

***Environmental Fate Constants for  
Organic Chemicals Under  
Consideration for  
EPA's Hazardous Waste Identification Rule (HWIR)***

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## FOREWORD

As it becomes more and more obvious that many thousands of potentially hazardous manmade 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 some 200 chemical constituents that may occur in the various wastes. This report explains some of the means by which these chemicals may be transformed and provides hydrolysis degradation pathways and fate constants for the selected chemicals.

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## **ABSTRACT**

Under Section 301 of the Resource Conservation and Recovery Act (RCRA), EPA's Office of Solid Waste has identified some 200 chemicals to be listed in a proposed rule called the Hazardous Waste Identification Rule (HWIR). This publication addresses the 189 organics listed in the HWIR. The environmental fate constants and the chemical hydrolysis pathways of these chemicals are listed. Chemical hydrolysis rate constants for parent compounds and products including structural presentation of the pathways are presented. Redox rate constants are given for selected compounds. Sorption coefficients are presented for parents and products 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.

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## Introduction

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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.

In the May 20, 1992, *Federal Register*, EPA proposed two approaches for amending its regulations under RCRA for hazardous waste identification. The proposed rule is called the Hazardous Waste Identification Rule (HWIR). The first proposed approach would establish Concentration-Based Exemption Criteria (CBEC) for listed hazardous wastes, waste mixtures, derivatives, and media (including soils and ground-water) contaminated with certain listed hazardous wastes for exiting RCRA Subtitle C management requirements. The second proposed approach is referred to as the Expanded CHaracteristics Option (ECHO). It would establish "characteristic" levels for listed hazardous wastes, waste mixtures, derivatives, and media (including soils and ground-water) contaminated with certain listed hazardous wastes for both entering and exiting RCRA Subtitle C via an expansion of the number of toxic constituents in the Toxicity Characteristics (TC) rule.

Under the CBEC approach, listed wastes and contaminated media meeting the established criteria would no longer be subject to some of the hazardous waste management requirements under Subtitle C of RCRA.

Under the ECHO approach, listed wastes and contaminated media that do not exhibit a hazardous characteristic would not be regulated by the hazardous waste management requirements under Subtitle C of RCRA.

The purpose of this rulemaking is 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. For establishing exemption criteria, the Agency has selected some 200 chemical constituents. The environmental fate constants and the chemical hydrolysis pathways of the organics are listed in Part I and Part II of this report, respectively. Inorganic compounds are not addressed in this publication.

For all organic compounds on the HWIR list, 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 either through laboratory experiments at ERL-Athens, literature searches, or computational techniques.
- d) to the extent that current scientific knowledge will permit, identify those that will be subject to other important degradation reactions and identify products of these reactions including rate constants.

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.

Polychlorinated biphenyls (PCBs) have been addressed here only as a class because of the many different congeners of these compounds. The given Chemical Abstract Service number 1336-36-3 is the number for the general class of Aroclors without designating any specific Aroclor. Because PCBs will not hydrolyze to any reasonable extent, our Pathway Analysis Team classified them as non-labile. The sorptive capacity, however, will be different from congener to congener. We have found reported  $\log K_{ow}$  values ranging from 2.59 to 11.20. Therefore, a single sorption value for the class of Aroclors was not assigned.

The chemical hydrolysis pathways of compounds with negative boiling points that exist as gases at room temperature were not addressed in this report.

Some compounds may exist in the environment as ionized species. The transformation pathways show these species in the neutral form for better identification. 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. The values in this document are for those conditions specified in the references.

A team of EPA scientists met several times to discuss the rates and probable pathways of transformation for hydrolysis and redox reactions. 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. For hydrolysis, the team's decisions are identified in Table 1 with a zero in the Reference column. Final stable products are identified as containing either no hydrolyzable functional group (NHFG) or a non-labile functional group (NLFG) in the Comment column.

Literature searches were conducted afterwards to find needed fate data for the intermediate products of hydrolysis. If the literature failed to provide the required data, they were determined in the laboratory for some compounds.

*This report is composed of two parts. Part I includes text and data on chemical hydrolysis, sorption, and redox reactions. Part II includes the chemical structures of all organic*

*compounds on the HWIR list and the pathways of chemical hydrolysis of those compounds that undergo this transformation. When a compound was identified as NHFG, the text with the structure will say that the compound will not hydrolyze. When a compound was identified as NLFG, the text with the structure will say that the compound will not hydrolyze to any reasonable extent. When a compound might be subject to other abiotic transformation processes, the text with the structure will point this out; however, these processes have not been identified.*



## Hydrolysis

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### General

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<sup>-</sup> with HO<sup>-</sup> 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.

Generally, hydrolysis of organic compounds in water under pH-buffered conditions is first-order in the concentration of the organic species ([RX]), where the rate of hydrolysis ( $d[\text{RX}]/dt$ ) is proportional to the concentration of pollutant RX:

$$\frac{d[\text{RX}]}{dt} = -k_{\text{obs}}[\text{RX}] \quad (2)$$

Where  $k_{\text{obs}}$  is the observed pseudo-first-order disappearance rate constant. The first-order dependence of the disappearance rate on [RX] is important, because it means that the half-life ( $t_{1/2}$ ) of the reaction described by Equation 2 is independent of [RX]. Thus, the results obtained at a high RX concentration can be extrapolated to lower RX concentrations if other reaction conditions are held constant. The half-life of the reacting compound is given by Equation 3:

$$t_{1/2} = \frac{\ln 2}{k_{\text{obs}}} = \frac{0.693}{k_{\text{obs}}} \quad (3)$$

where  $k_{\text{obs}}$  can include contributions from acid-catalyzed or base-mediated hydrolysis, nucleophilic attack by water, or catalysis by buffers in the reaction medium.

For abiotic hydrolysis, the general expression for  $k_{\text{obs}}$  is given by:

$$k_{\text{obs}} = k_a[\text{H}^+] + k_b[\text{HO}^-] + k_n + \sum_i k_{\text{HA}i}[\text{HA}_i] + \sum_j k_{\text{A}j}[\text{A}_j] \quad (4)$$

where  $k_a$  and  $k_b$  are the specific acid and base second-order rate constants, respectively;  $k_n$  is the neutral hydrolysis rate constant; and  $k_{\text{HA}i}$  and  $k_{\text{A}j}$  are the general acid-catalyzed and base-mediated hydrolysis rate constants, respectively. In Equation 4,  $[\text{H}^+]$  and  $[\text{HO}^-]$  are the hydrogen and hydroxyl ion concentrations, respectively, and  $[\text{HA}_i]$  and  $[\text{A}_j]$  are the

concentrations of the *i*th and the *j*th pair of general acids and bases in the reaction mixture, respectively.

In Table 1,  $k_a$ ,  $k_b$ , and  $k_n$  values are reported for the particular chemical at 25°C (+/-4°C). A half-life at 25°C can be calculated by using Equation 4 to calculate  $k_{obs}$ , followed by Equation 3 to calculate the time at 50% hydrolysis. Concentration and time units used are molar (M) and year (Y), respectively. Products of hydrolysis are listed indented under the parent compound, e.g., acetonitrile (parent): acetamide is the first hydrolysis product and it then becomes an intermediate by hydrolyzing to a secondary product, acetic acid. Both products are indented according to the order of their appearance in the hydrolysis pathway of the original parent.

Hydrolysis rate constants that were reported in the literature at an elevated temperature were reanalyzed with RATE<sup>28</sup> to extrapolate the values to 25°C. These reanalyzed values are identified by RATE in the Comment column. Those compounds that were identified as non-hydrolyzable or non-labile were designated as 'NHFG' and 'NLFG', respectively, in the Comment column.

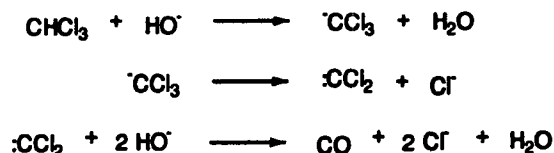
## Halogenated Aliphatics

### Simple halogenated aliphatics

Hydrolysis of the simple halogenated aliphatics (halogen substitution at one carbon atom) is generally pH independent, resulting in the formation of alcohols by nucleophilic substitution with water (Equation 1). Although a number of the simple halogenated aliphatics are susceptible to base-mediated hydrolysis, the rate term for the base-mediated process will not contribute to the overall hydrolysis rate under environmental conditions.

The halogenated methanes, except for the trihalomethanes, hydrolyze by direct nucleophilic displacement by water ( $S_N2$  mechanism). An increase in the number of halogen substituents on carbon increases the hydrolysis half-life because of the greater steric bulk about the site of nucleophilic attack. The type of halogen substituent also affects reactivity. For example, hydrolysis data indicate that the fluorinated aliphatics are much more stable than the chlorinated aliphatics, which in turn are more stable than the brominated aliphatics ( $F > Cl > Br$ ). This trend in reactivity reflects the strength of the carbon-halogen bond that is broken in the nucleophilic substitution reaction.

Hydrolysis of the trihalomethanes, or haloforms, is thought to occur initially by proton abstraction and subsequent formation of the carbene, which reacts with  $HO^-$  to form carbon monoxide and chloride ion:<sup>41</sup>



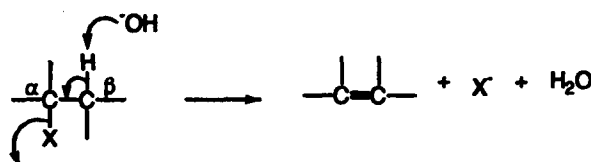


In contrast to the halogenated methanes which have hydrolysis half-lives on the order of years, the hydrolysis half-lives for allylic and benzylic halides are on the order of minutes to hours. The hydrolysis of these chemicals occurs through an indirect nucleophilic displacement by water ( $S_N1$  mechanism). The dramatic increase in reactivity is due to the structural features of these compounds that allow for delocalization, and thus, stabilization, of the carbonium ion intermediate. Resonance structures can be drawn for the allylic and benzyl carbonium ions that delocalize the positive charge over several carbon atoms.

The lack of reactivity observed for vinyl halides and halogenated aromatics is a reflection of the high energy pathway required for nucleophilic substitution at vinylic and aromatic carbons. Vinyl and phenyl carbonium ions have been observed, but their formation requires very reactive leaving groups.

### *Polyhalogenated aliphatics*

The hydrolysis kinetics for the polyhalogenated ethanes and propanes are somewhat more complex than for the simple halogenated aliphatics. In addition to nucleophilic substitution reactions, degradation of these compounds can occur through the base-mediated loss of HX. Depending on structure type, elimination or dehydrohalogenation may be the dominant reaction pathway at pH's characteristic of ambient environments. The loss of HX occurs through a bimolecular elimination ( $E2$ ) reaction in which abstraction of the hydrogen beta to the halogen (X) occurs simultaneously with cleavage of the C-X bond:



This process often results in the formation of halogenated alkenes, which can be more persistent and of more concern than substitution products<sup>42</sup>.

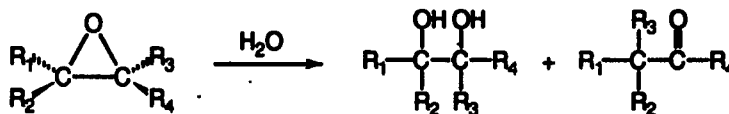
The distribution of reaction products resulting from the hydrolytic degradation of the polyhalogenated ethanes and propanes will depend on the relative rates for the nucleophilic substitution and dehydrohalogenation reaction pathways. Furthermore, because dehydrohalogenation is pH dependent, product distribution will also be pH dependent.

A wide range of reactivity is observed for these compounds; the environmental hydrolysis half-lives in years range over 7 orders of magnitude. For a number of the polyhalogenated aliphatics, it is apparent that both neutral and base-mediated hydrolysis will occur at ambient environmental pH values and that the relative contributions of these processes will be dependent on the degree and pattern of halogen substitution.

As with nucleophilic substitution reactions, rates of dehydrohalogenation reactions will be dependent on the strength of the C-X bond being broken in the elimination process. Accordingly, it is expected that the ease of elimination of X will follow the series  $\text{Br} > \text{Cl} > \text{F}$ .

## Epoxides

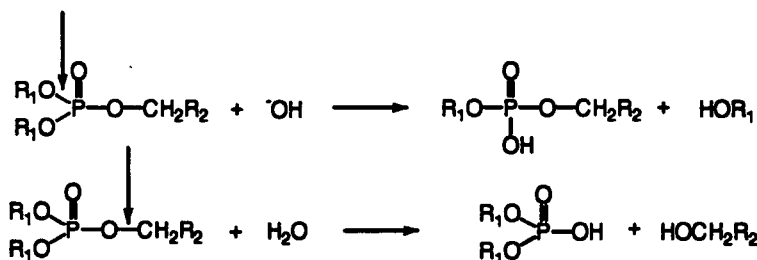
The hydrolysis of epoxides is pH dependent and can occur through acid-, neutral-, or base-promoted processes. Because the acid and neutral processes dominate over ambient environmental pH ranges, the base-mediated process can often be ignored. The products resulting from the hydrolysis of epoxides are diols, and to a lesser extent, rearrangement products:



## Organophosphorus Esters

Mechanistic studies of organophosphorus esters have demonstrated that hydrolysis occurs through direct nucleophilic displacement at the central phosphorus atom and does not involve formation of a pentavalent intermediate with  $\text{H}_2\text{O}$  or  $\text{HO}^-$ <sup>43,44</sup>. Accordingly, hydrolysis rates for phosphorus esters will be sensitive to electronic factors that alter the electrophilicity of the central phosphorus atom and steric interactions that impede nucleophilic attack. For example, substitution of sulfur ( $\text{P}=\text{S}$ ) for oxygen ( $\text{P}=\text{O}$ ) in the ester moiety will reduce the electrophilicity of the phosphorus center because of the weaker electron withdrawing effect of sulfur. Accordingly, phosphorothioate and phosphonothioate esters will exhibit greater stability towards neutral and base-mediated hydrolysis than their respective O-substituted counterparts.

An interesting feature of the hydrolytic degradation of phosphorus esters is that carbon-oxygen or carbon-sulfur cleavage may also occur. It is generally observed that base-mediated hydrolysis favors P-O cleavage, which is shown in the first chemical reaction below, and that neutral and acid catalysis favors C-O or C-S cleavage, which is shown in the second reaction below. As a result, hydrolysis mechanisms and product distribution for the organophosphorus esters will be pH dependent.



Because hydrolysis of phosphorus esters results in the formation of phosphate mono- and diesters, assessment of their hydrolytic activity is necessary. At any ambient environmental pH, the mono- and diesters will exist primarily as di- and monoacids, respectively. Accordingly, base hydrolysis of the anions will not be important, but neutral hydrolysis of these species must be considered. Hydrolysis of the dialkyl monoion to yield monoalkyl

products proceeds at a rate approximately a factor of 10 less than that of the triester. Hydrolysis of the resulting monoalkyl ester (dianion) proceeds at a rate of approximately one half that of the triester. Hydrolysis of the monoester has been shown to occur through nucleophilic attack on the phosphorus rather than carbon-oxygen cleavage<sup>66</sup>.

### Carboxylic Acid Esters

Hydrolysis of carboxylic acid esters results in the formation of a carboxylic acid and an alcohol:

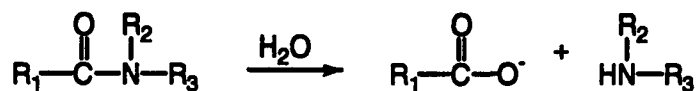


Hydrolysis mechanisms of carboxylic acid esters have been thoroughly investigated. Although nine distinct mechanisms have been proposed<sup>46</sup>, our comments will be limited to the two most common mechanisms involving acyl-oxygen bond cleavage by acid catalysis ( $\text{A}_{\text{AC}}2$ ) and base mediation ( $\text{B}_{\text{AC}}2$ ). Hydrolysis via the  $\text{A}_{\text{AC}}2$  mechanism involves initial protonation of the carbonyl oxygen. Protonation polarizes the carbonyl group, removing electron density from the carbon atom and making it more electrophilic and thus more susceptible to nucleophilic addition by water. The base-mediated mechanism ( $\text{B}_{\text{AC}}2$ ) proceeds via the direct nucleophilic addition of  $\text{HO}^-$  to the carbonyl group. Base mediation occurs because the hydroxide ion is a stronger nucleophile than water. Although neutral hydrolysis of carboxylic acid esters does occur, the base-mediated reaction will be the dominant pathway in most natural waters. Generally, acid hydrolysis will dominate in acidic waters with pH values below 4.

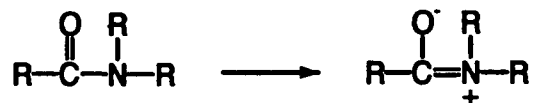
Both electronic and steric effects can significantly alter the reactivity of carboxylic acid esters. Because the acid-catalyzed process for both aliphatic and aromatic esters is relatively insensitive to structural changes, observed changes in the magnitude of  $k_{\text{obs}}$  with structure are due primarily to changes of  $k_{\text{b}}$ , and to a lesser extent,  $k_{\text{n}}$ . Based on the mechanism for base mediation ( $\text{B}_{\text{AC}}2$ ), we would expect that electronic factors that enhance the electrophilicity of the carbon atom of the carbonyl group would make it more susceptible to nucleophilic attack by  $\text{HO}^-$ . The electron-withdrawing groups can be substituents of either the acyl group  $\{\text{RC}(\text{O})\}$  or the alcohol portion of the ester.

### Amides

Hydrolytic degradation of amides results in the formation of a carboxylic acid and an amine:



In general, amides are much less reactive towards hydrolysis than esters. Typically, half-lives for amides at ambient environmental conditions are measured in hundreds to thousands of years<sup>5</sup>. This observation can be explained by the ground-state stabilization of the carbonyl group by the electron donating properties of the nitrogen atom:



This stabilization is lost in the transition state leading to the formation of the tetrahedral intermediate. The result is that the hydrolysis of amides generally requires base or acid catalysis, both of which can compete at neutral pH.

### Carbamates

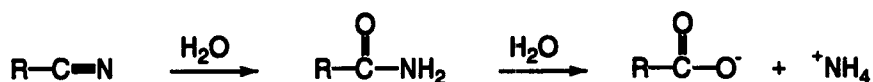
A carbamate is hydrolyzed to an alcohol, carbon dioxide, and an amine:



Carbamates are susceptible to acid, neutral and base hydrolysis, although in most cases, base hydrolysis will dominate at environmental conditions. In an analogous manner to carboxylic acid ester and amide hydrolysis, electron-withdrawing substituents on either oxygen or nitrogen will accelerate the rate of hydrolysis. The most dramatic differences in reactivities are observed when the hydrolysis half-lives of primary ( $\text{R}_1=\text{H}$ ,  $\text{R}_2=\text{alkyl}$ ) and secondary ( $\text{R}_1=\text{alkyl}$ ,  $\text{R}_2=\text{alkyl}$ ) carbamates are compared. The primary carbamates hydrolyze at rates that are approximately 6 to 7 orders of magnitude faster than the corresponding secondary carbamates.

### Nitriles

Nitriles are hydrolyzed to give a carboxylic acid and ammonium ion. Hydrolysis occurs through the intermediate amide:



Base-mediated hydrolysis appears to be the dominant hydrolysis pathway at pH 7.

## Sorption

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### *Neutral Organic Compounds*

Partitioning between water and natural soils, sediments, and aquifer materials is an important process affecting 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 chemical and the sorbent. Organic carbon content has been used almost exclusively as a measure of the hydrophobic nature of natural sedimentary material (organic matter or volatile solids content has also been used but not as widely). To quantitatively characterize the hydrophobic nature of organic compounds, researchers have used various measurable parameters, including octanol-water partition coefficients ( $K_{ow}$ ), water solubility (corrected for crystal energy), reverse phase HPLC retention, and topological parameters of the compounds such as calculated surface area. Generally, octanol-water partition coefficients have been used extensively for estimating the partitioning of organic compounds to sedimentary materials.

### *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 according to the following equations. For acids:

$$K_a = \frac{[H^+][A^-]}{[HA]} \quad (5)$$

and bases:

$$K_b = \frac{[H^+][B]}{[HB^+]} \quad (6)$$

where  $[H^+]$  is the hydrogen ion activity,  $[HA]$  is the neutral organic acid activity (or concentration),  $[A^-]$  is the organic acid anion activity,  $[B]$  is the neutral organic base activity,  $[HB^+]$  is the protonated organic base activity, and  $K_a$  is the acid dissociation or ionization constant.

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<sup>46</sup>.

Compounds with low  $pK_a$  values are more problematic. Adsorption of these compounds occurs predominantly by the anionic species through modified hydrophobic interactions<sup>47</sup>. Therefore, an estimate of a partition coefficient from the  $K_{ow}$  of the neutral species would

significantly overestimate the magnitude of adsorption. Jafvert et al.<sup>46</sup> and Jafvert<sup>47</sup> have investigated the partitioning behavior of these and similar compounds in the octanol-water system and in sediment- and soil-water systems. For example, Jafvert<sup>47</sup> has reported on the sediment-water distribution of silvex in 13 soils or sediments. If the partition coefficients (in which the pH of the slurry is greater than 7) are regressed versus the fraction organic carbon, a value of  $\log K_{oc} = 1.8$  is obtained for the organic-carbon-normalized partition coefficient,  $K_{oc}$ . The  $\log K_{ow}$  of the neutral form of silvex is 3.8. Similar results for pentachlorophenol and 4-chloro- $\alpha$ -(4-chlorophenyl)benzeneacetic acid (DDA) suggest that the partition coefficient (at pH 7.0) of the anionic form of these compounds is approximately two orders of magnitude less than the respective  $K_{ow}$  values of the neutral form of these compounds.

Unlike anionic organic compounds, which partition more weakly than their neutral counterparts, organic cations tend to partition more strongly than the corresponding unprotonated bases. Also, unlike organic anions, which partition largely through modified hydrophobic interactions, the organic cations can undergo cation (or ligand) exchange reactions. Pyridine, for example, is an organic base that has a  $pK_a$  value of 5.3. At pH 7, a small fraction (2.2%) will exist as an organic cation in aqueous solution. Because the cationic species is expected to adsorb more strongly to most natural soils, sediments, and aquifer materials than the neutral species, an organic-carbon-normalized partition coefficient ( $K_{oc}$ ) may severely underestimate the adsorption of this compound at near-neutral pH. Because no predictive methods exist for describing the partitioning of organic cations to natural matrices, however, the organic-carbon-normalized partition coefficient calculated from the  $K_{ow}$  of the neutral species (not accounting for ionization) is given in Table 1. For virtually every sediment and aquifer material, this constant will underpredict the true magnitude of adsorption of these compounds, with the error intensifying as the organic carbon content of a sediment or aquifer material decreases.

For neutral compounds and organic bases with  $pK_a$  values below 6, the organic-carbon-normalized partition coefficients in Table 1 have been calculated using the relationship,

$$\log K_{oc} = \log K_{ow} - 0.32 \quad (7)$$

given by Hassett et al.<sup>49</sup> 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%.

For organic acids, the  $pK_a$  must be considered in the computation of the  $K_{oc}$ . The following relationships were used according to the range of  $pK_a$  values:

$$pK_a > 9: K_{oc} = 1.05 K_{ow}^{(0.82)} \quad (8)$$

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

which simplifies at pH 7 to:

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

$$pK_a < 6: \log K_{oc} = \log K_{ow} - 2 \quad (11)$$

For organic bases, the  $pK_a$  value was considered in the computation of the  $K_{oc}$ , where  $pK_a = 14 - pK_b$ . Equation (7) was used for compounds with  $pK_a$  values of less than 6. For organic bases with  $pK_a$  values larger than 6, no  $K_{oc}$  values were calculated because the uncertainty is too great. When a  $K_{oc}$  value was needed for a complex ion with successive ionization constants, the first ionization constant ( $pK_1$ ) was used in the computation of the  $K_{oc}$  value. All ionization constants were computed with SPARC<sup>29</sup>.

### Estimated data

Most of the  $\log K_{ow}$  values in Table 1 were computed with QSAR<sup>4</sup> and SPARC<sup>29</sup>. QSAR is an interactive chemical database and hazardous assessment system designed to provide basic information for the evaluation of the fate and effects of chemicals in the environment. The QSAR<sup>4</sup> system is a composite of databases containing measured values obtained from the literature and a state-of-the-art QSAR model library capable of estimating chemical properties, behavior, and toxicity, based on conventional estimation techniques, many of which were derived from the work of Lyman et al.<sup>50</sup> The QSAR system contains automated estimation routines for 13 properties based upon modified structure-activity correlations.

SPARC<sup>29</sup> 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  $\pi$  electrons.

For example, SPARC computes the log of the octanol-water partition coefficient from activity coefficients in the octanol ( $\gamma_o^\infty$ ) and water ( $\gamma_w^\infty$ ) phases:

$$\log K_{ow} = \log \frac{\gamma_w^{\circ}}{\gamma_o^{\circ}} + \log \frac{M_o}{M_w} \quad (12)$$

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  $\log K_{ow}$  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 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.

## Redox

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### *Abiotic Redox Transformations of Organic Compounds*

Abiotic redox reactions will not generally mineralize large organic molecules, but the transformations will result in daughter products with different chemical and physical properties<sup>51</sup>. Furthermore, abiotic transformations can convert bio-resistant compounds to more bio-susceptible compounds. For example, redox reactions can result in oxidation or reduction of key functional groups on molecules that will render them labile to microbial transformations and ultimately mineralization or conversion to other environmentally innocuous components.

A large number of functional groups on organic compounds have been shown to undergo abiotic reduction under ambient environmental conditions. In general, these redox transformations encompass almost all chemical functional groups, utilize a large number of organic and inorganic redox agents, and result in an almost unlimited number of products<sup>52</sup>. Furthermore, the rates of redox reactions can be expected to span many orders of magnitude, depending upon the reaction type and redox agents' activities. Unfortunately, only a few of the reactions have been studied in enough detail to identify the system redox agents and provide kinetics data.

It is not currently possible to address redox transformations for all the listed compounds in soils, sediments and aquifer systems because of a lack of quantitative research in the area of environmental redox reactions. For the few classes of compounds where detailed studies have been carried out, it is possible to obtain reductive rate constants and apply them to environmental systems<sup>53,54</sup>. In these detailed studies, kinetic expressions and the reducing agents have been identified.

In this report, reduction of halogenated hydrocarbons and nitroaromatics, and the autooxidation of aldehydes and amines are addressed. Estimated rate constants for halogenated hydrocarbons and nitroaromatics are given in Table 2. These rate constants



were computed for soil-water systems in which the solids contained 1% and 0.02% organic carbon. The data clearly indicate the dependence of the reductive process on organic carbon. A 50-fold increase in organic carbon from a concentration of 0.02% decreases the half-lives by about 4 orders of magnitude for the halogenated hydrocarbons and about 1 order of magnitude for the nitroaromatics. For the QSAR computations of the halogenated hydrocarbons, either published sigma constants or estimated values were used. For the QSAR computations of the nitroaromatics, published sigma constants were used except for parathion and methyl parathion. For these two compounds, the sigma constants were estimated from 1-methoxy-*p*-nitrobenzene. Rate constants for the nitroso compounds were not computed. However, preliminary laboratory studies of some nitroso compounds indicated half-lives of less than 1 hour. It was not possible to identify products of degradation. We hope that the following will give the reader some insight into this difficult and unexplored area of heterogeneous redox reactions.

### ***Convention of Writing Redox Reactions***

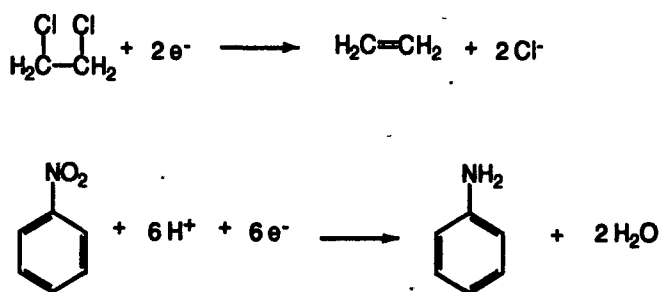
In the environmental literature, as well as in organic chemistry textbooks, the definitions of oxidation-reduction are often empirical and can result in ambiguities, especially when applied across classes of compounds<sup>52</sup>. Reactions that form new bonds with hydrogen are often referred to as reduction, whereas those forming new bonds with oxygen are often referred to as oxidation. Although this system may hold for specific classes of compounds, it is not generally applicable to the myriad of chemicals of environmental importance.

The overall reaction is not given because, for the most part, the activity of the reducing or oxidizing agent responsible for the transformation is not known. Thus it is not possible to sum up the two half-reactions and write the overall equation.

An unambiguous method for describing redox processes is to write the chemical equation for each half-reaction with the reactants on the left and the products on the right, balancing the equation by using hydrogen ions to provide needed hydrogen and hydroxide ions or water molecules to provide needed oxygen atoms. Electrons are then added to balance the charge (Figure 1). If electrons are added to the left side of the equation, it is a reduction reaction. If electrons are added to the right side of the equation, it is an oxidation reaction. Examples of half-reactions for reduction and oxidation are given below.

### ***Reduction***

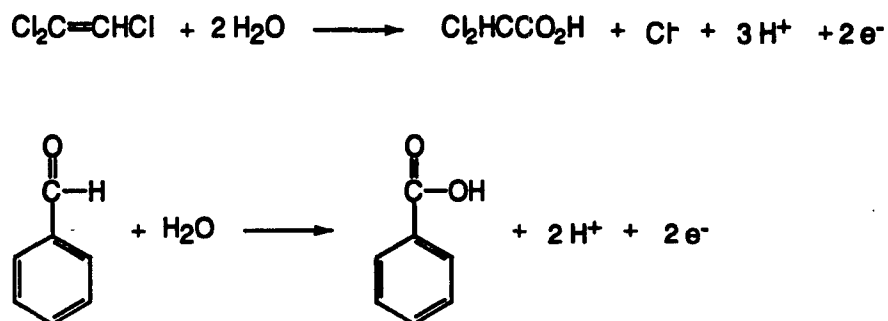
Figure 1 shows two examples of reductive transformations. The first is a two-electron transfer reaction for the reduction of 1,2-dichloroethane to ethene and chloride. The second is a six-electron reduction of nitrobenzene, requiring six protons that gives aniline and water as products.



**Figure 1.** Half-reactions for the reduction of 1,2-dichloroethane to ethene and the reduction of nitrobenzene to aniline.

### Oxidation

Figure 2 shows two examples of redox half-reactions. The first is a two-electron oxidation of 1,1,2-trichloroethylene to 1,1-dichloroacetic acid, chloride, and three protons. The second is a two-electron oxidation of benzaldehyde to benzoic acid. In this reaction, water provides the source of oxygen and results in two protons as a product.



**Figure 2.** Half-reactions for the oxidation of 1,1,2-trichloroethylene to 1,1-dichloroacetic acid and the oxidation of benzaldehyde to benzoic acid.

### Descriptions of Redox State of the System

#### *Eh*

When the *Eh* of the heterogeneous system, as measured by a platinum electrode, is above *Eh* 50 mv (relative to Ag:AgCl), the reductive reaction does not occur for the halogenated

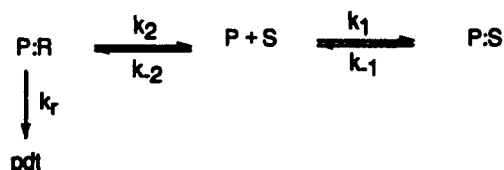
hydrocarbons and nitroaromatics<sup>55</sup>. When the Eh of the system is below 50 mv, the reaction occurs and the rate of reaction is independent of the magnitude of the Eh.

