

EPA/600/R-95/039
March 1995

ENVIRONMENTAL FATE CONSTANTS FOR
ADDITIONAL 27 ORGANIC CHEMICALS UNDER
CONSIDERATION FOR
EPA'S HAZARDOUS WASTE IDENTIFICATION PROJECTS

Compiled and edited by

Heinz P. Kollig

Contributors: J. Jackson Ellington
Samuel W. Karickhoff
Brenda E. Kitchens
Heinz P. Kollig
J. MacArthur Long
Eric J. Weber
N. Lee Wolfe

ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ATHENS, GA 30605-2700

DISCLAIMER

The information in this document has been funded by the United States Environmental Protection Agency. It has been subjected to the Agency's peer and administrative review and it has been approved for publication as an EPA document.

FOREWORD

As it becomes more and more obvious that many thousands of potentially hazardous man-made chemicals find their way into ambient environments, the need for a comprehensive understanding of the distribution of chemicals and their transport and transformation reaches a higher level of importance. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of chemical contaminants, the Chemistry Branch and the Measurements Branch determine the occurrence of unexpected organic chemicals in the environment, define mechanisms of transport and abiotic transformation, and develop and apply advanced methods to predict and measure physical and chemical transformation and equilibrium constants for use in exposure assessment.

Under Section 301 of the Resources Conservation and Recovery Act (RCRA), EPA's Office of Solid Waste is required to develop and promulgate criteria for identifying and listing hazardous wastes, taking into account, among other factors, persistence and degradability in the environment of selected chemicals. A requirement of the legislation is for EPA to take an initial step toward defining wastes that do not merit regulation under Subtitle C of RCRA and can be managed under other regimes. For establishing exemption criteria, the Agency has selected more than 200 chemical constituents that may occur in the various wastes. Some of the means by which these chemicals may be transformed, including hydrolysis degradation pathways and fate constants, were reported for 189 organic chemicals in a previous publication. This report is an addendum to this previous publication that provides an additional 27 chemicals with several more parameters added.

Rosemarie C. Russo, Ph.D.
Director
Environmental Research Laboratory
Athens, Georgia

ABSTRACT

Under Section 301 of the Resource Conservation and Recovery Act (RCRA), EPA's Office of Solid Waste is in the process of identifying chemicals to be considered in projects called the Hazardous Waste Identification Projects. A previous publication (EPA/600/R-93/132) addressed 189 organics in these projects. The environmental fate constants and chemical hydrolysis of an additional 27 organic chemicals are addressed in this report. Sorption coefficients are presented in terms of the octanol/water partition coefficient and the organic-carbon-normalized sediment/water partition coefficient. The ionization constant is given when this process affects sorption in the environmental pH range. Additionally, values for aqueous solubility, Henry's law constant, vapor pressure, and diffusivity are reported.

Table of Contents

Introduction	1
Definitions	3
Organic-carbon-normalized Sediment/water Partition Coefficient	3
Octanol/water Partition Coefficient	3
Water Solubility	3
Henry's law constant	4
Vapor Pressure	4
Diffusivity	4
Hydrolysis	4
Computation of log K_{oc}	5
Neutral Organic Compounds	5
Ionizable Organic Compounds	5
The Expert System SPARC	7
Data for Physical and Chemical Process Parameters.	8
References	10
Chemical Structures and Information on Hydrolysis.	11

Introduction

Assessment of potential risk posed to humans by man-made chemicals in the environment requires the prediction of environmental concentrations of those chemicals under various environmental reaction conditions. Whether mathematical models or other assessment techniques are employed, knowledge of equilibrium and kinetic constants (fate constants) is required to predict the transport and transformation of these chemicals.

Under section 301 of the Resource Conservation and Recovery Act (RCRA), EPA's Office of Solid Waste (OSW) has identified wastes that may pose a substantial hazard to human health and the environment. RCRA requires that EPA develop and promulgate criteria for identifying and listing hazardous wastes, taking into account, among other factors, persistence and degradability in the environment of selected chemicals.

EPA continues to believe that the Agency must assure continuity of the hazardous waste program while developing appropriate revisions. While fully preserving existing hazardous waste identification rules, EPA is considering alternatives to take an initial step towards defining wastes that do not merit regulation under Subtitle C and that can and will be safely managed under other regulatory regimes.

