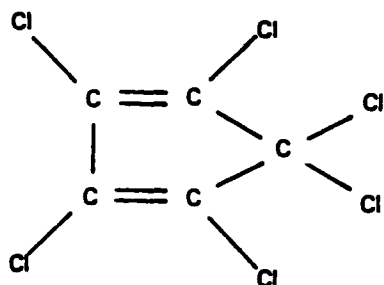


47. HEXACHLOROBUTADIENE

## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>WREF</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>&lt;10^3</math></u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>6</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-10}</math></u>	<u>E-KB</u>

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:

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

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	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

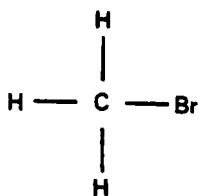
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [48-1]	Zepp, 1980
Reaction quantum yield, $\phi$ , at _____ nm	_____	_____
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	3.9	WREF
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<10^3$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	12	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	—	HPHI
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NACM
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$2.0 \times 10^{-3}$ (25°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	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 <sup>-1</sup> cm <sup>-1</sup> )
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

## 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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	4.2	C-KB f Kow

## Volatilization constants:

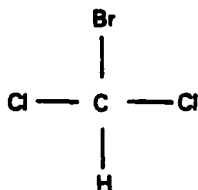
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	0.197	C-VP/S-20°
Vapor pressure, $P_v$ (torr)	$1.42 \times 10^3$ (20°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	0.737	C-DC.7

49. BROMOMETHANE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0.1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	—	HPII
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NACM
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$1.44 \times 10^{-3}$ (25°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	—	VF-NBD

E: Estimated value; see List of Source Codes.

50. BROMODICHLOROMETHANECAS No. 75-27-4

## 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)	$4.5 \times 10^3$	C-Sw f Kow
Octanol-water, $K_{ow}$ (unitless)	126	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	61	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	35	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$2.41 \times 10^{-3}$	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

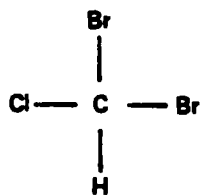
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0.2	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	5.76	WREF
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NACM
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$5.76 \times 10^{-8}$ (25°C)	E-AC-H
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	E-KB

E: Estimated value; see List of Source Codes.

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



51. DIBROMOCHLOROMETHANECAS No. 124-48-1

## 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)	$4.0 \times 10^3$	C-Sw f Kow
Octanol-water, $K_{ow}$ (unitless)	174	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	84	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	47	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$9.9 \times 10^{-4}$	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

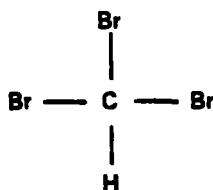
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0.5	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	2.88 (25°C)	WREF
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NACM
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$2.88 \times 10^{-8}$ (25°C)	E-AC-H
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	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

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

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$5.6 \times 10^{-4}$	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

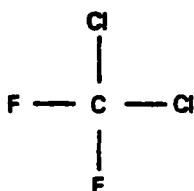
## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>UV-ATLAS</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0.5</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>1.15 (25°C)</u>	<u>WREF [52-1]</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u><math>2.5 \times 10^{-9}</math> (25°C)</u>	<u>[52-2]</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-10}</math></u>	<u>E-KB</u>

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. DICHLORODIFLUOROMETHANECAS No. 75-71-8

## 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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	33	C-KB f Kow

## Volatilization constants:

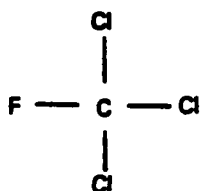
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	2.98	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$4.87 \times 10^3$ (25°C)	Jordan, 1954
Reaeration rate ratio, $k_v^C/k_v^O$	0.615	C-DC.7

53. DICHLORODIFLUOROMETHANE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	—	VF-NBD

E: Estimated value; see List of Source Codes.

54. TRICHLOROFLUOROMETHANECAS No. 75-69-4

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

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	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, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	—	VF-NBD

E: Estimated value; see List of Source Codes.

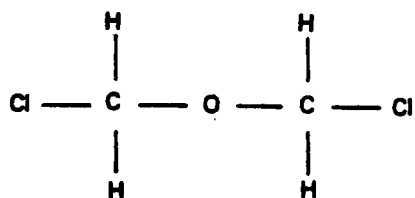


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### SECTION 3.5. HALOGENATED ETHERS

- 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) ETHERCAS No. 542-88-1

## 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)	$2.2 \times 10^4$ (25°C)	WREF
Octanol-water, $K_{ow}$ (unitless)	2.4	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	1.2	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	1.0	C-KB f Kow

## Volatilization constants:

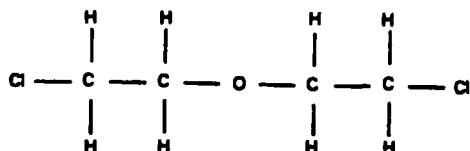
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$2.1 \times 10^{-4}$	C-VP22°/S25°
Vapor pressure, $P_v$ (torr)	30 (22°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

55. BIS(CHLOROMETHYL)ETHER

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	3	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	—	HPHI
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	—	HPHI
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	65 (20°C)	WREF
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	—	HF-NBD

E: Estimated value; see List of Source Codes.

56. BIS(2-CHLOROETHYL) ETHERCAS 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)	$1.02 \times 10^4$ [56-1]	WREF
Octanol-water, $K_{ow}$ (unitless)	29	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	13.9	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	9.2	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$1.3 \times 10^{-5}$	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

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>WREF</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>24</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>—</u>	<u>HPHI</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>—</u>	<u>HPHI</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u><math>4 \times 10^{-6}</math> (25°C)</u>	<u>[56-2]</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>3 \times 10^{-9}</math></u>	<u>E-KB</u>

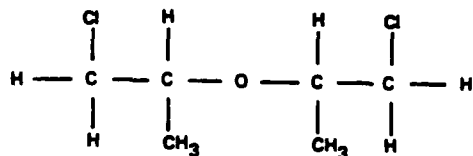
E: Estimated value; see List of Source Codes.

[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  $1.5 \times 10^{-5} \text{ min}^{-1}$  has been reported for bis(2-chloroethyl)ether in aqueous dioxane at  $100^\circ\text{C}$  (WREF). This rate constant corresponds to a half-life of 32 days. Allowing for a factor of two decrease in rate constant for each  $10^\circ\text{C}$  decrement, the half-life is calculated as 22 years (or 256 times slower) at  $20^\circ\text{C}$ . 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  $25^\circ\text{C}$  (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  $-\text{OCH}_2\text{CH}_2\text{Cl}$  group. Data have been obtained which show that aqueous solvolysis of 2-methoxyethyl iodide at  $60^\circ\text{C}$  is  $6.4 \times 10^{-3}$  times the rate of ethyl iodide under the same reaction conditions (Streitwieser, 1962). Assuming that this  $6.4 \times 10^{-3}$  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-chloroethyl)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  $4 \times 10^{-6} \text{ hr}^{-1}$ . The hydrolysis of bis(2-chloromethyl)ether should be independent of pH by analogy to other aliphatic halocarbons.

57. BIS(2-CHLOROISOPROPYL) ETHERCAS 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)	$1.7 \times 10^3$ [57-1]	WREF
Octanol-water, $K_{ow}$ (unitless)	126	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	61	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	35	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$1.1 \times 10^{-4}$	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	



57. BIS(2-CHLOROISOPROPYL)ETHER

## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>WREF</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>2</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>—</u>	<u>HPHI</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>—</u>	<u>HPHI</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u><math>4 \times 10^{-6}</math> (25°)</u>	<u>[57-2]</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-10}</math></u>	<u>E-KB</u>

E: Estimated value; see List of Source Codes.

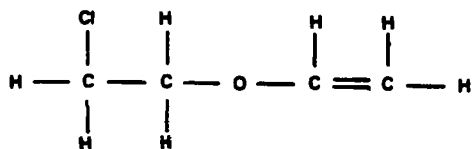
[57-1] Experimental water solubility data was generated at room temperature; no specific temperature was reported.  
This value was used in the calculation of Henry's constant.

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)	$1.5 \times 10^4$ (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, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	4.7	C-KB f Kow

## Volatilization constants:

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

## 58. 2-CHLOROETHYL VINYL ETHER

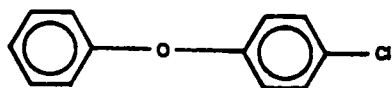
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$1 \times 10^{10}$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	34	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	—	HPHI
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	—	HPHI
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	$4 \times 10^{-6}$ (25°C)	[58-1]
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	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  $4 \times 10^{-6} \text{ hr}^{-1}$  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)	$1.2 \times 10^5$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$5.8 \times 10^4$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$1.8 \times 10^4$	C-KB f Kow

## Volatilization constants:

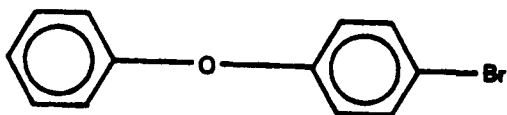
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$2.19 \times 10^{-4}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$2.7 \times 10^{-3}$	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

59. 4-CHLOROPHENYL PHENYL ETHER

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-7}$	E-KB

E: Estimated value; see List of Source Codes.

60. 4-BROMOPHENYL PHENYL ETHERCAS No. 101-55-3

## 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)	$8.7 \times 10^4$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$4.2 \times 10^4$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$1.3 \times 10^4$	C-KB f Kow

## Volatilization constants:

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

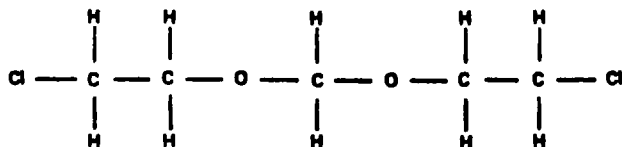
60. 4-BROMOPHENYL PHENYL ETHER

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

E: Estimated value; see List of Source Codes.



61. BIS(2-CHLOROETHOXY)METHANECAS 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:

Water solubility, $S_w$ (ppm)	$8.1 \times 10^4$ (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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	3.7	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$2.8 \times 10^{-7}$	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

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>WREF</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>52</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>—</u>	<u>HPHI</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>—</u>	<u>HPHI</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u><math>4 \times 10^{-6}</math> (25°C)</u>	<u>[61-1]</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>3 \times 10^{-12}</math></u>	<u>E-KB</u>

E: Estimated value; see List of Source Codes.

## 61. BIS(2-CHLOROETHOXY)METHANE

[61-1] A neutral hydrolysis rate constant,  $k_N$ , of  $4 \times 10^{-8} \text{ hr}^{-1}$  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 susceptible to hydrolysis. The acid-catalyzed hydrolysis rate constant,  $k_A$ , for this process has been measured at  $2.53 \times 10^{-6} \text{ M}^{-1} \text{ sec}^{-1}$  (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)	$1.78 \times 10^3$ (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, $K_B$ ( $(\mu\text{g/g})(\text{mg/l})^{-1}$ )	37	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$5.5 \times 10^{-3}$	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

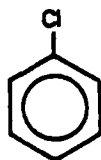
62. BENZENE

## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>UV-ATLAS</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;1</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NHFG</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NHFG</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	<u>NHFG</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-7}</math></u>	<u>E-KB</u>

E: Estimated value; see List of Source Codes.

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

63. CHLOROBENZENECAS 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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	164	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$3.58 \times 10^{-3}$	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



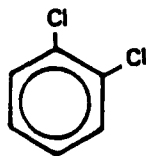
63. CHLOROBENZENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$\ll 360$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$\ll 1$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	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-DICHLOROBENZENECAS 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)	$3.6 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.7 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	730	C-KB f Kow

## Volatilization constants:

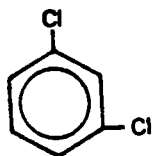
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$1.93 \times 10^{-3}$	C-VP/S-20°
Vapor pressure, $P_v$ (torr)	1.0 (20°C)	Verschueren, 1977
Reaeration rate ratio, $k_v^c/k_v^o$	0.495	C-DC.7

## 64. 1,2-DICHLOROBENZENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) , _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$\ll 360$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$\ll 1$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	E-KB

E: Estimated value; see List of Source Codes.

65. 1,3-DICHLOROBENZENECAS 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)	$3.6 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.7 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	730	C-KB f Kow

## Volatilization constants:

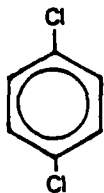
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$3.61 \times 10^{-3}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	2.28 (25°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	0.495	C-DC.7

## 65. 1,3-DICHLOROBENZENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	E-KB

E: Estimated value; see List of Source Codes.

66. 1,4-DICHLOROBENZENECAS 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)	$3.6 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.7 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	730	C-KB f Kow

## Volatilization constants:

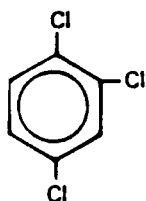
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$3.1 \times 10^{-3}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	1.18 (25°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	0.495	C-DC.7

66. 1,4-DICHLOROBENZENE

## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>E-P</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;1</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-10}</math></u>	<u>E-KB</u>

E: Estimated value; see List of Source Codes.

67. 1,2,4-TRICHLOROBENZENECAS 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)	$1.9 \times 10^4$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$9.2 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$3.3 \times 10^3$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$2.3 \times 10^{-3}$	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



67. 1,2,4-TRICHLOROBENZENE

## TRANSFORMATION DATA

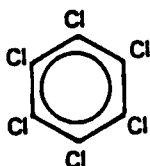
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [67-1]	Zepp, 1980
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	E-KB

E: Estimated value; 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 <sup>-1</sup> cm <sup>-1</sup> )
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. HEXACHLOROGENECAS 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)	$6 \times 10^{-3}$ (25°C)	WREF
Octanol-water, $K_{ow}$ (unitless)	$2.6 \times 10^6$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.2 \times 10^6$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$2.9 \times 10^5$	C-KB f Kow

## Volatilization constants:

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

68. HEXACHLOROBENZENE

## TRANSFORMATION DATA

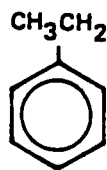
<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	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



## 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)	$2.2 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.1 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	470	C-KB f Kow

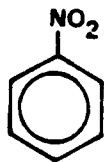
## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$6.6 \times 10^{-3}$	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

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	720	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

E: Estimated value; see List of Source Codes.

70. NITROBENZENECAS No. 98-95-3

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

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$1.31 \times 10^{-5}$	C-VP/S-20°
Vapor pressure, $P_v$ (torr)	0.15 (20°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

70. NITROBENZENE

## TRANSFORMATION DATA

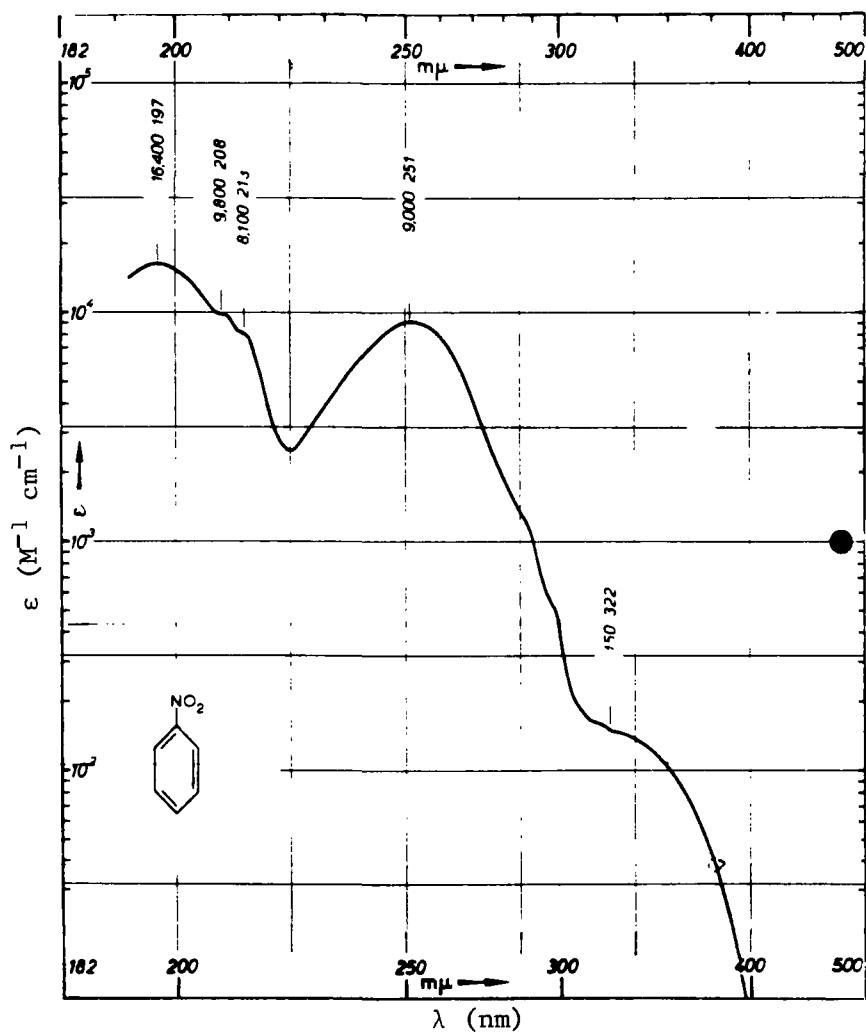
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [70-1]	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	_____	_____
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	_____	_____
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<1	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

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).