### **pH**

In general, in heterogenous systems, pH effects on the rates of abiotic reductions are minimal. This is partly because the solids tend to buffer the pH of the system<sup>56</sup>. For example, over the pH range of 5 to 9, the rate constant for reduction of nitrobenzene to aniline was independent of pH. The same has been observed for the reduction of halogenated hydrocarbons.

## **Kinetics of Reaction in Heterogenous Systems**

To carry out abiotic reactions in heterogenous systems such as soils, sediments and aquifer materials, requires an understanding of the kinetics of reaction. In these heterogenous systems, sorption of the compounds to the solids will affect the overall kinetics of reaction. A working model has been proposed to account for the observed kinetics of reduction of compounds in these types of heterogenous systems<sup>54,55,56,58</sup>. The model, which is shown below, assumes non-reactive and reactive sorptive sites on the solids.



Where P is pollutant concentration; S is sediment concentration (g/g);  $k_1$  and  $k_{-1}$  are the respective sorption-desorption rate constants to a non-reactive sink, P:S;  $k_2$  and  $k_{-2}$  are the respective sorption-desorption rate constants to the reactive sink, P:R;  $k_r$  is the first-order rate constant for reduction at reactive solid sites.

## **Calculation of Rate Constants**

### **Reductive Processes**

#### **Nitroaromatics**

Rate constants for the reduction of nitroaromatics can be calculated using the SAR based on Hammett sigma constants reported by Wolfe et al.<sup>58</sup> This relation provides selected, observed first-order disappearance rate constants for nitroaromatic compounds. These first-order rate constants have been shown by Wolfe et al.<sup>58</sup> to correlate with the organic carbon of the system.

#### **Halogenated hydrocarbons**

Wolfe and co-workers<sup>57,58</sup> developed a structure reactivity relationship that associates the reductive disappearance rate constants of halogenated hydrocarbons in anoxic sediments with readily available molecular descriptors. The correlation is based on disappearance

rate constants for the reductive transformation of 19 halogenated hydrocarbons. The compounds span a large cross section of chemical structures that includes halogenated methanes, ethanes, ethenes, and halogenated aromatics.

Wolfe and co-workers<sup>57,58</sup> also corrected the rate constants for hexachloroethane for sorption. These rate constants were obtained in 18 different sediment, soil and aquifer samples and correlated with the organic carbon.

## ***Oxidative Processes***

### ***Aldehydes***

In general, aldehydes will undergo autooxidation to the corresponding carboxylic acids in the presence of oxygen<sup>52,59</sup>. In sediments, soil and aquifer materials, aldehydes have been shown to undergo such oxidations even under anoxic conditions. No comprehensive data base of rate constants is available for these reactions and, furthermore, the autooxidation kinetics are too complex to extrapolate precise rate constants from laboratory to field conditions.

These reactions have been observed for a large number of aldehydes and, based on this qualitative data base, half-lives of less than 1 year are reasonable.

### ***Amines***

In general, amines undergo rapid autooxidation<sup>52,59</sup>. Their autooxidation mechanisms and transformation kinetics are complicated and not well understood. In the presence of oxygen in sediments and soils, they can form covalent bonds with the organic components of the solids and thus become bound residues. Under anoxic conditions in sediments and soils, however, they appear to be stable for long periods of time and tend not to bind irreversibly to the organic matter associated with the organic carbon.

No comprehensive data base of rate constants for these types of reactions has been compiled and, furthermore, the reaction kinetics are too complex to extrapolate precise rate constants from the laboratory to field conditions.

Because reactions have been observed for a large number of amines, it is reasonable to assume that these compounds will undergo autooxidation in the field. Based on the qualitative data base, half-lives for this class of compounds will be less than 1 year.

**TABLE 1. Chemical hydrolysis rate constants and sorption data for organic compounds.**

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
1. Acenaphthene	83-32-9	3.75	4.07	0	0	0	NHFG	/ 4 / 0
2. Acetone (2-propanone)	67-64-1	-0.568	-0.268	0	0	0	NHFG	/ 4 / 0
3. Acetonitrile (methyl cyanide)	75-05-8	-0.714	-0.394	0	0	45	RATE	/ 4 / 24
Acetamide	60-35-5	-1.55	-1.23	2.6E2	0	1.5E3		/ 4 / 5
Acetic acid ( $pK_a=4.65$ )	64-19-7	-2.23	-0.234	0	0	0	NHFG	/ 4 / 0
Ammonia	7664-41-7	NA	NA	0	0	0	NHFG	/ 0 / 0
4. Acetophenone	98-86-2	1.26	1.58	0	0	0	NHFG	/ 4 / 0
5. Acrolein	107-02-8	-0.219	0.101	NG	6.68E8	NG		/ 4 / 30
3-Hydroxy-1-propanal	2134-29-4	-1.3	-1.0	0	0	0	NHFG	/ 29 / 0
6. Acrylamide	79-06-1	-0.989	-0.669	31.5	1.8E-2	0	a	/ 4 / 6
Acrylic acid ( $pK_a=4.13$ )	79-10-7	-1.84	0.161	0	0	0	NHFG	/ 4 / 2
Ammonia	7664-41-7	NA	NA	0	0	0	NHFG	/ 0 / 0
7. Acrylonitrile	107-13-1	-0.089	0.231	5E2	0	5.2E3	RATE	/ 4 / 6
Acrylamide **	79-06-1	-0.989	-0.669	31.5	1.8E-2	0	a	/ 4 / 6
Acrylic acid ( $pK_a=4.13$ )	79-10-7	-1.84	0.161	0	0	0	NHFG	/ 4 / 2
Ammonia	7664-41-7	NA	NA	0	0	0	NHFG	/ 0 / 0
8. Aldrin	309-00-2	6.18	6.496	0	0	0	NLFG	/ 7 / 0
9. Aniline (benzenamine: $pK_b=9.3$ )	62-53-3	0.595	0.915	0	0	0	NHFG	/ 4 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
10. Antimony (and compounds N.O.S.)	7440-36-0							
11. Aramite	140-57-8	5.2	5.5	0	7.7	6.0E4	ff	/ 29 /
1-Methyl-2-[p-(1,1-dimethyl-ethyl)phenoxy]ethylhydrogensulfite	NG			0	7.7	6.0E4	gg	/ / 0
1-Methyl-2[p-(1,1-dimethyl-ethyl)phenoxy]ethanol	2416-30-0	3.15	3.47	0	0	0	NHFG	/ 4 / 0
Sulfuric acid	7664-93-9	NA	NA	0	0	0	NHFG	/ 0 / 0
1-Methyl-2[p-(1,1-dimethylethyl)-phenoxy]ethanol	2416-30-0	3.15	3.47	0	0	0	NLFG	/ 4 / 0
2-Chloroethylhydrogensulfite	NG			0	7.7	6.0E4	gg	/ / 0
Sulfuric acid	7664-93-9	NA	NA	0	6.0E40	0	NHFG	/ 0 / 0
2-Chloroethanol	107-07-3	-0.492	-0.172	0	3.9E-2	3.2E5		/ 4 / 3
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Ethylene oxide	75-21-8	-1.1	-0.792	2.9E5	21	0		/ 4 / 5
Ethylene glycol	107-21-1	-1.5	-1.2	0	0	0	NHFG	/ 29 / 0
2-Chloroethanol	107-07-3	-0.492	-0.172	0	3.9E-2	3.2E5		/ 4 / 3
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Ethylene oxide	75-21-8	-1.1	-0.792	2.9E5	21	0		/ 4 / 5
Ethylene glycol	107-21-1	-1.5	-1.2	0	0	0	NHFG	/ 29 / 0
12. Arsenic (and compounds N.O.S.)	7440-38-2							
13. Barium (and compounds N.O.S.)	7440-39-3							
14. Benz[a]anthracene	56-55-3	5.34	5.66	0	0	0	NHFG	/ 4 / 0
15. Benzene	71-43-2	1.80	2.12	0	0	0	NHFG	/ 37 / 0
16. Benzidine ( $pK_a=9.3$ )	92-87-5	1.26	1.58	0	0	0	NHFG	/ 4 / 0
17. Benzo[b]fluoranthene	205-99-2	5.8	6.12	0	0	0	NHFG	/ 4 / 0
18. Benzo[a]pyrene	50-32-8	5.8	6.12	0	0	0	NHFG	/ 4 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_n$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
19. Benzotrichloride	98-07-7	4.06	4.38	0	2.0E6	0		/ 29 / 5
Benzoic acid ( $pK_a=4.18$ )	65-85-0	-0.11	1.89	0	0	0	NHFG	/ 4 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
20. Benzyl alcohol ( $pK_a=15.1$ )	100-51-6	0.78	1.10	0	0	0	NHFG	/ 4 / 0
21. Benzyl chloride	100-44-7	2.84	3.16	0	4.1E2	0	RATE	/ 29 / 24
Benzyl alcohol **	100-51-6	0.78	1.10	0	0	0	NHFG	/ 4 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
22. Beryllium (and compounds N.O.S.)	7440-41-7							
23. Bis(2-chloroethyl)ether	111-44-4	0.80	1.12	0	0.23	0		/ 1 / 3
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
2-(2-chloroethoxy)ethanol	628-89-7	-0.186	-0.154	0	0.28	0		/ 4 / 3
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Bis(2-hydroxyethyl)ether	111-46-6	-1.62	-1.30	0	0	0	NHFG	/ 4 / 2
1,4-Dioxane **	123-91-1	-0.812	-0.492	0	0	0	NHFG	/ 4 / 2
24. Bis(2-chloroisopropyl)ether	39638-32-9	2.39	2.71	0		0	See Part II.	/ 4 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
(2-Hydroxyisopropyl-2-chloro-isopropyl)ether	NG	2.7	3.0				b	/ 29 / 0
Bis(2-hydroxyisopropyl) ether	72986-46-0	1.1	1.4	0	0	0	NHFG	/ 29 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_h$ $M^{-1}Y^{-1}$	$k_h$ $Y^{-1}$	$k_h$ $M^{-1}Y^{-1}$		
25. Bis(2-ethylhexyl)phthalate	117-81-7	7.13	7.453	0	0	1.4E3	RATE	/ 7 / 9
2-Ethylhexanol	104-76-7	2.56	2.88	0	0	0	NHFG	/ 29 / 0
2-Ethylhexyl hydrogen phthalate	4376-20-9	5.5	5.8	0	0	7E2	c	/ 29 / 0
2-Ethylhexanol	104-76-7	2.56	2.88	0	0	0	NHFG	/ 29 / 0
o-Phthalic acid ( $pK_a=3.03$ )	88-99-3	-1.27	0.732	0	0	0	NHFG	/ 4 / 0
26. Bromodichloromethane	75-27-4	1.77	2.09	NG	NG	5.0E4	t	/ 4 / 41
Carbon monoxide	630-08-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
27. Bromomethane (Flammable gas, $bp=4^\circ C$ )	74-83-9	0.76	1.08	0	9.46	0		/ 4 / 10
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
28. Butanol	71-36-3	0.503	0.823	0	0	0	NHFG	/ 4 / 0
29. Butyl benzyl phthalate	85-68-7	4.23	5.05	0	0	1.2E5	d	11 / 29 / 0
Benzyl alcohol **	100-51-6	0.78	1.10	0	0	0	NHFG	/ 4 / 0
Butyl hydrogen phthalate	131-70-4	3.43	3.75	0	0	6E4	c	/ 9 / 0
o-Phthalic acid ( $pK_a=3.03$ )	88-99-3	-1.27	0.732	0	0	0	NHFG	/ 4 / 0
n-Butanol **	71-36-3	0.503	0.823	0	0	0	NHFG	/ 4 / 0
n-Butanol **	71-36-3	0.503	0.823	0	0	0	NHFG	/ 4 / 0
Benzyl hydrogen phthalate	2528-16-7	3.63	3.95	0	0	6E4	c	/ 29 / 0
Benzyl alcohol **	100-51-6	0.78	1.10	0	0	0	NHFG	/ 4 / 0
o-Phthalic acid ( $pK_a=3.03$ )	88-99-3	-1.27	0.732	0	0	0	NHFG	/ 4 / 0
30. 2-sec-Butyl-4,6-dinitrophenol (Dinoseb; $pK_a=3.5$ )	88-85-7	2.02	4.02	0	0	0	NHFG	/ 4 / 0
31. Cadmium (and compounds N.O.S.)	7440-43-9							



Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_b$ $Y^{-1}$	$k_c$ $M^{-1}Y^{-1}$		
32. Carbon disulfide	75-15-0	1.84	2.16	0	0	3.15E4		/ 1 / 61
Carbonyl sulfide	463-58-1	0.4	0.7	NG	6.3E2	4.1E8		/ 29 / 40
Carbon dioxide	124-38-9	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
(Flammable gas: bp= -60°C; (pK <sub>a</sub> =7.0)								
33. Carbon tetrachloride	56-23-5	2.41	2.73	0	1.7E-2	0	RATE	/ 37 / 13
Carbon dioxide	124-38-9	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
34. Chlordane	57-74-9	5.89	6.21	0	0	37.7	y	/ 62 / 3
2,4,5,6,7,8,8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-methano-1H-indene	5103-65-1	6.2	6.5	0	0	0	NLFG	/ 29 / 2
35. <i>p</i> -Chloroaniline (pK <sub>a</sub> =10)	106-47-8	1.61	1.93	0	0	0	NLFG	/ 4 / 0
36. Chlorobenzene	108-90-7	2.578	2.898	0	0	0	NLFG	/ 7 / 1
37. Chlorobenzilate (pK <sub>a</sub> =13.6)	510-15-6	4.04	4.36	0	0	2.8E6	ff	/ 4 /
<i>Bis(p</i> -chlorophenyl)hydroxy-acetic acid (pK <sub>a</sub> =3.1)	23851-46-9	2.5	4.5	0	0	2.8E5	ff	/ 29 / 0
<i>p,p'</i> -Dichlorobenzophenone	90-98-2	4.43	4.75	0	0	0	NLFG	/ 4 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
38. 2-Chloro-1,3-butadiene (Chloroprene)	126-99-8	1.74	2.06	0	0	0	NLFG	/ 4 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
39. Chlorodibromomethane	124-48-1	1.91	2.23	NG	NG	2.5E4	1	/ 4 / 41
Carbon monoxide	630-08-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
40. Chloroform	67-66-3	1.58	1.90	0	1.0E-4	2.74E3		/ 37 / 13
Carbon monoxide	630-08-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
41. Chloromethane (Methyl Chloride: bp= -23.7°C)	74-87-3							
42. 2-Chlorophenol ( $pK_a=8.4$ )	95-57-8	1.82	2.20	0	0	0	NLFG	/ 4 / 0
43. 3-Chloropropene	107-05-1	1.13	1.45	0	40	0		/ 4 / 5
3-Hydroxypropene	107-18-6	-0.57	-0.250	0	0	0	NHFG	/ 4 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
44. Chromium (and compounds N.O.S.)	7440-47-3							
45. Chrysene	218-01-9	5.34	5.66	0	0	0	NHFG	/ 4 / 0
46. Cresols (See below)								
47. o-Cresol ( $pK_a=9.8$ )	95-48-7	1.76	2.12	0	0	0	NHFG	/ 4 / 1
48. m-Cresol ( $pK_a=10.0$ )	108-39-4	1.76	2.12	0	0	0	NHFG	/ 4 / 1
49. p-Cresol ( $pK_a=10.1$ )	106-44-5	1.76	2.12	0	0	0	NHFG	/ 4 / 1
50. Cumene	98-82-8	3.40	3.72	0	0	0	NHFG	/ 4 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
51. Cyanide (amenable)	57-12-5			0	29	0	e	/ / 27
Carbon dioxide	124-38-9	NA	NA	0	0	0	NHFG	/ 0 / 0
Ammonia	7664-41-7	NA	NA	0	0	0	NHFG	/ 0 / 0
52. 2,4-Dichlorophenoxyacetic acid (2,4-D: $pK_a=3.1$ )	94-75-7	0.68	2.68	0	0	0	NLFG	/ 4 / 1
53. DDD	72-54-8	5.89	6.21	0	2.5E-2	2.2E4	RATE	/ 4 / 24
2,2-Bis(4-chlorophenyl)-1-chloroethene (DDMU)	1022-22-6	6.47	6.79	0	0	0	NLFG	/ 29 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
54. DDE	72-55-9	6.64	6.956	0	0	0	NLFG	/ 7 / 12
55. <i>p,p'</i> -DDT	50-29-3	6.59	6.91	0	6.0E-2	3.1E5		/ 4 / 12
DDE **	72-55-9	6.64	6.956	0	0	0	NLFG	/ 7 / 12
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
56. Diallate	2303-16-4	4.17	4.49	0	0.10	8E3		/ 62 / 3
Diallate (Z-)	17708-57-5	3.8	4.1	0	3.2E-1	0	RATE	/ 29 / 24
Diallate (E-)	17708-58-6	3.8	4.1	0	7.8E-2	7.3E3	RATE	/ 29 / 24
Diisopropylamine ( $pK_b=11.5$ )	108-18-9	0.84	1.16	0	0	0	NHFG	/ 4 / 0
<i>trans</i> -2,3-Dichloro-2-propene-1-thiol ( $pK_a=8.2$ )	16714-72-0	2.4	2.84	0	0	0	NLFG	/ 29 / 0
<i>cis</i> -2,3-Dichloro-2-propene-1-thiol ( $pK_a=8.2$ )	16714-71-9	2.5	3.0	0	0	0	NLFG	/ 29 / 0
Carbon dioxide	124-38-9	NA	NA	0	0	0	NHFG	/ 0 / 0
57. Dibenz[a,h]anthracene	53-70-3	6.52	6.84	0	0	0	NHFG	/ 4 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
58. 1,2-Dibromo-3-chloropropane	96-12-8	1.94	2.26	0	4.0E-3	1.2E5	RATE	/ 4 / 31
.....( $k_a$ ).....								
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
2-Bromo-3-chloropropanol	73727-39-6	0.17	0.49	0	1.4	5.4E5	cc	/ 4 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
Epichlorohydrin	106-89-8	-0.53	-0.210	2.5E4	30.9	0		/ 4 / 5
1-Chloro-2,3-dihydroxypropane	96-24-2	-0.8	-0.5	0	0.46	1.8E5	f	/ 29 / 0
1-Hydroxy-2,3-propylene oxide	556-52-5	-1.7	-1.4	7.7E4	8.9	0		/ 29 / 5
Glycerol	56-81-5	-2.2	-1.9	0	0	0	NHFG	/ 29 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Glycerol	56-81-5	-2.2	-1.9	0	0	0	NHFG	/ 29 / 0
.....( $k_a$ ).....								
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
2,3-Dibromo-1-propanol	96-13-9	1.10	1.42	0	1.4	5.4E5	cc	/ 29 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
Epibromohydrin	3132-64-7	0.2	0.5	1.9E4	1.6E1	0		/ 29 / 41
1-Bromo-2,3-dihydroxypropane	4704-77-2	-1.2	-0.857	0	1.4	5.4E5	cc	/ 4 / 0
1-Hydroxy-2,3-propylene oxide	556-52-5	-1.7	-1.4	7.7E4	8.9	0		/ 29 / 5
Glycerol	56-81-5	-2.2	-1.9	0	0	0	NHFG	/ 29 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
Glycerol	56-81-5	-2.2	-1.9	0	0	0	NHFG	/ 29 / 0
.....( $k_a$ ).....								
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
2,3-Dibromopropene	513-31-5	2.39	2.71	0	29	0		/ 29 / 31
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
2-Bromo-3-chloropropene	16400-63-8	1.75	2.07	0	1.8	0		/ 4 / 31
2-Bromo-3-hydroxypropene	598-19-6	1.40	1.72	0	0	0	NLFG	/ 29 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
59. Dibromomethane (methylene bromide)	74-95-3	1.21	1.53	0	0	0	NLFG,w	/ 4 / 0
60. 1,2-Dichlorobenzene	95-50-1	3.08	3.40	0	0	0	NLFG	/ 37 / 1

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
61. 1,4-Dichlorobenzene	106-46-7	3.05	3.37	0	0	0	NLFG	/ 37 / 1
62. 3,3'-Dichlorobenzidine ( $pK_b=11.7$ )	91-94-1	3.32	3.64	0	0	0	NLFG	/ 4 / 0
63. Dichlorodifluoromethane (Freon 12: bp = -29°C)	75-71-8							
64. 1,1-Dichloroethane	75-34-3	1.46	1.78	0	1.13E-2	3.78E-1	RATE	/ 4 / 13
Acetaldehyde (bp = 20°C)	75-07-0	-0.544	-0.224	0	0	0	NHFG	/ 4 / 0
Vinyl chloride (bp = -13.37°C)	75-01-4	1.04	1.36	0	0	0	NLFG	/ 1 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
65. 1,2-Dichloroethane	107-06-2	1.13	1.45	0	9.61E-3	54.7		/ 37 / 13
Vinyl chloride (bp = -13.37°C)	75-01-4	1.04	1.36	0	0	0	NLFG	/ 1 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
2-Chloroethanol	107-07-3	-0.492	-0.172	0	3.9E-2	3.2E5		/ 4 / 3
Ethylene oxide	75-21-8	-1.1	-0.792	2.9E5	21	0		/ 4 / 5
Ethylene glycol	107-21-1	-1.52	-1.2	0	0	0	NHFG	/ 29 / 2
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
66. 1,1-Dichloroethylene (Vinylidene chloride: bp = 30-32°C)	75-35-4	1.79	2.11	0	0	0	NLFG	/ 1 / 2
67. <i>cis</i> -1,2-Dichloroethylene	156-59-2	1.7	2.0	0	0	0	NLFG	/ 29 / 0
68. <i>trans</i> -1,2-Dichloroethylene	156-60-5	1.60	1.92	0	0	0	NLFG	/ 29 / 0
69. Dichloromethane (Methylene Chloride)	75-09-2	0.93	1.25	0	1E-3	6E-1	aa	/ 4 / 63
Formaldehyde (bp = -19.5°C; HYDRATES RAPIDLY)	50-00-0	-1.3	-1.0	0	0	0	NHFG	/ 29 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
70. 2,4-Dichlorophenol ( $pK_a=7.9$ )	120-83-2	2.49	3.07	0	0	0	NLFG	/ 4 / 0
71. 1,2-Dichloropropane	78-87-5	1.67	1.99	0	4.6E-2	4.2	RATE	/ 4 / 24
1-Chloro-1-propene	590-21-6	1.7	2.0	0	0	0	NLFG	/ 29 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
2-Chloropropan-1-ol	19210-21-0	0.58	0.90	0	0.46	1.8E5	f	/ 29 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Propylene oxide	75-56-9	-0.59	-0.27	1.9E6	17	3E3		/ 4 / 5
1,2-Dihydroxypropane	57-55-6	-1.38	-1.06	0	0	0	NLFG	/ 4 / 0
72. 1,3-Dichloropropene (mixture of isomers)	542-75-6	1.43						14 / /
cis-1,3-Dichloropropene	10061-01-5	1.8	2.2	0	40	0	s	/ 29 / 0
cis-3-Chloro-2-propen-1-ol	4643-05-4	0.23	0.55	0	0	0	NLFG	/ 29 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
trans-1,3-Dichloropropene	10061-02-6	1.8	2.2	0	40	0	s	/ 29 / 0
trans-3-Chloro-2-propen-1-ol	4643-06-5	0.18	0.50	0	0	0	NLFG	/ 29 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
73. Dieldrin	60-57-1	5.08	5.401	0	6.3E-2	0	RATE	/ 7 / 6
cis-1,2,3,4,10,10-Hexachloro-6,7-dihydroxyexo-1,4,4a,5,6,7,8,8a-octahydroexo-1,4-endo-5,8-dimethanonaphthalene (Dieldrin diol)	64839-05-0	3.2	3.5	0	0	0	NLFG	/ 29 / 0
trans-1,2,3,4,10,10-Hexachloro-6,7-dihydroxyexo-1,4,4a,5,6,7,8,8a-octahydroexo-1,4-endo-5,8-dimethanonaphthalene (Dieldrin diol)	57345-89-8	3.2	3.5	0	0	0	NLFG	/ 29 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
74. Diethyl phthalate	84-66-2	1.99	2.57	0	0	3.1E5	RATE	11 / 4 / 9
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
Ethyl hydrogen phthalate	2306-33-4	2.18	2.50	0	0	1.6E5	c	/ 29 / 0
o-Phthalic acid ( $pK_a=3.03$ )	88-99-3	-1.27	0.732	0	0	0	NHFG	/ 4 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
75. Diethylstilbestrol ( $pK_a=9.3$ )	56-53-1	4.09	4.96	0	0	0	NHFG	/ 4 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_n$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
76. Dimethoate	60-51-5	0.132	0.452	0	1.68	4.48E6	RATE	/ 4 / 32
.....( $k_n$ at C).....								
O,O-Dimethylphosphorodithioic acid ( $pK_a=1.6$ )	756-80-9	-2.5	-0.5	0	0.2	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
O-Methylphosphorodithioic acid ( $pK_a=1.5$ )	106191-34-8	-0.7	1.3	0	1	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
Phosphorodithioic acid ( $pK_a=1.7$ )	15834-33-0	-3.6	-1.6	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
N-Methyl-2-hydroxyacetamide	5415-94-1	-0.8	-0.5	0	0	0	NLFG	/ 29 / 0
.....( $k_n$ at P).....								
O-Methyl-S-[2-(N-methylacetamide)]-phosphorodithioic acid ( $pK_a=1.6$ )	2700-77-8	-0.5	1.5	0	0.2	0		/ 29 / 0
N-Methyl-2-hydroxyacetamide	5415-94-1	-0.8	-0.5	0	0	0	NLFG	/ 29 / 0
O-Methylphosphorodithioic acid ( $pK_a=1.5$ )	106191-34-8	-0.7	1.3	0	1	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
Phosphorodithioic acid	15834-33-0	-3.6	-1.6	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 4 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
.....( $k_b$ ).....								
O,O-Dimethylphosphorothioic acid ( $pK_a=1.6$ )	1112-38-5	-3	-1	0	0.2	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
O-Methylphosphorothioic acid ( $pK_a=1.5$ )	1111-99-5	-4	-2.0	0	1	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
Phosphorothioic acid ( $pK_a=1.5$ )	13598-51-1	-5	-3.0	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
N-Methyl-2-mercaptoacetamide ( $pK_a=8.7$ )	20938-74-3	-0.8	-1.0	0	0	0	NLFG	/ 29 / 0



Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
77. 3,3'-Dimethoxybenzidine ( $pK_a=10.3$ )	119-90-4	1.49	1.81	0	0	0	NHFG	/ 4 / 0
78. 7,12-Dimethylbenz[a]anthracene	57-97-6	6.64	6.96	0	0	0	NHFG	/ 4 / 0
79. 3,3'-Dimethylbenzidine ( $pK_a=9.3$ )	119-93-7	2.55	2.87	0	0	0	NHFG	/ 4 / 0
80. 2,4-Dimethylphenol ( $pK_a=10.1$ )	105-67-9	2.29	2.77	0	0	0	NHFG	/ 4 / 0
81. Dimethyl phthalate	131-11-3	1.20	1.52	0	0	1.8E6	RATE	/ 4 / 9
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
Methyl hydrogen phthalate	4367-18-5	1.6	1.9	0	0	9E5	c	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
o-Phthalic acid ( $pK_a=3.03$ )	88-99-3	-1.27	0.732	0	0	0	NHFG	/ 4 / 0
82. 1,3-Dinitrobenzene	99-65-0	1.31	1.63	0	0	0	NHFG	/ 4 / 0
83. 2,4-Dinitrophenol ( $pK_a=3.3$ )	51-28-5	-0.09	1.91	0	0	0	NHFG	/ 4 / 0
84. 2,4-Dinitrotoluene	121-14-2	1.68	2.00	0	0	0	NHFG	/ 4 / 1
85. 2,6-Dinitrotoluene	606-20-2	1.40	1.72	0	0	0	NHFG	/ 4 / 0
86. Di-n-butyl phthalate	84-74-2	4.37	4.69	0	0	1.2E5	RATE	/ 4 / 9
n-Butanol **	71-36-3	0.503	0.832	0	0	0	NHFG	/ 4 / 0
n-Butyl hydrogen phthalate	131-70-4	3.43	3.75	0	0	6E4	c	/ 29 / 0
n-Butanol **	71-36-3	0.503	0.823	0	0	0	NHFG	/ 4 / 0
o-Phthalic acid ( $pK_a= 3.03$ )	88-99-3	-1.27	0.732	0	0	0	NHFG	/ 4 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
87. DI- <i>n</i> -octyl phthalate	117-84-0	7.6	7.9	0	0	5.2E5	RATE	/ 29 / 15
<i>n</i> -Octanol	111-87-5	2.77	3.09	0	0	0	NHFG	/ 29 / 0
<i>n</i> -Octyl hydrogen phthalate	5393-19-1	5.8	6.1	0	0	2.6E5	c	/ 29 / 0
<i>n</i> -Octanol	111-87-5	2.77	3.09	0	0	0	NHFG	/ 29 / 0
<i>o</i> -Phthalic acid ( $pK_a = 3.03$ )	88-99-3	-1.27	0.732	0	0	0	NHFG	/ 4 / 0
88. 1,4-Dioxane	123-91-1	-0.812	-0.492	0	0	0	NHFG	/ 4 / 0
89. 2378 TCDDioxin	1746-01-6	6.10	6.42	0	0	0	NLFG	/ 16 / 0
90. 2378 PeCDDioxins		6.9	7.2	0	0	0	NLFG	/ 29 / 0
91. 2378 HxCDDioxins		7.3	7.6	0	0	0	NLFG	/ 29 / 0
92. 2378 HpCDDioxins		7.8	8.1	0	0	0	NLFG	/ 29 / 0
93. OCDD (Octachlorodibenzo- <i>p</i> -dioxin)	3268-87-9	8.08	8.4	0	0	0	NLFG	/ 29 / 0
94. Diphenylamine ( $pK_b = 13.4$ )	122-39-4	3.30	3.62	0	0	0	NHFG	/ 4 / 0
95. 1,2-Diphenylhydrazine ( $pK_b = 13.2$ )	122-66-7	1.4	1.7	0	0	0	NHFG	/ 4 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_n$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_h$ $M^{-1}Y^{-1}$		
96. Disulfoton	298-04-4	2.94	3.26	0	2.3	5.4E4	RATE	/ 4 / 6
.....( $k_n$ at C).....								
O,O-Diethylphosphorodithioic acid ( $pK_a=1.5$ )	298-06-6	-2.2	-0.2	0	0.2	0	z	/ 29 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
O-Ethylphosphorodithioic acid ( $pK_a=1.6$ )	NG	-1	1.0	0	1	0	z	/ 29 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
Phosphorodithioic acid ( $pK_a=1.7$ )	15834-33-0	-3.6	-1.6	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
2-Hydroxyethylethylthioether	110-77-0	0.8	1.1	0	0	0	NLFG	/ 29 / 0
.....( $k_n$ at P).....								
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
O-Ethyl-S-[2-(ethylthio)ethyl]-phosphorodithioic acid ( $pK_a=1.6$ )	94139-29-4	-1.9	0.1	0	0.2	0	z	/ 29 / 0
2-Hydroxyethylethylthioether	110-77-0	0.8	1.1	0	0	0	NLFG	/ 29 / 0
O-Ethylphosphorodithioic acid ( $pK_a=1.6$ )	NG	-1	1.0	0	1	0	z	/ 29 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
Phosphorodithioic acid ( $pK_a=1.7$ )	15834-33-0	-3.6	-1.6	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
.....( $k_h$ ).....								
O,O-Diethylphosphorothioic acid ( $pK_a=1.5$ )	2465-65-8	-2	0	0	0.2	0	z	/ 29 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
O-Ethylphosphorothioic acid ( $pK_a=1.5$ )	14018-63-4	-1.5	0.5	0	1	0	z	/ 29 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
Phosphorothioic acid ( $pK_a=1.5$ )	13598-51-1	-5	-3.0	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
2-Thioethylethylthioether	26750-44-7	2.7	3.0	0	0	0	NLFG	/ 29 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_h$ $M^{-1}Y^{-1}$	$k_h$ $Y^{-1}$	$k_h$ $M^{-1}Y^{-1}$		
97. Endosulfan (Endosulfan I and II, mixture)	115-29-7							
Endosulfan I (alpha)	959-98-8	4.0	4.3	0	6.1E-2	1.7E8	RATE	/ 29 / 6
Endosulfan II (beta)	33213-65-9	4.0	4.3	0	8.9E-2	3.0E8	RATE	/ 29 / 6
Sulfuric acid	7664-93-9	NA	NA	0	0	0	NHFG	/ 0 / 0
1,4,5,6,7,7-Hexachloro-bicyclo-[2.2.1]hept-5-ene-2,3-dimethanol (Endosulfan diol)	2157-19-9	2.5	2.8	0	0	0	NLFG	/ 29 / 0
98. Endrin	72-20-8	4.60	4.92	0	5.5E-2	0		/ 62 / 1
cis-Endrin diol	34015-58-2	3.2	3.5	0	0	0	NLFG	/ 29 / 0
trans-Endrin diol	14737-72-5	3.2	3.5	0	0	0	NLFG	/ 29 / 0
99. Epichlorohydrin	106-89-8	-0.53	-0.210	2.5E4	30.9	0		/ 4 / 5
1-Chloro-2,3-dihydroxypropane	96-24-2	-0.8	-0.5	0	0.46	1.8E5	f	/ 29 / 0
1-Hydroxy-2,3-propylene oxide	556-52-5	-1.7	-1.4	7.7E4	8.9	0		/ 29 / 5
Glycerol	56-81-5	-2.2	-1.9	0	0	0	NHFG	/ 29 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Glycerol	56-81-5	-2.2	-1.9	0	0	0	NHFG	/ 29 / 0
100. 2-Ethoxyethanol ( $pK_a=15.1$ )	110-80-5	-0.54	-0.217	0	0	0	NHFG	/ 4 / 0
101. Ethyl acetate	141-78-6	0.351	0.671	3.5E3	4.8E-3	3.4E6		/ 4 / 5
Acetic acid ( $pK_a=4.65$ )	64-19-7	-2.23	-0.234	0	0	0	NHFG	/ 4 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 9 / 0
102. Ethylbenzene	100-41-4	3.00	3.32	0	0	0	NHFG	/ 4 / 0
103. Ethyl ether	60-29-7	0.55	0.870	0	0	0	NHFG	/ 4 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_n$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_h$ $M^{-1}Y^{-1}$		
104. Ethyl methacrylate	97-63-2	1.27	1.59	0	0	1.1E6	g	/ 4 / 0
Methacrylic acid ( $pK_a=4.45$ )	79-41-4	-1.53	0.470	0	0	0	NHFG	/ 4 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
105. Ethyl methanesulfonate	62-50-0	-0.27	0.051	0	1.25E3	0	RATE	/ 4 / 60
Methylsulfonic acid ( $pK_a = -0.39$ )	75-75-2	-2	0	0	0	0	NLFG	/ 29 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
106. Ethylene dibromide (1,2-Dibromoethane)	106-93-4	1.42	1.74	0	6.3E-1	0	RATE	/ 4 / 3
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
Vinyl bromide (bp=16°C)	593-60-2	1.23	1.55	0	0	0	NLFG	/ 4 / 0
2-Bromoethanol	540-51-2	-0.35	-3.2E-2	0	0.1	1E6	r	/ 4 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
Ethylene oxide	75-21-8	-1.1	-0.792	2.9E5	21	0		/ 4 / 5
Ethylene glycol	107-21-1	-1.5	-1.2	0	0	0	NLFG	/ 29 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_n$
				$k_a$ $M^{-1}Y^{-1}$	$k_h$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
107. Famphur	52-85-7	1.95	2.27	0	2.2	4.6E4	RATE	/ 4 / 6
-----( $k_n$ )-----								
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
O-Methyl-O- <i>p</i> -( <i>N,N</i> -dimethylsulfamoyl)-phenylphosphorothioic acid ( $pK_a=1.5$ )	15020-55-0	2	4.0	0	0.2	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
O- <i>p</i> -( <i>N,N</i> -Dimethylsulfamoyl)-phenylphosphorothioic acid ( $pK_a=1.5$ )	NG	0.5	2.5	0	1	0	z	/ 29 / 0
Phosphorothioic acid ( $pK_a=1.5$ )	13598-51-1	-5	-3.0	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
<i>p</i> -( <i>N,N</i> -Dimethylsulfamoyl)phenol ( $pK_a=8.4$ )	15020-57-2	1.6	2.0	0	0	0	NLFG	/ 29 / 0
-----( $k_n, k_b$ )-----								
<i>p</i> -( <i>N,N</i> -Dimethylsulfamoyl)phenol ( $pK_a=8.4$ )	15020-57-2	1.6	2.0	0	0	0	NLFG	/ 29 / 0
O,O-Dimethylphosphorothioic acid ( $pK_a=1.6$ )	1112-38-5	-3	-1	0	0.2	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
O-Methylphosphorothioic acid ( $pK_a=1.5$ )	1111-99-5	-4	-2.0	0	1	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
Phosphorothioic acid ( $pK_a=1.5$ )	13598-51-1	-5	-3.0	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
108. Fluoranthene	206-44-0	4.63	4.95	0	0	0	NHFG	/ 4 / 0
109. Fluorene	86-73-7	3.91	4.23	0	0	0	NHFG	/ 4 / 0
110. Formic acid ( $pK_a=3.8$ )	64-18-6	-2.7	-0.7	0	0	0	NHFG	/ 29 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
111. Furan	110-00-9	1.00	1.32	0	0	0	NHFG	/ 4 / 0
112. 2378 TCDFuran (2,3,7,8-Tetrachlorodibenzofuran)	51207-31-9	6.62	6.94	0	0	0	NLFG	/ 4 / 0
113. 12378 PeCDFuran (1,2,3,7,8-Pentachlorodibenzofuran)	57117-41-6	6.5	6.8	0	0	0	NLFG	/ 29 / 0
114. 23478 PeCDFuran (2,3,4,7,8-Pentachlorodibenzofuran)	57117-31-4	6.60	6.92	0	0	0	NLFG	/ 16 / 0
115. 2378 HxCDFurans		7.0	7.3	0	0	0	NLFG	/ 29 / 0
116. 2378 HpCDFurans		7.6	7.9	0	0	0	NLFG	/ 29 / 0
117. OCDF (Octachlorodibenzofuran)	39001-02-0	8.13	8.45	0	0	0	NLFG	/ 29 / 0
118. Heptachlor	76-44-8	5.21	5.53	0	61	0	RATE	/ 62 / 25
1-Hydroxychloridene	24009-05-0	4.5	4.8	0	0	0	NLFG	/ 29 / 2
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
119. Heptachlor epoxide	1024-57-3	4.9	5.2	0	6.3E-2	0	h	/ 29 / 0
Heptachlor diol	126959-40-8	3.7	4.0	0	3.9E-3	3.2E4	h	/ 29 / 0
Heptachlor triol	126959-41-9	2.2	2.5	0	0	0	NLFG	/ 29 / 0
120. Hexachlorobenzene	118-74-1	5.411	5.731	0	0	0	NLFG	/ 7 / 1
121. Hexachlorobutadiene	87-68-3	4.46	4.78	0	0	0	NLFG	/ 37 / 1

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_t$
				$k_a$ $M^{-1}Y^{-1}$	$k_b$ $Y^{-1}$	$k_c$ $M^{-1}Y^{-1}$		
122. <i>alpha</i> -HCH	319-84-6	3.43	3.75	0	1.05	1.74E6	I	/ 4 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
1,3,4,5,6-pentachlorocyclohexene	319-94-8	3.3	3.6	0	0.26	6.5E5		/ 29 / 2
1,2,3-Trichlorobenzene	87-61-6	3.96	4.28	0	0	0	NLFG	/ 4 / 6
1,2,4-Trichlorobenzene	120-82-1	3.96	4.28	0	0	0	NLFG	/ 4 / 6
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
123. <i>beta</i> -HCH	319-85-7	3.43	3.75	0	0	0	NLFG	/ 4 / 0
124. Hexachlorocyclopentadiene	77-47-4	4.72	5.04	0	24.8	0	J, RATE	/ 19 / 19
1,1-Dihydroxytetrachlorocyclopentadiene	NG						unstable	/ / 0
Polymers								/ / 0
125. Hexachloroethane	67-72-1	3.61	3.93	0	0	0	NLFG	/ 1 / 24
126. Hexachlorophene ( $pK_a=6.1$ )	70-30-4	5.0	7.3	0	0	0	NLFG	/ 29 / 0
127. Indeno[1,2,3- <i>cd</i> ]pyrene	193-39-5	6.26	6.58	0	0	0	NHFG	/ 4 / 0
128. Isobutyl alcohol ( $pK_a=15.8$ )	78-83-1	0.44	0.76	0	0	0	NHFG	/ 1 / 1
129. Isophorone	78-59-1	1.9	2.2	0	0	0	NHFG	/ 8 / 0
130. Kepone	143-50-0	4.15	4.47	0	0	0	k, NLFG	/ 4 / 0
131. Lead (and compounds N.O.S.)	7439-92-1							



Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_n$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
132. <i>gamma</i> -HCH (Lindane)	58-89-9	3.40	3.72	0	1.05	1.73E6		/ 1 / 4
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
1,3,4,5,6-pentachlorocyclo- hexene	319-94-8	3.3	3.6	0	0.26	6.5E5		/ 29 / 2
1,2,3-Trichlorobenzene	87-61-6	3.96	4.28	0	0	0	NLFG	/ 4 / 6
1,2,4-Trichlorobenzene	120-82-1	3.96	4.28	0	0	0	NLFG	/ 4 / 6
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
133. Mercury (and compounds N.O.S.)	7439-97-6							
134. Methacrylonitrile	126-98-7	0.22	0.540	5E2	0	5.2E3	I	/ 4 / 0
Methacrylamide	79-39-0	0.7	1.0	31.5	1.8E-2	0	I	/ 29 / 0
Methacrylic acid ( $pK_a=4.45$ )	79-41-4	-1.53	0.470	0	0	0	NHFG	/ 4 / 0
Ammonia	7664-41-7	NA	NA	0	0	0	NHFG	/ 0 / 0
135. Methanol	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
136. Methoxychlor	72-43-5	4.90	5.08	0	0.69	1.2E4		38 / 38 / 12
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
2,2-Bis( <i>p</i> -methoxyphenyl)- 1,1-dichloroethylene	2132-70-9	4.1	4.4	0	0	0	NLFG	/ 9 / 0
Anisoin	119-52-8	3.9	4.2	0	6E3	0	m	/ 9 / 0
Anisil	1226-42-2	3.38	3.70	0	0	0	NHFG	/ 4 / 0
137. 3-Methylcholanthrene	56-49-5	7.0	7.3	0	0	0	NHFG	/ 29 / 0
138. Methyl ethyl ketone	78-93-3	-0.03	0.29	0	0	0	NHFG	/ 65 / 1
139. Methyl isobutyl ketone	108-10-1	0.87	1.19	0	0	0	NHFG	/ 4 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_r$
				$k_a$ $M^{-1}Y^{-1}$	$k_b$ $Y^{-1}$	$k_c$ $M^{-1}Y^{-1}$		
140. Methyl methacrylate	80-62-6	0.74	1.06	0	0	1.9E6	RATE	/ 4 / 24
Methacrylic acid ( $pK_a=4.45$ )	79-41-4	-1.53	0.470	0	0	0	NHFG	/ 4 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
141. Methyl parathion	298-00-0	2.47	2.79	NG	2.8	NG	n	/ 4 / 39
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
O-Methyl-O-(p-nitrophenyl)- phosphorothioic acid ( $pK_a=1.3$ )	7699-30-1	-2.5	-0.5	0	0.2	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
O-(p-Nitrophenyl)phosphoro- thioic acid ( $pK_a=1.1$ )	18429-96-4			0	1	0	z	/ / 0
Phosphorothioic acid ( $pK_a=1.5$ )	13598-51-1	-5	-3.0	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
p-Nitrophenol ( $pK_a=7.0$ )	100-02-7	1.2	1.85	0	0	0	NHFG	/ 4 / 0
O,O-Dimethylphosphorothioic acid ( $pK_a=1.6$ )	1112-38-5	-3	-1	0	0.2	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
O-Methylphosphorothioic acid ( $pK_a=1.5$ )	1111-99-5	-4	-2.0	0	1	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
Phosphorothioic acid ( $pK_a=1.5$ )	13598-51-1	-5	-3.0	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
142. Naphthalene	91-20-3	3.11	3.36	0	0	0	NHFG	38 / 38 / 0
143. 2-Naphthylamine ( $pK_b=9.8$ )	91-59-8	1.77	2.09	0	0	0	NHFG	/ 4 / 0
144. Nickel (and compounds N.O.S.)	7440-02-0							

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
145. Nitrobenzene	98-95-3	1.51	1.83	0	0	0	NLFG	/ 37 / 1
146. 2-Nitropropane	79-46-9	0.23	0.554	0	0	0	NHFG	/ 4 / 0
147. <i>N</i> -Nitroso-di- <i>n</i> -butylamine ( $pK_a < 1$ )	924-16-3	2.09	2.41	0	0	0	NHFG	/ 29 / 0
148. <i>N</i> -Nitrosodiethylamine ( $pK_a < 1$ )	55-18-5	-0.03	0.290	0	0	0	NHFG	/ 29 / 0
149. <i>N</i> -Nitrosodimethylamine ( $pK_a < 1$ )	62-75-9	0.448	0.768	0	0	0	NHFG	/ 29 / 0
150. <i>N</i> -Nitrosodiphenylamine ( $pK_a < 0$ )	86-30-6	2.84	3.16	0	0	0	NHFG	/ 29 / 0
151. <i>N</i> -Nitroso-di- <i>n</i> -propylamine ( $pK_a < 1$ )	621-64-7	1.03	1.35	0	0	0	NHFG	/ 29 / 0
152. <i>N</i> -Nitrosomethylethylamine ( $pK_a < 1$ )	10595-95-6	1.03	1.35	0	0	0	NHFG	/ 29 / 0
153. <i>N</i> -Nitrosopiperidine	100-75-4	-0.02	0.305	0	0	0	NHFG	/ 4 / 0
154. <i>N</i> -Nitrosopyrrolidine	930-55-2	-0.57	-0.254	0	0	0	NHFG	/ 4 / 0
155. Octamethyl pyrophosphoramidate  <i>Bis</i> ( <i>N,N</i> -ethylamino)- phosphoric acid ( $pK_a 4.2$ )	152-16-9			1.9E3	NG	NG		/ / 34
	27972-73-2			0	0	0	NLFG	/ / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
156. Parathion (ethyl)	56-38-2	3.15	3.47	0	2.4	3.7E6		/ 4 / 21
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
O-Ethyl-O-(p-nitrophenyl)- phosphorothioic acid ( $pK_a=1.2$ )	15576-30-4			0	0.2	0	z	/ / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
O-(p-Nitrophenyl)phosphoro- thioic acid ( $pK_a=1.1$ )	18429-96-4			0	1	0	z	/ / 0
p-Nitrophenol ( $pK_a=7.0$ )	100-02-7	1.2	1.85	0	0	0	NHFG	/ 4 / 0
Phosphorothioic acid ( $pK_a=1.5$ )	13598-51-1	-5	-3.0	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
p-Nitrophenol ( $pK_a=7.0$ )	100-02-7	1.2	1.85	0	0	0	NHFG	/ 4 / 0
O,O-Diethylphosphorothioic acid ( $pK_a=1.5$ )	2465-65-8	-2	0	0	0.2	0	z	/ 29 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
O-Ethylphosphorothioic acid ( $pK_a=1.5$ )	14018-63-4	-1.5	0.5	0	1	0	z	/ 29 / 0
Phosphorothioic acid ( $pK_a=1.5$ )	13598-51-1	-5	-3.0	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
157. Pentachlorobenzene	608-93-5	5.39	5.183	0	0	0	NLFG	/ 7 / 0
158. Pentachloronitrobenzene (PCNB)	82-68-8	4.57	4.89	0	0	0	NLFG	/ 4 / 0
159. Pentachlorophenol ( $pK_a=4.8$ )	87-86-5	3.06	5.06	0	0	0	NLFG	/ 4 / 1
160. Phenol ( $pK_a=10$ )	108-95-2	1.23	1.48	0	0	0	NHFG	/ 4 / 1

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
161. Phenylenediamine:								
1,2-Phenylenediamine ( $pK_b=9.3$ )	95-54-5	-0.1	0.2	0	0	0	NHFG	/ 29 / 0
1,3-Phenylenediamine ( $pK_b=8.7$ )	108-45-2	-0.3	0.05	0	0	0	NHFG	/ 29 / 0
1,4-Phenylenediamine ( $pK_b=7.7$ )	106-50-3	NA	-0.4	0	0	0	NHFG	/ 29 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
162. Phorate	298-02-2	2.64	2.96	0	62	0	RATE	/ 4 / 25
-----( $k_h$ at P-O)-----								
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
O-Ethyl-S-[(ethylthio)methyl]-phosphorodithioic acid ( $pK_a=1.6$ )	NG	-2.5	-0.5	0	0.2	0	z	/ 29 / 0
O-Ethylphosphorodithioic acid ( $pK_a=1.6$ )	NG	-1	1.0	0	1	0	z	/ 29 / 0
Phosphorodithioic acid ( $pK_a=1.7$ )	15834-33-0	-3.6	-1.6	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
Hydroxymethylethylthio-ether	15909-30-5	0.2	0.5	0	0	0	NLFG	/ 29 / 0
-----( $k_a$ )-----								
Mercaptomethylethylthioether	29414-49-1	2.0	2.3	0	0	0	NLFG	/ 29 / 0
O,O-Diethylphosphorothioic acid ( $pK_a=1.5$ )	2465-65-8	-2	0	0	0.2	0	z	/ 29 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
O-Ethylphosphorothioic acid ( $pK_a=1.5$ )	14018-63-4	-1.5	0.5	0	1	0	z	/ 29 / 0
Phosphorothioic acid ( $pK_a=1.5$ )	13598-51-1	-5	-3.0	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
-----( $k_h$ at S-C)-----								
Hydroxymethylethylthioether	15909-30-5	0.2	0.5	0	0	0	NLFG	/ 29 / 0
O,O-Diethylphosphorodithioic acid ( $pK_a=1.5$ )	298-06-6	-2.2	-0.2	0	0.2	0	z	/ 29 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
O-Ethylphosphorodithioic acid ( $pK_a=1.6$ )	NG	-1	1.0	0	1	0	z	/ 29 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
Phosphorodithioic acid ( $pK_a=1.7$ )	15834-33-0	-3.6	-1.6	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 29 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
163. Phthalic anhydride	85-44-9		-0.62	0	4.9E5	0	u, RATE	/ 35 / 22
o-Phthalic acid ( $pK_a=3.03$ )	88-99-3	-1.27	0.732	0	0	0	NHFG	/ 4 / 0
164. Polychlorinated biphenyls (Aroclors)	1338-38-3			0	0	0	NLFG	/ / 0
165. Pronamide	23950-58-5	2.63	2.95	59	0	6.1E2	RATE	/ 4 / 6
3,5-Dichlorobenzoic acid ( $pK_a=3.46$ )	51-38-5	1.5	3.5	0	0	0	NLFG	/ 29 / 0
1,1-Dimethyl-2-propynylamine ( $pK_b=8.1$ )	2978-58-7	-0.63	-0.306	0	0	0	NHFG	/ 4 / 0
166. Pyrene	129-00-0	4.92	5.18	0	0	0	NHFG	/ 38 / 0
167. Pyridine ( $pK_b=8.7$ )	110-86-1	0.34	0.665	0	0	0	NHFG	/ 4 / 1
168. Safrole	94-59-7	2.34	2.66	0	0	0	NHFG	/ 4 / 24
169. Selenium (and compounds N.O.S.)	7782-49-2							
170. Silver (and compounds N.O.S.)	7440-22-4							
171. Strychnine and salts ( $pK_b=4.7$ )	57-24-9	NA	2.0	0	0	0	NLFG	/ 29 / 0
172. Styrene	100-42-5	2.84	3.16	0	0	0	NHFG	/ 37 / 0
173. 1,2,4,5-Tetrachlorobenzene	95-94-3	4.284	4.604	0	0	0	NLFG	/ 7 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
174. 1,1,1,2-Tetrachloroethane	630-20-6	2.71	3.03	0	1.37E-2	1.13E4	RATE	/ 1 / 13
1,1,2-Trichloroethylene **	79-01-6	2.10	2.42	0	0	0	NLFG	/ 37 / 2
2,2,2-Trichloroethanol ( $pK_a=3.7$ )	115-20-8	1.13	1.45	0	0.65	0	v	/ 29 / 0
Hydroxyacetic acid	79-14-1	-4	-2	0	0	0	NHFG	/ 29 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
175. 1,1,2,2-Tetrachloroethane	79-34-5	2.07	2.39	0	5.10E-3	1.59E7	RATE	/ 37 / 13
1,1,2-Trichloroethylene **	79-01-6	2.10	2.42	0	0	0	NLFG	/ 37 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
176. Tetrachloroethylene	127-18-4	2.21	2.53	0	0	0	NLFG	/ 37 / 0
177. 2,3,4,6-Tetrachlorophenol ( $pK_a=5.3$ )	58-90-2	2.32	4.32	0	0	0	NLFG	/ 4 / 1
178. Tetraethyl dithiopyrophosphate (Sulfotep)	3689-24-5	3.51	3.83	0	84	9E6	o	/ 62 / 36
O,O-Diethylphosphorothioic acid ( $pK_a=1.5$ )	2465-65-8	-2	0	0	0.2	0	z	/ 29 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
O-Ethylphosphorothioic acid ( $pK_a=1.5$ )	14018-63-4	-1.5	0.5	0	1	0	z	/ 29 / 0
Phosphorothioic acid ( $pK_a=1.5$ )	13598-51-1	-5	-3.0	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-04	NA	NA	0	0	0	NHFG	/ 0 / 0
Ethanol	64-17-5	-0.62	-0.30	0	0	0	NHFG	/ 29 / 0
179. Thallium (and compounds N.O.S.)	7440-2							
180. Toluene	108-88-3	2.43	2.75	0	0	0	NHFG	/ 29 / 1
181. 2,4-Toluenediamine ( $pK_b=9.0$ )	95-80-7	0.02	0.337	0	0	0	NHFG	/ 4 / 0



Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
182. 2,6-Toluenediamine ( $pK_b=8.9$ )	823-40-5	0.02	0.337	0	0	0	NHFG	/ 4 / 0
183. <i>o</i> -Toluidine ( $pK_b=9.3$ )	95-53-4	1.24	1.56	0	0	0	NHFG	/ 4 / 0
184. <i>p</i> -Toluidine ( $pK_b=8.9$ )	106-49-0	1.24	1.56	0	0	0	NHFG	/ 4 / 0
185. Toxaphene (chlorinated camphenes)	8001-35-2	4.31	4.63	0	7.0E-2	2.8E4	p	/ 62 / 24
186. Tribromomethane (Bromoform)	75-25-2	2.05	2.37	NG	NG	1E4	t	/ 4 / 1
Carbon monoxide	630-08-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
187. 1,2,4-Trichlorobenzene	120-82-1	3.96	4.28	0	0	0	NLFG	/ 4 / 2
188. 1,1,1-Trichloroethane	71-55-6	2.16	2.47	0	6.4E-1	2.4E6		/ 37 / 67
1,1-Dichloroethylene ** (bp=31.9°C)	75-35-4	1.79	2.11	0	0	0	NLFG	/ 1 / 2
Acetic acid ( $pK_a=4.73$ )	64-19-7	-2.23	-0.234	0	0	0	NHFG	/ 4 / 2
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
189. 1,1,2-Trichloroethane	79-00-5	1.73	2.05	0	2.73E-5	4.95E4	RATE	/ 4 / 13
1,1-Dichloroethylene ** (bp=31.9°C)	75-35-4	1.79	2.11	0	0	0	NLFG	/ 1 / 2
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Chloroacetaldehyde	107-20-0	0.07	0.389	0	7E-3	2.6E4		/ 4 / 2
Hydroxyacetaldehyde	141-46-8	-1.38	-1.06	0	0	0	NHFG	/ 4 / 2
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
190. Trichloroethylene (1,1,2-Trichloroethylene)	79-01-6	2.10	2.42	0	0	0	NLFG	/ 37 / 2

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_n$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
191. Trichlorofluoromethane (Freon 11: bp=24.1°C)	75-69-4	2.11	2.43	0	0	0	NLFG,ee	/ 4 / 0
192. 2,4,5-Trichlorophenol ( $pK_a=7.1$ )	95-95-4	2.93	3.85	0	0	0	NLFG	/ 4 / 1
193. 2,4,6-Trichlorophenol ( $pK_a=6.4$ )	88-06-2	2.25	3.57	0	0	0	NLFG	/ 4 / 1
194. 2,4,5-Trichlorophenoxyacetic acid ( $pK_a=3.0$ )	93-76-5	1.43	3.43	0	0	0	NLFG	/ 4 / 0
195. 2-(2,4,5-Trichlorophenoxy)propionic acid (Silvex: ( $pK_a=3.4$ ))	93-72-1	1.74	3.74	0	0	0	NLFG	/ 4 / 1
196. 1,2,3-Trichloropropane	96-18-4	1.66	1.98	0	1.7E-2	3.6E3	RATE	/ 4 / 6
----- $k_n$ -----								
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
2,3-Dichloro-1-propanol	616-23-9	0.5	0.8	0	0.46	1.8E5		/ 29 / 3
Epichlorohydrin	106-89-8	-0.53	-0.210	2.5E4	30.9	0		/ 4 / 5
1-Chloro-2,3-dihydroxypropane	96-24-2	-0.8	-0.5	0	0.46	1.8E5	f	/ 29 / 0
1-Hydroxy-2,3-propylene oxide	556-52-5	-1.7	-1.4	7.7E4	8.9	0		/ 29 / 5
Glycerol	56-81-5	-2.2	-1.9	0	0	0	NHFG	/ 29 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
Glycerol	56-81-5	-2.2	-1.9	0	0	0	NHFG	/ 29 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
----- $k_b$ -----								
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
2,3-Dichloropropene	78-88-6	1.8	2.1	0	1.8	0	x	/ 29 / 0
2-Chloro-3-hydroxypropene	5976-47-6	-0.1	0.25	0	0	0	NLFG	/ 4 / 0
Hydrochloric acid	7647-01-0	NA	NA	0	0	0	NHFG	/ 0 / 0
197. 1,1,2-Trichloro-1,2,2-trifluoroethane	76-13-1	2.97	3.29	0	0	0	NLFG	/ 4 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_h$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
198. <i>sym</i> -Trinitrobenzene (1,3,5-Trinitrobenzene)	99-35-4	1.05	1.37	0	0	0	NHFG	/ 4 / 0
199. <i>Tris</i> (2,3-dibromopropyl)phosphate	126-72-7	3.19	3.51	0	8.8E-2	3.0E5	RATE	/ 4 / 24
-----( $k_a$ )-----								
<i>O,O</i> -(2,3-Dibromopropyl)- phosphoric acid ( $pK_a=0.8$ )	5412-25-9			0	0.2	0	z	/ / 0
<i>O</i> -(2,3-Dibromopropyl)- phosphoric acid ( $pK_a=1.3$ )	5324-12-9			0	1	0	z	/ / 0
2,3-Dibromo-1-propanol	96-13-9	1.10	1.42	0	1.4	5.4E5	cc	/ 29 / 0
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
2,3-Dibromo-1-propanol	96-13-9	1.10	1.42	0	1.4	5.4E5	cc	/ 29 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
Epibromohydrin	3132-64-7	0.2	0.5	1.9E4	1.8E1	0		/ 29 / 41
1-Bromo-2,3- dihydroxypropane	4704-77-2	-1.18	-0.857	0	1.4	5.4E5	cc	/ 4 / 0
1-Hydroxy-2,3- propylene oxide	556-52-5	-1.7	-1.4	7.7E4	8.9	0		/ 29 / 5
Glycerol	56-81-5	-2.2	-1.9	0	0	0	NHFG	/ 29 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
Glycerol	56-81-5	-2.2	-1.9	0	0	0	NHFG	/ 29 / 0
2,3-Dibromo-1-propanol	96-13-9	1.10	1.42	0	1.4	5.4E5	cc	/ 29 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
2-Bromo-1,3-propanediol	4704-87-4	-1.4	-1.1	0	2	9E5	q	/ 29 / 0
Glycerol	56-81-5	-2.2	-1.9	0	0	0	NHFG	/ 29 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
-----( $k_b$ )-----								
<i>O,O</i> -(2,3-Dibromopropyl)- phosphoric acid ( $pK_a=0.8$ )	5412-25-9			0	0.2	0	z,dd	/ / 0
2,3-Dibromo-1-propanol	96-13-9	1.10	1.42	0	1.4	5.4E5	cc	/ 29 / 0
2-Bromo-2-propen-1-ol	598-19-6	0.43	0.75	0	0	0	NLFG	/ 29 / 0
Hydrobromic acid	10035-10-6	NA	NA	0	0	0	NHFG	/ 0 / 0
200. Vanadium	7440-62-2							
201. Vinyl chloride (Chloroethene: bp = -13.4°C)	75-01-4	1.04	1.36	0	0	0	NLFG	/ 1 / 0

Common Name	Chemical Abstract Service No.	Sorption Log $K_{oc}$	Sorption Log $K_{ow}$	Chemical Hydrolysis			Comment	References $K_{oc} / K_{ow} / k_n$
				$k_a$ $M^{-1}Y^{-1}$	$k_n$ $Y^{-1}$	$k_b$ $M^{-1}Y^{-1}$		
202. Xylenes (mixture of three isomers)	1330-20-7			0	0	0	NHFG	/ / 0
o-Xylene	95-47-6	3.02	3.34	0	0	0	NHFG	/ 29 / 0
m-Xylene	108-38-3	3.09	3.41	0	0	0	NHFG	/ 29 / 0
p-Xylene	106-42-3	3.12	3.44	0	0	0	NHFG	/ 29 / 0
203. Zinc (and compounds N.O.S.)	7440-66-6							

## COMMENT

RATE) Hydrolysis data were extrapolated with the RATE program to obtain rate constants at 25° C (see reference #28).