In the course of developing appropriate revisions, OSW is in the process of identifying chemicals to be considered in projects called the Hazardous Waste Identification Projects. At this time, there are more than 200 chemical constituents identified in these projects. The environmental fate constants and the chemical hydrolysis pathways of 189 organics were addressed in a previous report¹.

For the 27 selected organic compounds in this report, OSW requested that the Environmental Research Laboratory-Athens (ERL-Athens):

- a) identify those that do not hydrolyze.
- b) Identify those that do hydrolyze and list products of degradation including hydrolysis rate constants for parents and intermediates obtained either through laboratory experiments at ERL-Athens, literature searches, or pathway analyses.
- c) obtain sorption data as the organic-carbon-normalized sediment/water partition coefficient and the octanol/water partition coefficient either through laboratory experiments at ERL-Athens, literature searches, or computational techniques.
- d) obtain data for aqueous solubility, Henry's law constant, vapor pressure, and diffusivity.
- e) to the extent that current scientific knowledge will permit, identify those that will be subject to other important degradation reactions.

For compounds identified as having no hydrolyzable functional group (NHFG), hydrolysis will not occur by abiotic reaction pathways in the pH range of 5 to 9 at 25°C.

The compounds identified as having non-labile functional groups (NLFG) will not hydrolyze to any reasonable extent. Although a molecule with a non-labile functional group contains one or more heteroatoms, they react so slowly over the pH range of 5 to 9 at 25°C that their half-lives will be greater than 50 years, if they react at all.

Some compounds may exist in the environment as ionized species. The values given in this report are for the neutral form of these species. It should be understood that both the persistence and mobility of a chemical in the environment is influenced by many environmental factors that may change from environment to environment.

A team of EPA scientists met to discuss the rates and probable pathways of transformation for hydrolysis. The methods used to arrive at the reaction products were based primarily on the team's experience with similar compounds, their knowledge of the theory of these processes, and their understanding of structure-activity relationships.

This report includes:

1. A short definition for:

- a) Organic-carbon-normalized sediment/water partition coefficient (K_{oc})
- b) Octanol/water partition coefficient (K_{ow})
- c) Water solubility
- d) Henry's law
- e) Vapor pressure
- f) Diffusivity
- g) Hydrolysis

2. A short treatise on how the $\log K_{oc}$ was computed from the $\log K_{ow}$.

3. A short treatise on the computational expert system SPARC² (SPARC Performs Automated Reasoning in Chemistry) which was used to compute the values for the octanol/water partition coefficient, the water solubility, the Henry's law constant, the vapor pressure, and the diffusivity.

4. Table 1 containing the data for the individual parameters at 25°C.

5. A structural representation of each chemical including information on chemical hydrolysis.

For a more detailed treatise on chemical hydrolysis and sorption, the reader is referred to the previous publication (EPA/600/R-93/132).

Definitions

Organic-carbon-normalized Sediment/water Partition Coefficient (K_{oc})

The K_{oc} value for a chemical is given by:

$$K_{oc} = K_p / f_{oc}$$

where

$K_p = C_s / C_w$ = sediment/water partition coefficient

f_{oc} = fraction organic carbon (weight basis)

C_s = concentration of chemical on sediment

C_w = concentration of chemical in water

and is used to estimate the K_p value for a sediment of known organic carbon fraction, f_{oc} .

Because K_{oc} values are normalized for the organic carbon content in the sediment, they can be used to estimate the K_p values for other sediments. Some researchers use total organic matter for normalization and obtain K_{om} instead of K_{oc} .

Octanol/water Partition Coefficient (K_{ow})

The octanol/water partition coefficient (K_{ow}), is defined as the ratio of the equilibrium concentration of a dissolved substance in a system consisting of n-octanol and water, and is ideally dependent upon temperature and pressure.

$$K_{ow} = C_{oct} / C_w$$

where C_{oct} is the concentration of the substance in n-octanol and C_w is the concentration of the substance in water. The K_{ow} is useful in predicting soil adsorption, biological uptake, lipophilic storage and biomagnification. It is also useful in estimating the organic-carbon-normalized sediment/water partition coefficient (K_{oc}) and the water solubility (S_w) using property reactivity correlations, and is frequently reported in the form of its logarithm to base ten as $\log P$.