71. TOLUENECAS No. 108-88-3

## 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-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	148	C-KB f Kow

## Volatilization constants:

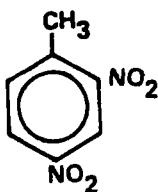
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$6.66 \times 10^{-3}$	C-VP20°/S25°
Vapor pressure, $P_v$ (torr)	28.7 (20°C)	Verschueren, 1977
Reaeration rate ratio, $k_v^c/k_v^o$	0.526	C-DC.7

71. TOLUENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	144	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-7}$	E-KB

E: Estimated value; see List of Source Codes.

72. 2,4-DINITROTOLUENECAS 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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	39	C-KB f Kow

## Volatilization constants:

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

72. 2,4-DINITROTOLUENE

## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	DATA-ATT	[72-1]
Reaction quantum yield, $\phi$ , at <u>313</u> nm	<u><math>7.5 \times 10^{-4}</math></u>	[72-1]
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) <u>summer</u> at <u>40°</u> latitude	<u><math>1.6 \times 10^{-2}</math></u>	[72-1]
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;360</u>	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>144</u>	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u><math>1 \times 10^{-7}</math></u>	[72-1]

E: Estimated value; see List of Source Codes.

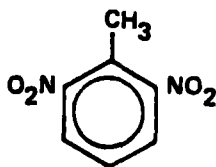
## 72. 2,4-DINITROTOLUENE

[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 ( $M^{-1} \text{ cm}^{-1}$ )
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-DINITROTOLUENECAS 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, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	51	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$7.9 \times 10^{-6}$	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	

73. 2,6-DINITROTOLUENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	144	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	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)	$9.3 \times 10^4$ (25°C)	WREF
Octanol-water, $K_{ow}$ (unitless)	30	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	14.2	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	9.4	C-KB f Kow

Volatilization constants:

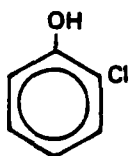
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$4.54 \times 10^{-7}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	0.341 (25°C)	Biddiscombe & Martin, 1958
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

74. PHENOL

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	E-P
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<7 \times 10^5$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$1 \times 10^7$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-6}$	E-KB

E: Estimated value; see List of Source Codes.

75. 2-CHLOROPHENOLCAS 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)	$2.85 \times 10^4$ (20°C)	WREF
Octanol-water, $K_{ow}$ (unitless)	151	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	73	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	41	C-KB f Kow

## Volatilization constants:

Henry's constant, $H^c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$1.03 \times 10^{-5}$	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	

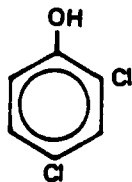
75. 2-CHLOROPHENOL

## TRANSFORMATION DATA

Property or Process [75-1]	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<7 \times 10^5$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$1 \times 10^7$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-7}$	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-DICHLOROPHENOLCAS 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)	$4.6 \times 10^3$ (20°C)	Verschueren 1977
Octanol-water, $K_{ow}$ (unitless)	790	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	380	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	186	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$2.8 \times 10^{-6}$	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	

76. 2,4-DICHLOROPHENOL

## TRANSFORMATION DATA

Property or Process [76-1]	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	[76-4]	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<7 \times 10^5$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$1 \times 10^7$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-7}$	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

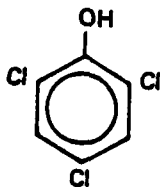
- [76-3] The Henry's Law constant was obtained by extrapolating the data beyond the melting point and adjusting by

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

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 been reported for the photolysis of 2,4-dichlorophenol (WREF). One paper reports that, after 10 days exposure to sunlight, 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

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

Partition constants:

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

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$4 \times 10^{-6}$	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	

77. 2,4,6-TRICHLOROPHENOL

## TRANSFORMATION DATA

<u>Property or Process [77-1]</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<7 \times 10^4$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$1 \times 10^6$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

E: Estimated value; see List of Source Codes.

[77-1] All data are calculated for the neutral form unless otherwise stated.

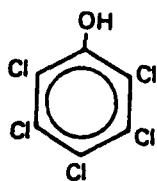
[77-2] No temperature is reported for the ionization constant.

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)	$1.1 \times 10^5$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$5.3 \times 10^4$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$1.6 \times 10^4$	C-KB f Kow

Volatilization constants:

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

78. PENTACHLOROPHENOL

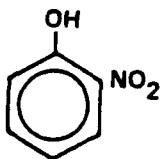
## TRANSFORMATION DATA

<u>Property or Process [78-1]</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<7 \times 10^3$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$1 \times 10^5$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

E: Estimated value; 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-NITROPHENOLCAS No. 88-75-5

## 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)	$2.1 \times 10^3$ (20°C)	Verschueren, 1977
Octanol-water, $K_{ow}$ (unitless)	56	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	27	C-Koc f Kow
Microorganisms-water, $K_B ((\mu\text{g/g})(\text{mg/l})^{-1})$	17	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$7.56 \times 10^{-6}$	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, $\phi$ , at _____ nm	_____	_____
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	_____	_____
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<2 \times 10^5$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$2 \times 10^6$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	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-NITROPHENOL

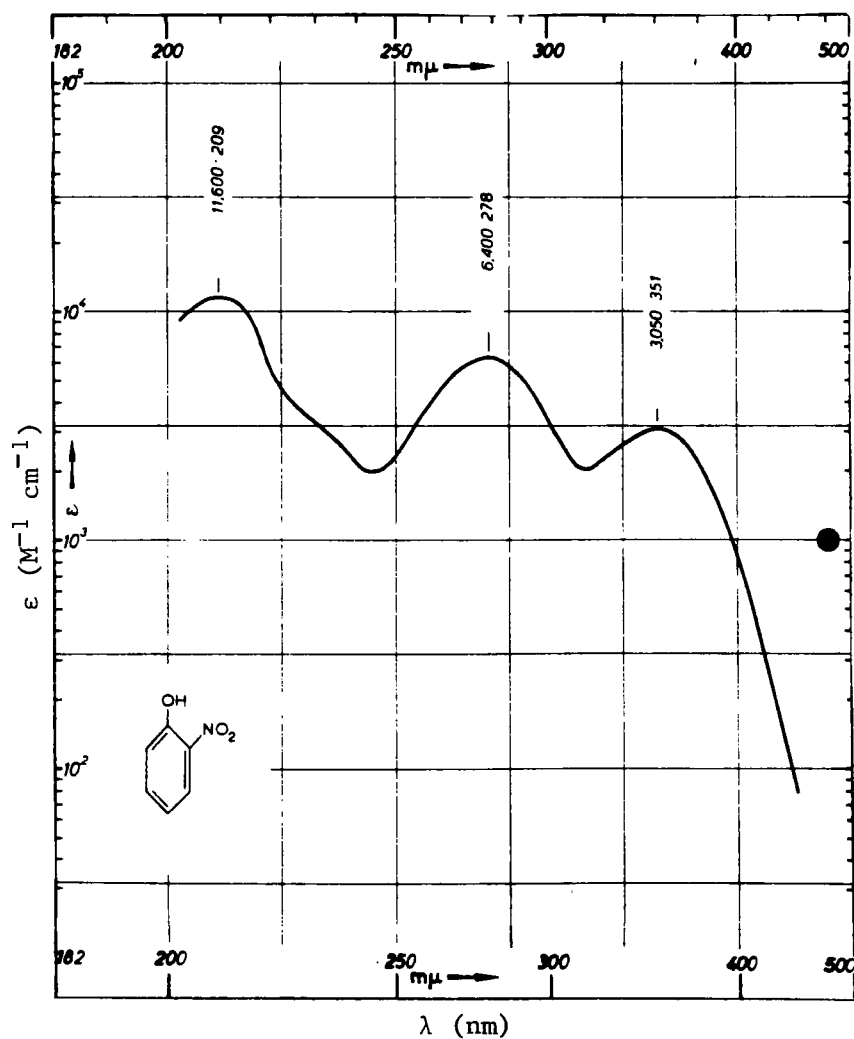
[79-2] The Henry's Law constant was obtained by extrapolating the data beyond the melting point and adjusting by

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

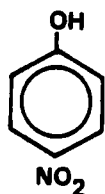
where  $T_M$  is the melting point in °C and  $T$  is the temperature at which  $H_c$  is being estimated.

[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).







80. 4-NITROPHENOL

CAS No. 100-07-7

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)	$1.6 \times 10^4$ (25°C)	Verschueren, 1977
Octanol-water, $K_{ow}$ (unitless)	93	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	45	C-Koc f Kow
Microorganisms-water, $K_B$ $((\mu\text{g/g})(\text{mg/l})^{-1})$	27	C-KB f Kow

Volatilization constants:

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

## 80. 4-NITROPHENOL

## TRANSFORMATION DATA

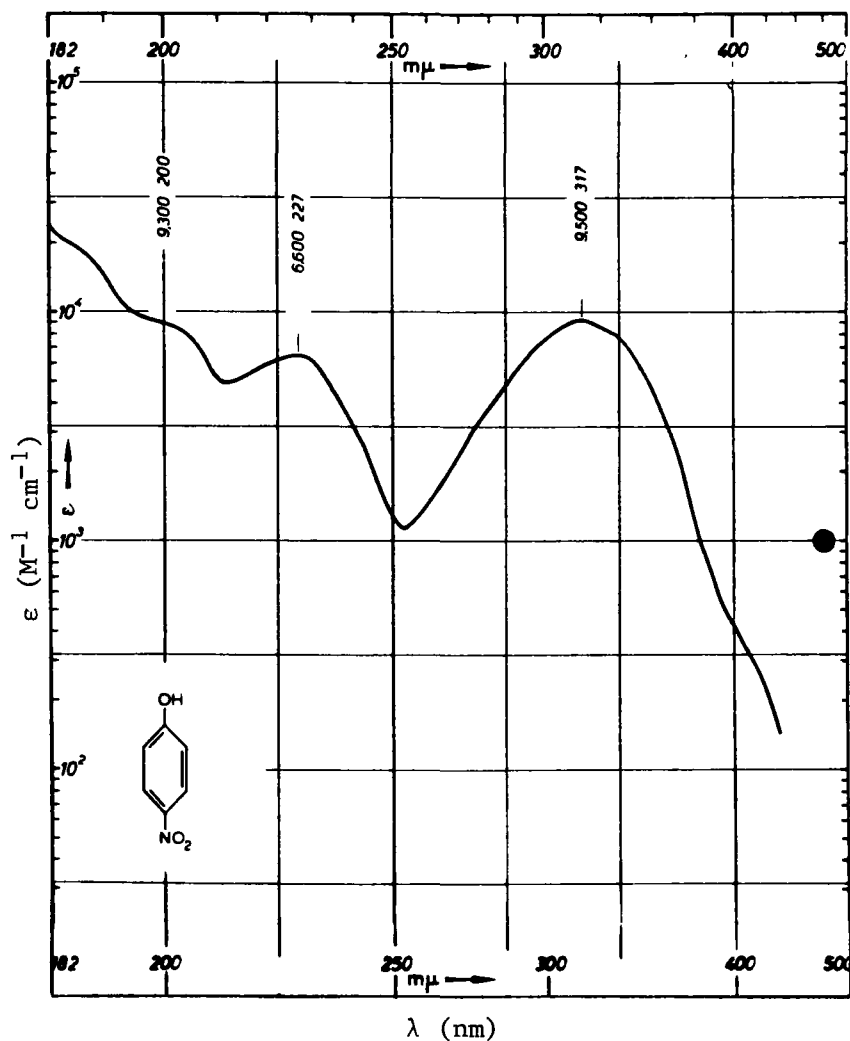
Property or Process [80-1]	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [80-2]	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	_____	_____
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	[80-3]	_____
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<2 \times 10^5$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$2 \times 10^6$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-7}$	E-KB

E: Estimated value; see List of Source Codes.

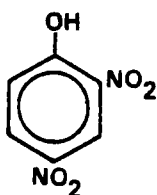
[80-1] All data are calculated for the neutral form unless otherwise stated.

80. 4-NITROPHENOL

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



[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)	$5.6 \times 10^3$ (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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	15.4	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$6.45 \times 10^{-10}$	C-VP/S-18°
Vapor pressure, $P_v$ (torr)	$1.49 \times 10^{-5}$ (18°C)	Hoyer & Peperle, 1958
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

81. 2,4-DINITROPHENOL

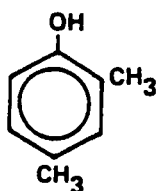
## TRANSFORMATION DATA

Property or Process [81-1]	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$3 \times 10^4$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$5 \times 10^5$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

E: Estimated value; see List of Source Codes.

## 82. 2,4-DIMETHYLPHENOL

CAS No. 105-67-9



## 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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	75	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$1.7 \times 10^{-5}$	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

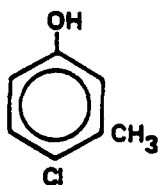
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<4 \times 10^6$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$1.1 \times 10^8$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-7}$	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)	$3.85 \times 10^3$ (20°C)	Verschueren, 1977
Octanol-water, $K_{ow}$ (unitless)	1259	Pomona
Sediment-water, $K_{oc}$ (unitless)	604	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	400	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$2.5 \times 10^{-6}$	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	



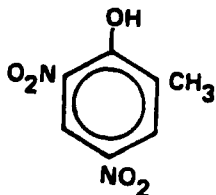
83. p-CHLORO-m-CRESOL

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<7 \times 10^5$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$1 \times 10^7$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	122	C-KB f Kow

#### Volatilization constants:

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

## 84. 4,6-DINITRO-o-CRESOL

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$3 \times 10^4$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$5 \times 10^5$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

E: Estimated value; see List of Source Codes.

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

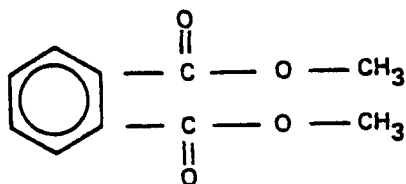
[84-2] Vapor pressure value assigned by analogy; no data were available.

### References for 3.6

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### SECTION 3.7. 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



# 85. DIMETHYL PHTHALATE

CAS No. 131-11-3

## 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)	$5.00 \times 10^3$ (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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	16.0	C-KB f Kow

### Volatilization constants:

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

85. DIMETHYL PHTHALATE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [85-1]	Zepp, 1980
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0.05	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	248 (30°C)	WREF
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0.025 (30°C)	C-KBASE
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	$5.2 \times 10^{-6}$	Wolfe et al., 1980

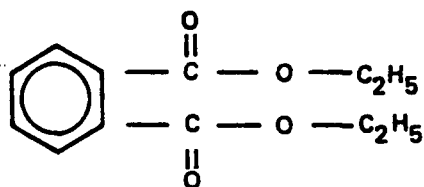
E: Estimated value; see List of Source Codes.

# 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 <sup>-1</sup> cm <sup>-1</sup> )
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	0.8000E-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

PHYSICAL AND TRANSPORT DATA

Property or Process	Value	Data Source
Molecular weight	222.2	
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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	107	C-KB f Kow

Volatilization constants:

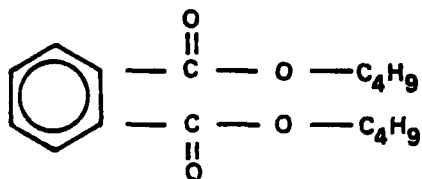
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$1.2 \times 10^{-6}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$3.5 \times 10^{-3}$ (25°C)	C-CT/CRC
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

86. DIETHYL PHTHALATE

## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>WREF</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>1.4</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>43.2 (30°C)</u>	<u>WREF</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>4.32 \times 10^{-3}</math> (30°C)</u>	<u>C-KBASE</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-7}</math></u>	<u>E-KB</u>

E: Estimated value; see List of Source Codes.



87. DI-n-BUTYL PHTHALATE

CAS No. 84-74-2

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)	$3.6 \times 10^5$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.7 \times 10^5$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$4.7 \times 10^4$	C-KB f Kow

Volatilization constants:

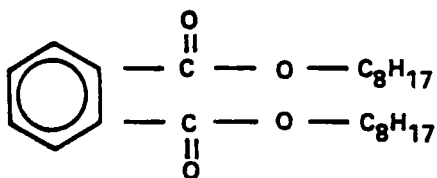
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$2.8 \times 10^{-7}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$1.0 \times 10^{-5}$ (25°C)	Jaber, 1982
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

87. DI-n-BUTYL PHTHALATE

## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	<u>PNES</u>	<u>WREF</u>
Reaction quantum yield, $\phi$ , at _____ nm	<u>PNER</u>	<u>                    </u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	<u>PNER</u>	<u>                    </u>
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>1.4</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>79.2 (30°C)</u>	<u>WREF</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>7.92 \times 10^{-3}</math> (30°C)</u>	<u>C-KBASE</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u><math>(1.9-4.4) \times 10^{-8}</math></u>	<u>Steen et al., 1979</u>

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)	$7.4 \times 10^9$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$3.6 \times 10^9$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$3.9 \times 10^8$	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$1.7 \times 10^{-5}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$1.4 \times 10^{-4}$ (25°C)	[88-1]
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

88. DI-n-OCTYL PHTHALATE

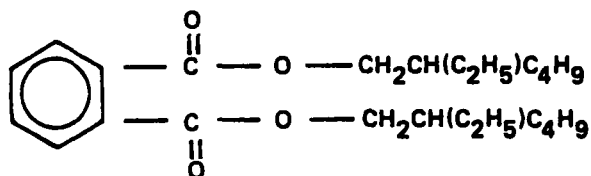
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	1.4	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	79.2 (30°C)	[88-2]
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$7.92 \times 10^{-3}$ (30°C)	[88-2]
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	$3.1 \times 10^{-10}$	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) PHTHALATECAS No. 117-81-7

## 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)	$4.1 \times 10^9$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$2.0 \times 10^9$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$2.3 \times 10^8$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$3 \times 10^{-7}$	C-VP20°/S25°
Vapor pressure, $P_v$ (torr)	$2 \times 10^{-7}$ (20°C)	C-CT/CRC
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

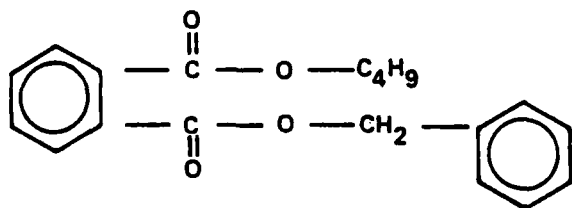
89. BIS(2-ETHYLHEXYL) PHTHALATE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<<360$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	7.2	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0.4 (30°C)	WREF
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$4.0 \times 10^{-5}$ (30°C)	C-KBASE
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	$4.2 \times 10^{-12}$	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)	$3.6 \times 10^5$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.7 \times 10^5$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$4.7 \times 10^4$	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$8.3 \times 10^{-6}$	C-VP/S [90-2]
Vapor pressure, $P_v$ (torr)	$6 \times 10^{-5}$	[90-3]
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

## 90. BUTYL BENZYL PHTHALATE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	280	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	79.2 (30°C)	[90-4]
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$7.92 \times 10^{-3}$ (30°C)	[90-4]
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	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

Jaber, H. 1982. SRI International, unpublished analysis.