NG) A rate constant was *not given* in the publication or a CAS number was not assigned in the CAS Registry.

\*\* ) This product appears as a parent compound elsewhere in the alphabetically arranged table.

NA) When NA (not applicable) appears in one of the sorption columns, the compound is either an inorganic compound or an organic base that is ionized within the environmental pH range with a  $pK_a$  value greater than 6. A value cannot be computed.



Shaded rows contain inorganic compounds which are not addressed in this work.

- At an alkaline pH and concentrations above 2 ppm for acrylamide, cloudiness was observed in the laboratory hydrolysis experiment. Cloudiness was thought to have been polymerization.
- The hydrolysis rate constant was assumed to be the same as the parent compound's by analogy to *bis*(2-chloroethyl)ether and its product 2-(2-chloroethoxy)ethanol (see text in Part II).
- The hydrolysis rate constant was assumed to be half the parent's.
- The hydrolysis rate constant was assumed to be the same as the one for di-*n*-butyl phthalate for both pathways.
- Cyanide will not sorb onto sediments at a detectable rate.
- The hydrolysis rate constants for 2-chloropropan-1-ol and 1-chloro-2,3-dihydroxypropane were assumed by analogy to be the same as those of 2,3-dichloro-1-propanol (see #196).

- g) The hydrolysis rate constant was estimated by analogy to be 0.6 of methyl methacrylate's.
- h) The hydrolysis rate constant for heptachlor epoxide was assumed by analogy to be the same as dieldrin's. The reaction to the final product heptachlor triol occurs through the intermediate heptachlor diol, for which a rate estimate was assumed to be 1/10 the rate of 2-chloro-ethanol.
- i) The hydrolysis rate constants were assumed by analogy to be the same as lindane's.
- j) Hydrolysis of hexachlorocyclopentadiene results in the formation of 1,1-dihydroxytetrachlorocyclopentadiene which is an unstable product. Its degradation leads to the formation of polymers which cannot be identified.
- k) Kepone hydrates in an aqueous medium. The sorption coefficient of the hydrated form may be orders of magnitude lower than the coefficient of the unhydrated form. The given log values are for the unhydrated form. A value for the hydrated form cannot be estimated.
- l) The hydrolysis rate constants for methacrylonitrile and its product methacrylamide were assumed by analogy to be the same as those for acrylonitrile and its product acrylamide.
- m) The product of methoxychlor, anisoin, degrades to anisil by autooxidation with an estimated half-life of one hour.
- n) The hydrolysis rate was determined at a pH<8.
- o) The hydrolysis rate constants for tetraethyl dithiopyrophosphate were based by analogy on the rate constants of tetraethyl pyrophosphate and tetraethyl monothiopyrophosphate. The rate constants of tetraethyl pyrophosphate were divided by 10 as an adjustment for the two sulfur substituents in tetraethyl dithiopyrophosphate.
- p) Toxaphene is produced by the chlorination of camphene and is a complex mixture of at least 177 C<sub>10</sub> polychloro- derivatives. It has an approximate overall empirical formula of C<sub>10</sub>H<sub>10</sub>Cl<sub>8</sub> (The Merck Index, Eleventh Edition). Products can, therefore, not be identified.
- q) The hydrolysis rate constants for 2-bromo-1,3-propanediol were estimated by analogy to be five times those of 2,3-dichloropropanol's (see #196) because of the two hydroxide groups and the greater reactivity of bromine.
- r) The hydrolysis rate constants for 2-bromoethanol were estimated by analogy to be three times larger than those of 2-chloroethanol because of the greater reactivity of bromine.
- s) The hydrolysis rate constants for the *cis*- and *trans*-1,3-dichloropropene were assumed by analogy to be the same as 3-chloropropene's (#43).
- t) The hydrolysis rate constants for bromodichloromethane, chlorodibromomethane, and tribromomethane were determined in 66.67% (v/v) dioxane/water.
- u) Phthalic anhydride hydrolyzes to *o*-phthalic acid with a half-life of less than one minute. A  $K_{\infty}$  value for the anhydride would be meaningless.
- v) The hydrolysis rate constant for 2,2,2-trichloroethanol was assumed by analogy to be the same as 1,1,1-trichloroethane's (see #188).
- w) QSAR model computations have indicated that the half-life of this halogenated methane is several thousand years. Its hydrolysis process was, therefore, designated as NLFG.
- x) The hydrolysis rate constant for 2,3-dichloropropene was assumed by analogy to be the same as 2-bromo-3-chloropropene's (see #58).

- y) The log  $K_{ow}$  value for technical grade chlordane was calculated by averaging the measured values of the *cis*- and *trans*- isomers. The hydrolysis rate constant given is for the *cis*- isomer only. The *trans*- isomer will not hydrolyze.
- z) The hydrolysis rate constant for the degradation of the organophosphorus diester to the monoester was estimated to be smaller than the parent's by a factor of ten, whereas the rate constant for the degradation of the monoester to the acid was estimated to be half the rate of the parent's<sup>5</sup>. These estimated rate constants were based on the average of the neutral rate constants of five organophosphorus compounds.
- aa) The hydrolysis rate constants for dichloromethane were extrapolated to 25°C from elevated temperatures.
- bb) The hydrolysis rate constant was estimated by extrapolation. Because the value was estimated, no distinction was made of the fact that hydrolysis of the phosphorodithioic acid is slightly faster than the monoacid.
- cc) The hydrolysis rate constants for 2-bromo-3-chloropropanol, 2,3-dibromo-1-propanol, and 1-bromo-2,3-dihydroxypropane were estimated by analogy to be three times larger than those of 2,3-dichloro-1-propanol (see #196) because of the greater reactivity of bromine.
- dd) The alkaline hydrolysis pathway of the diester is identical to its neutral pathway.
- ee) Half-lives of polyhalogenated methanes are usually larger than 50 years. The half-life of trichlorofluoromethane is estimated to be larger than 50 years. Its hydrolysis process is, therefore, designated as NLFG.
- ff) The hydrolysis rate constants for aramite and chlorobenzilate were determined experimentally in ERL-Athens' laboratory. Products, except the hydrogen sulfites, were confirmed by spectral analyses. The hydrolysis rate constants for the products were estimated.
- gg) The hydrolysis rate constants were assumed to be the same as the parent's.

**TABLE 2. SAR computed reductive rate constants for selected halogenated aliphatics and nitroaromatics.**

Halogenated Aliphatics	Chemical Abstract Service No.	1% Organic Carbon $k(\text{year}^{-1})$	0.02% Organic Carbon $k(\text{year}^{-1})$
26. Bromodichloromethane	75-27-4	1.2E3	1.9E-1
27. Bromomethane	74-83-9	1.4E2	2.2E-2
33. Carbon tetrachloride	56-23-5	5.8E1	9.3E-3
39. Chlorodibromomethane	124-48-1	1.2E3	1.8E-1
40. Chloroform	67-66-3	2.6E1	4.2E-3
58. 1,2-Dibromo-3-chloropropane	96-12-8	2.4E2	3.8E-2
59. Dibromomethane	74-95-3	4.0E2	6.4E-2
64. 1,1-Dichloroethane	75-34-3	1.1E1	1.7E-3
65. 1,2-Dichloroethane	107-06-2	4.0	6.5E-4
69. Dichloromethane	75-09-2	8.7	1.4E-3
71. 1,2-Dichloropropane	78-87-5	5.4	8.5E-4
72. 1,3-Dichloropropene	542-75-6	6.7	1.1E-3
106. Ethylene dibromide	106-93-4	1.7E2	2.7E-2
125. Hexachloroethane	67-72-1	2.8E1	4.5E-3
174. 1,1,1,2-Tetrachloroethane	630-20-6	7.0	1.1E-3
175. 1,1,2,2-Tetrachloroethane	79-34-5	7.5	1.2E-3
186. Tribromomethane	75-25-2	1.2E3	1.8E-1
188. 1,1,1-Trichloroethane	71-55-6	1.5E1	2.4E-3
189. 1,1,2-Trichloroethane	79-00-5	5.4	8.5E-4
191. Trichlorofluoromethane	75-69-4	5.8E1	9.3E-3
196. 1,2,3-Trichloropropane	96-18-4	4.3	6.8E-4
197. 1,1,2-Trichloro-1,2,2-trifluoroethane	76-13-1	4.0E1	6.4E-3
Nitroaromatics	Chemical Abstract Service No.	1% Organic Carbon $k(\text{year}^{-1})$	0.02% Organic Carbon $k(\text{year}^{-1})$
30. Dinoseb	88-85-7	5.0E3	8.8E1
82. 1,3-Dinitrobenzene	99-65-0	8.0E2	1.4E2
83. 2,4-Dinitrophenol	51-28-5	2.2E3	3.9E2
84. 2,4-Dinitrotoluene	121-14-2	6.6E2	1.2E2
85. 2,6-Dinitrotoluene	606-20-2	8.0E2	1.4E2
141. Methyl parathion	298-00-0	1.2E2	2.2E1
145. Nitrobenzene	98-95-3	3.0E2	5.2E1
156. Parathion	56-38-2	1.2E2	2.2E1
198. <i>sym</i> -Trinitrobenzene	99-35-4	2.2E3	3.9E2





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58. Wolfe, N.L., W. Peijnenburg, H. d Hollander, H. Verboom, and D. v d Meent. Structure reactivity relationships for predicting reductive transformation rate constants of halogenated hydrocarbons in anoxic sediment systems. *Environ. Toxicol. Chem.* Submitted for publication, 1993.
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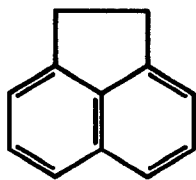
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## 1. Acenaphthene

---

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

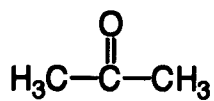


Acenaphthene

## 2. Acetone

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Acetone will not hydrolyze; however, it may undergo other abiotic transformation processes.

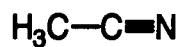


Acetone

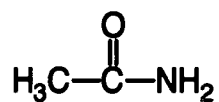
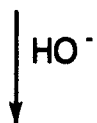
### 3. Acetonitrile

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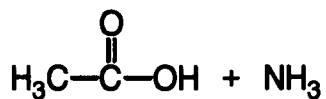
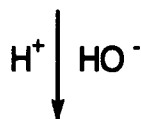
Acetonitrile is resistant to hydrolysis. Hydroxide or hydronium is required to facilitate hydrolysis. Hydrolysis proceeds through the intermediate amide to the final product, acetic acid.



Acetonitrile



Acetamide



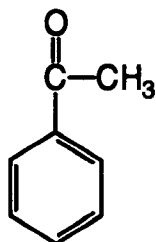
Acetic acid



## 4. Acetophenone

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Acetophenone will not hydrolyze; however, it may undergo other abiotic transformation processes.

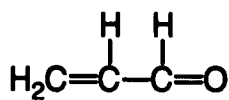


Acetophenone

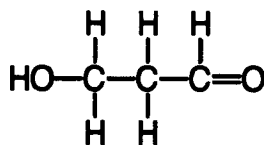
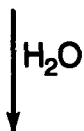
## 5. Acrolein

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



Acrolein

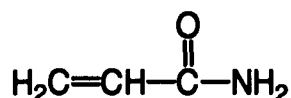


3-Hydroxy-1-propanal

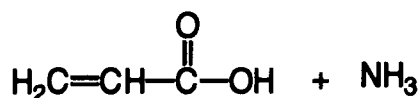
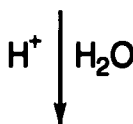
## 6. Acrylamide

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Acrylamide is an intermediate in the hydrolysis of acrylonitrile to acrylic acid. At high concentrations of hydroxide, acrylamide polymerizes. The reported neutral hydrolysis rate constant was determined at pH 7 by monitoring the disappearance of acrylamide from the solution. This constant, together with the acid hydrolysis rate constant, can be used to calculate persistence. The end product of hydrolysis is acrylic acid.



Acrylamide



Acrylic acid

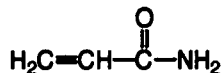
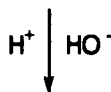
## 7. Acrylonitrile

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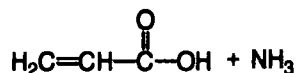
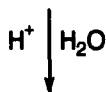
See compounds #3 and #6. Acrylonitrile hydrolyzes to acrylic acid through the intermediate acrylamide.



Acrylonitrile



Acrylamide

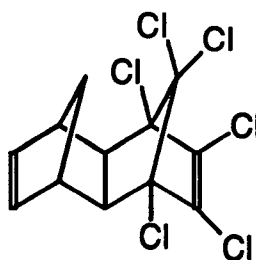


Acrylic acid

## 8. Aldrin

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The chlorinated bicyclic structure of aldrin is common to several persistent pesticides. All aldrin chlorine atoms are either protected from nucleophilic attack (bridgehead carbon) or are nonreactive (on the  $sp^2$  carbon). The previously reported hydrolysis rate constant for aldrin in reference 6 was based on disappearance kinetics without confirmation of hydrolysis products. For this report, the hydrolysis experiments were repeated in sealed glass ampules, and no disappearance of the aldrin was observed after 2 weeks at pH 11 and 85°C. Aldrin has been designated the assignment of NLFG.

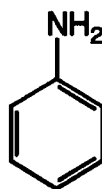


Aldrin

## 9. Aniline

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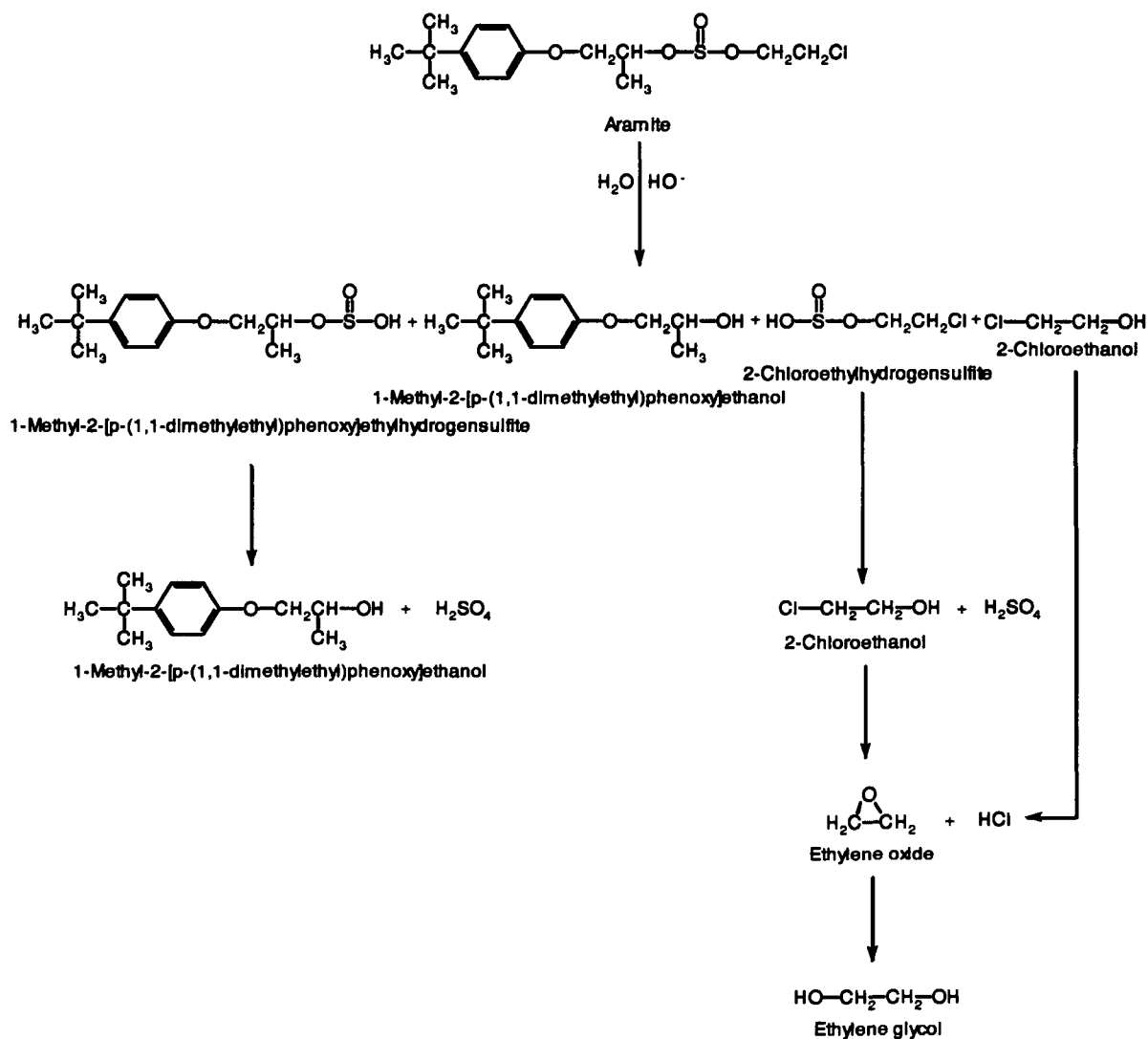
Aniline will not hydrolyze; however, it may undergo other abiotic transformation processes.



Aniline

## 11. Aramite

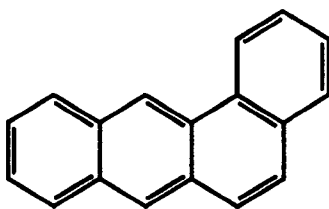
The sulfite bond in Aramite is very susceptible to hydrolysis (see endosulfan, #97). Initial hydrolysis of Aramite proceeds with cleavage of either of two sulfoxide bonds. This initial hydrolysis yields four products, two alcohols and two hydrogen sulfites. Hydrolysis of the hydrogen sulfites continues at a rate comparable to that of Aramite. Hydrolysis of 2-chloroethanol is discussed with 1,2-dichloroethane, #65.



#### 14. Benz[a]anthracene

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Benz[a]anthracene will not hydrolyze. It has no hydrolyzable functional group.

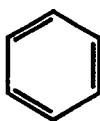


Benz[a]anthracene

#### 15. Benzene

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

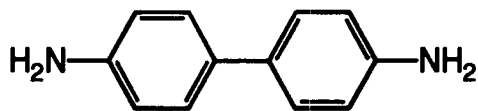


Benzene

## 16. Benzidine

---

Benzidine will not hydrolyze; however, it may undergo other abiotic transformation processes.

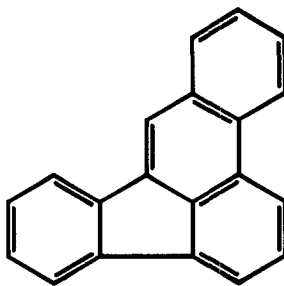


Benzidine

## 17. Benzo[*b*]fluoranthene

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

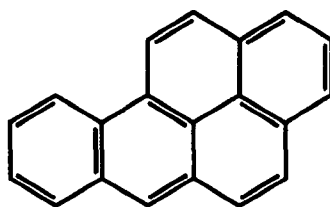


Benzo[*b*]fluoranthene

## 18. Benzo[a]pyrene

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Benzo[a]pyrene will not hydrolyze. It has no hydrolyzable functional group.

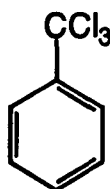


Benzo[a]pyrene

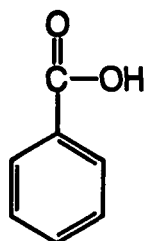
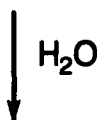
## 19. Benzotrichloride

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Hydrolysis of benzotrichloride proceeds through nucleophilic substitution of chlorine by  $\text{H}_2\text{O}$ . The halohydrin formed by this displacement is unstable and reacts further to yield benzoic acid.



Benzotrichloride



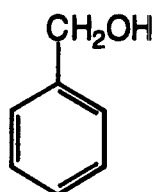
Benzoic acid

+ HCl

## 20. Benzyl alcohol

---

Benzyl alcohol will not hydrolyze. It has no hydrolyzable functional group.

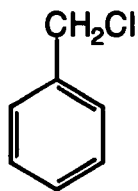


Benzyl alcohol

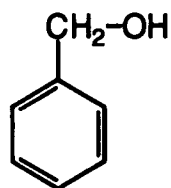
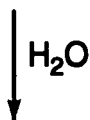
## 21. Benzyl chloride

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Hydrolysis of benzyl chloride occurs through nucleophilic displacement of chlorine by  $\text{H}_2\text{O}$ . Hydrolysis is not mediated by hydroxide.



Benzyl chloride



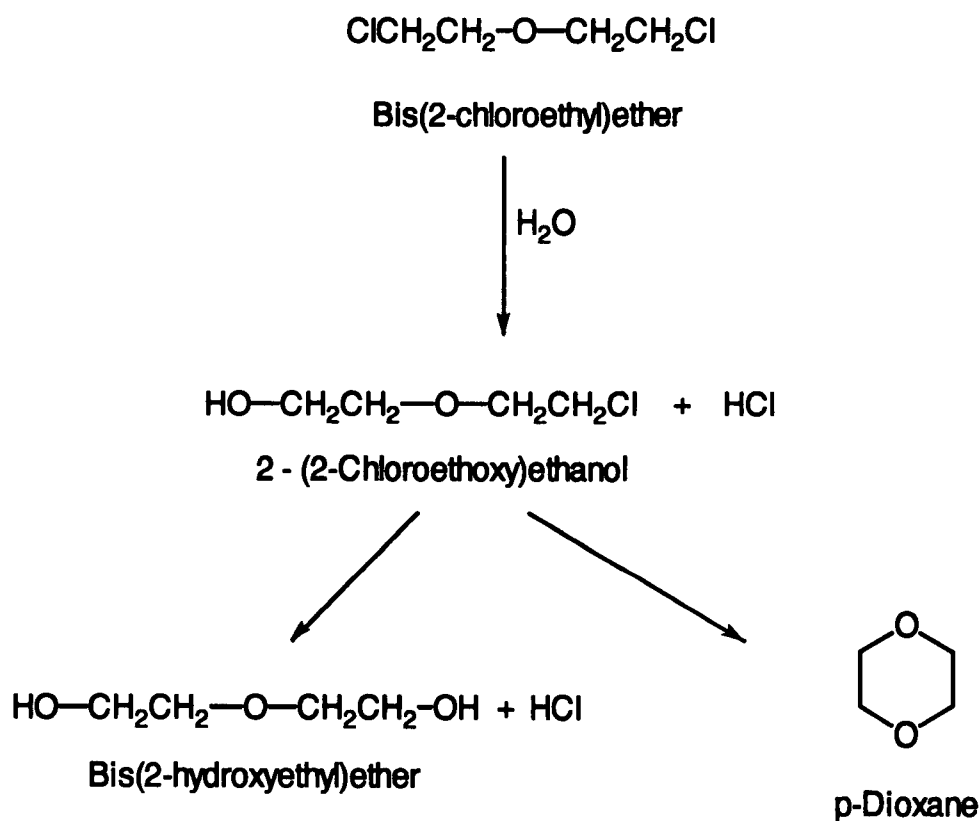
Benzyl alcohol

+ HCl



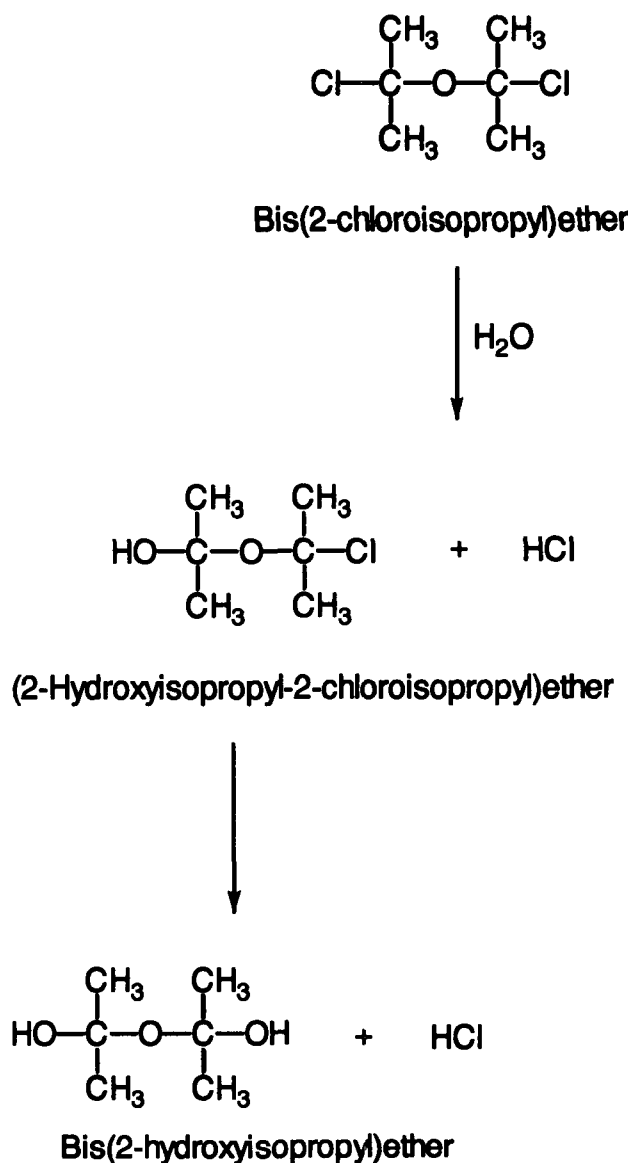
### 23. *Bis*(2-chloroethyl)ether

Hydrolysis of *bis*(2-chloroethyl)ether occurs through nucleophilic displacement of chlorine with  $\text{H}_2\text{O}$ . The monochloroether formed by this reaction will undergo a second substitution by  $\text{H}_2\text{O}$  to yield *bis*(2-hydroxyethyl)ether and intramolecular displacement of chlorine to yield dioxane.



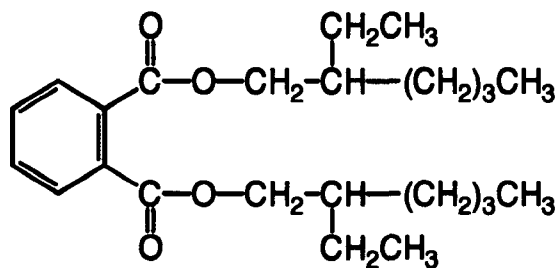
## 24. *Bis*(2-chloroisopropyl)ether

The literature hydrolysis rate constant for *bis*(2-chloroisopropyl)ether seems to be questionable. This value was estimated by analogy to *bis*(2-chloroethyl)ether by Mabey et al.<sup>8</sup> The value for *bis*(2-chloroethyl) ether was determined in aqueous dioxane at 100°C and extrapolated to 20°C by Mabey et al.<sup>8</sup> However, Mabey et al.<sup>8</sup> named the compound *bis*(2-chloroisopropyl)ether but give the Chemical Abstract Service number and structure for *bis*(1-chloroisopropyl)ether. Moreover, it is questionable whether *bis*(2-chloroisopropyl)ether should be the compound on the HWIR list or whether it should be *bis*(1-chloroisopropyl)ether. Our Pathway Analysis Team deliberated and concluded that *bis*(2-chloroisopropyl)ether is a halohydrin and is, thus, unstable. If the intended compound on the HWIR list is *bis*(1-chloroisopropyl)ether, the hydrolysis rate should be the one given by Mabey et al.<sup>8</sup> ( $k_a = 3.5\text{E-}2 \text{ Y}^{-1}$ ). However, if the intended compound is *bis*(2-chloroisopropyl)ether, its half-life is on the order of minutes because of its instability.

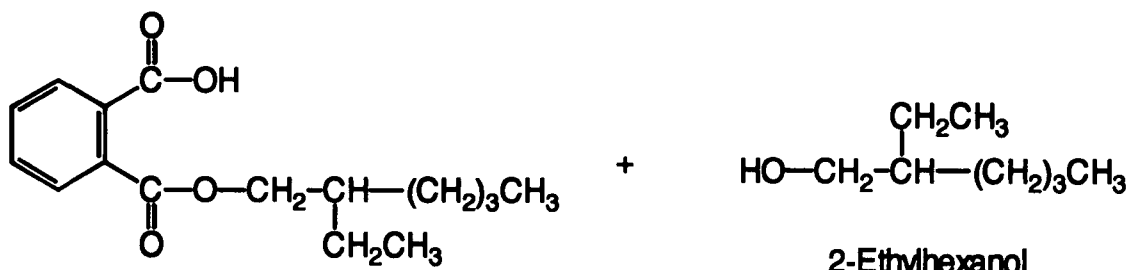
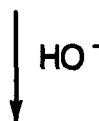


## 25. *Bis*(2-ethylhexyl)phthalate

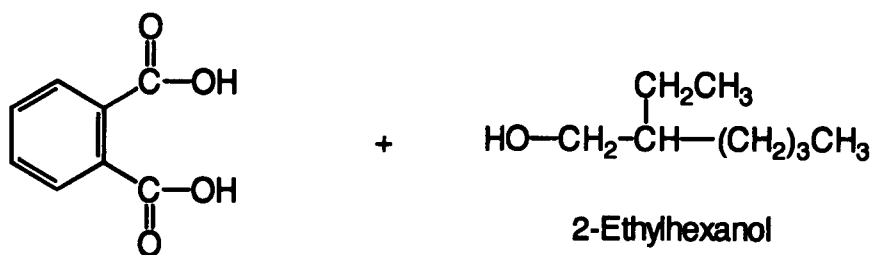
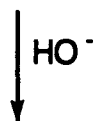
*Bis*(2-ethylhexyl)phthalate will hydrolyze by nucleophilic attack of  $\text{HO}^-$  at the ester carbonyl group to give 2-ethylhexyl hydrogen phthalate and 2-ethylhexanol. The monoester will undergo further base-mediated hydrolysis to *o*-phthalic acid and 2-ethylhexanol.



*Bis*(2-ethylhexyl)phthalate



2-Ethylhexyl hydrogen phthalate

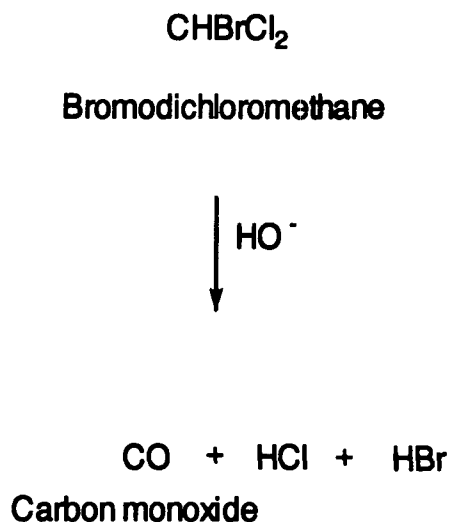


*o*-Phthalic acid

## 26. Bromodichloromethane

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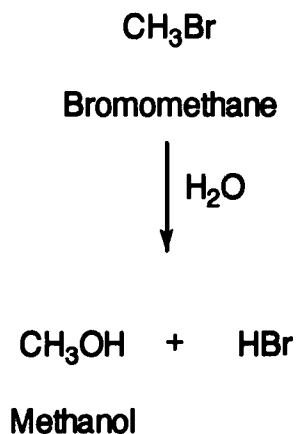
Hydrolysis of bromodichloromethane occurs initially by proton abstraction followed by formation of the carbene, which reacts with  $\text{HO}^-$  to form carbon monoxide and the mineral acids.