Water Solubility (S_w)

Water solubility is defined as the quantity of solute present in a given amount of saturated water, at a certain temperature. S_w of a chemical is an important characteristic for that chemical's potential environmental movement and distribution. A number of processes can be affected by S_w such as adsorption and desorption on soils, hydrolysis, photolysis, oxidation/reduction, and biodegradation. S_w values are often used for estimating Henry's law constants for calculating volatilization rate constants. A good correlation has been established between solubilities of organic compounds and their octanol/water partition coefficients.

Henry's law constant (H_c)

Henry's law states that the solution of a gas in a liquid is directly proportional to the pressure of the gas above the liquid at a definite temperature and is given by: $H_c = PX^{-1}$, where P is the partial pressure and X is the mole fraction. Hence, H_c data are often used to calculate vapor pressure and the rate of volatilization and can be regarded as the ratio of vapor pressure to water solubility.

Vapor Pressure (P_v)

Vapor pressure is defined as the pressure exerted by a vapor when a state of equilibrium has been reached between a liquid, solid, or solution, respectively, and its vapor. P_v increases as the temperature increases, and P_v values for certain compounds (e.g. chlorinated benzenes and phenols) can be estimated graphically from the boiling points and the boiling point/vapor pressure relationship for homologous series. P_v data can also be estimated using: $P_v = H_c S_w$, where H_c is Henry's law constant and S_w is water solubility. P_v values are used for the calculation of volatilization rates.

Diffusivity

Diffusivity or coefficient of diffusion represents the quantity of gas travelling one centimeter per second through a surface of one square centimeter.

Hydrolysis

In general, hydrolysis is a bond-making, bond-breaking process in which a molecule, RX , reacts with water forming a new $R-O$ bond with the oxygen atom from water and cleaving an $R-X$ bond in the original molecule. One possible pathway is the direct displacement of X^- with HO^- as shown in Equation 1.



The detailed mechanisms of hydrolytic processes are well defined and have been shown to involve the formation of intermediates such as protonated species, anions and carbonium ions, as well as combinations of these intermediates.

Computation of $\log K_{oc}$

Neutral Organic Compounds

Partitioning between water and natural soils, sediments, and aquifer materials is an important process affecting transport, transformation rates, toxicity, and the ultimate disposition of organic chemicals in the environment. Research focusing on the partitioning of neutral organic compounds has shown that adsorption of these compounds is usually controlled by hydrophobic interactions. As a result, the affinity that a natural sorbent has for neutral organic solutes, in most cases, can be reliably estimated from characterization (quantification) of the hydrophobicity of the chemical and the sorbent.

For neutral compounds, the organic-carbon-normalized sediment/water partition coefficients in Table 1 have been calculated using the relationship,

$$\log K_{oc} = \log K_{ow} - 0.32 \quad (2)$$

given by Hassett et al³. This correlation was calculated from adsorption isotherms of 13 organic chemicals, representing several classes of compounds, using 14 different sediment and soil samples. This correlation adequately predicts partitioning of several classes of organic compounds, including chlorinated and nonchlorinated aromatic and alkyl hydrocarbons. Use of this correlation will generally be valid for soils, sediments, and aquifer materials that have organic carbon contents greater than 0.1%.

Ionizable Organic Compounds

Predicting the partitioning of ionizable organic compounds is not as straightforward as for the neutral compounds. These compounds, whether they are acids or bases, can exist as ions in solution depending upon the pH of the solution.

In general, more effort has been expended investigating the sorption of organic acids than the sorption of organic bases. For organic acids, adsorption can be modeled to sediments, soils, and aquifer materials in a similar manner to that of the neutral compounds, after taking into account ionization, as long as the pH is not more than one unit above the pK_a of the compound^{4,5}.

For organic acids, the pK_a must be considered in the computation of the K_{oc} . The following relationship was used:

$$6 < \text{p}K_a < 9: K_{oc} = 1.05K_{ow}^{(0.82)} \frac{1}{1.0 + \frac{K_a}{[H^+]}} \quad (3)$$

which simplifies at pH 7 to:

$$K_{oc} = \frac{1.05 \times 10^{-7} \times K_{ow}^{(0.82)}}{10^{-7} + K_a} \quad (4)$$

The Expert System SPARC

All values in Table 1, including pK_a , were computed with SPARC² (SPARC Performs Automated Reasoning in Chemistry) except values for the $\log K_{ow}$, which were computed manually from the $\log K_{ow}$ values.