Pomona College Medicinal Data Base, June 1982.

Steen, W. C., D. F. Paris and G. L. Baughman. 1979. 177th National Meeting of American Chemical Society, Honolulu, 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. Correlation of Microbial Degradation Rates with Chemical Structure. Environmental Sci. Technol. 14:1143-4.

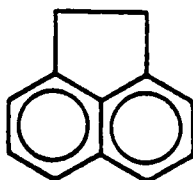
Zepp, R. G. 1980. Private communication.

### 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)	$9.6 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$4.6 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$1.8 \times 10^3$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$9.1 \times 10^{-5}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$1.55 \times 10^{-3}$ (25°C)	Hoyer & Peperle, 1958
Reaeration rate ratio, $k_v^C/k_v^O$	NAV	

## 91. ACENAPHTHENE

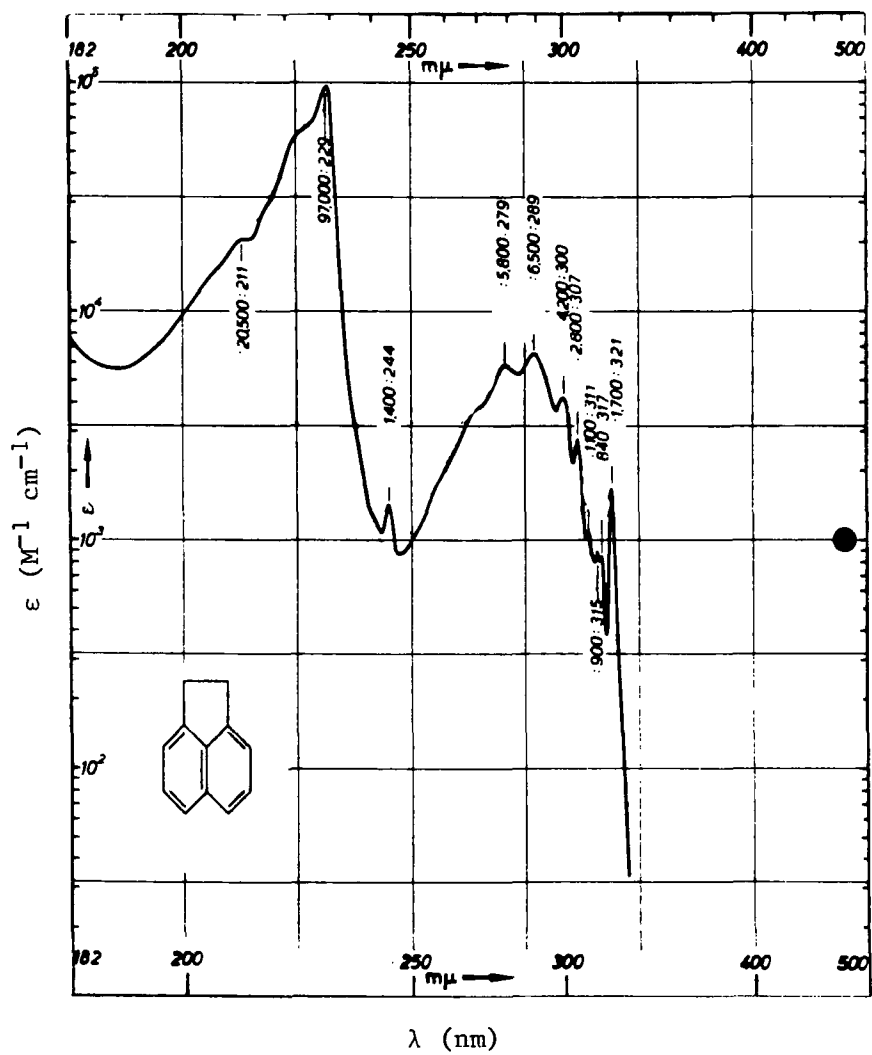
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [91-1]	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	(E) $5 \times 10^{-3}$	E-APAH
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	< 3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$8 \times 10^3$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

E: Estimated value; see List of Source Codes.

# 91. ACENAPHTHENE

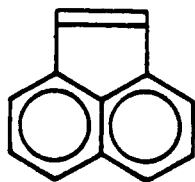
[91-1] UV spectrum of acenaphthene in heptane solvent is shown below (UV Atlas, 1966).





## 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)	$5.3 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$2.5 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$1.0 \times 10^3$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$1.45 \times 10^{-3}$	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

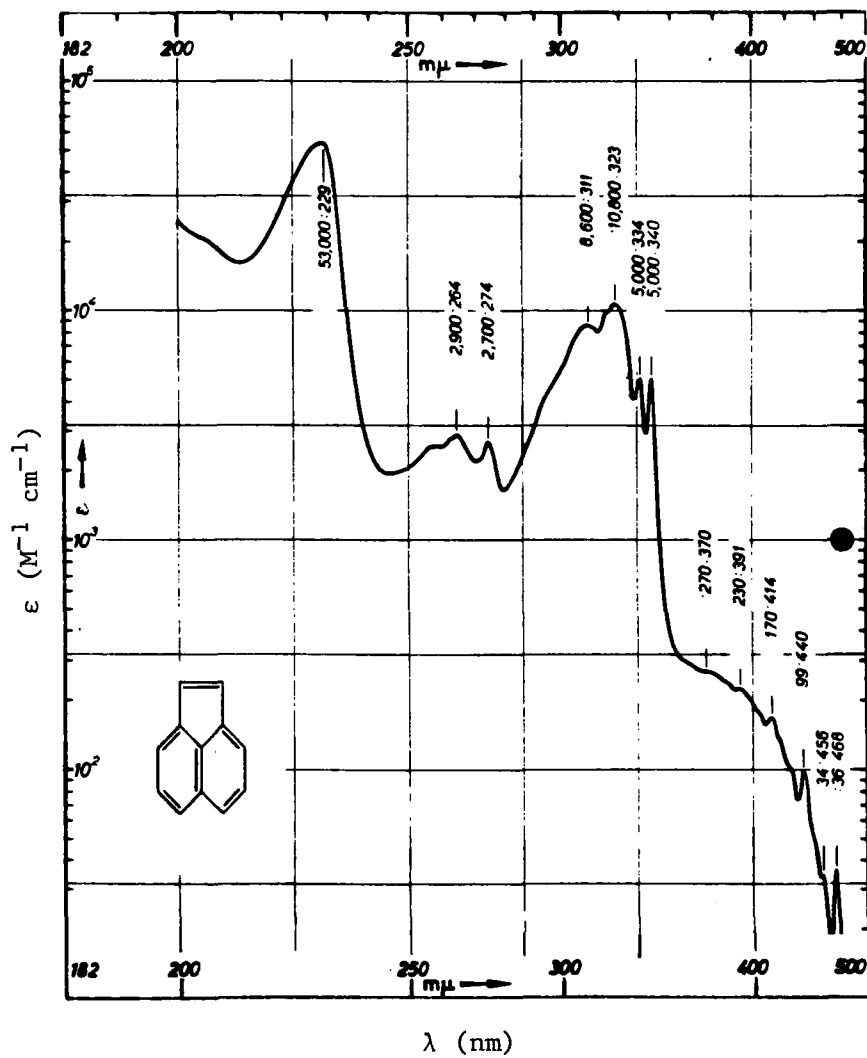
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [92-2]	UV ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	(E) $5 \times 10^{-3}$	E-APAH
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$\sim 4 \times 10^7$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$5 \times 10^3$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

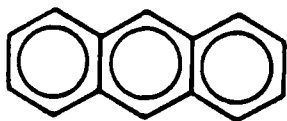
E: Estimated value; see List of Source Codes.

[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).



93. ANTHRACENECAS 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)	$2.8 \times 10^4$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.4 \times 10^4$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$4.7 \times 10^3$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$8.6 \times 10^{-5}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$1.7 \times 10^{-5}$ (25°C)	Jaber, 1982
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

## 93. ANTHRACENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [93-2]	Zepp, 1980
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ (hr <sup>-1</sup> )		
<u>winter</u> at <u>35°</u> latitude	0.15	WREF
Oxidation constants at 25°C:		
For <sup>1</sup> O <sub>2</sub> (singlet oxygen), $k_{OX}$ (M <sup>-1</sup> hr <sup>-1</sup> )	$5 \times 10^8$	C-OX
For RO <sub>2</sub> (peroxy radical), $k_{OX}$ (M <sup>-1</sup> hr <sup>-1</sup> )	$2.2 \times 10^5$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ (M <sup>-1</sup> hr <sup>-1</sup> )	0	NHFG
For acid-promoted process, $k_A$ (M <sup>-1</sup> hr <sup>-1</sup> )	0	NHFG
For neutral process, $k_N$ (hr <sup>-1</sup> )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ (ml cell <sup>-1</sup> hr <sup>-1</sup> )	(E) $3 \times 10^{-9}$	E-KB

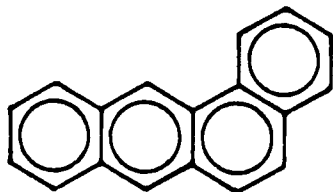
E: Estimated value; see List of Source Codes.

[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 ( $M^{-1} \text{ cm}^{-1}$ )
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]ANTHRACENECAS 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)	$5.7 \times 10^{-3}$ (20°C)	Smith et al, 1978
Octanol-water, $K_{ow}$ (unitless)	$4.1 \times 10^5$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$2.0 \times 10^5$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$5.3 \times 10^4$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$1 \times 10^{-6}$	C-VP/S-20°
Vapor pressure, $P_v$ (torr)	$2.2 \times 10^{-8}$ (20°C)	Hoyer & Peperle, 1958
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

94. BENZO[a]ANTHRACENE

## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	DATA-ATT [94-1]	Smith et al, 1978
Reaction quantum yield, $\phi$ , at <u>313</u> nm	<u><math>3.3 \times 10^{-3}</math></u>	Smith et al, 1978
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) midday <u>summer</u> at <u>40°</u> latitude	<u>1.39</u>	Smith et al, 1978
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>5 \times 10^8</math></u>	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>2 \times 10^4</math></u>	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-10}</math></u>	E-KB

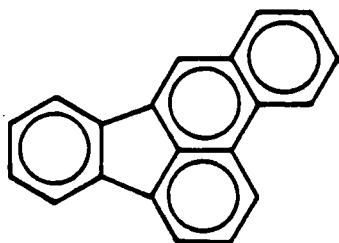
E: Estimated value; see List of Source Codes.



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 <sup>-1</sup> cm <sup>-1</sup> )
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)	$1.15 \times 10^6$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$5.5 \times 10^5$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$1.4 \times 10^5$	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$1.22 \times 10^{-5}$	C-VP20°/S25°
Vapor pressure, $P_v$ (torr)	$5 \times 10^{-7}$ (20°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

95. BENZO[b]FLUORANTHENE

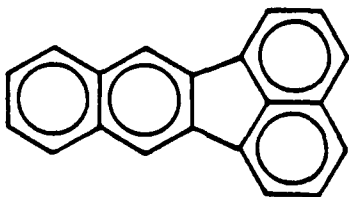
## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$4 \times 10^7$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$5 \times 10^3$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

## 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)	$4.3 \times 10^{-3}$ (25°C)	C-Sw f Kow
Octanol-water, $K_{ow}$ (unitless)	$1.15 \times 10^6$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$5.5 \times 10^5$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$1.4 \times 10^5$	C-KB f Kow

## Volatilization constants:

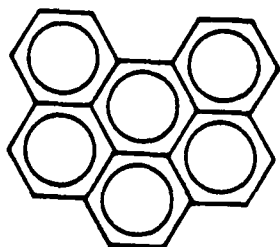
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$3.87 \times 10^{-5}$	C-VP20°/S25°
Vapor pressure, $P_v$ (torr)	$5 \times 10^{-7}$ (20°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	0.374	C-DC.7

## 96. BENZO[k]FLUORANTHENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$4 \times 10^7$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$5 \times 10^3$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

97. BENZO[ghi]PERYLENECAS 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)	$2.6 \times 10^{-4}$ (25°C)	WREF
Octanol-water, $K_{ow}$ (unitless)	$3.2 \times 10^6$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.6 \times 10^6$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$3.5 \times 10^5$	C-KB f Kow

## Volatilization constants:

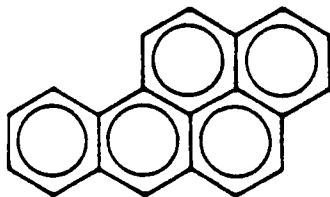
Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$1.44 \times 10^{-7}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$1.03 \times 10^{-10}$ (25°C)	Murray et al, 1974
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

97. BENZO[ghi]PERYLENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<36	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E)3 x 10 <sup>-12</sup>	E-KB

E: Estimated value; see List of Source Codes.

98. BENZO[a]PYRENECAS 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)	$3.8 \times 10^{-3}$ (25°C)	WREF
Octanol-water, $K_{ow}$ (unitless)	$1.15 \times 10^6$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$5.5 \times 10^6$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$1.4 \times 10^5$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$4.9 \times 10^{-7}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$5.6 \times 10^{-9}$ (25°C)	Murray et al, 1974
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	



98. BENZO[a]PYRENE

## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	DATA-ATT [98-1]	Smith et al, 1978
Reaction quantum yield, $\phi$ , at 313 nm	$8.9 \times 10^{-4}$	Smith et al, 1978
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) winter, at 40° latitude midday	0.58 [98-2]	Smith et al, 1978
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$5 \times 10^8$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$2 \times 10^4$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	E-KB

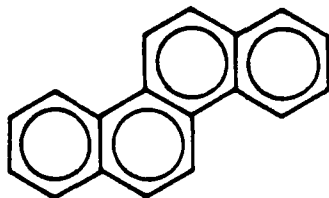
E: Estimated value; see List of Source Codes.

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 <sup>-1</sup> cm <sup>-1</sup> )
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. CHRYSENECAS 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)	$1.8 \times 10^{-3}$ (25°C)	May, 1978
Octanol-water, $K_{ow}$ (unitless)	$4.1 \times 10^5$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$2.0 \times 10^5$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$5.3 \times 10^4$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$1.05 \times 10^{-6}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$6.3 \times 10^{-9}$ (25°C)	Hoyer & Peperle, 1958
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

## 99. CHRYSENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [99-2]	Zepp, 1980
Reaction quantum yield, $\phi$ , at _____ nm	$2.8 \times 10^{-3}$	Zepp & Schlotzhauer, 1979
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	_____	_____
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$>1 \times 10^6$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$1 \times 10^3$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	E-KB

E: Estimated value; see List of Source Codes.

[99-1] No pressure is reported for the boiling point.

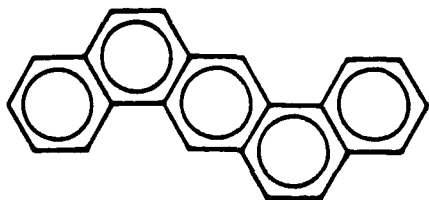
## 99. CHRYSENE

[99-2] Table of absorption coefficients and the corresponding wavelengths of chrysene is given below (Zepp, 1980).