## 27. Bromomethane

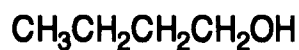
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Hydrolysis of bromomethane proceeds through nucleophilic substitution of bromine by  $\text{H}_2\text{O}$  to yield methanol and hydrobromic acid.



## 28. Butanol

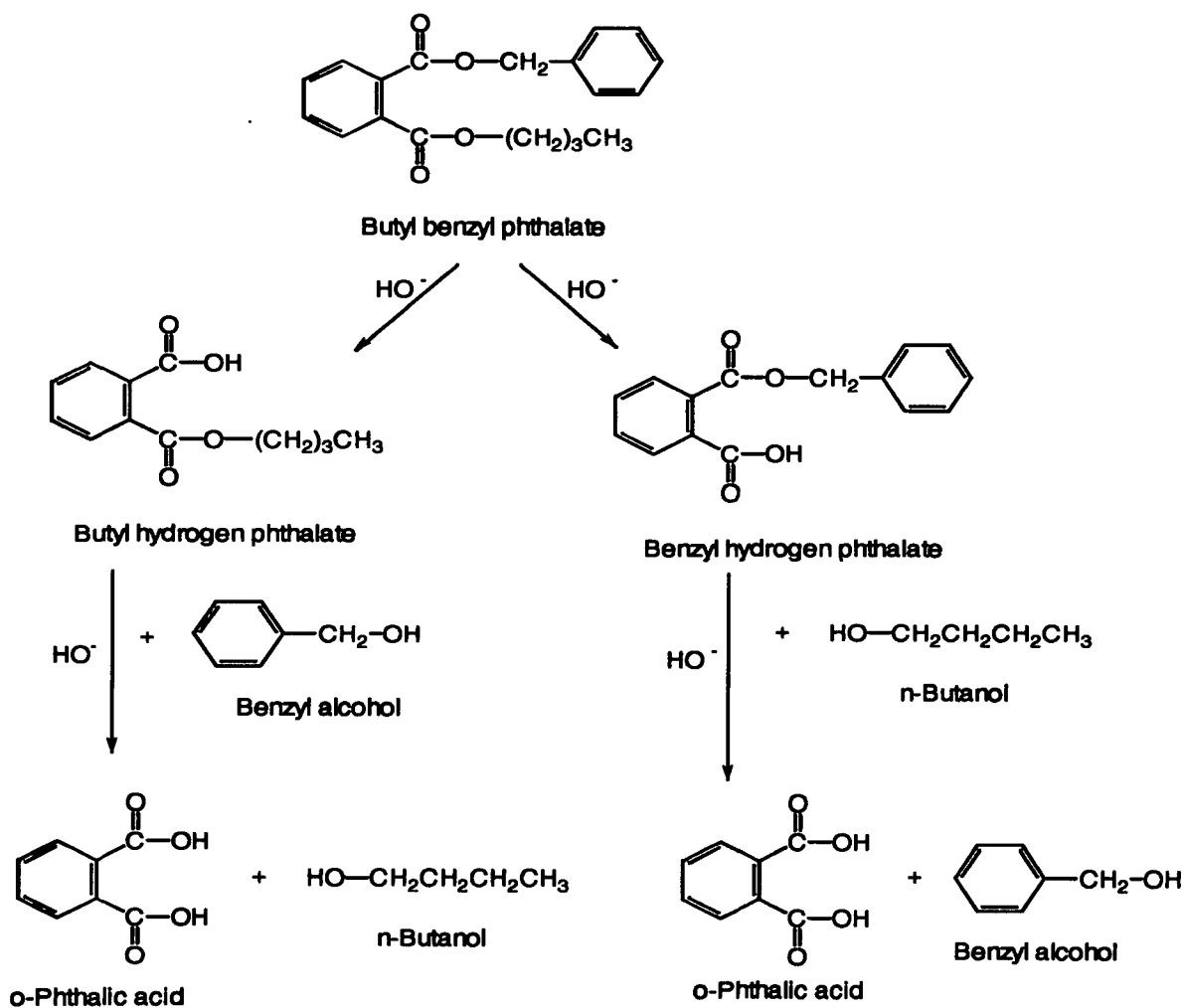
Butanol will not hydrolyze. It has no hydrolyzable functional group.



Butanol

## 29. Butyl benzyl phthalate

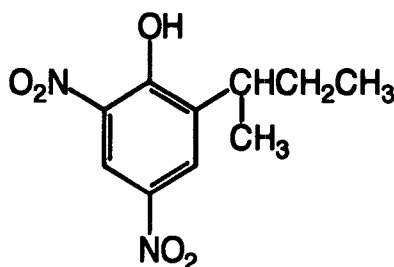
Butyl benzyl phthalate is a mixed ester formed by condensation of phthalic acid with two different alcohols. The hydrolysis mechanism is the same as described for *bis*(2-ethyl-hexyl)phthalate (#25) with the two resulting monoesters undergoing further hydrolysis to *o*-phthalic acid and the corresponding alcohols.



### 30. 2-sec-Butyl-4,6-dinitrophenol

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2-sec-Butyl-4,6-dinitrophenol will not hydrolyze; however, it may undergo other abiotic transformation processes.

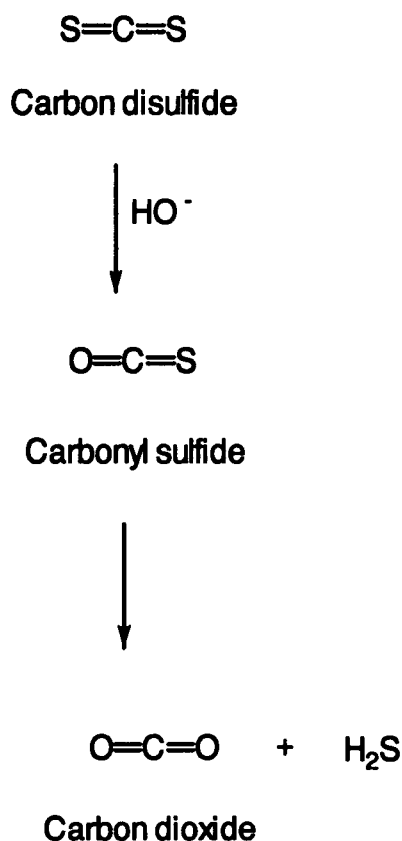


2-sec-Butyl-4,6-dinitrophenol

### 32. Carbon disulfide

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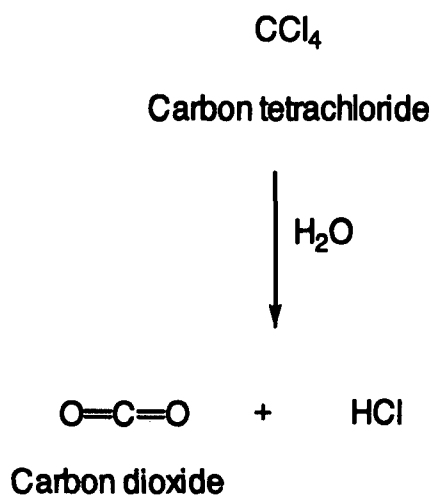
Hydrolysis of carbon disulfide occurs by nucleophilic attack of  $\text{HO}^-$ . The initial hydrolysis product is carbonyl sulfide, which reacts further with  $\text{H}_2\text{O}$  or  $\text{HO}^-$  to give carbon dioxide and hydrogen sulfide.



### 33. Carbon tetrachloride

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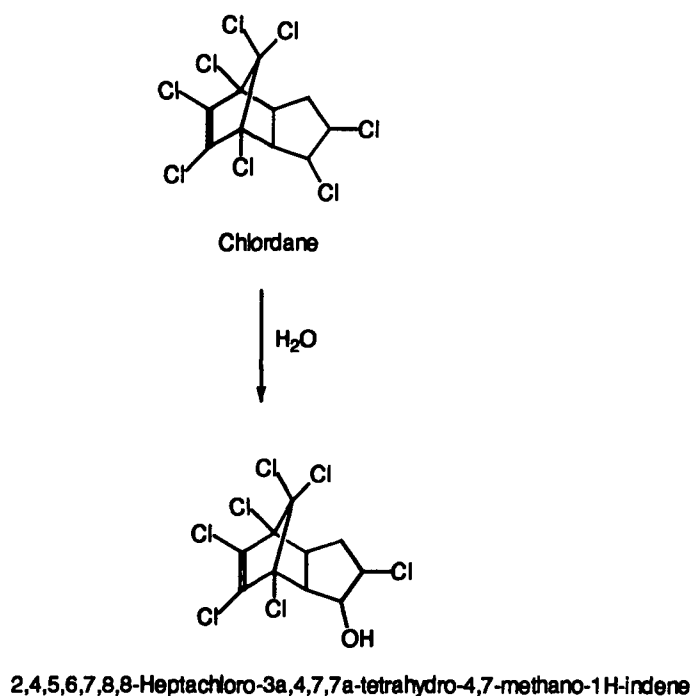
Hydrolysis of carbon tetrachloride occurs by reaction with  $\text{H}_2\text{O}$  to yield carbon dioxide and the mineral acid.



### 34. Chlordane

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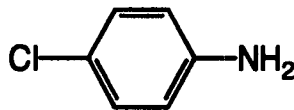
Hydrolysis of chlordane proceeds by nucleophilic substitution of chlorine by  $\text{HO}^-$  to give 2,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-4,7-methano-1H-indene, which will not be susceptible to further hydrolysis.



### 35. *p*-Chloroaniline

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*p*-Chloroaniline will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.

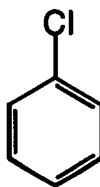


*p*-Chloroaniline

### 36. Chlorobenzene

---

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

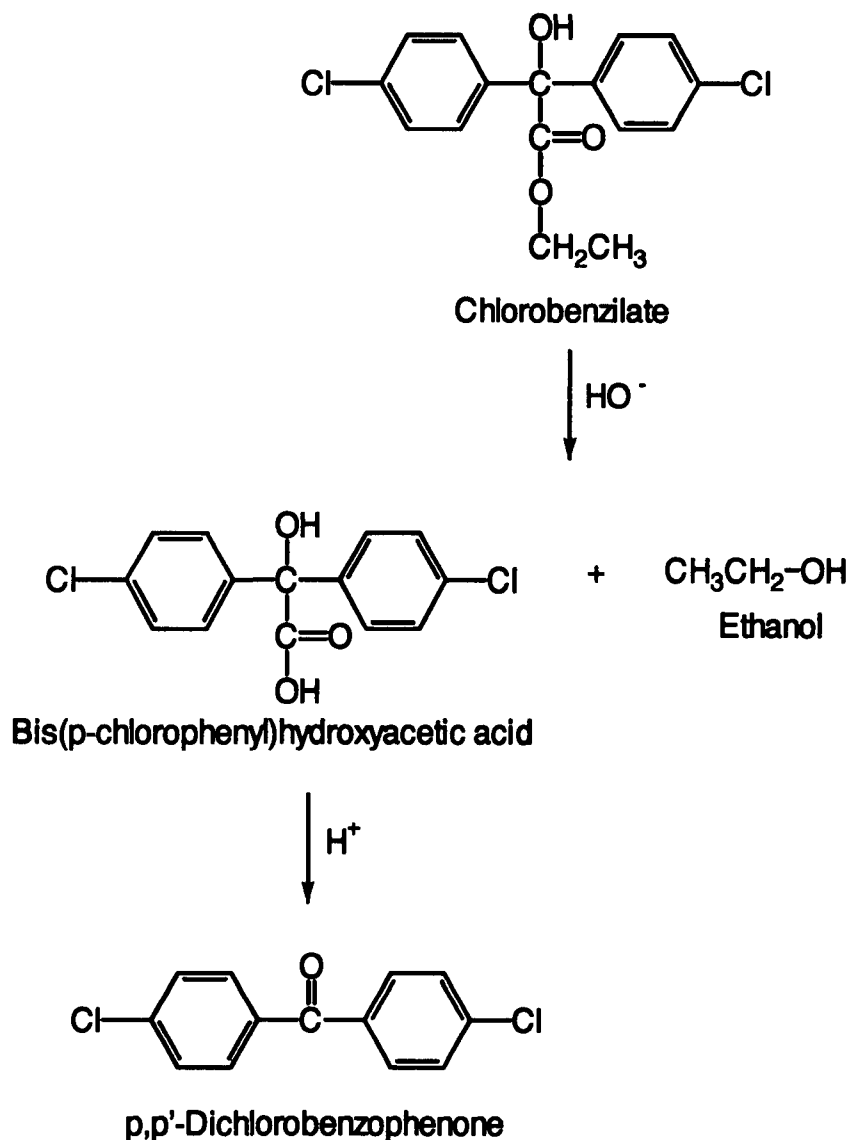


Chlorobenzene



### 37. Chlorobenzilate

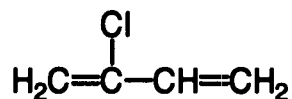
Hydrolysis of chlorobenzilate is analogous to the phthalate esters and proceeds through nucleophilic attack of  $\text{HO}^-$  at the ester carbonyl. The resulting acid is stable in the ionic form, but the protonated form that would exist at acidic pH values will decarboxylate with concurrent oxidation to yield carbon dioxide and *p,p'*-dichlorobenzophenone. The conversion of *bis(p-chlorophenyl)hydroxyacetic acid* to *p,p'*-dichlorobenzophenone was estimated to proceed at 10% of the hydrolysis rate of the parent.



### 38. 2-Chloro-1,3-butadiene

---

2-Chloro-1,3-butadiene will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.

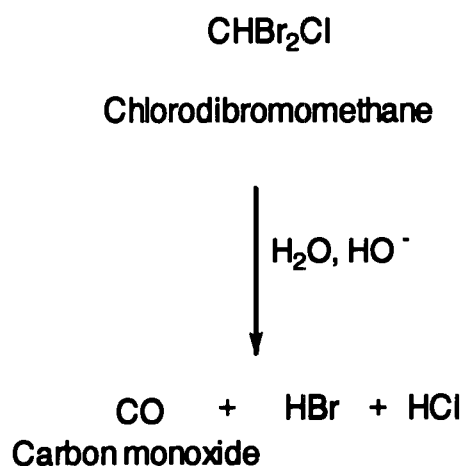


2-Chloro-1,3-butadiene

### 39. Chlorodibromomethane

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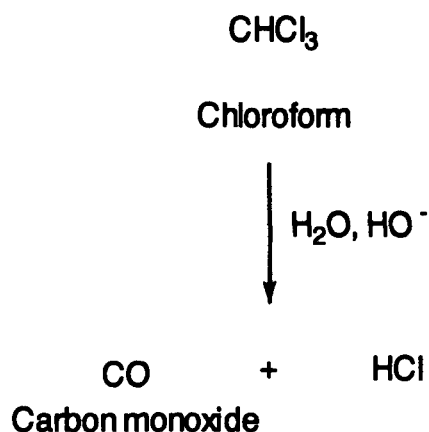
Hydrolysis of chlorodibromomethane occurs initially by proton abstraction followed by formation of the carbene, which reacts with  $\text{HO}^-$  to form carbon monoxide and the mineral acids.



## 40. Chloroform

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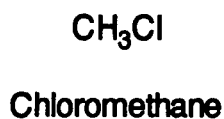
Hydrolysis of chloroform occurs initially by proton abstraction followed by formation of the carbene, which reacts with  $\text{HO}^-$  to form carbon monoxide and the mineral acid.



## 41. Chloromethane

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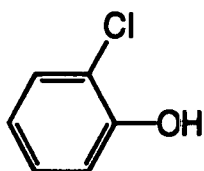
Chloromethane has a negative boiling point and exists in a gaseous state at room temperature. Its hydrolysis pathway has not been addressed.



## 42. 2-Chlorophenol

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

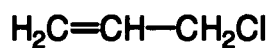


2-Chlorophenol

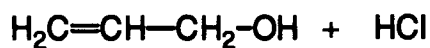
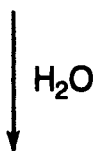
## 43. 3-Chloropropene

---

Neutral hydrolysis of 3-chloropropene occurs through the formation of the allylic carbonium ion, which reacts with  $\text{H}_2\text{O}$  to give 3-hydroxypropene and the mineral acid.



3-Chloropropene

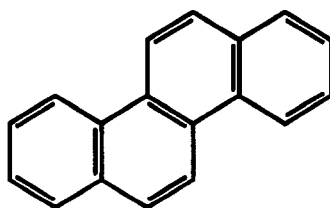


3-Hydroxypropene

## 45. Chrysene

---

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

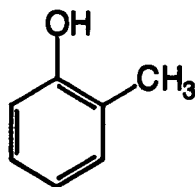


Chrysene

## 47. o-Cresol

---

o-Cresol will not hydrolyze. It has no hydrolyzable functional group.

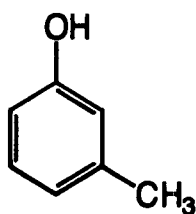


o-Cresol

**48. *m*-Cresol**

---

*m*-Cresol will not hydrolyze. It has no hydrolyzable functional group.

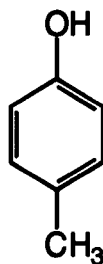


*m*-Cresol

**49. *p*-Cresol**

---

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

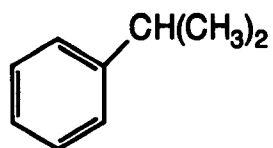


*p*-Cresol

## 50. Cumene

---

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

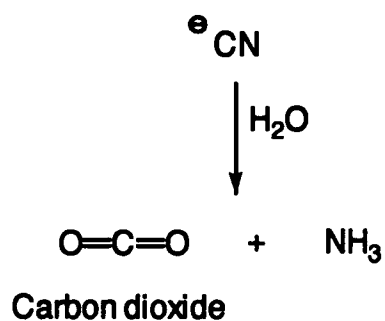


Cumene

## 51. Cyanide

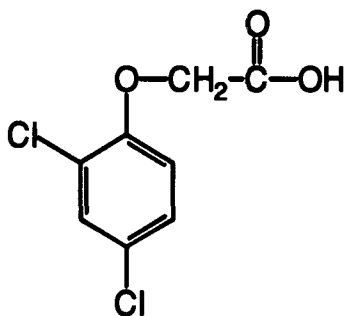
---

Cyanide will hydrolyze by nucleophilic attack of  $\text{H}_2\text{O}$  resulting in carbon dioxide and ammonia.



## 52. 2,4-Dichlorophenoxyacetic acid

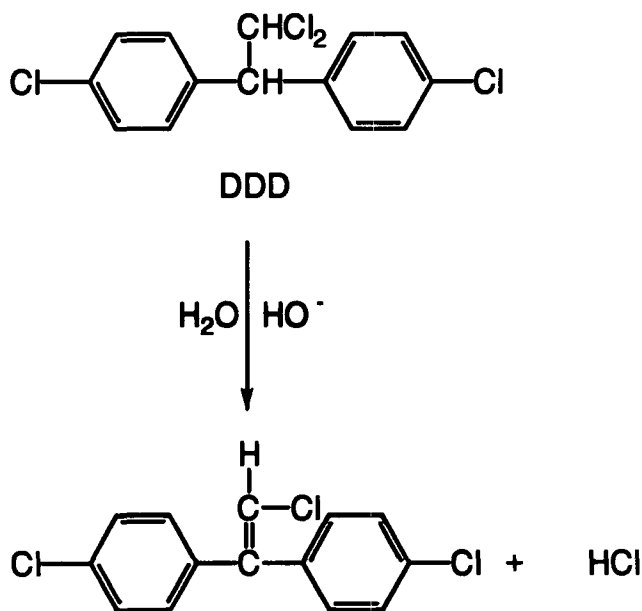
2,4-Dichlorophenoxyacetic acid will not hydrolyze to any reasonable extent.



2,4-Dichlorophenoxyacetic acid

## 53. DDD

The reaction of DDD occurs by the elimination of chlorine (dehydrochlorination) to give 2,2-bis(4-chlorophenyl)-1-chloroethene (DDMU). This process will occur by reaction with either  $\text{H}_2\text{O}$  or  $\text{HO}^\cdot$ .

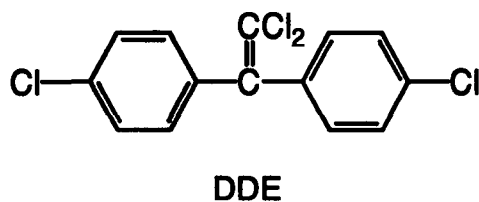


2,2-Bis(4-chlorophenyl)-1-chloroethene



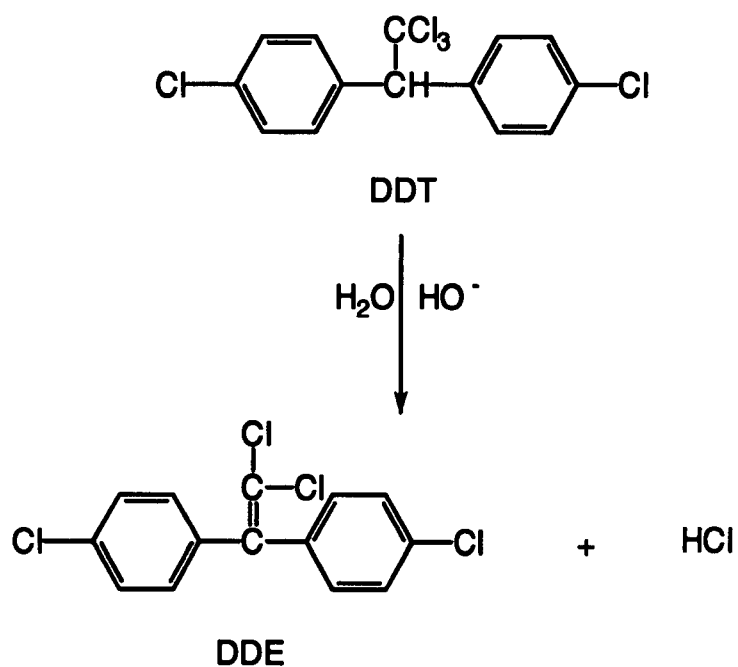
## 54. DDE

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



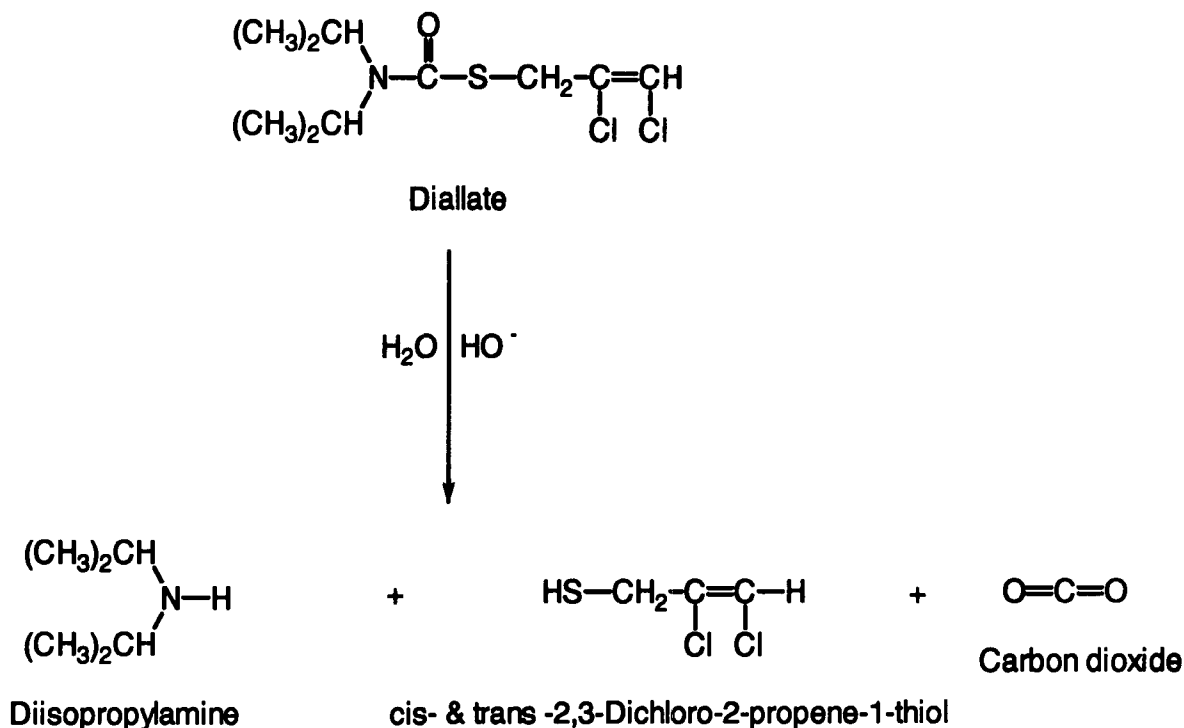
## 55. *p,p'*-DDT

The reaction of *p,p'*-DDT occurs in a manner analogous to that previously described for DDD. The reaction products resulting from dehydrochlorination are DDE and the mineral acid.



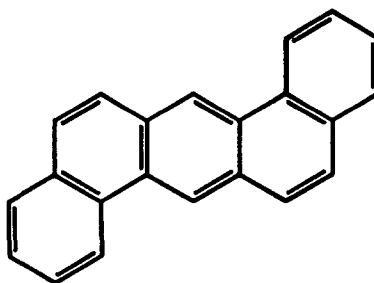
## 56. Diallate

Diallate will hydrolyze by nucleophilic attack of  $\text{H}_2\text{O}$  and  $\text{HO}^-$  at the carbonyl group resulting in the formation of diisopropylamine and *cis*- and *trans*-2,3-dichloro-2-propene-1-thiol.



## 57. Dibenz[*a,h*]anthracene

Dibenz[*a,h*]anthracene will not hydrolyze. It has no hydrolyzable functional group.

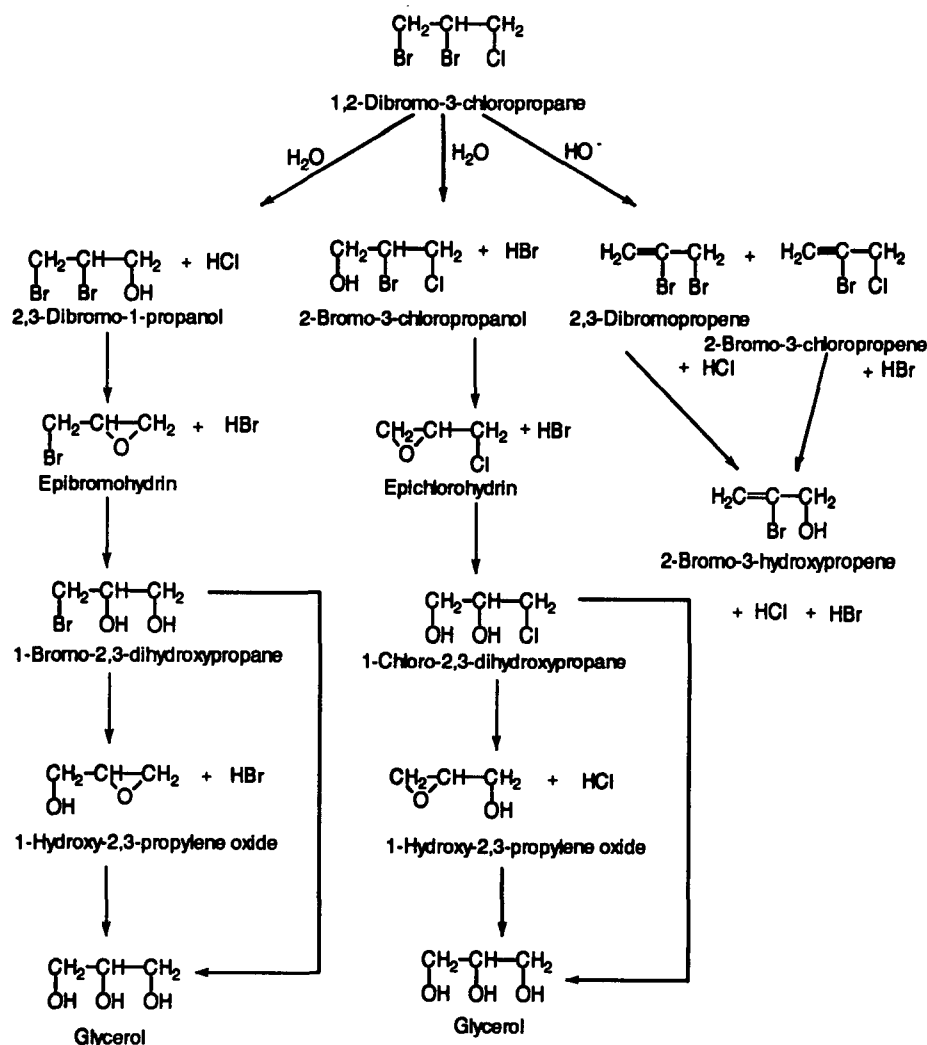


Dibenz[*a,h*]anthracene

## 58. 1,2-Dibromo-3-chloropropane

1,2-Dibromo-3-chloropropane is subject to both neutral and base-mediated hydrolysis. Neutral hydrolysis occurs initially by nucleophilic displacement of either chlorine or bromine. Nucleophilic attack at the carbon bearing the chlorine results in the formation of 2,3-dibromopropanol, which will react further to give 2,3-dihydroxybromopropane through the intermediate epoxide, epibromohydrin. 2,3-Dihydroxybromopropane will undergo further hydrolysis through the intermediate epoxide, 1-hydroxy-2,3-propylene oxide, which reacts with  $\text{H}_2\text{O}$  to give glycerol. Nucleophilic displacement of bromine from 1,2-dibromo-3-chloropropane gives 2-bromo-3-chloropropanol, which will react further through epoxide intermediates eventually to give glycerol, as described previously for the hydrolysis of 2,3-dibromopropanol.

The base-mediated hydrolysis of 1,2-dibromo-3-chloropropane will occur by dehydrohalogenation to give two initial products, 2-bromo-3-chloropropene and 2,3-dibromo-1-propene. 2-Bromo-3-chloropropene is expected to be the major reaction product because bromine is a better leaving group than chlorine. Both products, however, will undergo facile hydrolysis through formation of an allylic carbonium ion, which will react with  $\text{H}_2\text{O}$  to give 2-bromo-3-hydroxypropene. This product will be stable to further hydrolysis.



## 59. Dibromomethane

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Dibromomethane should not hydrolyze to any reasonable extent. QSAR model computations have indicated that the half-life of this halogenated methane is several thousand years.

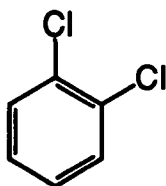


Dibromomethane

## 60. 1,2-Dichlorobenzene

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1,2-Dichlorobenzene will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.

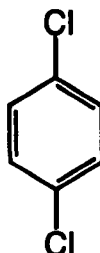


1,2-Dichlorobenzene

## 61. 1,4-Dichlorobenzene

---

1,4-Dichlorobenzene will not hydrolyze to any reasonable extent, however, it may undergo other abiotic transformation processes.

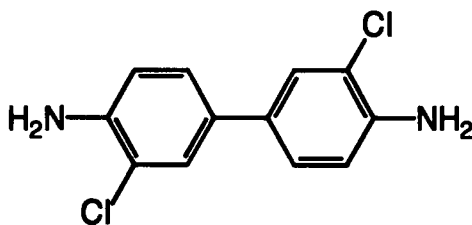


1,4-Dichlorobenzene

## 62. 3,3'-Dichlorobenzidine

---

3,3'-Dichlorobenzidine will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



3,3'-Dichlorobenzidine

### 63. Dichlorodifluoromethane

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Dichlorodifluoromethane has a negative boiling point and exists in a gaseous state at room temperature. Its hydrolysis pathway has not been addressed.