SPARC is a computational expert system that predicts chemical reactivity. The system has the capability of crossing chemical boundaries to cover all organic chemicals and uses algorithms based on fundamental chemical structure theory to estimate parameters. SPARC quantifies reactivity by classifying molecular structures and selecting appropriate "mechanistic" models. It uses an approach that combines principles of quantitative structure-activity relationships, linear free energy theory (LFET), and perturbed molecular orbital (PMO) or quantum chemistry theory. In general, SPARC utilizes LFET to compute thermal properties and PMO theory to describe quantum effects such as delocalization energies or polarizabilities of π electrons.

For example, SPARC computes the log of the octanol-water partition coefficient from activity coefficients in the octanol (γ_o^∞) and water (γ_w^∞) phases:

$$\log K_{ow} = \log \frac{\gamma_w^\infty}{\gamma_o^\infty} + \log \frac{M_o}{M_w} \quad (5)$$

where M_o and M_w are solvent molecularities of octanol and water, respectively. Activity coefficients for either solvent or solute are computed by solvation models that are built from structural constituents requiring no data besides the structures.

A goal for SPARC is to compute values that are as accurate as values obtained experimentally for a fraction of the cost required to measure them. Because SPARC does not depend on laboratory measurements conducted on compounds with structures closely related to that of the solute of interest, it does not have, for instance, the inherent problems of phase separation encountered in measuring highly hydrophobic compounds ($\log K_{ow} > 5$). For these compounds, SPARC's computed value should, therefore, be more reliable than a measured one. However, at this time no SPARC version has been assigned for the physical property calculator. Data computed after future refinement in the calculator may, therefore, be slightly different. The number of significant figures reflects the certainty in the computation of the calculator.

TABLE 1. Data for Physical and Chemical Process Parameters.

Common Name	Chemical Abstract Service No.	Water Solubility (mg/L)	Sorption Log K_{oc}	Sorption Log K_{ow}	Henry's law constant (atm ³ /mol)	Vapor Pressure (torr)	Diffusivity in Air (cm ² /s)	Hydrolysis
1. Anthracene	120-12-7	7.6E-2	4.21	4.53	1.9E-5	6.1E-6	0.055	NHFG
2. Benzenethiol ^a pK _a = 6.5	108-98-5	7.6E2	1.32	2.35	4.4E-4	2.4	0.076	NLFG (OXIDIZES)
3. Benzo[<i>g,h,i</i>]perylene	191-24-2	1.2E-4	6.28	6.60	1.2E-7	4.0E-11	0.039	NHFG
4. Benzo[<i>k</i>]fluoranthene	207-08-9	9.4E-4	6.0	6.3	5.0E-7	1.4E-9	0.041	NHFG
5. Bromobenzene	108-86-1	4.1E2	2.43	2.75	2.1E-3	4.2	0.073	NLFG ^b
6. <i>n</i> -Butylbenzene	104-51-8	21	3.8	4.1	9.7E-3	1.1	0.060	NHFG
7. <i>sec</i> -Butylbenzene	135-98-8	38	3.6	3.9	9.8E-3	2.1	0.061	NHFG
8. Carbazole	86-74-8	4.0E-1	3.3	3.6	8.6E-7	1.6E-6	0.062	NHFG
9. Crotonaldehyde	4170-30-3	1.3E5	-0.06	0.26	3.1E-5	4.5E1	0.093	SEE PAGE 13
10. Dibenzofuran	132-64-9	4.3	3.8	4.1	1.4E-4	2.7E-3	0.059	NHFG
11. 1,2,3,4,6,7,8- Heptachlorodibenzo- furan	67562-39-4	9.5E-7	8.20	8.52	3.7E-5	6.5E-11	0.043	NLFG
12. 1,2,3,4,7,8,9- Heptachlorodibenzo- furan	55673-89-7	1.3E-6	8.2	8.5	3.8E-5	9.5E-11	0.043	NLFG