WAVELENGTH (nm)	EPSILON (M <sup>-1</sup> cm <sup>-1</sup> )
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	270	WREF
Boiling point, °C		
Ionization constant	pK-NER	

Partition constants:

Water solubility, $S_w$ (ppm)	$5 \times 10^{-4}$ (25°C)	WREF
Octanol-water, $K_{ow}$ (unitless)	$6.9 \times 10^6$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$3.3 \times 10^6$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$6.9 \times 10^5$	C-KB f Kow

Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$7.3 \times 10^{-8}$	C-VP20°/S25°
Vapor pressure, $P_v$ (torr)	$1 \times 10^{-10}$ (20°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

100. DIBENZO[a,h]ANTHRACENE

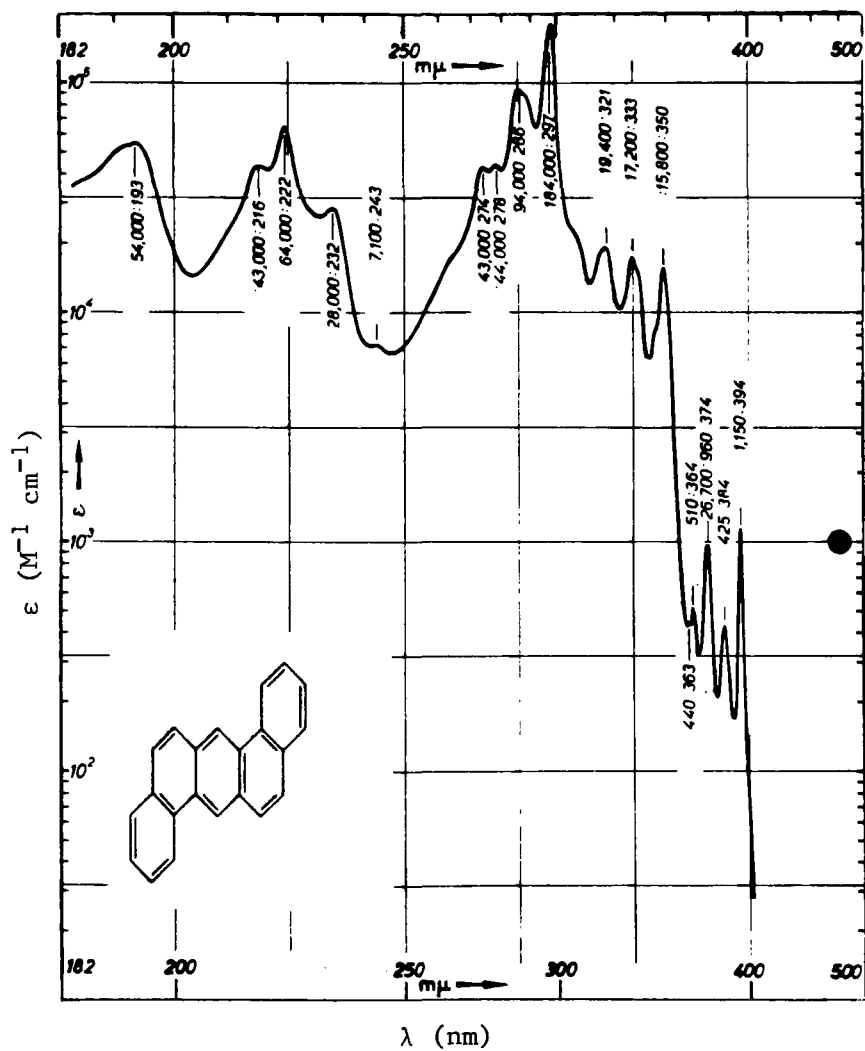
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [100-1]	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm	_____	_____
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	_____	_____
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$5 \times 10^8$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$1.5 \times 10^4$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	E-KB

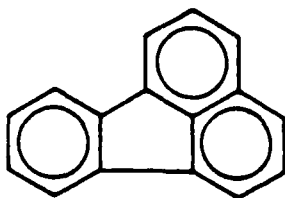
E: Estimated value; see List of Source Codes.

100. DIBENZO[a,h]ANTHRACENE

[100-1] UV spectrum of dibenzo[a,h]anthracene in heptane solvent is shown below (UV Atlas, 1966).





101. FLUORANTHENECAS 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)	$7.9 \times 10^4$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$3.8 \times 10^4$	C-Koc f Kow
Microorganisms-water, $K_B ((\mu\text{g/g})(\text{mg/l})^{-1})$	$1.2 \times 10^4$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$6.5 \times 10^{-6}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$5.0 \times 10^{-6}$ (25°C)	Hoyer & Peperle, 1958
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

101. FLUORANTHENE

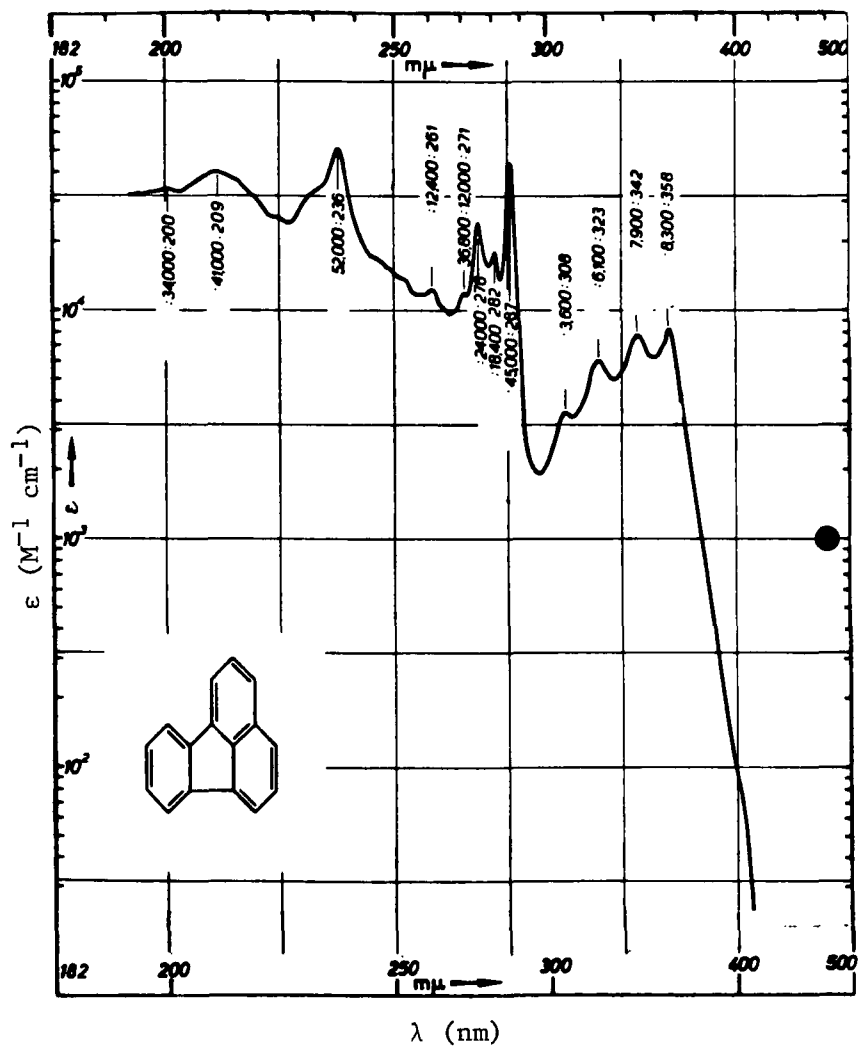
## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum	<u>SPEC-ATT [101-1]</u>	<u>UV-ATLAS</u>
Reaction quantum yield, $\phi$ , at <u>313</u> nm	<u><math>1.2 \times 10^{-4}</math> [101-2]</u>	<u>Zepp &amp; Schlotzhauer, 1979</u>
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) at _____ latitude	_____	_____
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;3600</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;360</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NHFG</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NHFG</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	<u>NHFG</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-10}</math></u>	<u>E-KB</u>

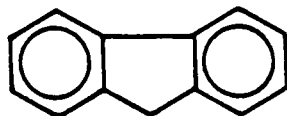
E: Estimated value; see List of Source Codes.

# 101. FLUORANTHENE

[101-1] UV spectrum of fluoranthene in methanol solvent is shown below (UV Atlas, 1966).



[101-2] At 366 nm, the quantum yield is  $2 \times 10^{-6}$ .

102. FLUORENECAS 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)	$1.5 \times 10^4$	Pomona
Sediment-water, $K_{oc}$ (unitless)	$7.3 \times 10^3$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$3.8 \times 10^3$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H$ ( $\text{atm m}^3 \text{ mol}^{-1}$ ) <sup>c</sup>	$6.4 \times 10^{-5}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$7.1 \times 10^{-4}$	Irwin, 1982
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

## 102. FLUORENE

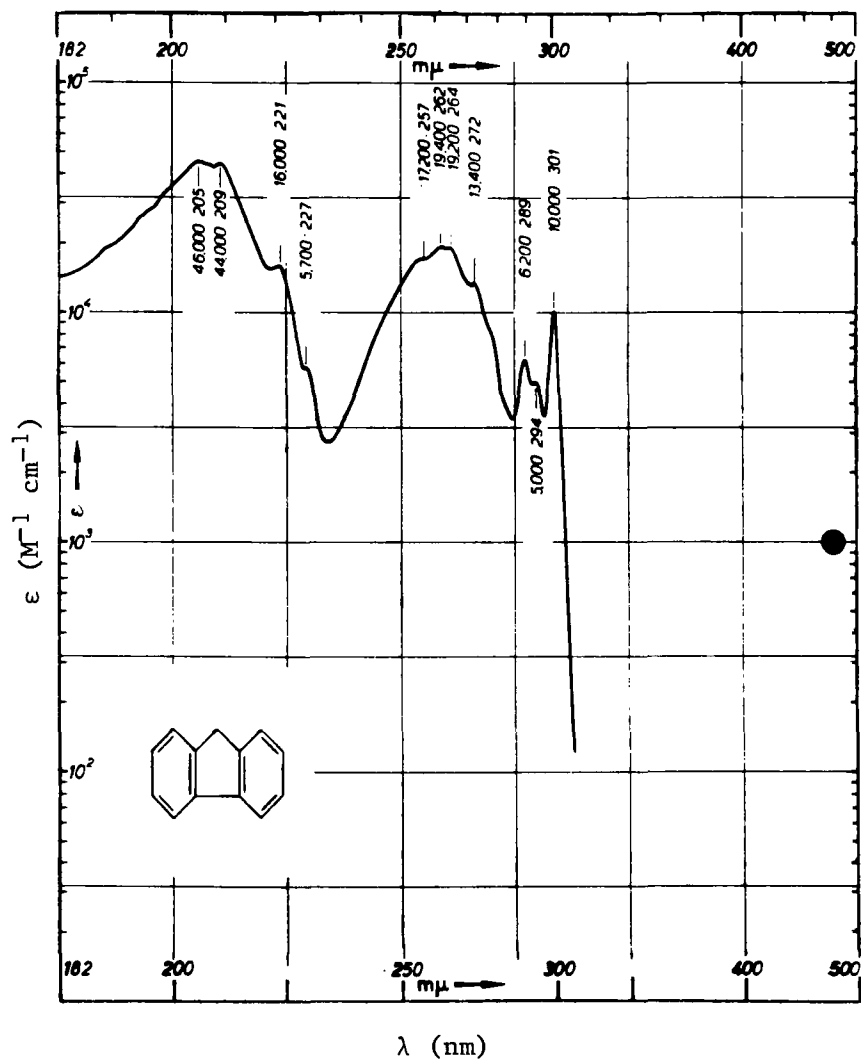
## TRANSFORMATION DATA

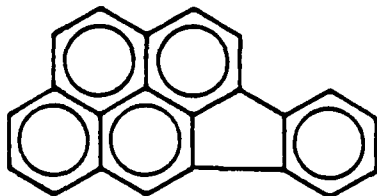
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	SPEC-ATT [102-1]	UV-ATLAS
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$3 \times 10^3$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	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).



103. INDENO[1,2,3-cd]PYRENECAS 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)	$5.3 \times 10^{-4}$ (25°C)	C-Sw f Kow
Octanol-water, $K_{ow}$ (unitless)	$3.2 \times 10^6$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.6 \times 10^6$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	$3.5 \times 10^5$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$6.95 \times 10^{-8}$	C-VP20°/S25°
Vapor pressure, $P_v$ (torr)	$1.0 \times 10^{-10}$ (20°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

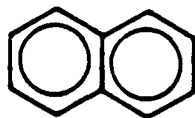
103. INDENO[1,2,3-cd]PYRENE

## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>5 \times 10^8</math></u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>2 \times 10^4</math></u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NHFG</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NHFG</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	<u>NHFG</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>3 \times 10^{-12}</math></u>	<u>E-KB</u>

E: Estimated value; see List of Source Codes.



104. NAPHTHALENECAS 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)	$1.95 \times 10^3$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	940	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	420	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$4.6 \times 10^{-4}$	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

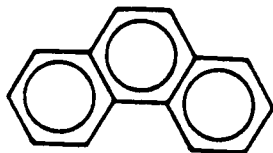
Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [104-1]	Zepp, 1980
Reaction quantum yield, $\phi$ , at <u>313</u> nm	<u><math>1.5 \times 10^{-2}</math></u>	Zepp & Schlotzhauer, 1979
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	_____	_____
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;360</u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>&lt;1</u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NHFG</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>NHFG</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	<u>NHFG</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-7}</math></u>	<u>E-KB</u>

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 <sup>-1</sup> cm <sup>-1</sup> )
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. PHENANTHRENECAS 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)	$2.8 \times 10^4$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$1.4 \times 10^4$	C-Koc f Kow
Microorganisms-water, $K_B ((\mu\text{g/g})(\text{mg/l})^{-1})$	$4.7 \times 10^3$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$2.26 \times 10^{-4}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$9.6 \times 10^{-4}$ (25°C)	C-CT/CRC
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

## 105. PHENANTHRENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [105-1]	Zepp, 1980
Reaction quantum yield, $\phi$ , at 313 nm	0.01	Zepp & Schlotzhauer, 1979
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) at latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<360	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<36	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	$1.6 \times 10^{-7}$	Paris et al., 1980

E: Estimated value; see List of Source Codes.

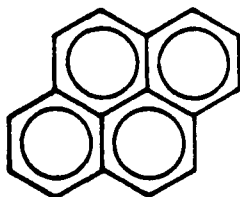
105. PHENANTHRENE

[105-1] Table of absorption coefficients and the corresponding wavelengths for phenanthrene is given below (Zepp, 1980).

WAVELENGTH (nm)	EPSILON (M <sup>-1</sup> cm <sup>-1</sup> )
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)	$8.0 \times 10^4$	CC-Kow
Sediment-water, $K_{oc}$ (unitless)	$3.8 \times 10^4$	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	$1.2 \times 10^4$	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$5.1 \times 10^{-6}$	C-VP/S-25°
Vapor pressure, $P_v$ (torr)	$2.5 \times 10^{-6}$ (25°C)	Hoyer & Peperle 1958
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

## 106. PYRENE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	DATA-ATT [106-1]	Zepp, 1980
Reaction quantum yield, $\phi$ , at 313 nm	$2.1 \times 10^{-3}$ [106-2]	Zepp & Schlotzhauer, 1979
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) at latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$5 \times 10^8$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$2.2 \times 10^4$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	E-KB

E: 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 <sup>-1</sup> cm <sup>-1</sup> )
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  $2.1 \times 10^{-3}$ .

### References for 3.8

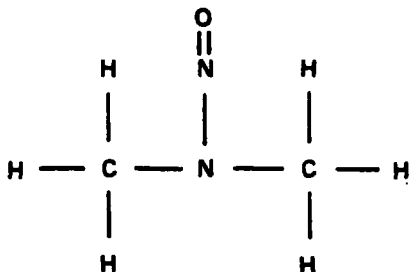
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### SECTION 3.9. NITROSAMINES AND OTHER NITROGEN-CONTAINING CHEMICALS

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

## 107. DIMETHYL NITROSAMINE

CAS No. 62-75-9



## 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-NER	

## 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, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	0.11	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$3.3 \times 10^{-5}$	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	

107. DIMETHYL NITROSAMINE

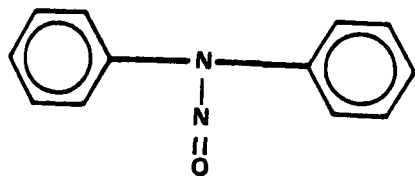
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	[107-2]	WREF
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	E-KB

E: Estimated value; see List of Source Codes.

[107-1] A water solubility value of  $6.3 \times 10^4$  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 NITROSAMINECAS 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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	426	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$6.6 \times 10^{-4}$	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	

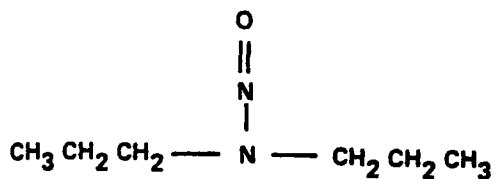
108. DIPHENYL NITROSAMINE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	see [107-2]	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	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 NITROSAMINECAS No. 621-64-7

## 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, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	9.8	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$6.3 \times 10^{-6}$	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	



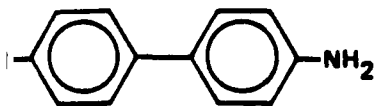
109. DI-n-PROPYL NITROSAMINE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	see [107-2]	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<3600	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	E-KR

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. BENZIDINECAS No. 92-87-5

## 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, $K_B$ $(\mu\text{g/g})(\text{mg/l})^{-1}$	10.1	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$3 \times 10^{-7}$	C-VP-/S12° [110-2]
Vapor pressure, $P_v$ (torr)	$5 \times 10^{-4}$	[110-2]
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

110. BENZIDINE

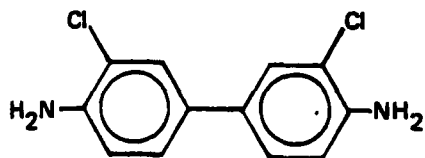
## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<4 \times 10^7$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$1.1 \times 10^8$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	NHFG
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	NHFG
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $1 \times 10^{-10}$	E-KB

E: Estimated value; see List of Source Codes.