Dichlorodifluoromethane

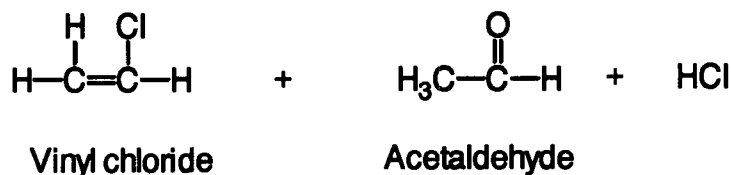
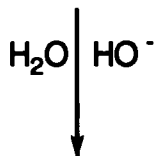
### 64. 1,1-Dichloroethane

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The reaction of 1,1-dichloroethane occurs by both nucleophilic substitution and dehydrochlorination. The reaction products resulting from nucleophilic substitution by  $\text{H}_2\text{O}$  and  $\text{HO}^-$  are acetaldehyde and  $\text{HCl}$ , whereas dehydrochlorination gives vinyl chloride and the mineral acid.

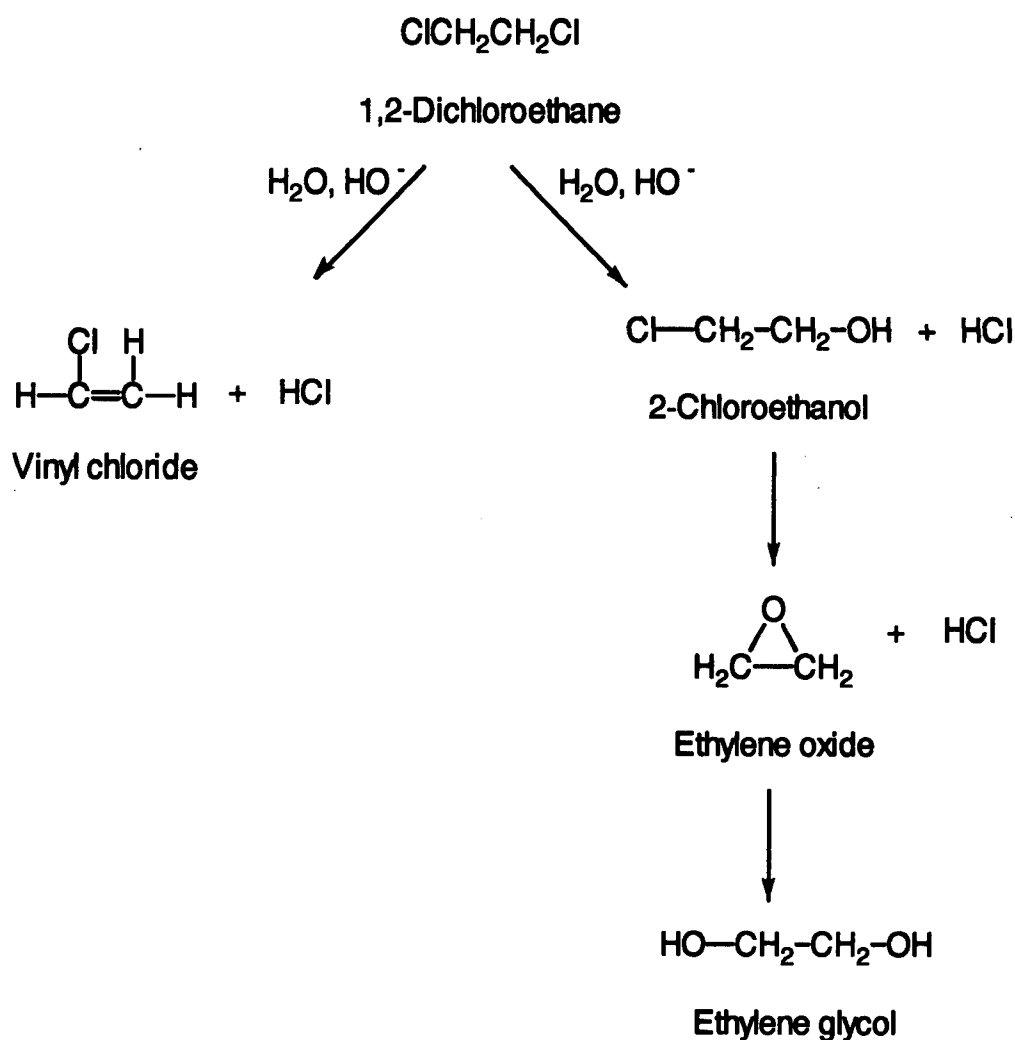


1,1-Dichloroethane



## 65. 1,2-Dichloroethane

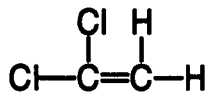
The reaction of 1,2-dichloroethane by  $\text{H}_2\text{O}$  and  $\text{HO}^-$  occurs by both nucleophilic substitution and dehydrochlorination. Hydrolysis by nucleophilic substitution will lead to the formation of 2-chloroethanol and  $\text{HCl}$ , whereas dehydrochlorination results in vinyl chloride and the mineral acid. 2-Chloroethanol will react further producing ethylene oxide, which will hydrolyze by reaction with  $\text{H}_2\text{O}$  to yield ethylene glycol.



**66. 1,1-Dichloroethylene**

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1,1-Dichloroethylene will not hydrolyze to any reasonable extent.

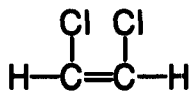


1,1-Dichloroethylene

**67. *cis*-1,2-Dichloroethylene**

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*cis*-1,2-Dichloroethylene will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



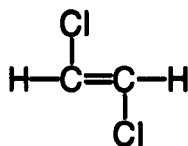
*cis*-1,2-Dichloroethylene



## 68. *trans*-1,2-Dichloroethylene

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*trans*-1,2-Dichloroethylene will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.

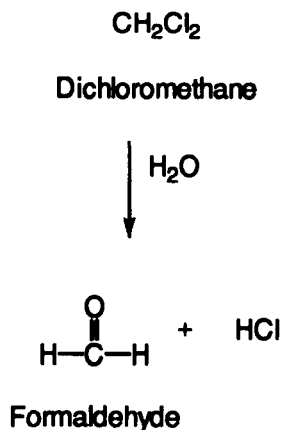


*trans*-1,2-Dichloroethylene

## 69. Dichloromethane

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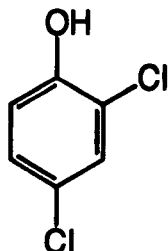
Hydrolysis of dichloromethane occurs by nucleophilic substitution with  $\text{H}_2\text{O}$  (neutral hydrolysis) resulting in the displacement of chlorine with  $\text{HO}^-$ . The resulting chlorohydrin is a transient intermediate that immediately loses chlorine to yield formaldehyde, the final hydrolysis product.



## 70. 2,4-Dichlorophenol

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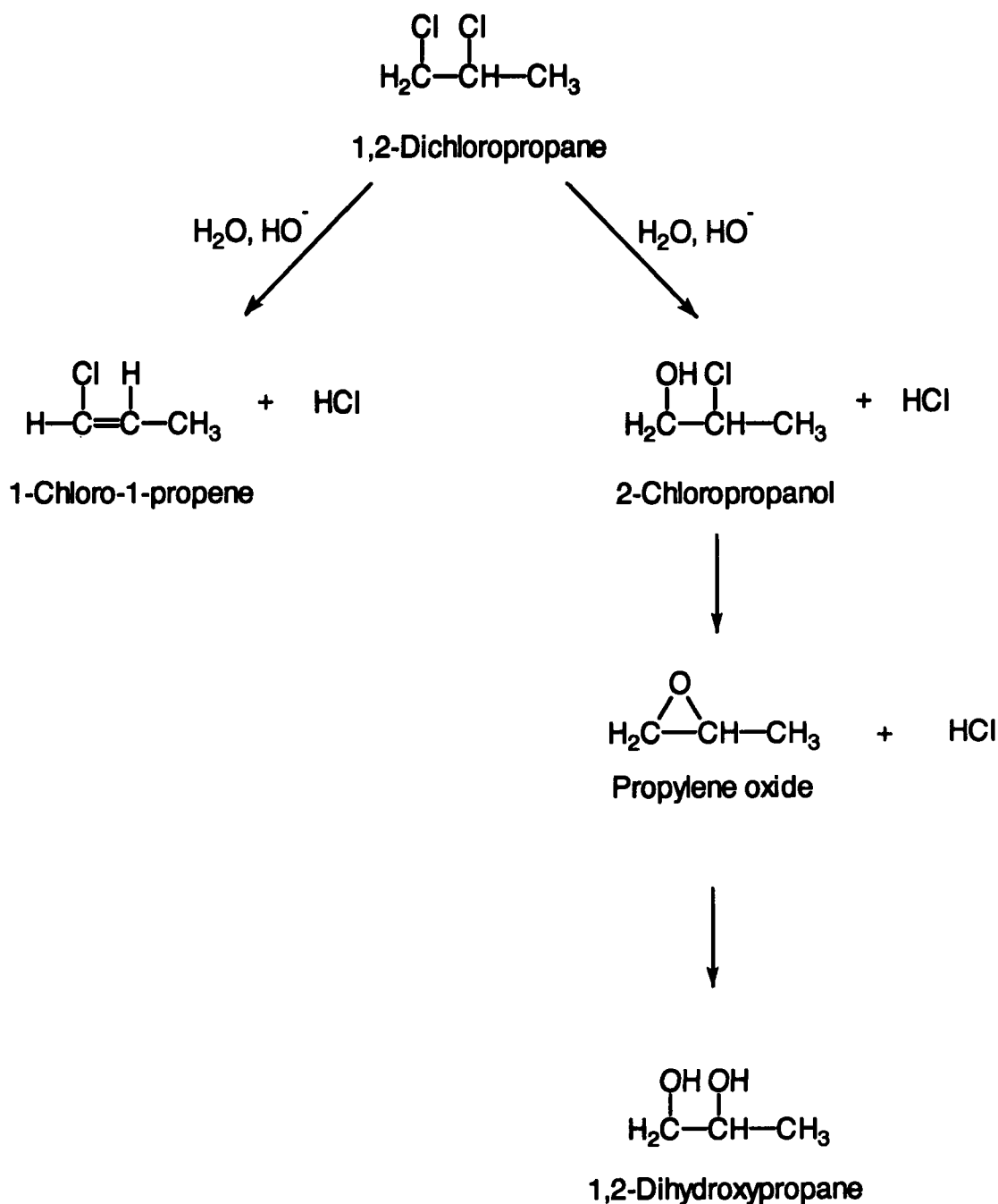
2,4-Dichlorophenol will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



2,4-Dichlorophenol

## 71. 1,2-Dichloropropane

The reaction of 1,2-dichloropropane with  $\text{H}_2\text{O}$  or  $\text{HO}^\cdot$  will proceed through competing reaction pathways (nucleophilic substitution and dehydrohalogenation). Nucleophilic substitution will occur at the primary carbon resulting in the formation of 2-chloropropanol. This intermediate will degrade by intramolecular nucleophilic displacement of the chlorine atom by the adjacent hydroxyl group resulting in the formation of propylene oxide. Propylene oxide will undergo predominantly neutral hydrolysis to give 1,2-dihydroxypropane. Base-mediated elimination of chlorine will result in the formation of 1-chloro-1-propene, which will be stable to further hydrolysis.

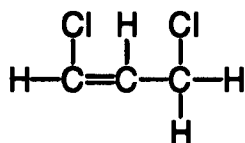


## 72. 1,3-Dichloropropene

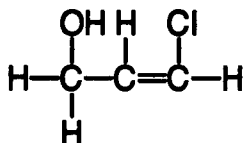
Hydrolysis of 1,3-dichloropropene will occur by reaction with  $\text{H}_2\text{O}$  through nucleophilic substitution resulting in the formation of 3-chloro-2-propene-1-ol. Because the stereochemistry about the carbon-carbon double bond is not affected in this hydrolysis reaction, the *trans* isomer of 1,3-dichloropropene will give the *trans* isomer of the allylic alcohol and the *cis* isomer of 1,3-dichloropropene will lead to the formation of the *cis* isomer of the allylic alcohol.



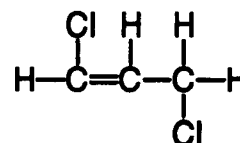
1,3-Dichloropropene



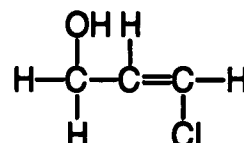
cis-1,3-Dichloropropene



cis-3-Chloro-2-propen-1-ol



trans-1,3-Dichloropropene

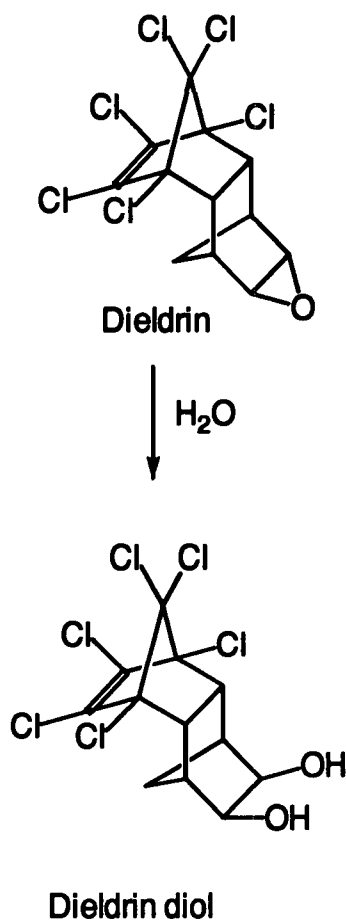


trans-3-Chloro-2-propen-1-ol

## 73. Dieldrin

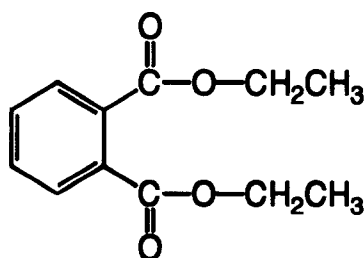
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Hydrolysis of dieldrin will occur through nucleophilic substitution with  $\text{H}_2\text{O}$  at the epoxide moiety resulting in the formation of the diol. The diol will be stable to further hydrolysis.

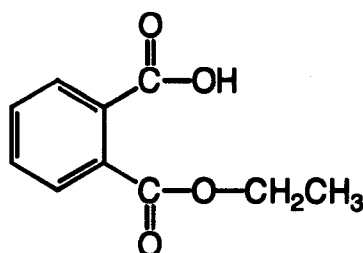
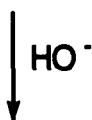


## 74. Diethyl phthalate

The base-mediated hydrolysis of diethyl phthalate will initially result in formation of the monoester, which will undergo further hydrolysis to *o*-phthalic acid. The hydrolysis of the monoester will occur at a rate approximately half that of the parent compound.



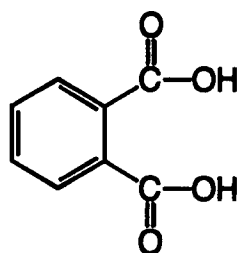
Diethyl phthalate



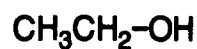
Ethyl hydrogen phthalate



Ethanol



*o*-Phthalic acid

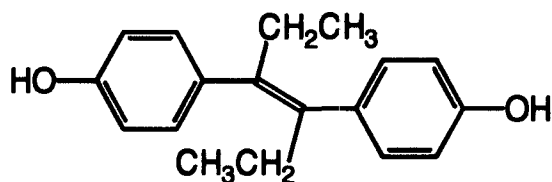


Ethanol

## 75. Diethylstilbestrol

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



Diethylstilbestrol

## 76. Dimethoate (opposite page)

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Hydrolysis of dimethoate may occur through either reaction with H<sub>2</sub>O (neutral hydrolysis) or reaction with HO<sup>-</sup> (base-mediated hydrolysis). Nucleophilic substitution by water can occur at either the methylene carbon of the thio substituent, which gives *O,O*-dimethylphosphorodithioic acid and *N*-methyl-2-hydroxyacetamide, or the carbon of the methoxy substituent to give *O*-methyl-*S*-[2-(*N*-methylacetamide)]phosphorodithioic acid and methanol. In either case, the diester that is formed will be much more persistent than the parent compound. Because the diesters are ionized at pH 7, they are approximately a factor of 10 less reactive towards hydrolysis than the triesters. Hydrolysis of *O,O*-dimethylphosphorodithioic acid will occur through formation of the monoester, *O*-methylphosphorodithioic acid, which hydrolyzes further to eventually give phosphoric acid and hydrogen sulfide. Likewise, hydrolysis of *O*-methyl-*S*-[2-(*N*-methylacetamide)]phosphorodithioic acid will result in the formation of the monoester, *O*-methylphosphorodithioic acid, in addition to *N*-methyl-2-hydroxyacetamide. Hydrolysis of the monoester, which occurs by nucleophilic attack at the phosphorus atom, will proceed at a rate of approximately one half that of the parent triester.

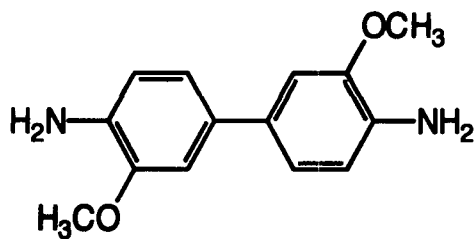
Base-mediated hydrolysis of dimethoate will occur by nucleophilic attack of HO<sup>-</sup> at the central phosphorus atom to give *O,O*-dimethylphosphorothioic acid and *N*-methyl-2-mercaptoacetamide. Further hydrolysis of *O,O*-dimethylphosphorothioic acid may occur as previously described.



## 77. 3,3'-Dimethoxybenzidine

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3,3'-Dimethoxybenzidine will not hydrolyze; however, it may undergo other abiotic transformation processes.

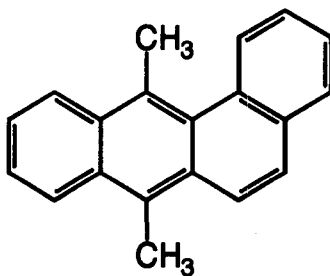


3,3'-Dimethoxybenzidine

## 78. 7,12-Dimethylbenz[a]anthracene

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7,12-Dimethylbenz[a]anthracene will not hydrolyze. It has no hydrolyzable functional group.



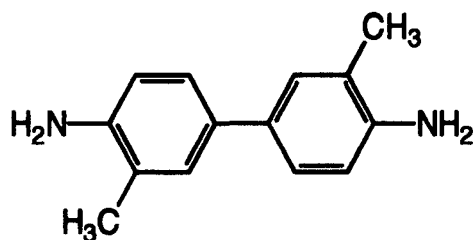
7,12-Dimethylbenz[a]anthracene



**79. 3,3'-Dimethylbenzidine**

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3,3'-Dimethylbenzidine will not hydrolyze; however, it may undergo other abiotic transformation processes.

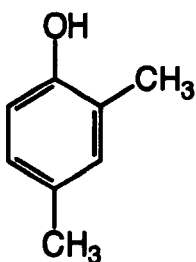


3,3'-Dimethylbenzidine

**80. 2,4-Dimethylphenol**

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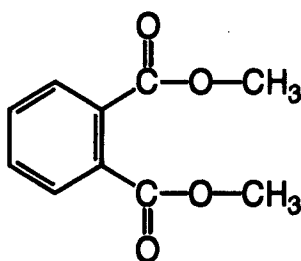
2,4-Dimethylphenol will not hydrolyze. It has no hydrolyzable functional group.



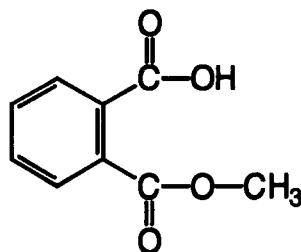
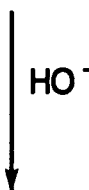
2,4-Dimethylphenol

## 81. Dimethyl phthalate

Dimethyl phthalate will hydrolyze by nucleophilic attack of  $\text{HO}^-$  at the ester carbonyl group resulting in methyl hydrogen phthalate and methanol, which can undergo further base-mediated hydrolysis to *o*-phthalic acid.



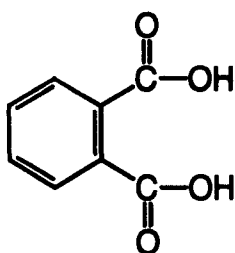
Dimethyl phthalate



Methyl hydrogen phthalate



Methanol



*o*-Phthalic acid

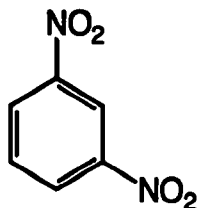


Methanol

## 82. 1,3-Dinitrobenzene

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1,3-Dinitrobenzene will not hydrolyze; however, it may undergo other abiotic transformation processes.

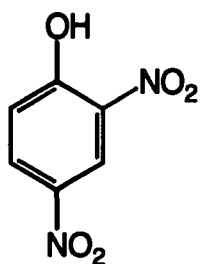


1,3-Dinitrobenzene

## 83. 2,4-Dinitrophenol

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2,4-Dinitrophenol will not hydrolyze; however, it may undergo other abiotic transformation processes.

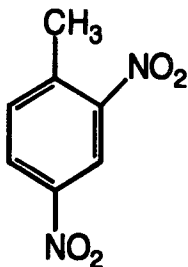


2,4-Dinitrophenol

## 84. 2,4-Dinitrotoluene

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2,4-Dinitrotoluene will not hydrolyze; however, it may undergo other abiotic transformation processes.

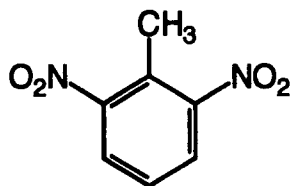


2,4-Dinitrotoluene

## 85. 2,6-Dinitrotoluene

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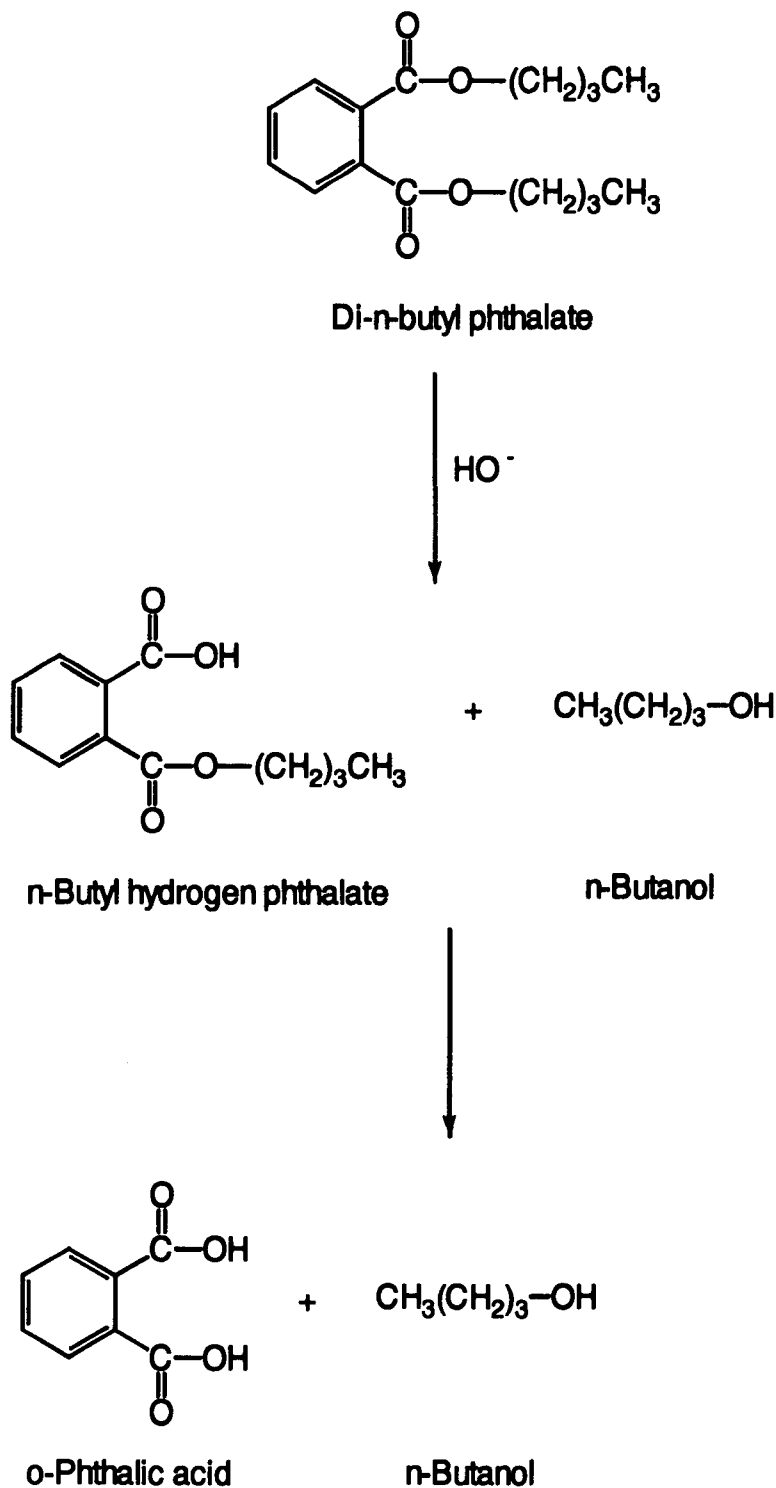
2,6-Dinitrotoluene will not hydrolyze; however, it may undergo other abiotic transformation processes.



2,6-Dinitrotoluene

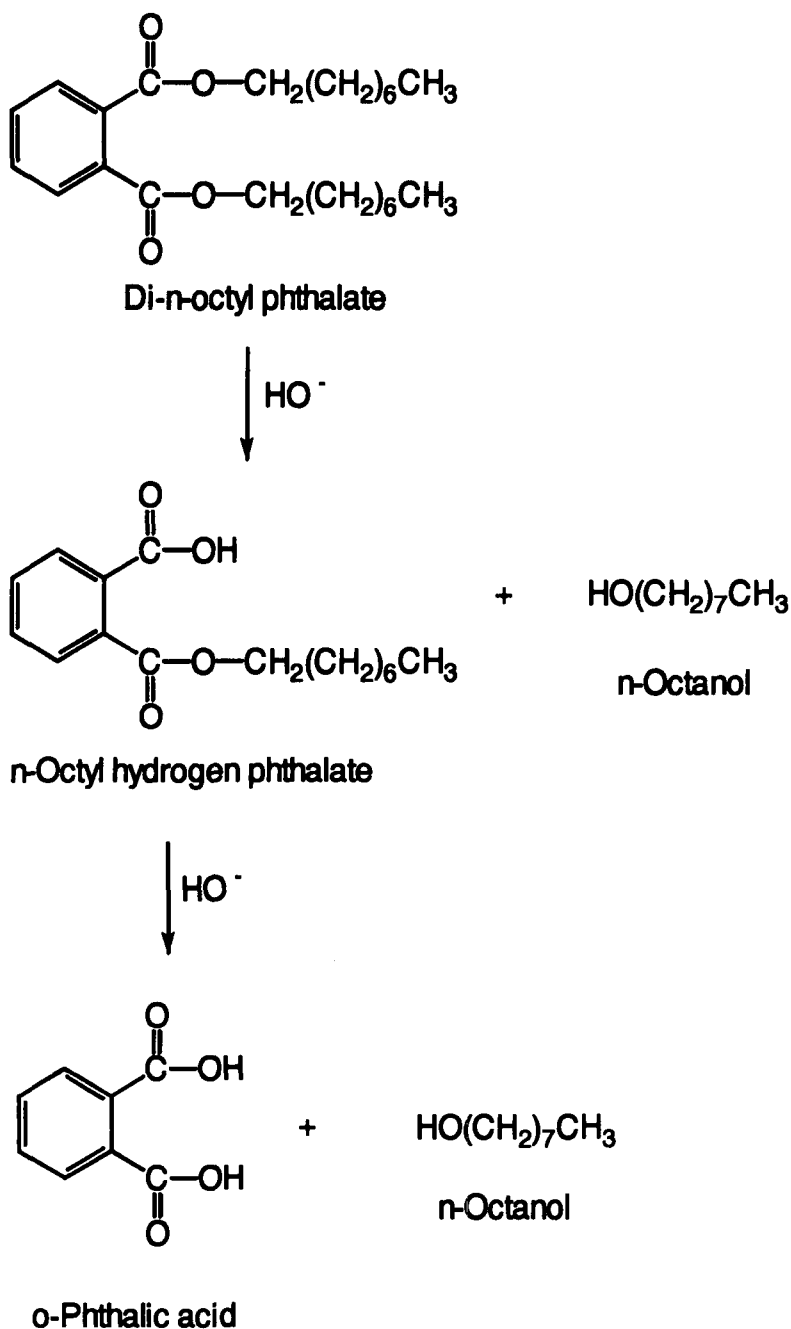
## 86. Di-*n*-butyl phthalate

The reaction pathway for the hydrolysis of di-*n*-butyl phthalate is identical to that described previously for dimethyl phthalate (#81).



## 87. Di-*n*-octyl phthalate

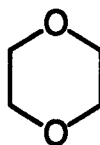
The reaction pathway for the hydrolysis of di-*n*-octyl phthalate is identical to that described previously for dimethyl phthalate (#81).



**88. 1,4-Dioxane**

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

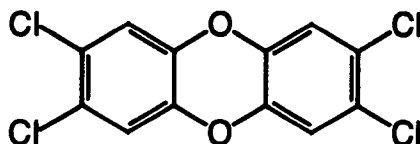


1,4-Dioxane

**89. 2,3,7,8-TCDDioxin**

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

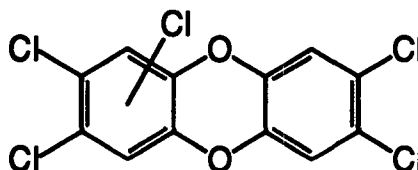


2,3,7,8-TCDDioxin

## 90. 2,3,7,8-PeCDDioxins

---

2,3,7,8-PeCDDioxins will not hydrolyze to any reasonable extent; however, they may undergo other abiotic transformation processes.

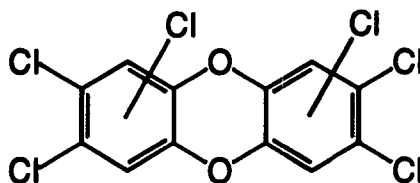


2,3,7,8-PeCDD

## 91. 2,3,7,8-HxCDDioxins

---

2,3,7,8-HxCDDioxins will not hydrolyze to any reasonable extent; however, they may undergo other abiotic transformation processes.

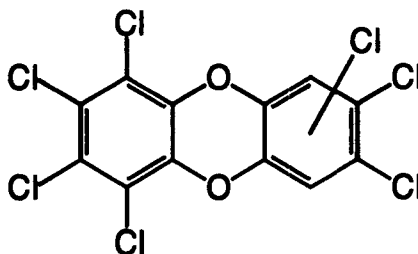


2,3,7,8-HxCDD

## 92. 2,3,7,8-HpCDDioxins

---

2,3,7,8-HpCDDioxins will not hydrolyze to any reasonable extent; however, they may undergo other abiotic transformation processes.