Common Name	Chemical Abstract Service No.	Water Solubility (mg/L)	Sorption Log K_{oc}	Sorption Log K_{ow}	Henry's law constant (atm ³ /mol)	Vapor Pressure (torr)	Diffusivity in Air (cm ² /s)	Hydrolysis
13. 1,2,3,4,6,7,8-Heptachlorodibenzo- <i>p</i> -dioxin	35822-46-9	1.9E-7	8.53	8.85	4.1E-5	1.4E-11	0.043	NLFG
14. 1,2,3,4,7,8-Hexachlorodibenzo-furan	70648-26-9	7.3E-6	7.54	7.86	4.2E-5	6.3E-10	0.045	NLFG
15. 1,2,3,6,7,8-Hexachlorodibenzo-furan	57117-44-9	6.9E-6	7.55	7.87	4.2E-5	5.9E-10	0.045	NLFG
16. 1,2,3,7,8,9-Hexachlorodibenzo-furan	72918-21-9	7.3E-6	7.55	7.87	4.3E-5	6.4E-10	0.045	NLFG
17. 2,3,4,6,7,8-Hexachlorodibenzo-furan	60851-34-5	7.6E-6	7.54	7.86	4.1E-5	6.3E-10	0.045	NLFG
18. 2-Hexanone	591-78-6	1.8E4	1.0	1.3	8.7E-5	1.2E1	0.072	NHFG
19. Indene	95-13-6	3.9E2	2.5	2.8	5.0E-4	1.3	0.071	NHFG
20. <i>p</i> -Isopropyltoluene	99-87-6	28	3.7	4.0	9.3E-3	1.5	0.060	NHFG
21. 2-Methylchrysene	3351-32-4	8.5E-4	5.82	6.14	1.2E-6	3.1E-9	0.044	NHFG
22. 1-Methylnaphthalene	90-12-0	40	3.52	3.84	2.8E-4	6.6E-2	0.060	NHFG
23. 2-Methylnaphthalene	91-57-6	33	3.54	3.86	3.0E-4	5.8E-2	0.061	NHFG
24. Phenanthrene	85-01-8	1.1	4.25	4.57	2.3E-5	1.0E-4	0.055	NHFG
25. <i>n</i> -Propylbenzene	103-65-1	57	3.35	3.67	9.9E-3	3.6	0.065	NHFG

Common Name	Chemical Abstract Service No.	Water Solubility (mg/L)	Sorption Log K _{oc}	Sorption Log K _{ow}	Henry's law constant (atm·m ³ /mol)	Vapor Pressure (torr)	Diffusivity in Air (cm ² /s)	Hydrolysis
26. 1,2,4-Trimethylbenzene	95-63-6	70	3.28	3.60	4.9E-3	2.2	0.065	NHFG
27. 1,3,5-Trimethylbenzene	108-67-8	67	3.37	3.69	6.3E-3	2.7	0.065	NHFG

a. Values reported are for neutral species.

b. Bromobenzene was tested in the laboratory for hydrolysis. No disappearance was noted after 29 days at 85°C in 0.1N sodium hydroxide and 0.1N hydrochloric acid.

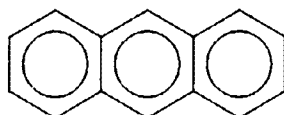
References

1. Kollig, H.P. 1993. Environmental Fate Constants for Organic Chemicals Under Consideration for EPA's Hazardous Waste Identification Projects. U.S. EPA, Environmental Research Laboratory, Athens, GA, EPA/600/R-93/132.
2. Karickhoff, S.W., L.A. Carreira, C. Melton, V.K. McDaniel, A.N. Vellino, and D.E. Nute. 1989. Computer Prediction of Chemical Reactivity--The Ultimate SAR. U.S. Environmental Protection Agency, Athens, GA. EPA/600/M-89/017.
3. Hassett, J.J., J.C. Means, W.L. Banwart, and S.G. Wood. 1980. Sorption Properties of Sediments and Energy-related Pollutants. U.S. Environmental Protection Agency, Athens, GA, EPA-600/3-80-041.
4. Schellenberg, K., C. Leuenberger, and R.P. Schwarzenbach. 1984. Sorption of chlorinated phenols by natural sediments and aquifer materials. *Environ. Sci. Technol.* 18(9):652-657.
5. Jafvert, C.T. 1990. Sorption of organic acid compounds to sediments: initial model development. *Environ. Toxicol. Chem.* 9:1259-1268.