[110-1] The two ionization constants are  $\text{pK}_{\text{a}1} = 4.66$  and  $\text{pK}_{\text{a}2} = 3.57$  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'-DICHLOROBENZIDINECAS 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)	$3.236 \times 10^3$	Pomona
Sediment-water, $K_{oc}$ (unitless)	1553	C-Koc f Kow
Microorganisms-water, $K_B ((\mu\text{g/g})(\text{mg/l})^{-1})$	941	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$8 \times 10^{-7}$	C-VP/S-22° [111-1]
Vapor pressure, $P_v$ (torr)	$1 \times 10^{-5}$ (22°C)	[111-1]
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

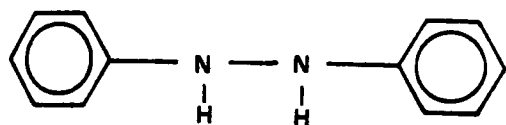
111. 3,3'-DICHLOROBENZIDINE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) <u>summer</u> at <u>40°</u> latitude	$2.1 \times 10^{-6}$	WREF
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<4 \times 10^7$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$4 \times 10^7$	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-12}$	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-DIPHENYLHYDRAZINECAS 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)	$1.84 \times 10^3$	C-Sw f Kow
Octanol-water, $K_{ow}$ (unitless)	871	Pomona
Sediment-water, $K_{oc}$ (unitless)	418	C-Koc f Kow
Microorganisms-water, $K_B \left( (\mu\text{g/g})(\text{mg/l})^{-1} \right)$	286	C-KB f Kow

## Volatilization constants:

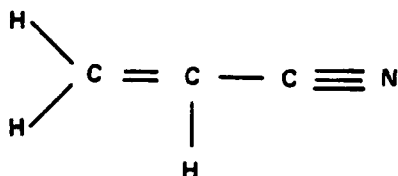
Henry's constant, $H^c$ ( $\text{atm m}^3 \text{mol}^{-1}$ )	$3.4 \times 10^{-9} (25^\circ\text{C})$	C-VP/S
Vapor pressure, $P_v$ (torr)	$2.6 \times 10^{-5} (25^\circ\text{C})$	Jaber, 1981
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	

112. 1,2-DIPHENYLHYDRAZINE

## TRANSFORMATION DATA

<u>Property or Process</u>	<u>Value</u>	<u>Data Source</u>
Photolysis data:		
Absorption spectrum		
Reaction quantum yield, $\phi$ , at _____ nm		
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude		
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>&lt;4 \times 10^7</math></u>	<u>C-OX</u>
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u><math>1 \times 10^9</math></u>	<u>C-OX</u>
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	<u>0</u>	<u>HNES</u>
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	<u>(E) <math>1 \times 10^{-10}</math></u>	<u>E-KB</u>

E: Estimated value; see List of Source Codes.

113. ACRYLONITRILECAS No. 107-13-1

## 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)	$7.9 \times 10^4$ (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, $K_B \left( (\mu\text{g/g}) (\text{mg/l})^{-1} \right)$	1.04	C-KB f Kow

## Volatilization constants:

Henry's constant, $H_c$ ( $\text{atm m}^3 \text{ mol}^{-1}$ )	$8.8 \times 10^{-5}$	C-VP22.8°/S25°
Vapor pressure, $P_v$ (torr)	100 (22.8°C)	WREF
Reaeration rate ratio, $k_v^c/k_v^o$	NAV	



113. ACRYLONITRILE

## TRANSFORMATION DATA

Property or Process	Value	Data Source
Photolysis data:		
Absorption spectrum	PNES	WREF
Reaction quantum yield, $\phi$ , at _____ nm	PNER	
Direct photolysis rate constant, $k_p$ ( $\text{hr}^{-1}$ ) _____ at _____ latitude	PNER	
Oxidation constants at 25°C:		
For $^1\text{O}_2$ (singlet oxygen), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	$<1 \times 10^8$	C-OX
For $\text{RO}_2$ (peroxy radical), $k_{\text{OX}}$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	36	C-OX
Hydrolysis rate constants:		
For base-promoted process, $k_B$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For acid-promoted process, $k_A$ ( $\text{M}^{-1} \text{hr}^{-1}$ )	0	HNES
For neutral process, $k_N$ ( $\text{hr}^{-1}$ )	0	HNES
Biotransformation rate constant:		
For bacterial transformation in water, $k_b$ ( $\text{ml cell}^{-1} \text{hr}^{-1}$ )	(E) $3 \times 10^{-9}$	E-KB

E: Estimated value; see List of Source Codes.

### References for 3.9

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## 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 partitioning of a chemical is given by the equation

$$K_p = C_p / C_w \quad (4.1)$$

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

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:

$$K_{oc} = K_p / f_{oc} \quad (4.2)$$

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 partition 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.

#### 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).<sup>\*</sup> 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):

$$\log K_{oc} = 1.00 \log K_{ow} - 0.21 \quad (4.3)$$

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:

$$\log S_w = -1.08 \log K_{ow} + 3.70 + \log MW \quad (4.4)$$

where MW is the molecular weight of the pollutant ( $\text{g mole}^{-1}$ ). For organic pollutants that are solid in their pure state at 25°C:

$$\log S_w = -1.08 \log K_{ow} + 3.70 + \log MW - \left( \frac{\Delta S_f}{1360} \right) (\text{mp}-25) \quad (4.5)$$

where mp is the melting point of the pollutant (°C) and  $\Delta S_f$  is the entropy of fusion of the pollutant ( $\text{cal mol}^{-1} \text{ deg}^{-1}$ ). If  $\Delta S_f$  is not known, it may be approximated by (Yalkowsky and Valvani, 1980):

$$\Delta S_f \sim 13.6 + 2.5 (n - 5) \quad (4.6)$$

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.

---

<sup>\*</sup>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):

$$\log K_{oc} = -0.55 \log S_w + 3.64 \quad (4.7)$$

$K_B$  can be correlated with  $K_{ow}$  by

$$K_B = 0.16 K_{ow} \quad (4.8)$$

#### 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

$$x = n / (n + n_w)$$

$$\sim n / n_w \text{ for } n_w \gg n \quad (4.9)$$

- (2) Molarity,  $S$ , expressed in moles of solute per liter of solution (M):

$$S(M) = n(\text{mol}) / \text{liter of solution} \quad (4.10)$$

- (3) Weight fraction, expressed in milligrams of solute per liter of water, or parts per million, ppm

$$S_w (\text{ppm}) = \frac{n (\text{mol}) \text{ MW } (\text{g mol}^{-1}) 1000 (\text{mg g}^{-1})}{\text{liter of water}} \quad (4.11)$$

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

$$x = \frac{S}{55.5 + S} \sim \frac{S}{55.5} \text{ for } S < 1 \text{ M} \quad (4.12)$$

or

$$S = \frac{55.5 x}{(1 - x)} \sim 55.5 x \text{ for } x < 10^{-2} \quad (4.13)$$

To convert from molarity to ppm is straightforward by substituting Equation (4.10) into equation (4.11)

$$\text{ppm} \sim S(\text{MW}) (1000) \text{ for } S < 1 \text{ M} \quad (4.14)$$

Thus to convert from mole fractions to ppm follows from equations (4.11) and (4.13)

$$\begin{aligned} \text{ppm} &= \frac{55.5 x}{(1 - x)} (\text{MW}) (1000) \\ &\sim 55.5(x) (\text{MW}) (1000) \text{ for } x < 10^{-2} \end{aligned} \quad (4.15)$$

These conversion factors are summarized in Table 4.1.

Table 4.1  
CONVERSION FACTORS FOR COMPOSITION UNITS

FROM	TO	x (mole fraction)	M (Molarity)
ppm	---	$\frac{1.80 \times 10^{-5}}{\text{MW}}$	$\frac{10^{-3}}{\text{MW}}$
(mole fraction)	$5.55 \times 10^4 (\text{MW})$	---	55.5
M (Molarity)	$(\text{MW}) (10^3)$	$\frac{1}{55.5}$	---

Concentration in aqueous solution is preferably given in mole fraction or molarity units since these units are measures of the amount of solute per amount of solution. The weight fraction or ppm, on the other hand, expresses the weight of solute per weight of solution and is thus a function of the molecular weight of the molecule, which is not relevant to environmental or toxicological effects.

#### 4.3 CALCULATION OF $K_{oc}$ and $S_w$ FROM $K_{ow}$

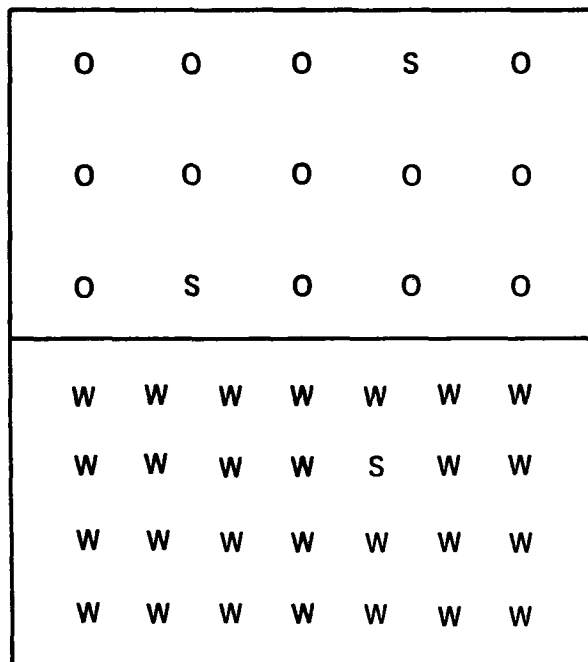
The sediment partition coefficient, normalized for organic carbon content ( $K_{oc}$ ), and aqueous solubility ( $S_w$ ) of an organic pollutant are critical to its environmental fate. Because  $K_{oc}$  and  $S_w$  values may be unmeasured or unreliable, it is important to be able to correlate these environmental parameters with other experimental quantities, namely, to predict unmeasured values and appraise the reliability of measured values.

It is useful to correlate these parameters with octanol/water partition coefficients ( $K_{ow}$ ) for practical as well as theoretical reasons. Practically,  $K_{ow}$  values are easier to measure and, where  $K_{ow}$  measurements have not been made, calculated values may be used with confidence. The theoretical basis for expecting correlations of  $K_{oc}$  and  $S_w$  with  $K_{ow}$  is described below. The correlation of  $K_B$  with other partitioning constants is not discussed in this section since a recent review of the subject is available.

##### 4.3.1 Partitioning Thermodynamics

This discussion first considers the partitioning of a chemical between octanol and water, with octanol being a representative organic phase. If a small amount of a chemical is added to a closed vessel containing n-octanol and water, the vessel is shaken, and the octanol and water are allowed to separate, the chemical will partition between the two phases (see Figure 4.1). By convention, the small amount of chemical in each phase is called the solute. The partitioning of the solute molecules between the two phases can be understood in terms of a simple lattice model. If we assume that every molecule (water, octanol,

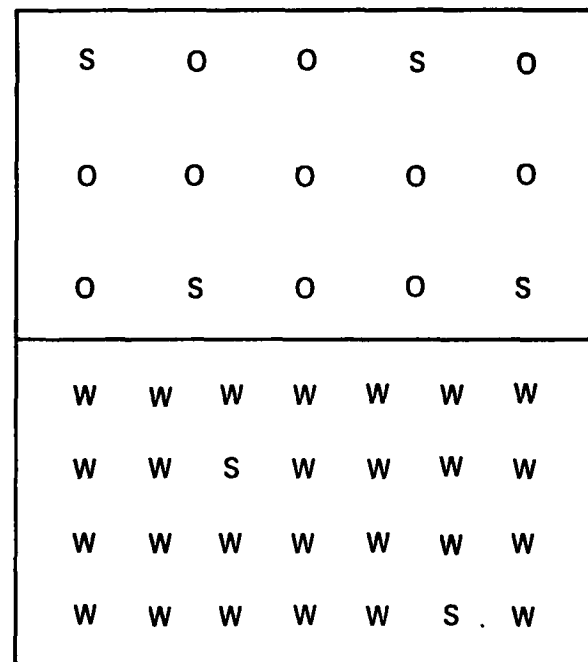




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FIGURE 4.1 LATTICE MODEL OF A SOLUTE (S) PARTITIONING BETWEEN OCTANOL (O) AND WATER (W) PHASES

$$K_{ow} = C_o / C_w = 2$$



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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.

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 proportional 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:

$$f = Hx \quad (4.16)$$

where  $H$  is a constant representing the forces exerted on the solute by the solvent. At higher solute mole fractions, where solute-solute interactions 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  $x$ :

$$f = H(x) x \quad (4.17)$$

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<sup>\*</sup> 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).

$$f_w = (f^R \gamma_w) x_w \quad (4.18)$$

$$f_o = (f^R \gamma_o) x_o \quad (4.19)$$

where subscripts w and o refer, respectively, to the water and octanol phases, and  $f^R$  and  $\gamma_i$  are, respectively, the reference fugacity and activity coefficient, which together represent the forces acting on the solute in the  $i^{\text{th}}$  phase. At equilibrium

$$f_w = f_o \quad (4.20)$$

so that

$$x_o/x_w = \frac{f^R \gamma_w}{f^R \gamma_o} = \frac{\gamma_w}{\gamma_o} \quad (4.21)$$

In general, at constant pressure,  $f^R$  depends only on the temperature and  $\gamma_i$  depends on the composition as well as the temperature of the  $i^{\text{th}}$  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

$$(f^R \gamma_i) = H_i \quad (4.22)$$

where  $H_i$  is the Henry's constant for a very dilute solution of the solute in phase  $i$ . Thus

$$x_o/x_w = H_w/H_o \quad (4.23)$$

is a function only of temperature. However, if  $x_o$  or  $x_w$  is large enough that  $\gamma_o$  or  $\gamma_w$  is not constant, then  $K_{ow}$  will also no longer be constant.

Because composition is commonly measured in moles liter<sup>-1</sup>(M), it is convenient to define:

$$K_{ow} = C_o / C_w = r_{wo} (x_o / x_w) = r_{wo} (H_w / H_o) \quad (4.25)$$

where  $r_{wo}$  is a constant equal to the ratio of the molar volume of water

$$r_{wo} = v_w / v_o \quad (= 0.115) \quad (4.26)$$

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

$$K_{pw} = r_{wp} (H_w / H_p) \quad (4.27)$$

From equation (4.25) for partitioning between octanol and water

$$H_w = K_{ow} H_o / r_{wo} \quad (4.28)$$

thus

$$K_{pw} = (r_{wp} / r_{wo}) (H_o / H_p) K_{ow} = r_{op} (H_o / H_p) K_{ow} \quad (4.29)$$

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)

$$\log K_{pw} = \log K_{ow} + \log (r_{op} H_o / H_p) \quad (4.30)$$

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

$$K_{ow} = (C_o/C_w)_{\text{dilute}} = (C_o/C_w)_{\text{saturated}} \quad (4.31)$$

From equation (4.21), this means that the ratio of activity coefficients  $\gamma_w/\gamma_o$  remains constant up to saturation. As explained above, however, the ratio  $\gamma_x/\gamma_o$  will depend on solute concentration,\* particularly if  $C_w$  (saturated) is large enough that solute-solute interactions become

---

\*Because of the chemical similarity of a neutral organic solute with n-octanol, it is expected that  $\gamma_o$  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

$$K_{ow} = S_o / S_w \quad (4.32)$$

where  $S_o$  and  $S_w$  are solubilities in moles liter<sup>-1</sup>(M) in pure octanol and pure water, respectively.

To correlate aqueous solubility with  $K_{ow}$ , many authors have proposed an equation of the form:

$$\log S_w = -(1/a) \log K_{ow} + c \quad (4.33)$$

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:

$$K_{ow} = (S_o / S_w)^a \quad (4.34)$$

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:

$$\log S_w = - (1/a) \log K_{ow} + (1/a) \log S_o \quad (4.35)$$

If  $S_o$  is assumed constant for a set of solutes in octanol, equation (4.35) becomes

$$\log S_w = - (1/a) \log K_{ow} + c \quad (4.36)$$

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  $\underline{a}$  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:

$$\log S_w = - (1/a) \log K_{ow} + c - (1/a) \frac{\Delta H_f}{2.303 RT_f} \frac{T_f - T}{T} \quad (4.37)$$

where  $\Delta H_f$  is the enthalpy of fusion,  $R$  is the gas constant, and  $T_f$  is the melting temperature of the solute. At the melting point,

$$\Delta H_f = T_f \Delta S_f \quad (4.38)$$

Therefore at 25°C, equation (4.38) becomes

$$\log S_w = - (1/a) \log K_{ow} + c - \frac{\Delta S_f}{a(1360)} (mp-25) \quad (4.39)$$

where  $mp$  is the melting point (in °C) and  $\Delta S_f$  is the entropy of fusion (in cal deg<sup>-1</sup> mole<sup>-1</sup>). 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  $\underline{a}$  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<sup>-1</sup> mol<sup>-1</sup>).