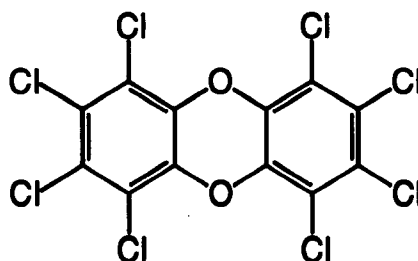
2,3,7,8-HpCDD



### 93. OCDD

---

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

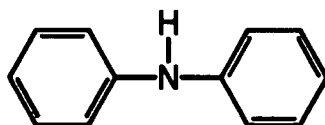


OCDD

### 94. Diphenylamine

---

Diphenylamine will not hydrolyze; however, it may undergo other abiotic transformation processes.

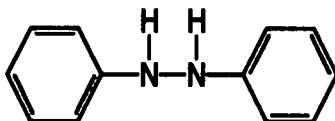


Diphenylamine

### 95. 1,2-Diphenylhydrazine

---

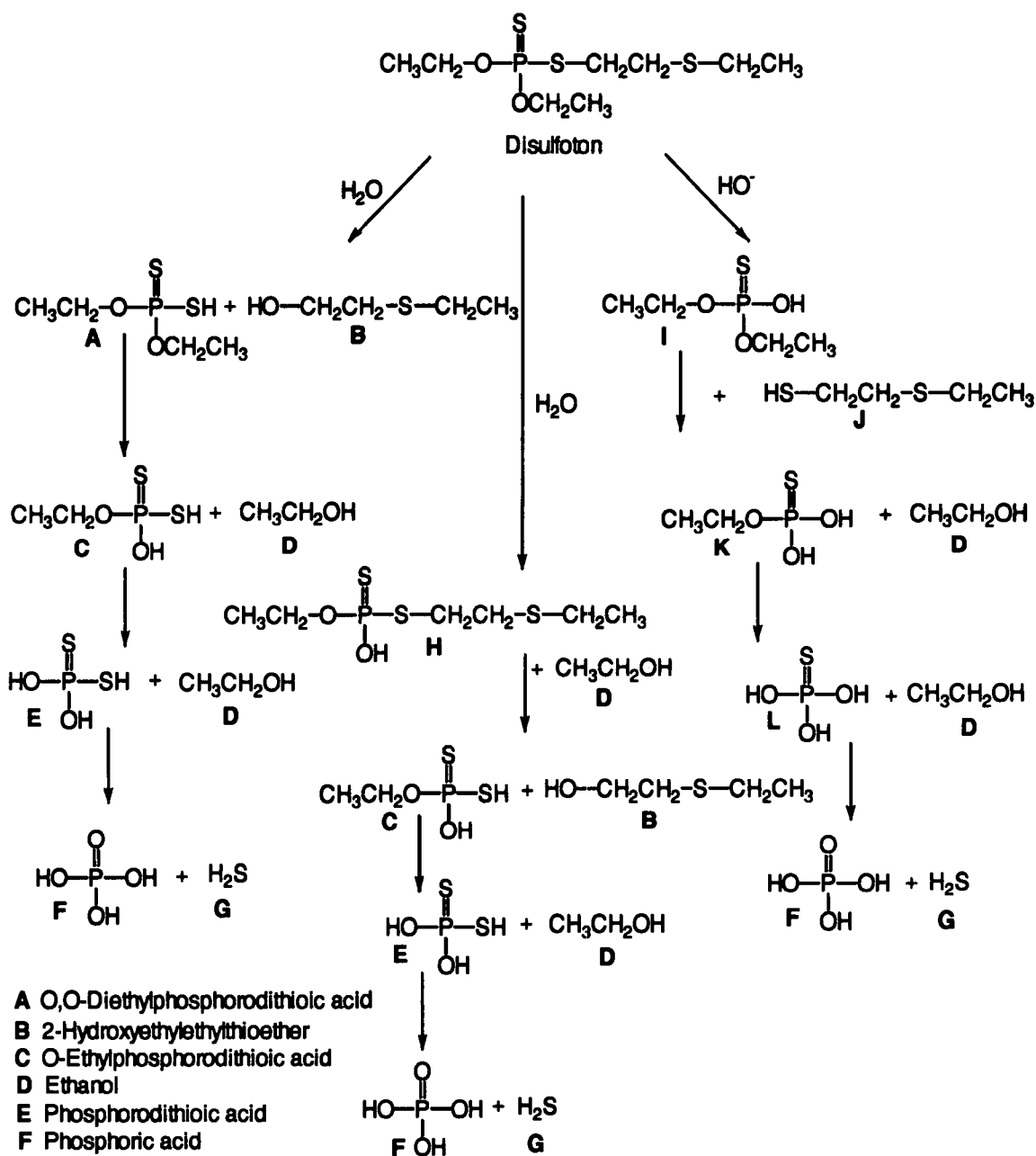
1,2-Diphenylhydrazine will not hydrolyze; however, it may undergo other abiotic transformation processes.



1,2-Diphenylhydrazine

## 96. Disulfoton

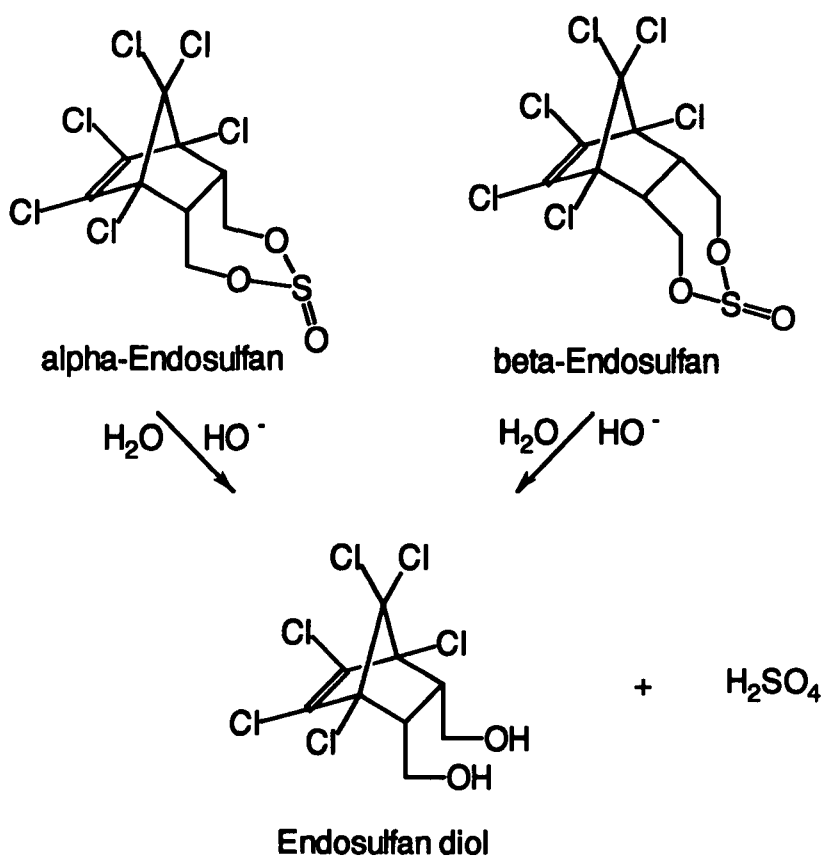
The reaction pathways for the hydrolysis of disulfoton are quite similar to those already discussed for the hydrolysis of dimethoate (#76). Neutral hydrolysis can occur at two sites resulting in the formation of phosphorus diesters, which will hydrolyze through the phosphate monoester to eventually give phosphoric acid and hydrogen sulfide. As with dimethoate, base-mediated hydrolysis will occur by nucleophilic attack of  $\text{HO}^-$  at the central phosphorus atom resulting in 2-thioethylethylthioether and *O,O*-diethylphosphorothioic acid, which will hydrolyze further to phosphoric acid and hydrogen sulfide.



- A O,O-Diethylphosphorodithioic acid  
 B 2-Hydroxyethylthioether  
 C O-Ethylphosphorodithioic acid  
 D Ethanol  
 E Phosphorodithioic acid  
 F Phosphoric acid  
 G Hydrogen sulfide  
 H O-Ethyl-S-[(2-(ethylthio)ethyl)]phosphorodithioic acid  
 I O,O-Diethylphosphorothioic acid  
 J 2-Thioethylthioether  
 K O-Ethylphosphorothioic acid  
 L Phosphorothioic acid
- $$\text{HO}-\text{P}(=\text{O})(\text{OH})_2 + \text{H}_2\text{S}$$

## 97. Endosulfan

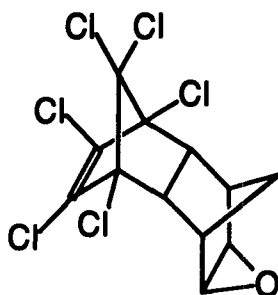
Endosulfan, which is a mixture of the *alpha* (Endosulfan I) and *beta* (Endosulfan II) isomers, will hydrolyze by nucleophilic attack of  $\text{H}_2\text{O}$  or  $\text{HO}^-$  at the sulfur atom resulting in the *alpha* and *beta* isomers of endosulfan diol. The ratio of the *alpha* to the *beta* isomers of endosulfan diol will reflect the ratio of Endosulfan I to Endosulfan II in the parent compound.



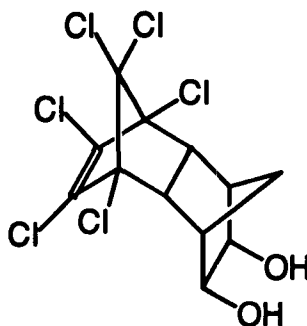
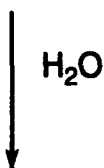
## 98. Endrin

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Hydrolysis of endrin will proceed by nucleophilic attack of  $\text{H}_2\text{O}$  at the epoxide moiety resulting in the formation of endrin diol, which will be stable to further hydrolysis.



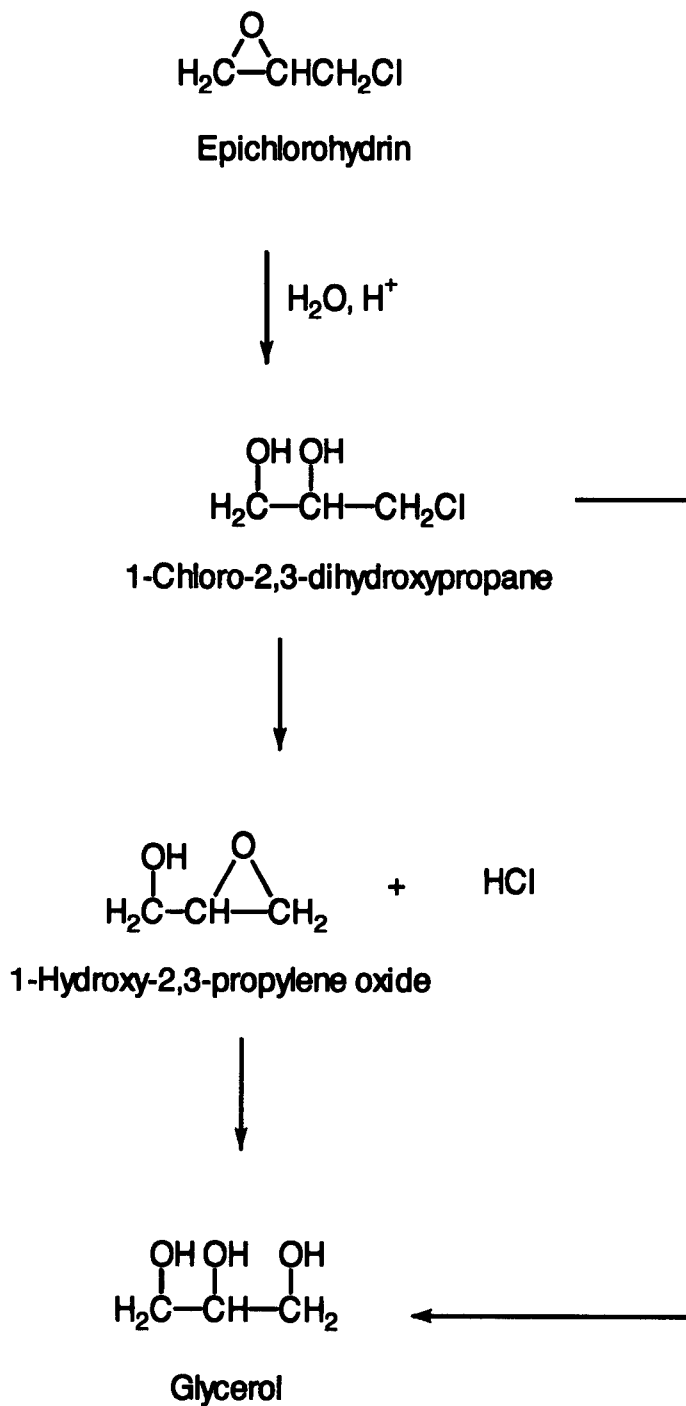
Endrin



Endrin diol

## 99. Epichlorohydrin

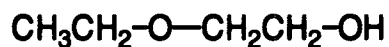
Hydrolysis of epichlorohydrin will occur initially by attack of  $\text{H}_2\text{O}$  at the epoxide moiety resulting in the formation of 1-chloro-2,3-dihydroxypropane. Subsequently, loss of chlorine will occur through the intramolecular attack of  $\text{HO}^-$  on the adjacent carbon to give 1-hydroxy-2,3-propylene oxide, which will undergo further hydrolysis by attack of  $\text{H}_2\text{O}$  at the epoxide moiety to give glycerol.



## 100. 2-Ethoxyethanol

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

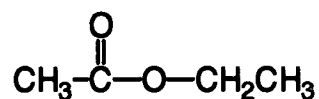


2-Ethoxyethanol

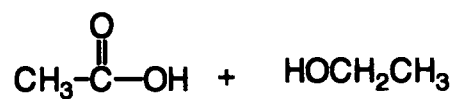
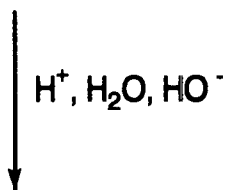
## 101. Ethyl acetate

---

Hydrolysis of ethyl acetate will occur by acyl-oxygen bond cleavage by  $\text{H}_2\text{O}$  and acid catalysis and base mediation resulting in the formation of acetic acid and ethanol.



Ethyl acetate



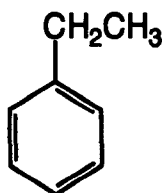
Acetic acid

Ethanol

## 102. Ethylbenzene

---

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

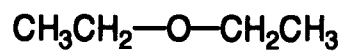


Ethylbenzene

## 103. Ethyl ether

---

Ethyl ether will not hydrolyze. It has no hydrolyzable functional group.

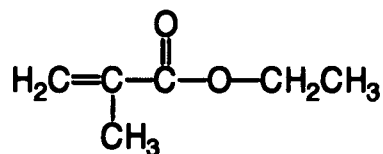


Ethyl ether

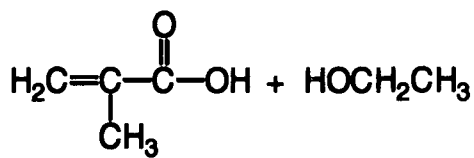
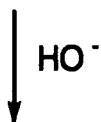
## 104. Ethyl methacrylate

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Hydrolysis of ethyl methacrylate will occur by the base-mediated cleavage of the acyl-oxygen bond resulting in methacrylic acid and ethanol.



Ethyl methacrylate



Methacrylic acid

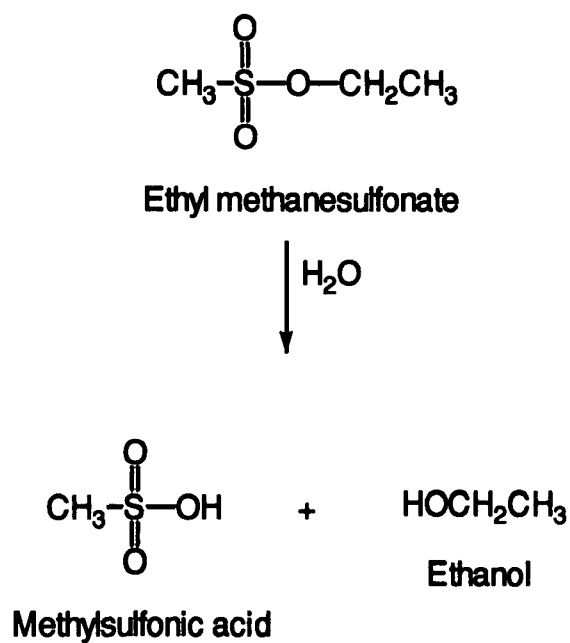
Ethanol



## 105. Ethyl methanesulfonate

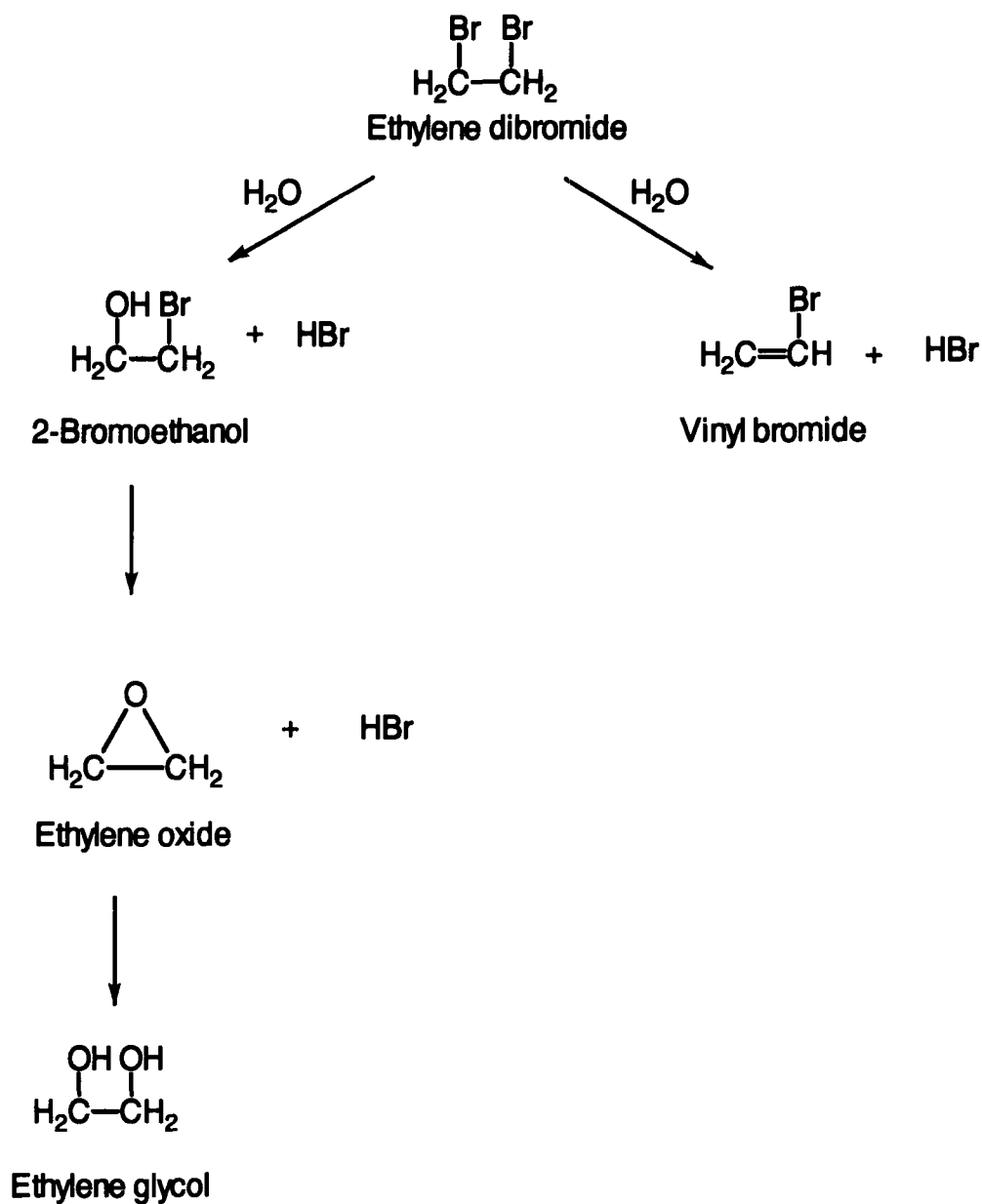
---

Hydrolysis of ethyl methanesulfonate will occur in a manner analogous to the hydrolysis of carboxylic acid esters. Nucleophilic attack of  $\text{H}_2\text{O}$  at the carbon results in the formation of methanesulfonic acid and ethanol.



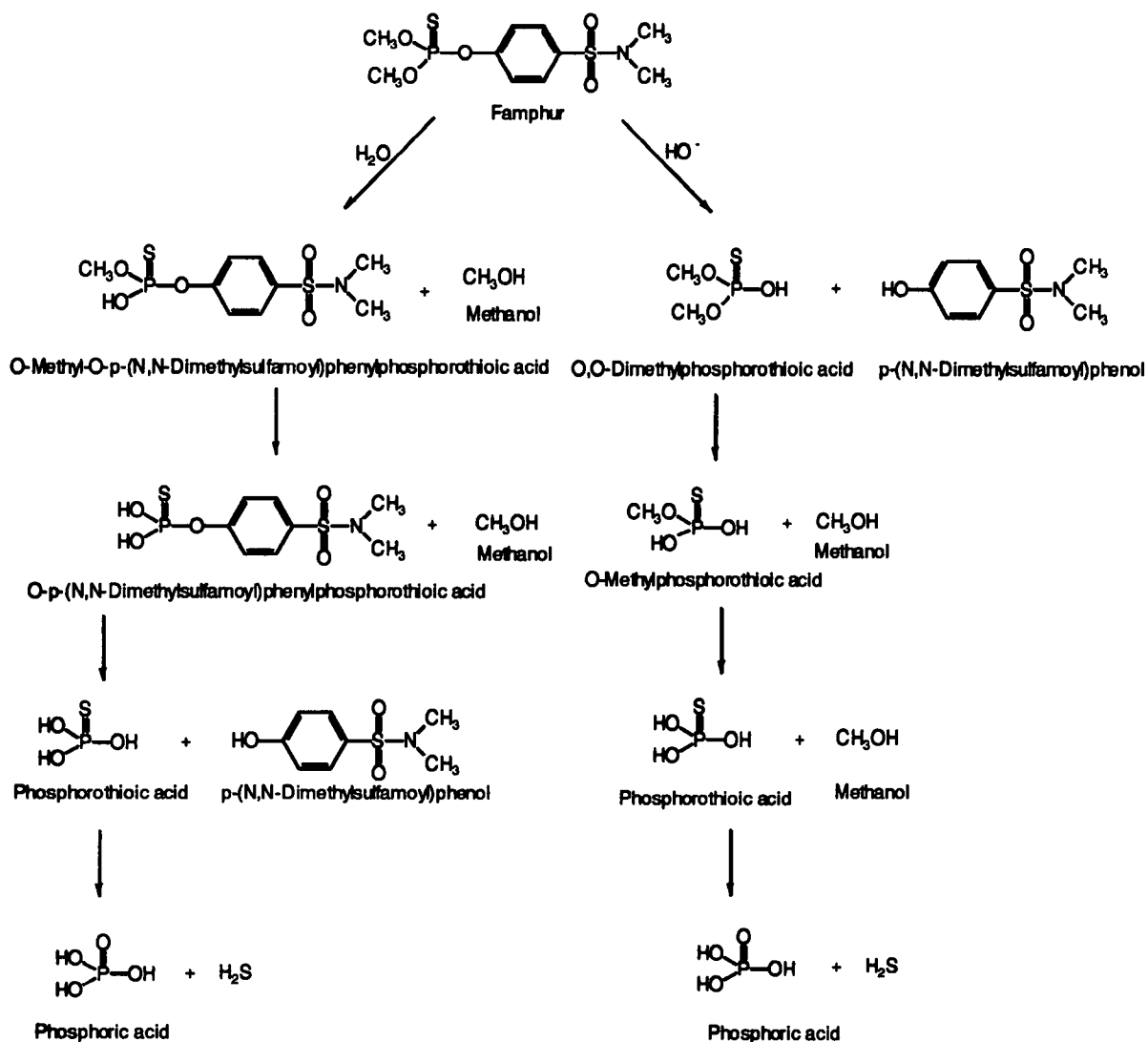
## 106. Ethylene dibromide

The reaction of ethylene dibromide proceeds by either nucleophilic substitution or dehydrohalogenation. Nucleophilic displacement of bromine by  $\text{H}_2\text{O}$  results in 2-bromoethanol, which will react further through the epoxide intermediate to yield ethylene glycol. Dehydrohalogenation results in the formation of vinyl bromide, which will be stable to further hydrolysis.



## 107. Famphur

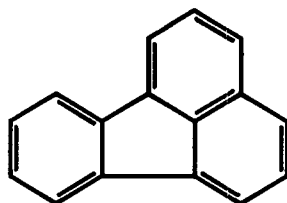
The reaction pathways for the hydrolysis of famphur are similar to the organophosphorus esters previously discussed. Both base and neutral hydrolysis can occur by nucleophilic attack at the phosphorus atom resulting in the formation of phosphorous diesters, which will hydrolyze through the phosphate monoester eventually to result in phosphoric acid and hydrogen sulfide, and *p*-(*N,N*-dimethylsulfamoyl)phenol.



## 108. Fluoranthene

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

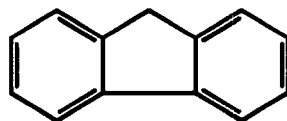


Fluoranthene

## 109. Fluorene

---

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

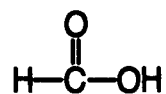


Fluorene

### 110. Formic acid

---

Formic acid will not hydrolyze. It has no hydrolyzable functional group.

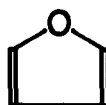


Formic acid

### 111. Furan

---

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

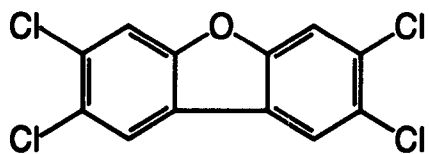


Furan

## 112. 2,3,7,8-TCDFuran

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

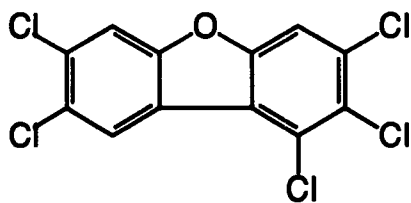


2,3,7,8-TCDFuran

## 113. 1,2,3,7,8-PeCDFuran

---

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

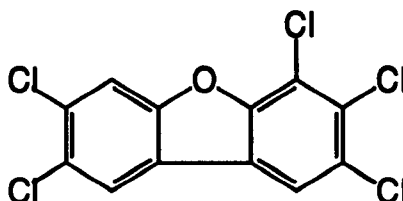


1,2,3,7,8-PeCDFuran

#### 114. 2,3,4,7,8-PeCDFuran

---

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

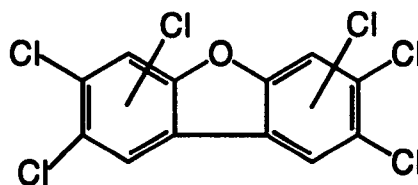


2,3,4,7,8-PeCDFuran

#### 115. 2,3,7,8-HxCDFurans

---

2,3,7,8-HxCDFurans will not hydrolyze to any reasonable extent; however, they may undergo other abiotic transformation processes.

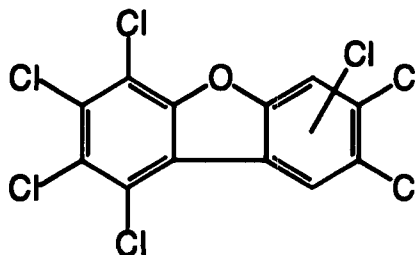


2,3,7,8-HxCDFuran

## 116. 2,3,7,8-HpCDFurans

---

2,3,7,8-HpCDFurans will not hydrolyze to any reasonable extent; however, they may undergo other abiotic transformation processes.

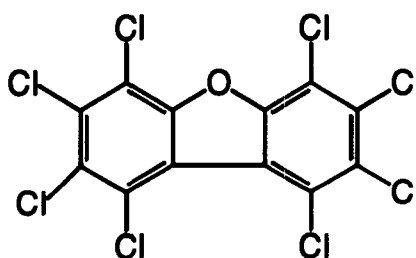


2,2,7,8-HpCDFuran

## 117. OCDF

---

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

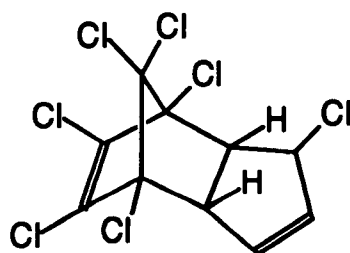


OCDF

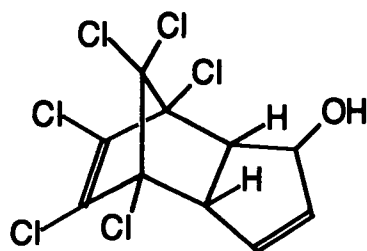
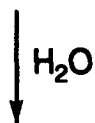


## 118. Heptachlor

Hydrolysis of heptachlor will occur by nucleophilic substitution of  $\text{H}_2\text{O}$  at the allylic-carbon-bearing chlorine resulting in the formation of 1-hydroxychlordehene, which will be stable to further hydrolysis.



Heptachlor

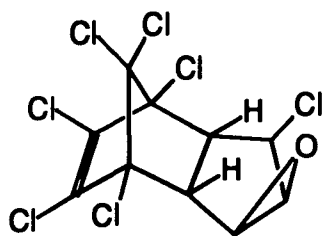


1-Hydroxychlordehene

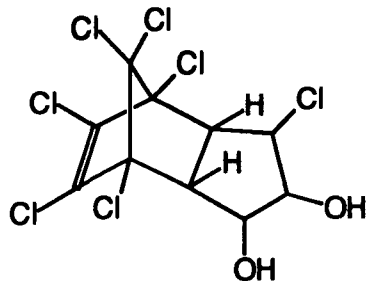
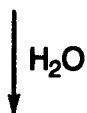


## 119. Heptachlor epoxide

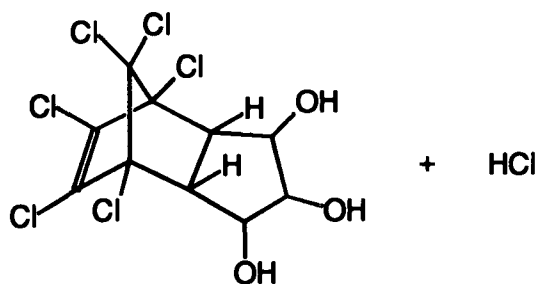
Heptachlor epoxide will hydrolyze by nucleophilic attack of  $\text{H}_2\text{O}$  at the epoxide moiety resulting in heptachlor diol. Further hydrolysis of the diol can occur by nucleophilic substitution of  $\text{H}_2\text{O}$  at the chlorine-bearing carbon adjacent to the hydroxyl groups. The resulting triol will be stable to further hydrolysis.