Chemical Structures and Information on Hydrolysis.

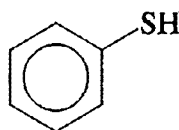
1. Anthracene (120-12-7)

Anthracene will not hydrolyze. It has no hydrolyzable functional group.



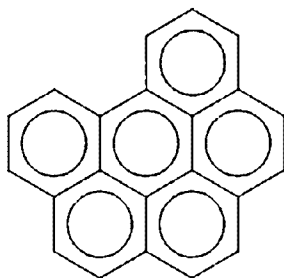
2. Benzenethiol (108-98-5)

Benzenethiol will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



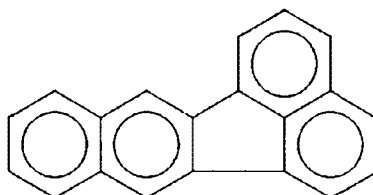
3. Benzo[g,h,i]perylene (191-24-2)

Benzo[g,h,i]perylene will not hydrolyze. It has no hydrolyzable functional group.



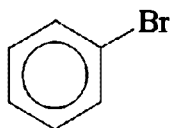
4. Benzo[k]fluoranthene (207-08-9)

Benzo[k]fluoranthene will not hydrolyze. It has no hydrolyzable functional group.



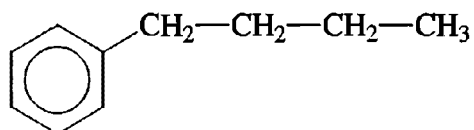
5. Bromobenzene (108-86-1)

Bromobenzene will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



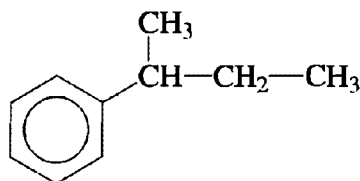
6. n-Butylbenzene (104-51-8)

n-Butylbenzene will not hydrolyze. It has no hydrolyzable functional group.



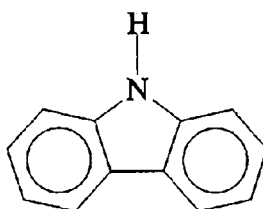
7. sec-Butylbenzene (135-98-8)

sec-Butylbenzene will not hydrolyze. It has no hydrolyzable functional group.



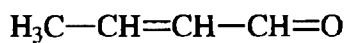
8. Carbazole (86-74-8)

Carbazole will not hydrolyze. It has no hydrolyzable functional group.

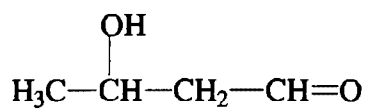


9. Crotonaldehyde (4170-30-3)

Crotonaldehyde undergoes a rapid addition of water across the double bond (Michael addition) to yield 3-hydroxy-1-butanal.



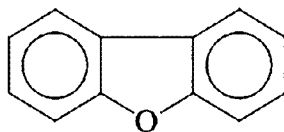
Crotonaldehyde



3-Hydroxy-1-butanal

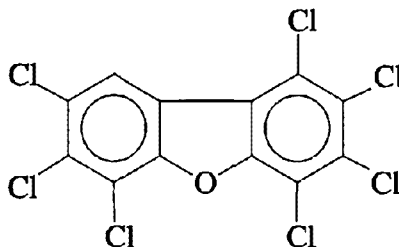
10. Dibenzofuran (132-64-9)

Dibenzofuran will not hydrolyze. It has no hydrolyzable functional group.



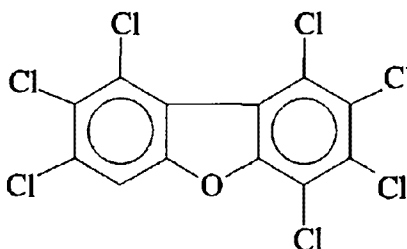
11. 1,2,3,4,6,7,8-heptachlorodibenzofuran (67562-39-4)

1,2,3,4,6,7,8-Heptachlorodibenzofuran will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