Table 4.2

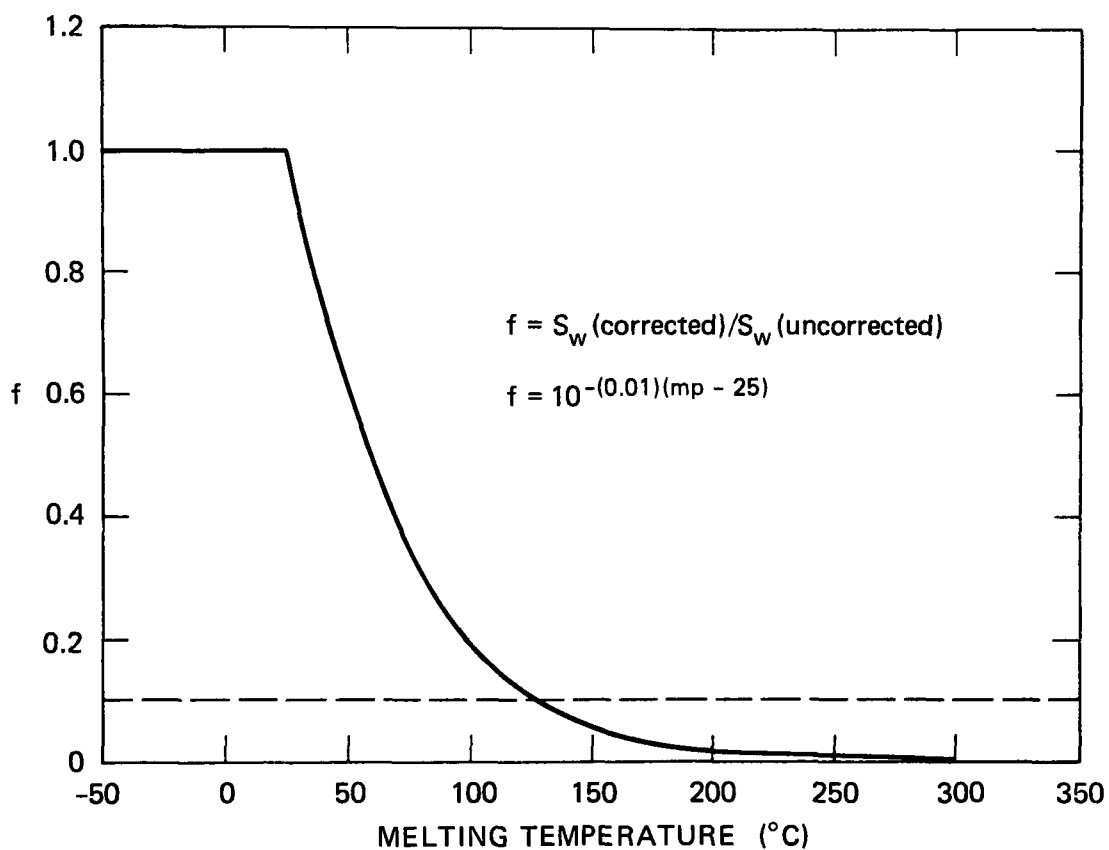
EFFECT OF MELTING POINT CORRECTION  
ON WATER SOLUBILITY VALUES

Solubility (uncorrected) (ppm)	Melting Point (°C)	Solubility <sup>*</sup> (corrected) (ppm)
100	25	100
100	50	56
100	100	18
100	200	2
100	300	0.2

---

\*  $\log S_w (\text{corrected}) = \log S_w (\text{uncorrected}) - 0.01 (\text{mp}-25)$  at  $25^\circ\text{C}$ ,  
 where  $\Delta S_f = 13.6$  and  $a = 1$  are assumed in equation (4.39) and  $S_w$   
 is the water solubility in ppm.





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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.

$\frac{K_{oc}}{K_{ow}}$ . 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:

$$K_p = K_{oc}(f_{oc}) = C_s / C_w \quad (4.40)$$

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	Equation	Eq.	Data Base*	Authors
$K_{oc} - K_{ow}$	$\log K_{oc} = 0.544 \log K_{ow} + 1.377$	(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)
$K_{oc} - K_{ow}$	$\log K_{oc} = 1.00 \log K_{ow} - 0.21$	(4.3)	Pollutants Polycyclic aromatics (8) Chlorinated hydrocarbons (2)	Karickhoff et al. (1979)
$S_w - K_{ow}$	$\log S_w = -0.922 \log K_{ow} + 4.184$ $S_w$ in ppm	(4.42)	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)
$S_w - K_{ow}$	$\log x_s = -1.08 \log K_{ow} - 1.04$ $- \left[ \frac{\Delta S_f}{1360} (mp - 25) \right]$ $x_s$ is the mole fraction solubility at 25°C $\Delta S_f$ is the entropy of fusion in cal deg <sup>-1</sup> mol <sup>-1</sup> mp is the melting point in °C (if mp ≤ 25 then the term in brackets is zero)	(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)

\* 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)
$K_{oc} - S_w^*$	$\log K_{om} = - 0.56 \log S_w + 0.70$	(4.44)	Pollutants	Chiou et al. (1979)
	$\log K_{oc} = - 0.56 \log S_w + 0.93$	(4.45)	Polychlorinated biphenyls (3) Pesticides (4) Halogenated ethanes and propanes (6) Tetrachloroethene 1,2-Dichlorobenzene Adsorbents Willamette silt loam Miscellaneous other soils	
$K_{oc} - S_w$	$\log K_{oc} = - 0.54 \log x_s + 0.44$ $x_s$ 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.

The theoretical equation of Table 4.4,

$$\log K_{oc} = 1.00 \log K_{ow} + \text{constant} \quad (4.47)$$

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  $K_{oc}$  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.

$\frac{S_w}{K_{ow}}$ . Several comparisons of the equations of Kenaga and Goring (1978) 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

	<u>Kenaga and Goring (1978)</u>	<u>Karickhoff et al. (1979)</u>	<u>Theoretical</u>
$\log K_{oc} =$	$0.54 \log K_{ow} + 1.38$	$1.00 \log K_{ow} - 0.21$	$1.00 \log K_{ow} + \text{constant}$
$K_{ow}$	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

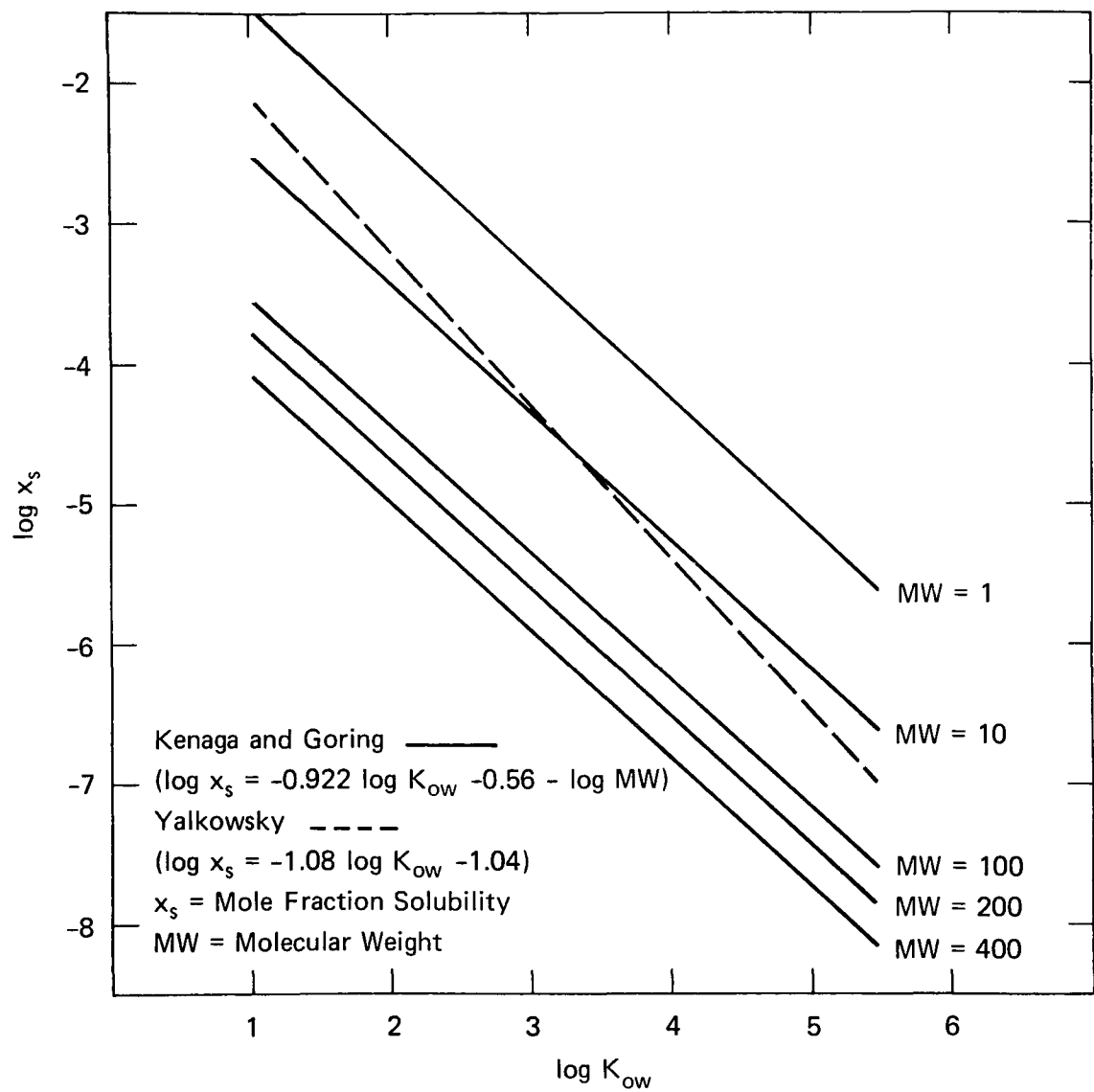
$$\log x_s = - 0.922 \log K_{ow} - 0.56 - \log MW \quad (4.48)$$

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 sublimates) are liquid at 25°C. Furthermore, it 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 of 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.



SA-6729-11

FIGURE 4.4 COMPARISON OF SOLUBILITY  $K_{ow}$  EQUATIONS FOR LIQUID SOLUTES



Table 4.5

## CALCULATED VERSUS MEASURED SOLUBILITIES FOR CHLORINATED METHANES AND ETHANES

	<u>log K<sub>ow</sub></u>	<u>mp (°C)</u>	<u>log S<sub>w</sub> (M)</u>		
			<u>Kenaga and Goring</u>	<u>Yalkowsky</u>	<u>Measured</u> <sup>a</sup>
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	2.96	-23	-3.70	-2.49	-2.29
Hexachloroethane	4.62	Sublimes	-5.45	-4.29	-3.68

<sup>a</sup> 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°C, Yalkowsky included an entropy of melting correction term. Thus the equation of Yalkowsky, assuming accurate known values of the entropy of fusion ( $\Delta S_f$ ) 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°C, then the solid will be less soluble than the liquid by a factor of

$$\exp [-2.303(\Delta S_f/1360)(\text{mp}-25)] \quad (4.49)$$

where  $\Delta S_f$  is the entropy of fusion and mp is the melting point (°C). If  $\Delta S_f$  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  $\alpha$ -,  $\beta$ -,  $\delta$ -, and  $\gamma$ -BHC.

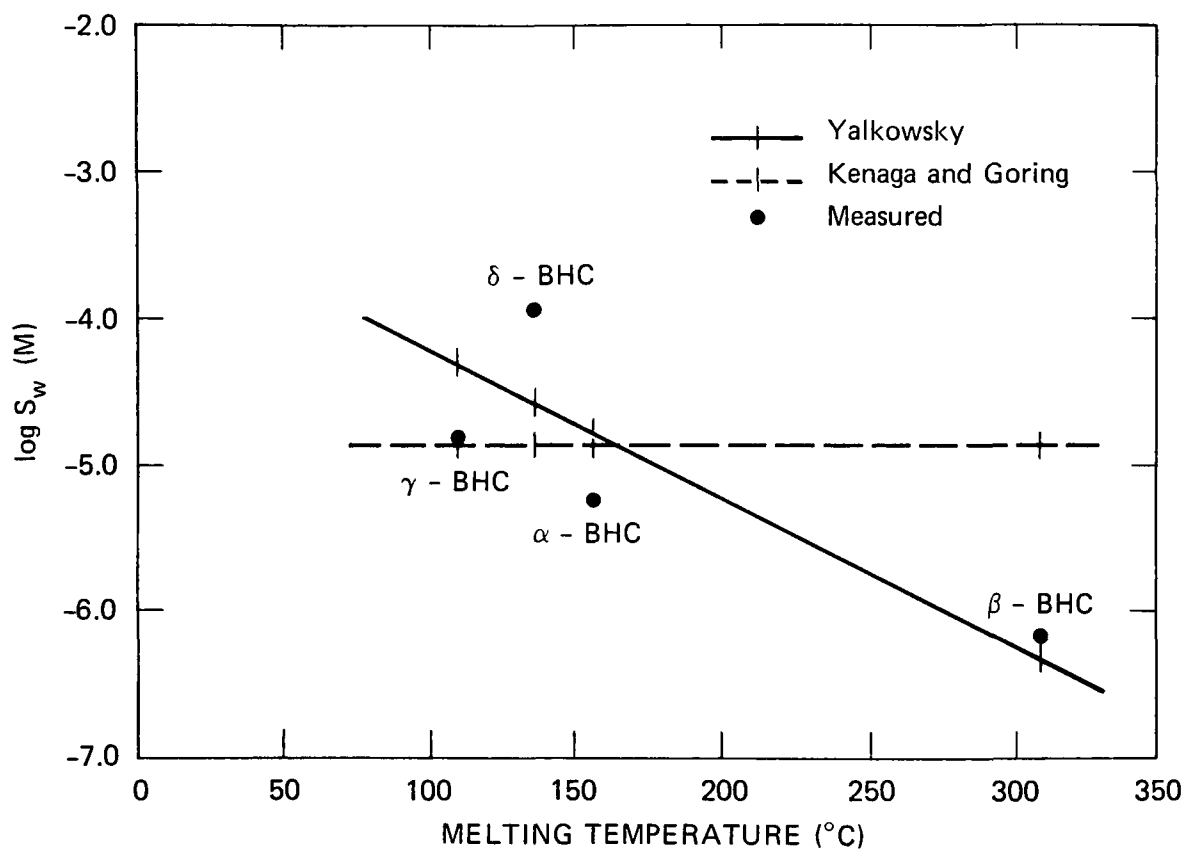
Figure 4.5 also indicates that implicit in equation (4.42) of Kenaga and Goring is an empirical average of the solid solute correction term. Because the solubilities of liquid solutes predicted by equation (4.42) are approximately an order of magnitude lower than measured values, we can assume that this 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°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°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

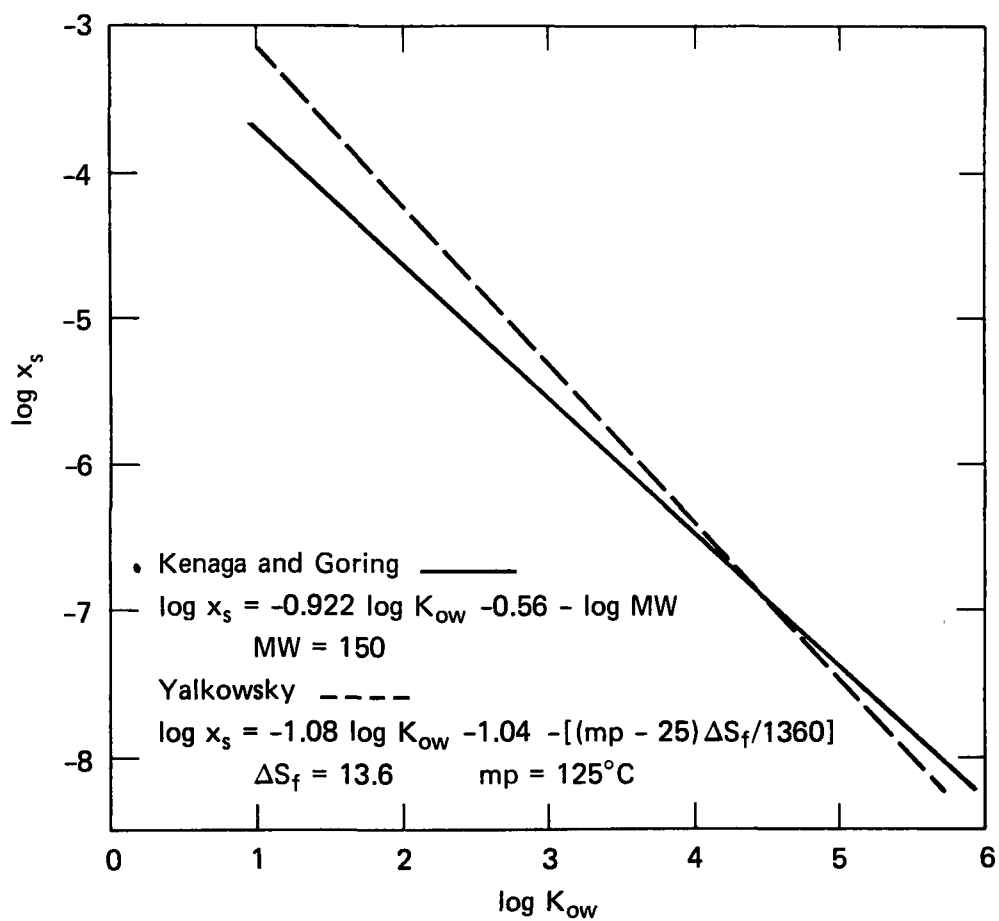
	log K <sub>ow</sub>	mp (°C)	log S <sub>w</sub> (M)		
			Kenaga and Goring	Yalkowsky	Measured <sup>a</sup>
Nitrobenzene	1.87	5.6	-2.63	-1.32	-1.82
Benzene	2.13	5.5	-2.63	-1.60	-1.64
Toluene	2.79	-95	-3.35	-2.31	-2.24
Chlorobenzene	2.84	-45	-3.48	-2.37	-2.37
Ethylbenzene	3.34	-94.9	-3.92	-2.90	-2.85
1,2-Dichlorobenzene	3.56	-17	-4.26	-3.14	-3.00

<sup>a</sup> Sources for measured values are given on data sheet for each chemical  
(see Section 3)



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FIGURE 4.5 SOLUBILITIES OF HEXACHLOROCYCLOHEXANES ( $\alpha$ -,  $\beta$ -,  $\delta$ -,  $\gamma$ -BHC) AS A FUNCTION OF MELTING TEMPERATURE



SA-6729-13

FIGURE 4.6 COMPARISON OF SOLUBILITY -  $K_{ow}$  EQUATIONS FOR SOLID SOLUTES

Table 4.7

## CALCULATED VERSUS MEASURED SOLUBILITIES FOR SELECTED PESTICIDES

	<u>log K<sub>ow</sub></u>	MP (°C)	log S <sub>w</sub> (M)		
			<u>Kenaga and Goring</u>	<u>Yalkowsky</u>	<u>Measured</u>
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

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<sup>a</sup> Sources of measured values are given on the data sheets for each chemical (see Section 3).

that for selected pesticides with melting points around 110°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°C. Table 4.8 indicates that, indeed, measured solubilities of chemicals with melting points above 200°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°C range, but equation (4.43) of Yalkowsky, because it includes a melting point correction factor is not limited by melting point restrictions.