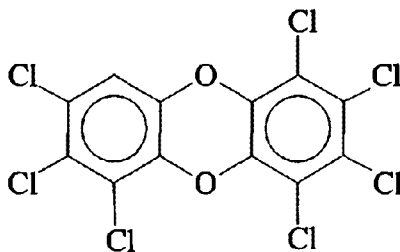
12. 1,2,3,4,7,8,9-Heptachlorodibenzofuran (55673-89-7)

1,2,3,4,7,8,9-Heptachlorodibenzofuran will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



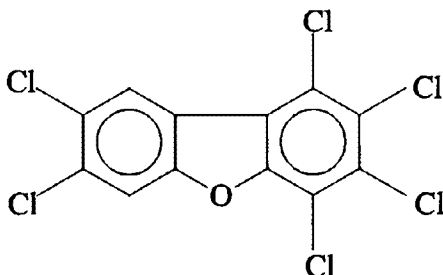
13. 1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin (35822-46-9)

1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



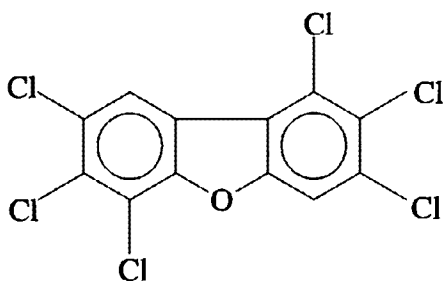
14. 1,2,3,4,7,8-Hexachlorodibenzofuran (70648-26-9)

1,2,3,4,7,8-Hexachlorodibenzofuran will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



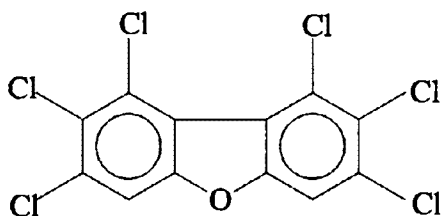
15. 1,2,3,6,7,8-Hexachlorodibenzofuran (57117-44-9)

1,2,3,6,7,8-Hexachlorodibenzofuran will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



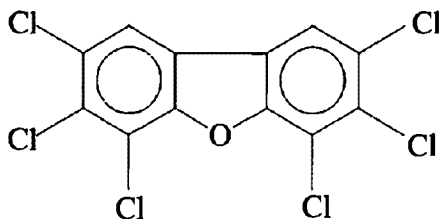
16. 1,2,3,7,8,9-Hexachlorodibenzofuran (72918-21-9)

1,2,3,7,8,9-Hexachlorodibenzofuran will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



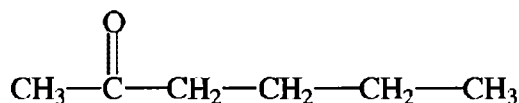
17. 2,3,4,6,7,8-Hexachlorodibenzofuran (60851-34-5)

2,3,4,6,7,8-Hexachlorodibenzofuran will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



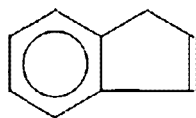
18. 2-Hexanone (591-78-6)

2-Hexanone will not hydrolyze. It has no hydrolyzable functional group.



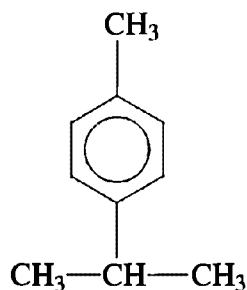
19. Indene (95-13-6)

Indene will not hydrolyze. It has no hydrolyzable functional group.



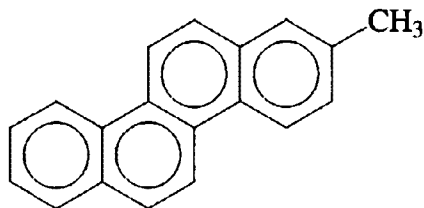
20. p-Isopropyltoluene (99-87-6)

p-Isopropyltoluene will not hydrolyze. It has no hydrolyzable functional group.



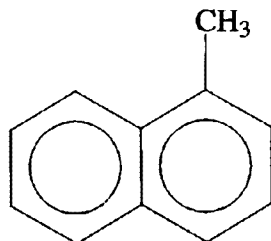
21. 2-Methylchrysene (3351-32-4)

2-Methylchrysene will not hydrolyze. It has no hydrolyzable functional group.