$\frac{K_{oc}}{S_w}$ . 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

$$\log K_{oc} = - 0.55 \log x_s - 0.23 \quad (\text{Kenaga and Goring, 1978}) \quad (4.50)$$

$$\log K_{oc} = - 0.56 \log x_s - 0.04 \quad (\text{Chiou et al., 1979}) \quad (4.51)$$

$$\log K_{oc} = - 0.54 \log x_s + 0.44 \quad (\text{Karickhoff et al., 1979}) \quad (4.46)$$

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

$$K_{oc} = (\text{constant}) x_s^{-0.55(\pm 0.01)} \quad (4.52)$$

Table 4.8

## AQUEOUS SOLUBILITIES OF HIGH MELTING POINT CHEMICALS

Chemical Name	Melting Point (°C)	Solubilities (ppm)	
		Measured	Predicted by Equation (4.42) <sup>a</sup>
Benzo[k]fluoranthene	217	$5.6 \times 10^{-4}$	0.04
Anthracene	219	0.045	1.2
Benzo[g,h,i]perylene	222	$2.6 \times 10^{-4}$	0.015
Chrysene	258	$1.8 \times 10^{-3}$	0.1
Dibenz[a,h]anthracene	270	$5 \times 10^{-4}$	$9 \times 10^{-3}$
TCDD	303	$2 \times 10^{-4}$	$7.5 \times 10^{-3}$
B-BHC	309	0.24	4.0

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<sup>a</sup> 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)],

$$\log K_{oc} = a \log K_{ow} + \text{constant} \quad (4.53)$$

and

$$\log K_{ow} = -a \log x_s + \text{constant} \quad (4.54)$$

where  $a \sim 1$ , then by substituting equation (4.54) into equation (4.53)

$$\log K_{oc} = -a^2 \log x_s + \text{constant} \quad (4.55)$$

$$\sim -1.0 \log x_s + \text{constant}$$

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.

$K_B - K_{ow}$ . 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  $K_B$

$$K_B = 0.16 K_{ow} \quad (4.8)$$

which is the simplified version of the equation given by Baughman and Paris (1981),

$$\log K_B = 0.907 \log K_{ow} - 0.21 \quad (4.56)$$

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

$$\log P = \sum_{n=1}^n a_n f_n \quad (4.57)$$

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 $K_{ow} \pm S.D.$ <sup>a</sup>	Computer-Calculated	
		$K_{ow}$	$r$ <sup>b</sup>
Pyrene	124,000 $\pm$ 11,000	79,400	1.6
7,12-Dimethylbenz[a]anthracene	953,000 $\pm$ 59,000	871,000	1.1
Dibenz[a,h]anthracene	3,170,000 $\pm$ 883,000	5,890,000	0.54
3-Methylcholanthrene	2,632,000 $\pm$ 701,000	9,330,000	0.28
Dibenzothiophene	24,000 $\pm$ 2,200	33,900	0.71
Acridine	4,200 $\pm$ 940	2,570	1.6
13H-Dibenzo[a,i]carbazole	2,514,000 $\pm$ 761,000	692,000	3.6
Acetophenone	38.6 $\pm$ 1.2	38.9	0.99
1-Napthol	700 $\pm$ 62	417	1.7
Benzidine	46.0 $\pm$ 2.2	35.5	1.3
2-Aminoanthracene	13,400 $\pm$ 930	1,660	8.1
6-Aminochrysene	96,600 $\pm$ 4,200	24,000	4.0
Anthracene-9-carboxylic acid	1,300 $\pm$ 130	15,500	0.08

<sup>a</sup> Hassett et al. (1980).

<sup>b</sup> 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.

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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 reaeration rate ratio, which are used to calculate volatilization data in many aquatic fate models, plus the vapor pressure. The calculation 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 theoretical 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, only 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

$$R_v = - \frac{d[C_w]}{dt} = k_v [C_w] \quad (5.1)$$

where  $[C_w]$  is the concentration of the chemical in moles liter<sup>-1</sup> (M) in water and  $k_v$  is the volatilization rate constant in units of time<sup>-1</sup> (usually hr<sup>-1</sup> or day<sup>-1</sup>). The full expression for estimating the volatilization rate constant of the chemical from a natural water body is

$$k_v^C = \frac{1}{L} \left[ \frac{1}{k_\ell^O \left( D_\ell^C / D_\ell^O \right)^m} + \frac{RT}{H_c k_g^W \left( D_g^C / D_g^W \right)^n} \right]^{-1} \quad (5.2)$$

where

$L$  = mixing depth of the water body (cm)

$k_\ell^O$  = liquid phase mass transport coefficient of oxygen in the water body (cm hr<sup>-1</sup>)

$D_\ell$  = liquid phase diffusion coefficient of the chemical (C) or oxygen (O) in water (cm<sup>2</sup> sec<sup>-1</sup>)

$m$  = 0.5 to 1.0, depending on the liquid phase turbulence

$R$  = gas constant, 62.4 torr deg<sup>-1</sup> M<sup>-1</sup> or 8.205 x 10<sup>-5</sup> m<sup>3</sup> atm deg<sup>-1</sup> mol<sup>-1</sup>

$T$  = temperature (K)

$H_c$  = Henry's constant (torr M<sup>-1</sup> or m<sup>3</sup> atm mol<sup>-1</sup>)

$k_g^W$  = gas phase mass transport coefficient for water (cm hr<sup>-1</sup>)

$D_g$  = gas phase diffusion coefficient for the chemical (C) or water (W) in air (cm<sup>2</sup> sec<sup>-1</sup>)

$n$  = 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  $k_\ell^O$  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

$$P_i = H_c [C_{wi}] \quad (5.3)$$

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  $\text{torr M}^{-1}$  can be converted to  $\text{atm m}^3 \text{ mole}^{-1}$  by the following equation:

$$H_c (\text{atm m}^3 \text{ mole}^{-1}) = \frac{H_c (\text{torr M}^{-1})}{760 \times 1000} = 1.32 \times 10^{-6} H_c (\text{torr M}^{-1}) \quad (5.4)$$

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  $20^\circ\text{C}$ , is:

$$H (\text{unitless}) = \frac{H_c (\text{torr M}^{-1})}{RT} = 5.47 \times 10^{-5} H_c (\text{torr M}^{-1}) \quad (5.5)$$

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 ( $T_m$ ,  $^\circ\text{C}$  and  $\text{K}$ )
- Solubility in water at  $20^\circ\text{C}$  ( $S_w$ ,  $\text{g liter}^{-1}$  and  $\text{mole liter}^{-1}$ )
- Vapor pressure at  $20^\circ\text{C}$  ( $P_v$ ,  $\text{torr}$ )
- Heat of fusion,  $\Delta H_f$ , is required if the chemical is a solid at  $20^\circ\text{C}$  and if the vapor pressure used to calculate  $H_c$  is for the liquid. If a measured value of  $\Delta H_f$  is not available, an estimation method can be used.

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  $S_w$

$$H_c = P/S_w \quad (5.6)$$

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

$$P_{2\ell} = P_{1\ell} \left[ \exp \frac{\Delta H_v}{R} \left( \frac{1}{T_1} - \frac{1}{T_2} \right) \right] \quad (5.7)$$

$P_{2\ell}$  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

$$\log_{10} P_{2\ell} = (-0.2185 A/T_2) + B \quad (5.8)$$

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

$$P_{2sl} = P_1 \left[ \exp \frac{\Delta H_f}{R} \left( \frac{1}{T_1} - \frac{1}{T_2} \right) \right] \quad (5.9)$$

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 ( $P_{2sl}$ ) by

$$P_{2s} = P_{2sl} \left[ \exp \frac{\Delta H_f}{R} \left( \frac{1}{T_m} - \frac{1}{T_2} \right) \right] \quad (5.10)$$

where  $\Delta H_f$  is the heat of fusion for the chemical ( $\text{cal mol}^{-1}$ ),  $R$  is the gas constant ( $1.987 \text{ cal K}^{-1} \text{ mol}^{-1}$ ), 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  $T_2$ :

$$P_{2l} = P_{1l} \left[ \exp \frac{\Delta H_v}{1.987} \left( \frac{1}{T_1} - \frac{1}{T_2} \right) \right] \quad (5.11)$$

or

$$\log_{10} P_{2l} = (-0.2185 A/T_2) + B \quad (5.8)$$

$$H_c = P_{2l}/S_w \quad (5.12)$$

For solids, at  $20^\circ\text{C}$ , when a value for  $\Delta H_f$  is available:

$$P_{2s} = P_{1l} \left[ \exp \frac{\Delta H_v}{1.987} \left( \frac{1}{T_1} - \frac{1}{T_2} \right) \right] \left[ \exp \frac{\Delta H_f}{1.987} \left( \frac{1}{T_m} - \frac{1}{T_2} \right) \right] \quad (5.13)$$

$$H_c = P_{2s}/S_w \quad (5.14)$$

The value of  $T_2$  is chosen as  $20^\circ\text{C} = 293\text{ K}$ , or equal to the same temperature as reported for the solubility data.

Yalkowski and Valvani (1979) have suggested that  $\Delta H_f$  be calculated from the melting temperature and entropy of fusion,  $\Delta S_f$ , using equation (5.15)

$$\Delta H_f = T_m \Delta S_f \quad (5.15)$$

where  $\Delta S_f = 13.5$  entropy units and is nearly constant for rigid molecules. If the value of  $\Delta H_f$  is not available, equation (5.16) is used to calculate  $P_{2s}$  for solids.

$$P_{2s} = P_{1l} \left[ \exp \frac{\Delta H_v}{1.987} \left( \frac{1}{T_1} - \frac{1}{T_2} \right) \right] \left[ \exp \frac{\Delta S_f}{1.987} \left( 1 - \frac{T_m}{T_2} \right) \right] \quad (5.16)$$

### 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 Laudie modification of the Othmer and Thakar relation (Reid et al., 1977, p. 573)

$$D_l = \frac{13.26 \times 10^{-5}}{\eta_w^{1.4} V_b^{0.589}} \quad (5.17)$$

where  $\eta_w$  is the viscosity of water (centipoise) and  $V_b$  is the molar volume at the normal boiling point ( $\text{cm}^3 \text{ mol}^{-1}$ ). The ratio of liquid diffusion constants for the chemical and oxygen in water,  $D_l^C/D_l^O$ , becomes

$$D_l^C/D_l^O = \left( V_b^O/V_b^C \right)^{0.589} \quad (5.18)$$

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,  $25.6 \text{ cm}^3 \text{ mol}^{-1}$ , which was calculated from diffusion coefficient data (Reid et al., 1977, p. 58).

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

$$D_g = \frac{0.001 T^{1.75} (1/M_1 + 1/M_2)^{1/2}}{P \left[ (\Sigma v)_1^{1/3} + (\Sigma v)_2^{1/3} \right]^2} \quad (5.19)$$

where  $M$  is the molecular weight and  $\Sigma v$  is the atomic diffusion volume. The subscripts 1 and 2 refer to the chemical or water and to air, respectively. The value of  $\Sigma v$  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

$$D_g^C/D_g^W = 85 \frac{(1/M_c + 0.0347)^{1/2}}{\left[ (\Sigma v)_c^{1/3} + 2.72 \right]^2} \quad (5.20)$$

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

$$t_{1/2} \text{ (hr)} = (\ln^2)/k_v^C \quad (5.21)$$

The rationales for the choices of  $k_g^O$ ,  $m$ ,  $k_g^W$ , 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)

<u>Constant/value</u>	<u>Rivers</u>	<u>Lakes</u>
L (cm)	200	200
$k_{\ell}^O$ (cm hr <sup>-1</sup> )	8	1.8
m	0.7	1.0
T (K)	293	293
RT (torr M <sup>-1</sup> )	18,283	18,283
RT (m <sup>3</sup> atm mol <sup>-1</sup> )	$2.40 \times 10^{-2}$	$2.40 \times 10^{-2}$
$k_g^W$ (cm hr <sup>-1</sup> )	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<sup>-1</sup> at 20°C or 9.88 x 10<sup>-4</sup> 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  $\Delta H_v = 13.55 \text{ kcal mol}^{-1}$  and that the boiling point is 285°C (where the vapor pressure must equal 760 torr). The heat of fusion,  $\Delta H_f$ , 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.

$$\begin{aligned} P_{2s} &= 760 \left[ \exp \frac{13,550}{1.987} \left( \frac{1}{285 + 273} - \frac{1}{293} \right) \right] \left[ \exp \frac{13.5}{1.987} \left( 1 - \frac{65 + 273}{293} \right) \right] \\ &= 4.2 \times 10^{-3} \text{ torr} \end{aligned}$$

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<sup>-4</sup> torr. The agreement is reasonable, considering the range of extrapolation of the vapor pressure data and that a value for  $\Delta H_f$  is not available. Using Pella's vapor pressure data, Henry's constant is

$$\begin{aligned} H_c &= P_{2s}/S_w \\ &= 3.5 \times 10^{-4} / 9.88 \times 10^{-4} = 0.35 \text{ torr M}^{-1} \end{aligned} \quad (5.14)$$

To convert  $H_c$  in torr M<sup>-1</sup> to atm m<sup>3</sup> mol<sup>-1</sup>,

$$\begin{aligned} H_c (\text{atm m}^3 \text{ mol}^{-1}) &= \frac{1}{760} \left( \frac{\text{atm}}{\text{torr}} \right) \frac{1}{10^3} \left( \frac{\text{m}^3}{\text{liter}} \right) H_c (\text{torr M}^{-1}) \\ &= 1.32 \times 10^{-6} H_c (\text{torr M}^{-1}) \end{aligned}$$

For 2,6-DNT,

$$H_c = 0.35 \times 1.32 \times 10^{-6} = 4.6 \times 10^{-7} \text{ atm m}^3 \text{ mol}^{-1}$$

Calculation of the Diffusion Constant Ratios for 2,6-DNT. The liquid phase diffusion constant for 2,6-DNT was calculated from equation (5.18),

$$D_\ell^C/D_\ell^O = \left( V_b^O/V_b^C \right)^{0.589} \quad (5.18)$$

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  $25.6 \text{ cm}^3 \text{ mol}^{-1}$ . 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

$$\begin{aligned} (\Sigma v)^{1/3} &= [(7 \times 16.5) + (6 \times 1.98) + (4 \times 5.48) + (2 \times 5.69) - 20.2]^{1/3} \\ &= 140.48^{1/3} = 5.20 \text{ cm}^3 \text{ mol}^{-1} \end{aligned}$$

Then,

$$\begin{aligned} D_g^C/D_g^W &= 85 \frac{(1/182 + 0.0347)^{1/2}}{[5.20 + 2.72]^2} \\ &= 85 \times (0.200/62.7) = 0.271 \end{aligned}$$



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,

$$k_v^C = \frac{1}{200} \left[ \frac{1}{1.8 \times (0.322)^{1.0}} + \frac{62.4 \times 293}{0.35 \times 2100 \times (0.271)^{0.7}} \right]^{-1}$$

$$= \frac{1}{200} (1.72 + 62.0)^{-1} = 7.84 \times 10^{-5} \text{ hr}^{-1}$$

$$t_{1/2} = (\ln 2)/7.84 \times 10^{-5} = 8.84 \times 10^3 \text{ hr} = 368 \text{ days}$$

For rivers,

$$k_v^C = \frac{1}{200} \left[ \frac{1}{8 \times (0.322)^{0.7}} + \frac{62.4 \times 293}{0.35 \times 2100 \times (0.271)^{0.7}} \right]^{-1}$$

$$= \frac{1}{200} (0.276 + 62.0)^{-1} = 8.02 \times 10^{-5} \text{ hr}^{-1}$$

$$t_{1/2} = (\ln 2)/8.02 \times 10^{-5} = 8.64 \times 10^3 \text{ hr} = 360 \text{ days}$$

### 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  $D_{\ell}^C/D_{\ell}^0$  and  $D_g^C/D_g^W$  were calculated using equations (5.18) and (5.20). The values for  $D_{\ell}^C/D_{\ell}^0$  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  $m^3 \text{ mol}^{-1}$ ), when liquid phase mass transport resistance controls about 80% of the volatilization rate for lakes or ponds and 14% for rivers.

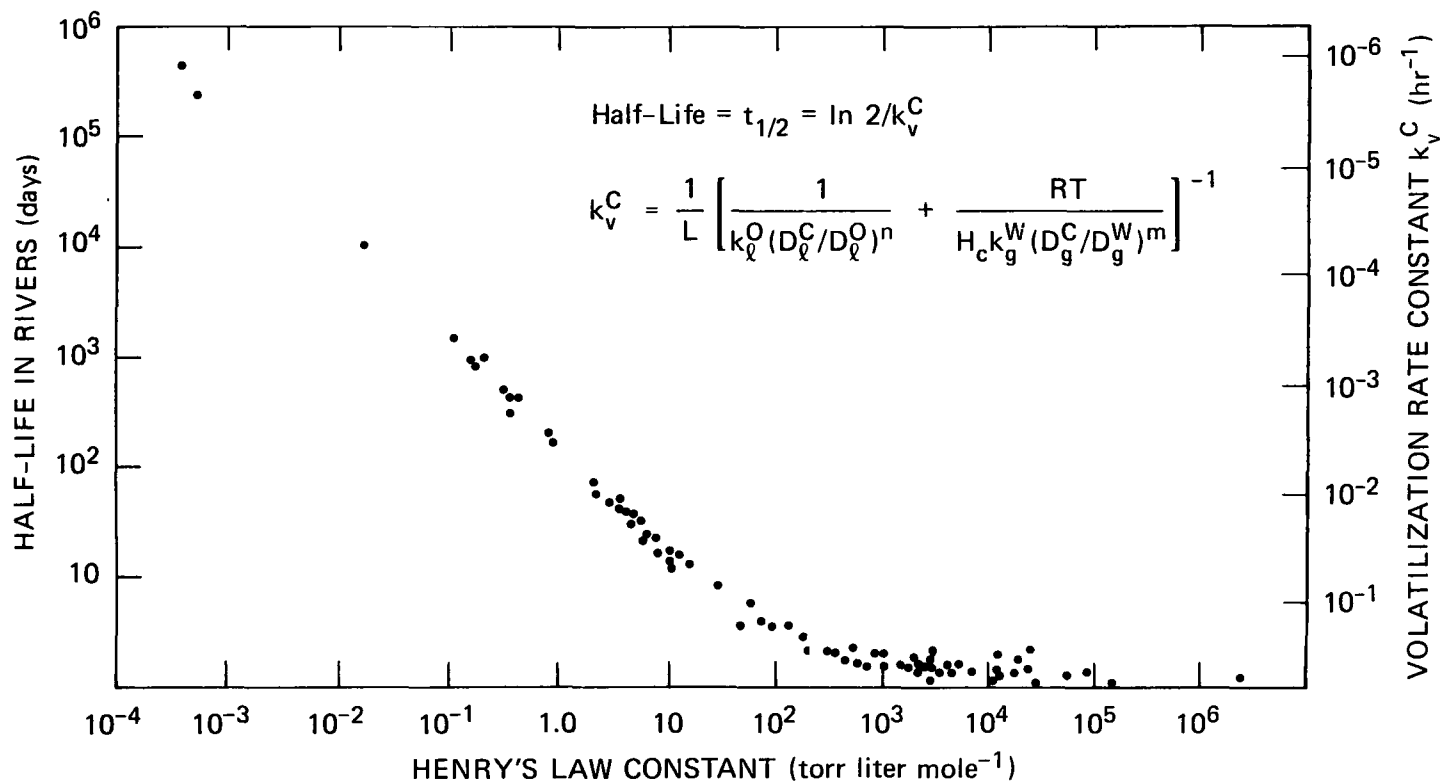
Aroclors. The seven aroclors consist of various proportions of chlorinated biphenyls, which include components with chlorine substitution ranging from zero to nine. The diffusion coefficient ratios  $D_{\ell}^C/D_{\ell}^0$  and  $D_g^C/D_g^W$  for each component of the mixtures (e.g., the  $Cl_2$  component) were first calculated. Overall diffusion coefficient ratios for each of the seven mixtures were then determined by

$$D_{\ell}^C/D_{\ell}^0 = \sum_{i=1}^9 f_i (D_{\ell}^C/D_{\ell}^0)_i$$

and

$$D_g^C/D_g^W = \sum_{i=1}^9 f_i (D_g^C/D_g^W)_i$$

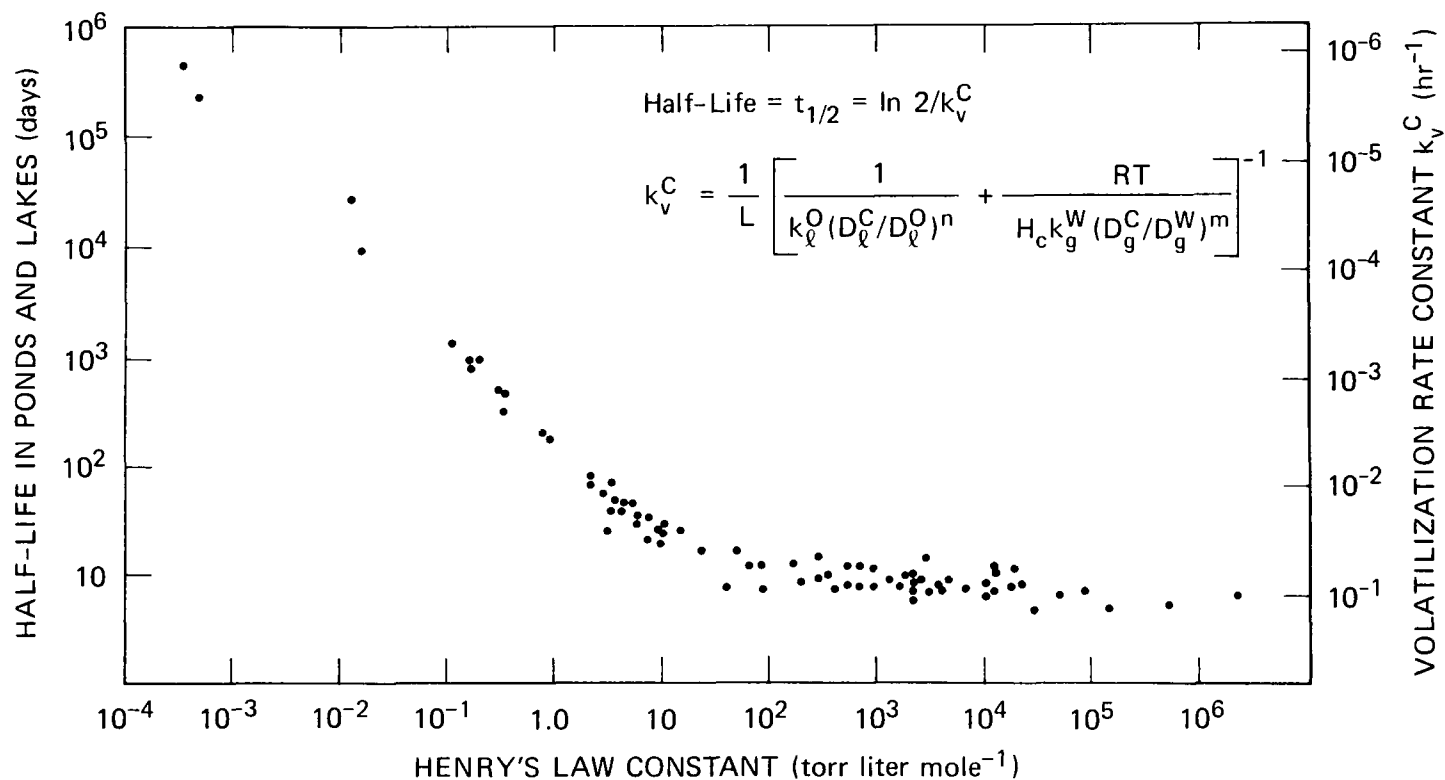
where  $f_i$  is the fraction of the  $i^{\text{th}}$  component of the mixture and  $(D_{\ell}^C/D_{\ell}^0)_i$  and  $(D_g^C/D_g^W)_i$  are the diffusion coefficient ratios of the  $i^{\text{th}}$  components. The Henry's constants for the aroclors were calculated from solubility and vapor pressure data of the complete mixture.



SA-6729-4B

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<sup>-1</sup>,  $k_g^W = 2100$  cm hr<sup>-1</sup>,  $n = m = 0.7$ )



SA-6729-3B

FIGURE 5.2 ESTIMATED HALF-LIVES VERSUS HENRY'S CONSTANT FOR THE PRIORITY POLLUTANTS IN LAKES OR PONDS

(Values used:  $L = 200$  cm,  $k_\ell^O = 1.8$  cm hr<sup>-1</sup>,  $k_g^W = 2100$  cm hr<sup>-1</sup>,  $n = 1$ ;  $m = 0.7$ .)

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 chlordane 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

$$R_v = - \frac{d[C_w]}{dt} = k_v [C_w] \quad (5.1)$$

$$k_v = \frac{1}{L} \left[ \frac{1}{k_\ell} + \frac{RT}{H_c k_g} \right]^{-1} \quad (5.22)$$

where

$R_v$  = volatilization rate of a chemical, C  
(moles liter<sup>-1</sup> hr<sup>-1</sup>)

$C_w$  = concentration of C in water  
 $k_v$  = volatilization rate constant ( $\text{hr}^{-1}$ )  
 $L$  = depth (cm)  
 $k$  = liquid phase mass transport coefficient  
 (cm  $\text{hr}^{-1}$ )  
 $H_c$  = Henry's law constant (torr  $M^{-1}$ )  
 $k_g$  = gas phase mass transport coefficient  
 (cm  $\text{hr}^{-1}$ )

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  $k_\ell$  and  $H_c k_g$ . Liss and Slater (1974) estimated values of  $k_\ell$  for  $\text{CO}_2$  (20 cm  $\text{hr}^{-1}$ ) and of  $k_g$  for water (1000 to 3000 cm  $\text{hr}^{-1}$ ). These values were assumed to be typical and substituted into equation (5.22). Then, the ratio of the first term 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  $M^{-1}$  ( $4.6 \times 10^{-3} \text{ atm m}^3 \text{ mol}^{-1}$ ). We have called chemicals that meet this requirement high volatility compounds. A similar calculation shows that if  $H_c$  is less than 10 torr  $M^{-1}$  ( $1.3 \times 10^{-5} \text{ atm m}^3 \text{ mol}^{-1}$ ), 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  $H_c > 3500 \text{ torr } M^{-1}$ ,  $R_v$  is determined by the value of  $k_\ell$  and is limited by diffusion through the liquid phase boundary layer since

$$k_v = k_\ell / L \quad (5.23)$$

For low volatility compounds, where  $H_c < 10 \text{ torr M}^{-1}$ , only the second term in equation (5.22) is significant. Then

$$k_v = \frac{H_c k_g}{LRT} \quad (5.24)$$

and the volatilization rate is limited by gas phase mass transport resistance. For intermediate volatility compounds, where  $3500 < H_c < 10 \text{ torr M}^{-1}$ , 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

$$k_\ell = D_\ell / \delta_\ell \quad (5.25)$$

$$k_g = D_g / \delta_g \quad (5.26)$$

where  $D$  is the diffusion coefficient and  $\delta$  is the boundary layer thickness. These equations suggest that the liquid and gas phase mass transport coefficients of the chemical,  $k_\ell^C$  and  $k_g^C$ , are proportional to the gas and liquid phase diffusion coefficients,  $D_\ell^C$  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).

$$k_\ell^A / k_\ell^B = f(D_\ell^A / D_\ell^B) \quad (5.27)$$

$$k_g^A / k_g^B = f(D_g^A / D_g^B) \quad (5.28)$$

In the liquid phase, oxygen is a convenient choice for a reference chemical since  $H_c$  for oxygen is  $1.2 \times 10^5 \text{ torr M}^{-1}$  at  $25^\circ\text{C}$  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

$$k_v^C/k_v^O = k_\ell^C/k_\ell^O = f(D_\ell^C/D_\ell^O) = \text{constant} \quad (5.29)$$

laboratory conditions (see Smith et al. 1980 and references therein).

Smith et al. (1980) have shown that

$$f(D_\ell^C/D_\ell^O) = (D_\ell^C/D_\ell^O)^m \quad (5.30)$$

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 (Treibal, 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  $M^{-1} = 4.6 \times 10^{-3} \text{ atm m}^3 \text{ mol}^{-1}$

$$(k_v^C)_{\text{env}} = (k_v^C/k_v^O)_{\text{lab}} (k_v^O)_{\text{env}} \quad (5.31)$$

where  $k_v^C$  is the volatilization rate constant for the chemical ( $\text{hr}^{-1}$ ) and  $k_v^O$  is the oxygen reaeration rate constant ( $\text{hr}^{-1}$ ) in the laboratory or the environment. The ratio  $k_v^C/k_v^O$  for benzene is independent of turbulence, salt concentration (seawater), temperature ( $4^\circ\text{--}50^\circ\text{C}$ ), or the presence of a surface-active compound (Smith et al., 1980). Also the value of  $(k_v^C/k_v^O)_{\text{lab}}$  can be predicted using

$$\left( \frac{k_v^C}{k_v^O} \right)_{\text{lab}} = \left( \frac{D_\ell^C}{D_\ell^O} \right)^{0.61} \quad (5.32)$$

where  $D_\ell$  is the liquid phase diffusion coefficient. This equation was also tested using laboratory measurements of  $k_v^C/k_v^O$  and estimates of  $D_\ell^C$  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)

$$k_g^A/k_g^B = f(D_g^A/D_g^B) = \text{a constant} \quad (5.33)$$

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

$$(k_g^C/k_g^W)_{\text{env}} = (k_g^C/k_g^W)_{\text{lab}} = f(D_g^C/D_g^W) = \text{a constant} \quad (5.34)$$

If classical two-film theory were a valid description of the mass transport, equation (5.33) would become

$$k_g^C/k_g^W = f(D_g^C/D_g^W) = (D_g^C/D_g^W)^m = \text{a constant} \quad (5.35)$$

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

$$k_\ell^C = k_\ell^O (D_\ell^C/D_\ell^O)^m \quad (5.36)$$

$$k_g^C = k_g^W (D_g^C/D_g^W)^n \quad (5.37)$$

If we know or can estimate  $k_\ell^O$ ,  $k_g^W$ , 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).

$$k_v^C = \frac{1}{L} \left[ \frac{1}{k_\ell^C} + \frac{RT}{H_c^C k_g^C} \right]^{-1} \quad (5.22)$$

$$= \frac{1}{L} \left[ \frac{1}{k_\ell^O (D_\ell^C/D_\ell^O)^m} + \frac{RT}{H_c^C k_g^W (D_g^C/D_g^W)^n} \right]^{-1} \quad (5.2)$$

This equation was used to estimate the volatilization rate constants of the priority pollutants.

#### 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  $k_\ell^0$  were calculated from literature estimates of  $k_v^0$ , which are summarized in Table 5.2.

Table 5.2

#### OXYGEN REAERATION RATES IN REPRESENTATIVE WATER BODIES

	Literature values (day <sup>-1</sup> )	Values used in Smith et al. <sup>a</sup> $k_v^0$			Corresponding value of $k_\ell^0$ (cm hr <sup>-1</sup> ) <sup>l</sup>
		(day <sup>-1</sup> )	(hr <sup>-1</sup> )	1 (cm)	
Pond	0.11 - 0.23 <sup>b</sup>	0.19	0.008	200	1.6
River	0.2, <sup>c</sup> 0.1 - 9.3 <sup>d</sup>	0.96	0.04	300	12
Lake	0.10 - 0.30 <sup>b</sup>	0.24	0.01	500	5

<sup>a</sup>Smith et al. (1977).

<sup>b</sup>Metcalf and Eddy (1972).

<sup>c</sup>Grenney et al. (1976).

<sup>d</sup>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  $k_v^0$  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

$$N^W = k_g^W \left( \frac{P_s^W - P^W}{RT} \right) \quad (5.38)$$

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  $0.59 \text{ cm sec}^{-1} = 2100 \text{ cm hr}^{-1}$ . 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 ( $\text{cm sec}^{-1} \times 10^6$ )	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, EXAMS 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  $k_\ell^O$  (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 overridden 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.

$$k_v^C/k_v^O = k_\ell^C/k_\ell^O = KVOG = (D_\ell^C/D_\ell^O)^{0.7} \quad (5.39)$$

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.

In EXAMS, the value of  $k_g^C$  is calculated from the wind speed, which is used to calculate  $k_g^W$  from

$$\text{WAT}(k_g^W) = 0.1857 + 11.36 \text{ WINDG} \quad (5.40)$$

where WINDG is the wind speed 10 cm above the water surface. The default value of WINDG is  $2 \text{ m sec}^{-1}$ , which gives a value of  $k_g^W = 2290 \text{ cm hr}^{-1}$ , in good agreement with the value of  $2100 \text{ cm hr}^{-1}$  that was estimated from the field data for water evaporation summarized in Table 5.3.

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# **TECHNICAL REPORT DATA**

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