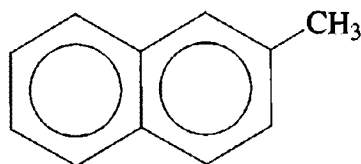
22. 1-Methylnaphthalene (90-12-0)

1-Methylnaphthalene will not hydrolyze. It has no hydrolyzable functional group.



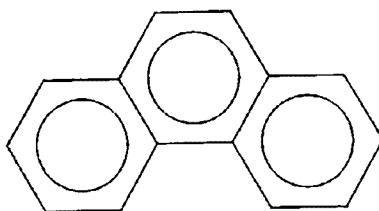
23. 2-Methylnaphthalene (91-57-6)

2-Methylnaphthalene will not hydrolyze. It has no hydrolyzable functional group.



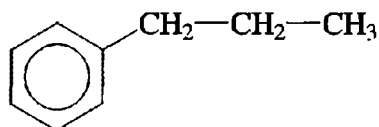
24. Phenanthrene (85-01-8)

Phenanthrene will not hydrolyze. It has no hydrolyzable functional group.



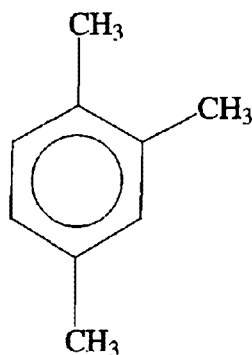
25. n-Propylbenzene (103-65-1)

n-Propylbenzene will not hydrolyze. It has no hydrolyzable functional group.



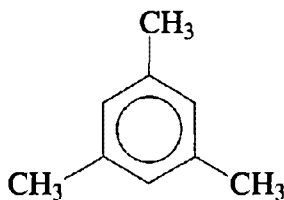
26. 1,2,4-Trimethylbenzene (95-63-6)

1,2,4-Trimethylbenzene will not hydrolyze. It has no hydrolyzable functional group.



27. 1,3,5-Trimethylbenzene (108-67-8)

1,3,5-Trimethylbenzene will not hydrolyze. It has no hydrolyzable functional group.



TECHNICAL REPORT DATA
(Please read Instructions on the reverse before comp)

1. REPORT NO. EPA/600/R-95/039		2.	
4. TITLE AND SUBTITLE ENVIRONMENTAL FATE CONSTANTS FOR ADDITIONAL 27 ORGANIC CHEMICALS UNDER CONSIDERATION FOR EPA'S HAZARDOUS WASTE IDENTIFICATION PROJECTS		5. REPORT DATE March 1995	
7. AUTHOR(S) Heinz P. Kollig		6. PERFORMING ORGANIZATION CODE	
9. PERFORMING ORGANIZATION NAME AND ADDRESS Environmental Research Laboratory U.S. Environmental Protection Agency Athens GA 30605		8. PERFORMING ORGANIZATION REPORT NO.	
12. SPONSORING AGENCY NAME AND ADDRESS Environmental Research Laboratory - Athens, GA Office of Research and Development U.S. Environmental Protection Agency Athens GA 30605-2700		10. PROGRAM ELEMENT NO. CC5D1A	
		11. CONTRACT/GRANT NO.	
15. SUPPLEMENTARY NOTES		13. TYPE OF REPORT AND PERIOD COVERED	
16. ABSTRACT <p>Under Section 301 of the Resource Conservation and Recovery Act (RCRA), EPA's Office of Solid Waste is in the process of identifying chemicals to be considered in projects called the Hazardous Waste Identification Projects. A previous publication (3PA/600/R-93/132) addressed 189 organics in these projects. The environmental fate constants and chemical hydrolysis of an additional 27 organic chemicals are addressed in this report. Sorption coefficients are presented in terms of the octanol/water partition coefficient and the organic-carbon-normalized sediment/water partition coefficient. The ionization constant is given when this process affects sorption in the environmental pH range. Additionally, values for aqueous solubility, Henry's law constant, vapor pressure, and diffusivity are reported.</p>		14. SPONSORING AGENCY CODE EPA/600/01	
17. KEY WORDS AND DOCUMENT ANALYSIS			
a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group	
Hydrolysis Hazardous waste Sorption coefficients Fate constants			
18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS (This Report) UNCLASSIFIED	21. NO. OF PAGES 24	
	20. SECURITY CLASS (This page) UNCLASSIFIED	22. PRICE	