Heptachlor epoxide



Heptachlor diol

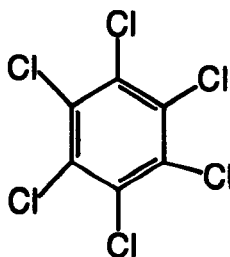


Heptachlor triol

## 120. Hexachlorobenzene

---

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

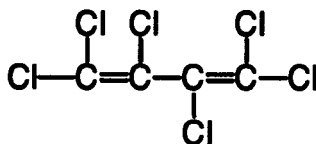


Hexachlorobenzene

## 121. Hexachlorobutadiene

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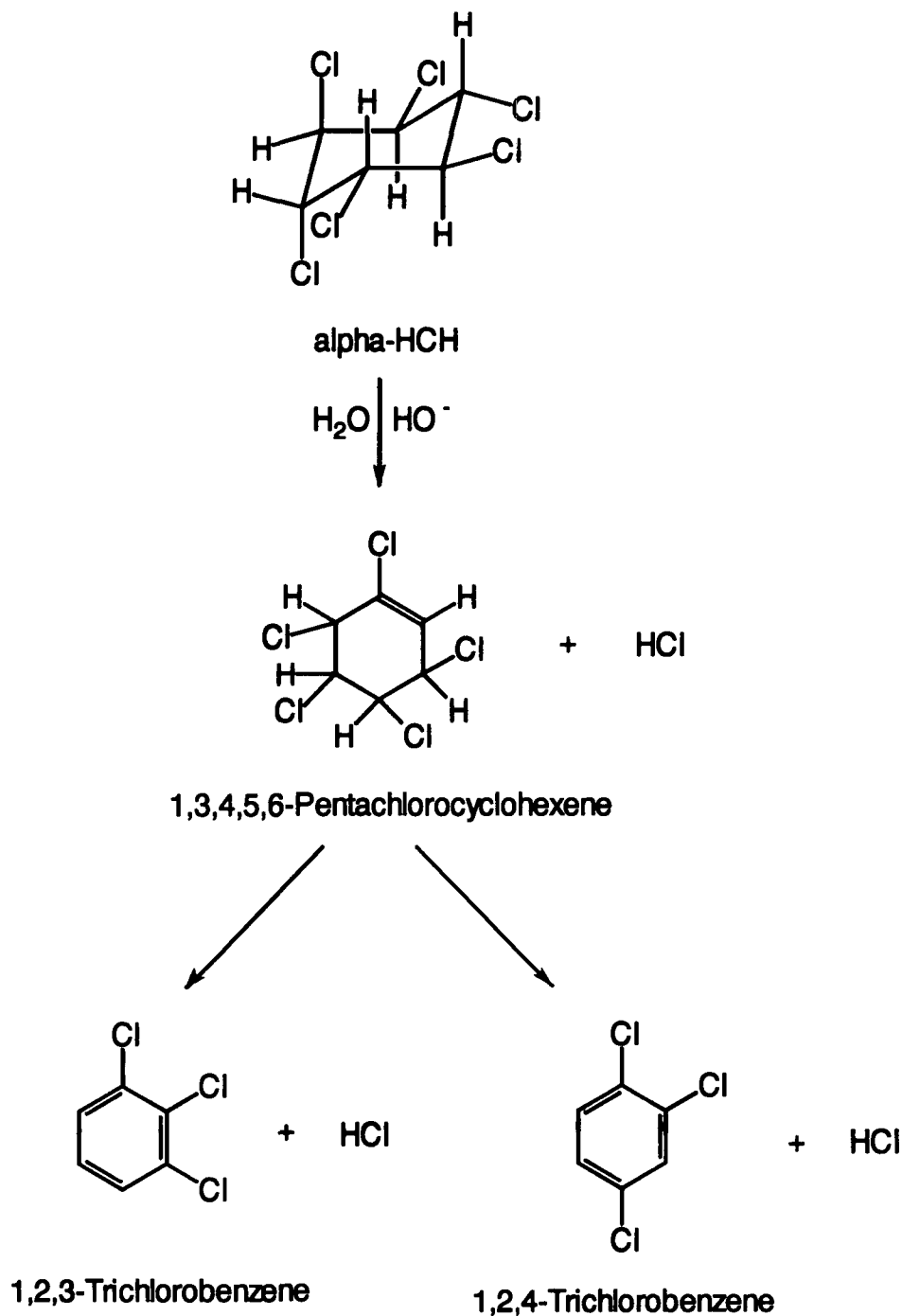
Hexachlorobutadiene will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



Hexachlorobutadiene

## 122. *alpha*-HCH

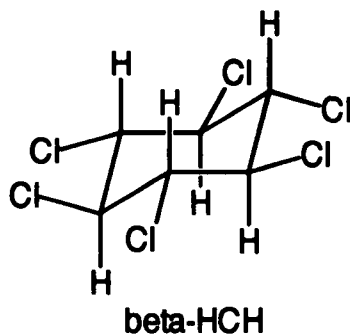
The reaction of *alpha*-HCH occurs by *trans*-dehydrochlorination of the axial chlorines resulting in the intermediate 1,3,4,5,6-pentachlorocyclohexene. This cyclohexene will react further with either  $\text{H}_2\text{O}$  or  $\text{HO}^-$  through sequential dehydrochlorination steps to give a mixture of the regioisomers, 1,2,3-trichlorobenzene and 1,2,4-trichlorobenzene.



### 123. *beta*-HCH

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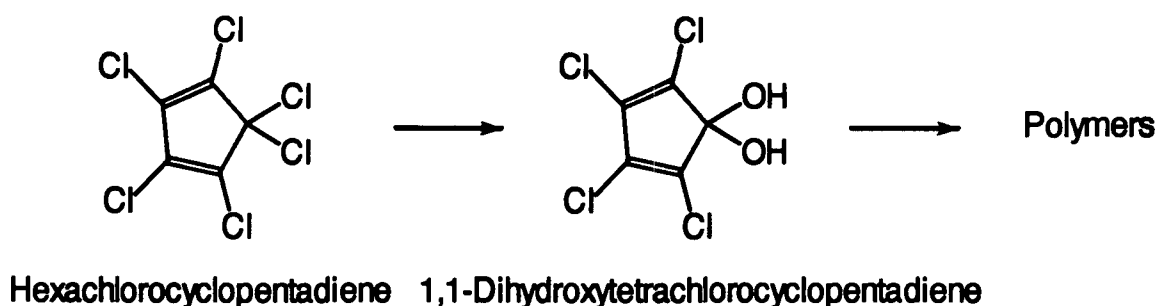
*beta*-HCH will not hydrolyze to any reasonable extent (NLFG). The six equatorial chlorines do not permit initial *trans*-dehydrochlorination to yield the intermediate pentachlorocyclohexene as occurs in the *alpha*- (#122.) and *gamma*-isomers (#132).



## 124. Hexachlorocyclopentadiene

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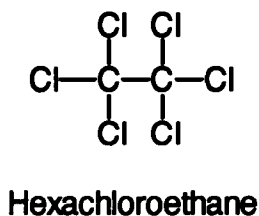
Hydrolysis of hexachlorocyclopentadiene results in the formation of 1,1-dihydroxy-tetrachlorocyclopentadiene, which is an unstable product. Its degradation leads to the formation of polymers.



## 125. Hexachloroethane

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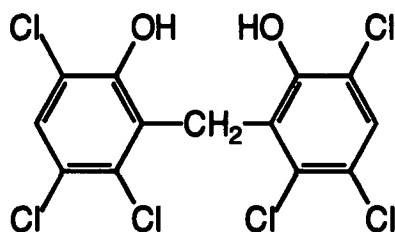
Hexachloroethane will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



## 126. Hexachlorophene

---

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

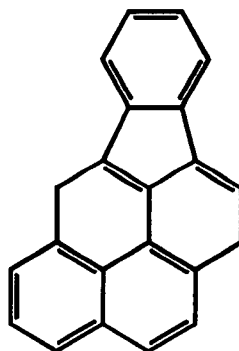


Hexachlorophene

## 127. Indeno[1,2,3-*cd*]pyrene

---

Indeno[1,2,3-*cd*]pyrene will not hydrolyze. It has no hydrolyzable functional group.

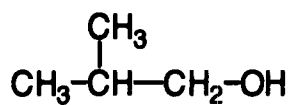


Indeno[1,2,3-*cd*]pyrene

## 128. Isobutyl alcohol

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Isobutyl alcohol will not hydrolyze. It has no hydrolyzable functional group.

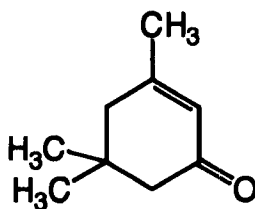


Isobutyl alcohol

## 129. Isophorone

---

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

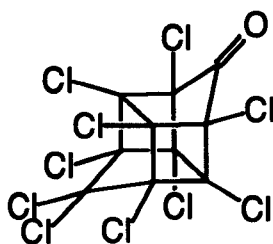


Isophorone



### 130. Kepone

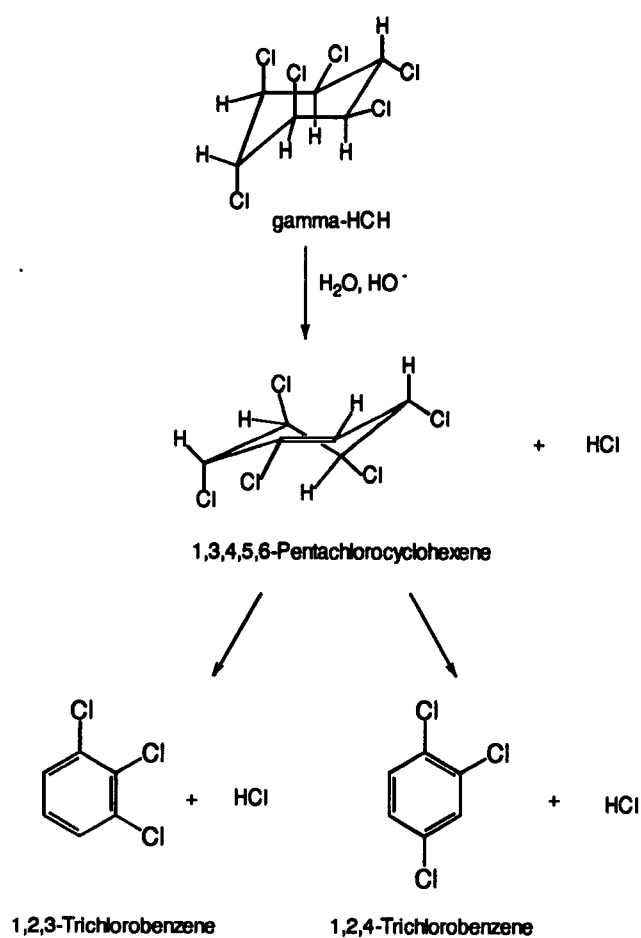
Kepone will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



Kepone

### 132. *gamma*-HCH

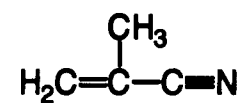
The reaction pathway for the hydrolysis of *gamma*-HCH (lindane) is identical to that described for *alpha*-HCH (#122).



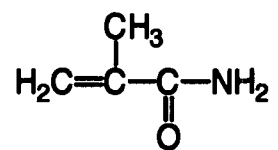
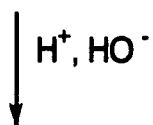
## 134. Methacrylonitrile

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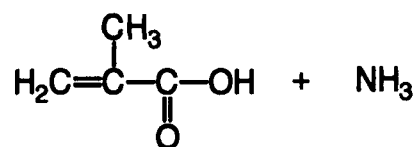
Hydrolysis of methacrylonitrile will occur by the acid-catalyzed or base-mediated hydrolysis of the nitrile moiety to give methacrylic acid and ammonia.



Methacrylonitrile



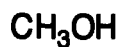
Methacrylamide



Methacrylic acid

### 135. Methanol

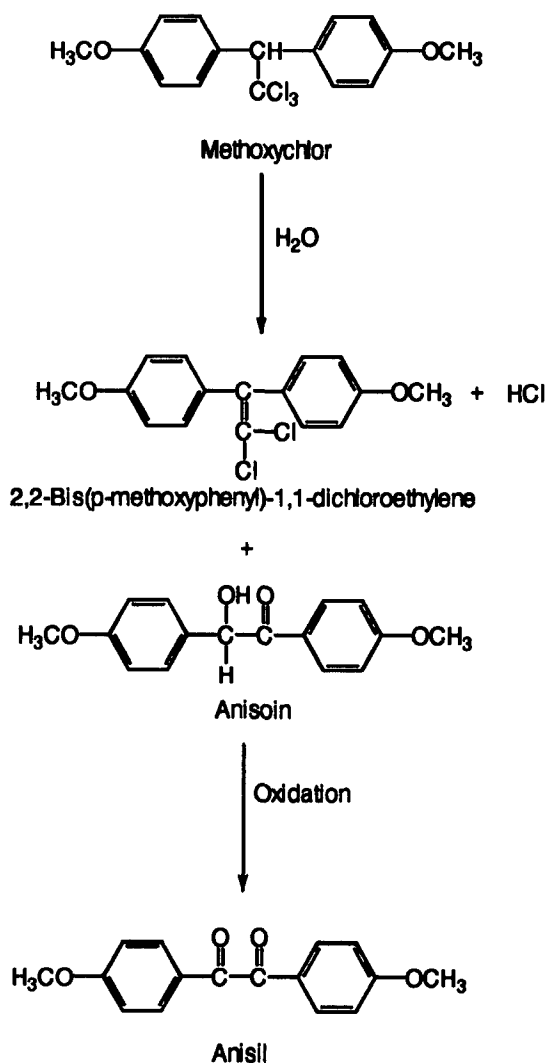
Methanol will not hydrolyze. It has no hydrolyzable functional group.



Methanol

### 136. Methoxychlor

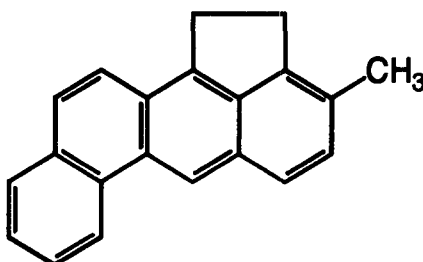
The products formed during aqueous hydrolysis of methoxychlor are influenced by the pH of the system. Above pH 10, 2,2-bis(*p*-methoxyphenyl)-1,1-dichloroethylene (DMDE) is the only reported product. Below pH 10 a second product, anisoin, is observed. Anisoin is the major product formed by hydrolysis when the system is below pH 8; however, it is unstable and will oxidize to anisil. Hydrolysis is not an important pathway in further degradation of DMDE and anisil.



### 137. 3-Methylcholanthrene

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3-Methylcholanthrene will not hydrolyze. It has no hydrolyzable functional group.

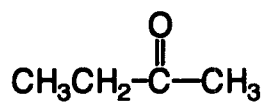


3-Methylcholanthrene

### 138. Methyl ethyl ketone

---

Methyl ethyl ketone will not hydrolyze. It has no hydrolyzable functional group.

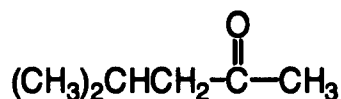


Methyl ethyl ketone

### 139. Methyl isobutyl ketone

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Methyl isobutyl ketone will not hydrolyze. It has no hydrolyzable functional group.

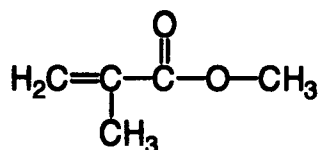


Methyl isobutyl ketone

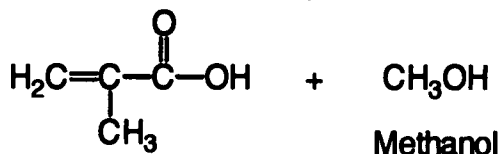
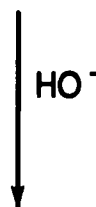
### 140. Methyl methacrylate

---

Hydrolysis of methyl methacrylate proceeds through nucleophilic attack by  $\text{HO}^-$  at the ester carbonyl to yield methacrylic acid and methanol. The second order alkaline hydrolysis rate constant and the corresponding calculated half-life are in the range of values reported for esters of similar structure.



Methyl methacrylate

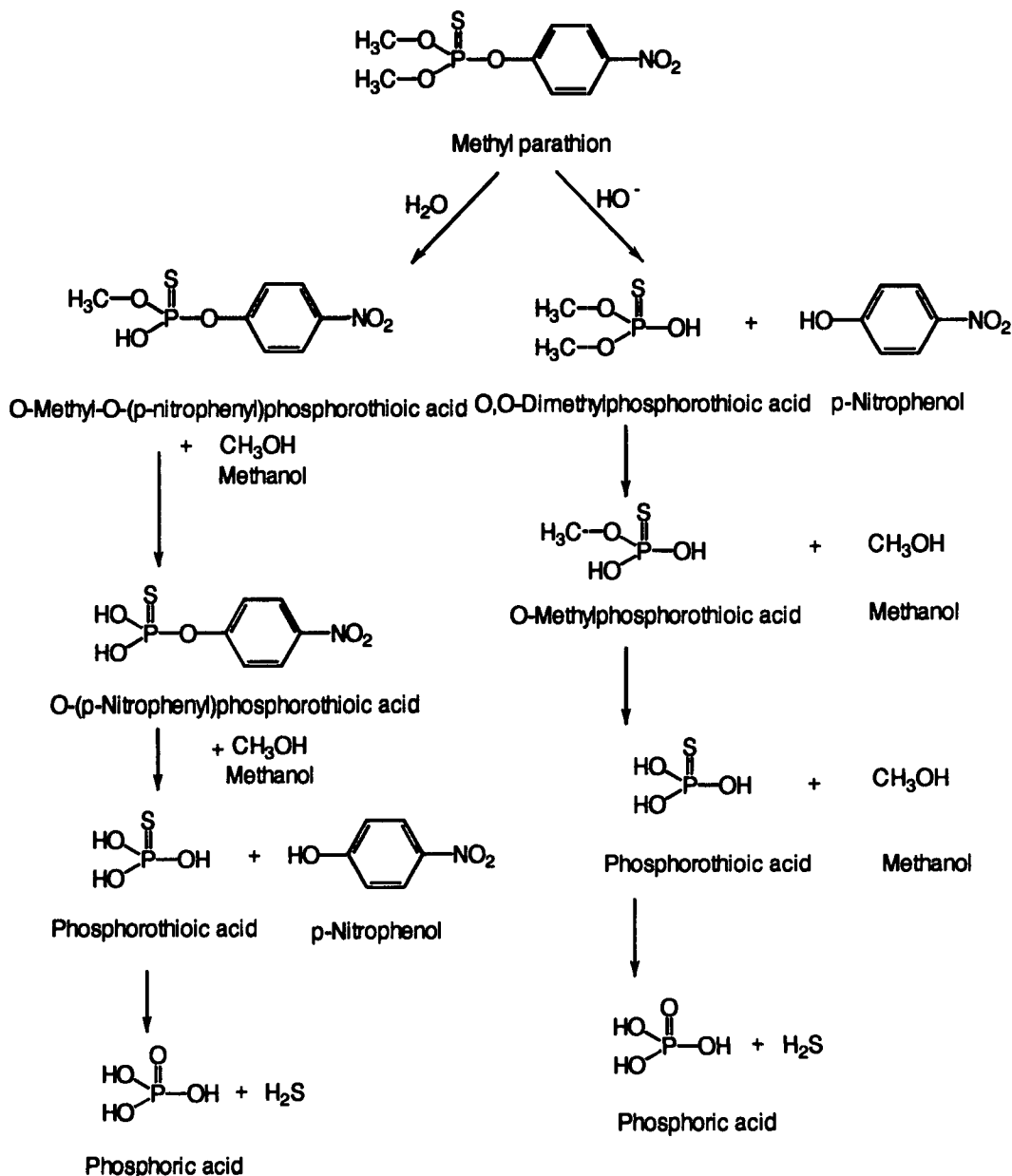


Methacrylic acid

Methanol

## 141. Methyl parathion

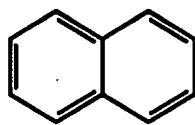
Hydrolysis of methyl parathion may occur through either reaction with  $\text{H}_2\text{O}$  (neutral hydrolysis) or reaction with  $\text{HO}^-$  (base-mediated hydrolysis). Nucleophilic substitution by  $\text{H}_2\text{O}$  occurs in sequence at the two methoxy carbons to yield *O*-methyl-*O*-(*p*-nitrophenyl)phosphorothioic acid (diester) and *O*-(*p*-nitrophenyl)phosphorothioic acid (monoester), respectively. Loss of the second methyl group from the disubstituted ester would be at a rate approximately a factor of 10 less than the loss of the methyl group from the triester. Hydrolysis of the monosubstituted ester [*O*-(*p*-nitrophenyl)phosphorothioic acid] would proceed through cleavage of the P-O bond at a rate of approximately one-half the rate of the parent triester. Hydroxide-ion-mediated hydrolysis of methyl parathion proceeds through initial attack of the hydroxide ion on the phosphorus atom with displacement of the *p*-nitrophenylate ion. Loss of the two methyl groups from the *O,O*-dimethylphosphorothioic acid will proceed as described above. The phosphorothioic acid generated in each hydrolytic pathway will eventually degrade to phosphoric acid and hydrogen sulfide.



## 142. Naphthalene

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

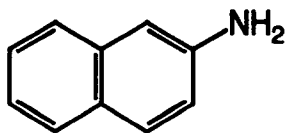


Naphthalene

## 143. 2-Naphthylamine

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2-Naphthylamine will not hydrolyze; however, it may undergo other abiotic transformation processes.

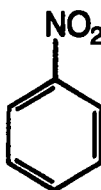


2-Naphthylamine

## 145. Nitrobenzene

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Nitrobenzene will not hydrolyze; however, it may undergo other abiotic transformation processes.

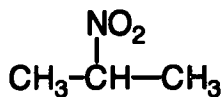


Nitrobenzene

## 146. 2-Nitropropane

---

2-Nitropropane will not hydrolyze; however, it may undergo other abiotic transformation processes.



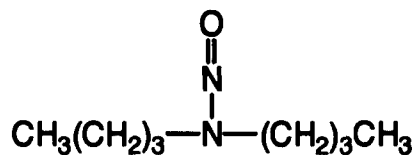
2-Nitropropane



**147. *N*-Nitroso-di-*n*-butylamine**

---

*N*-Nitroso-di-*n*-butylamine will not hydrolyze; however, it may undergo other abiotic transformation processes.

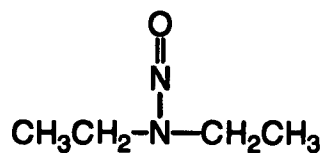


*N*-Nitroso-di-*n*-butylamine

**148. *N*-Nitrosodiethylamine**

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*N*-Nitrosodiethylamine will not hydrolyze; however, it may undergo other abiotic transformation processes.

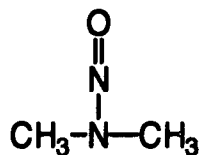


*N*-Nitrosodiethylamine

## 149. *N*-Nitrosodimethylamine

---

*N*-Nitrosodimethylamine will not hydrolyze; however, it may undergo other abiotic transformation processes.

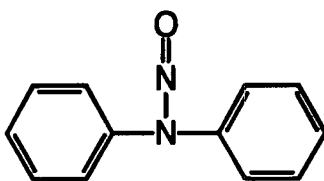


*N*-Nitrosodimethylamine

## 150. *N*-Nitrosodiphenylamine

---

*N*-Nitrosodiphenylamine will not hydrolyze; however, it may undergo other abiotic transformation processes.

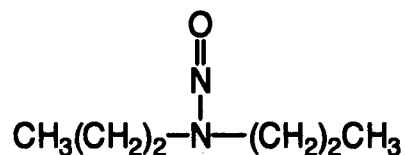


*N*-Nitrosodiphenylamine

### 151. *N*-Nitroso-di-*n*-propylamine

---

*N*-Nitroso-di-*n*-propylamine will not hydrolyze; however, it may undergo other abiotic transformation processes.

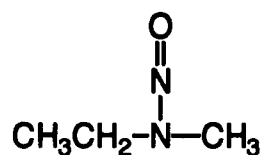


*N*-Nitroso-di-*n*-propylamine

### 152. *N*-Nitrosomethylethylamine

---

*N*-Nitrosomethylethylamine will not hydrolyze; however, it may undergo other abiotic transformation processes.

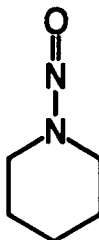


*N*-Nitrosomethylethylamine

### 153. *N*-Nitrosopiperidine

---

*N*-Nitrosopiperidine will not hydrolyze; however, it may undergo other abiotic transformation processes.

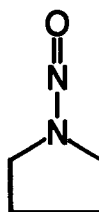


*N*-Nitrosopiperidine

### 154. *N*-Nitrosopyrrolidine

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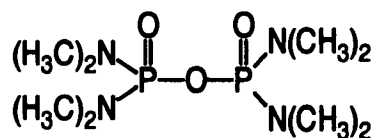
*N*-Nitrosopyrrolidine will not hydrolyze; however, it may undergo other abiotic transformation processes.



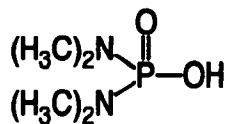
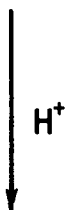
*N*-Nitrosopyrrolidine

### 155. Octamethyl pyrophosphoramidate

Hydrolysis of octamethyl pyrophosphoramidate (OMPP) proceeds through cleavage of the P-O-P bond. OMPP is stable to attack by the hydroxide ion and the neutral water molecule, but is degraded under acidic conditions.



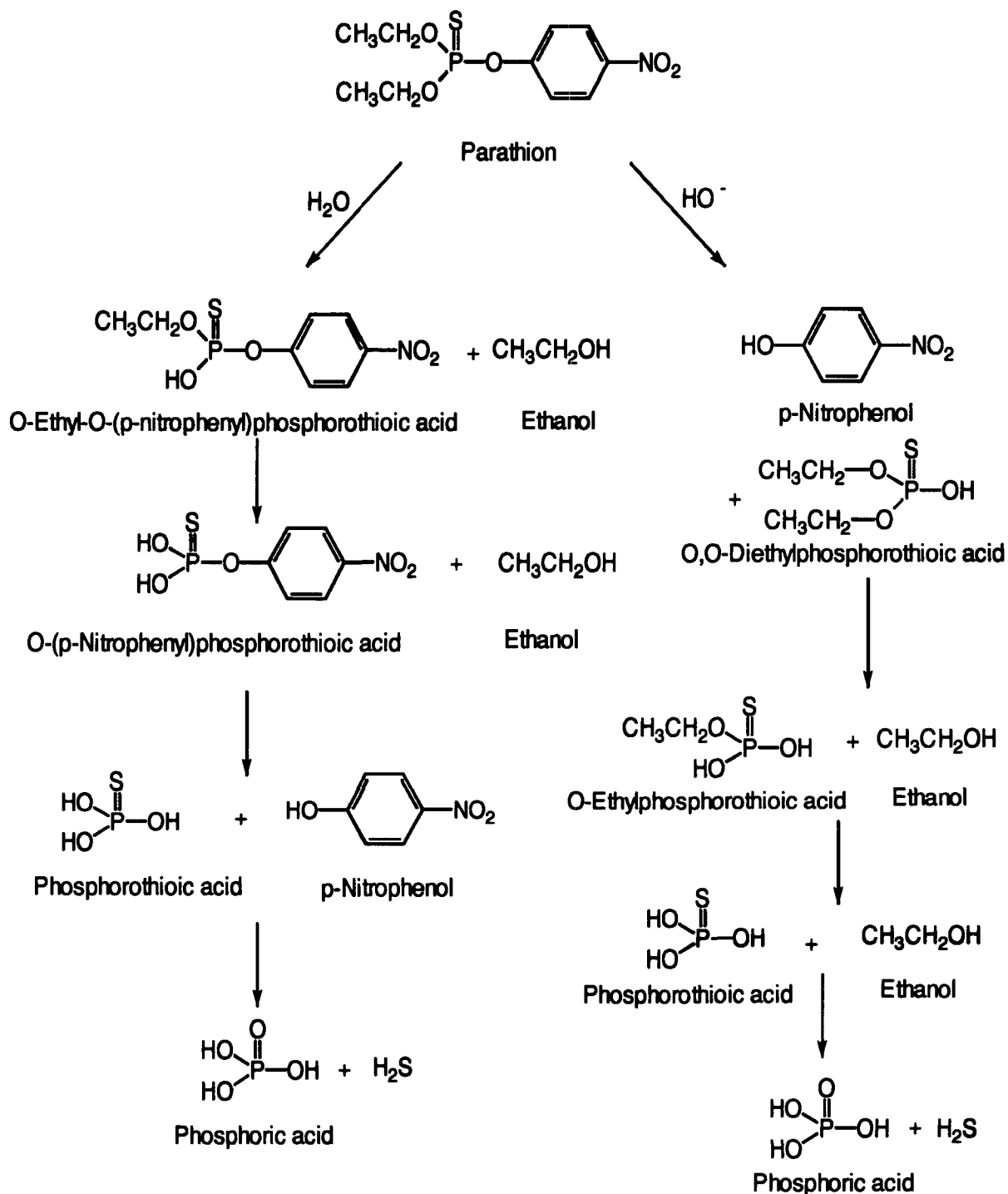
Octamethyl pyrophosphoramidate



Bis(N,N-dimethylamino)phosphoric acid

## 156. Parathion

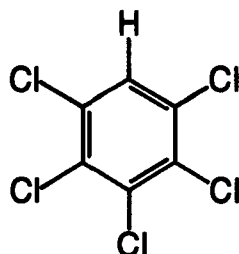
Parathion is the ethyl analog of methyl parathion. The products formed and mechanisms of hydrolysis parallel those of methyl parathion (#141) but hydrolysis proceeds at a slower rate typical for triethyl phosphates compared to trimethyl phosphates.



## 157. Pentachlorobenzene

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

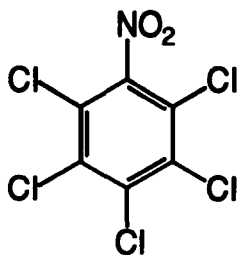


Pentachlorobenzene

## 158. Pentachloronitrobenzene

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The previously reported hydrolysis rate constant for pentachloronitrobenzene (PCNB) in reference 6 was based on disappearance kinetics without confirmation of hydrolysis products. For this report, the hydrolysis experiment was repeated in glass-sealed ampules. No disappearance of PCNB was observed after 33 days at pH 11 and 85°C. PCNB has, therefore, been designated as NLFG.

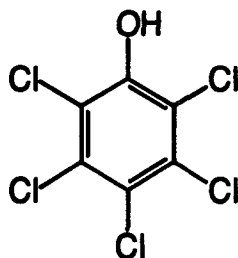


Pentachloronitrobenzene

### 159. Pentachlorophenol

---

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

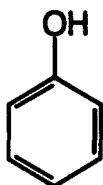


Pentachlorophenol

### 160. Phenol

---

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

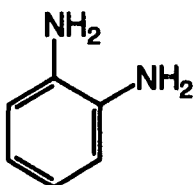


Phenol

### 161. Phenylenediamine

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The three isomers of phenylenediamine, *ortho*-, *meta*-, and *para*-, will not hydrolyze; however, they may undergo other abiotic transformation processes.

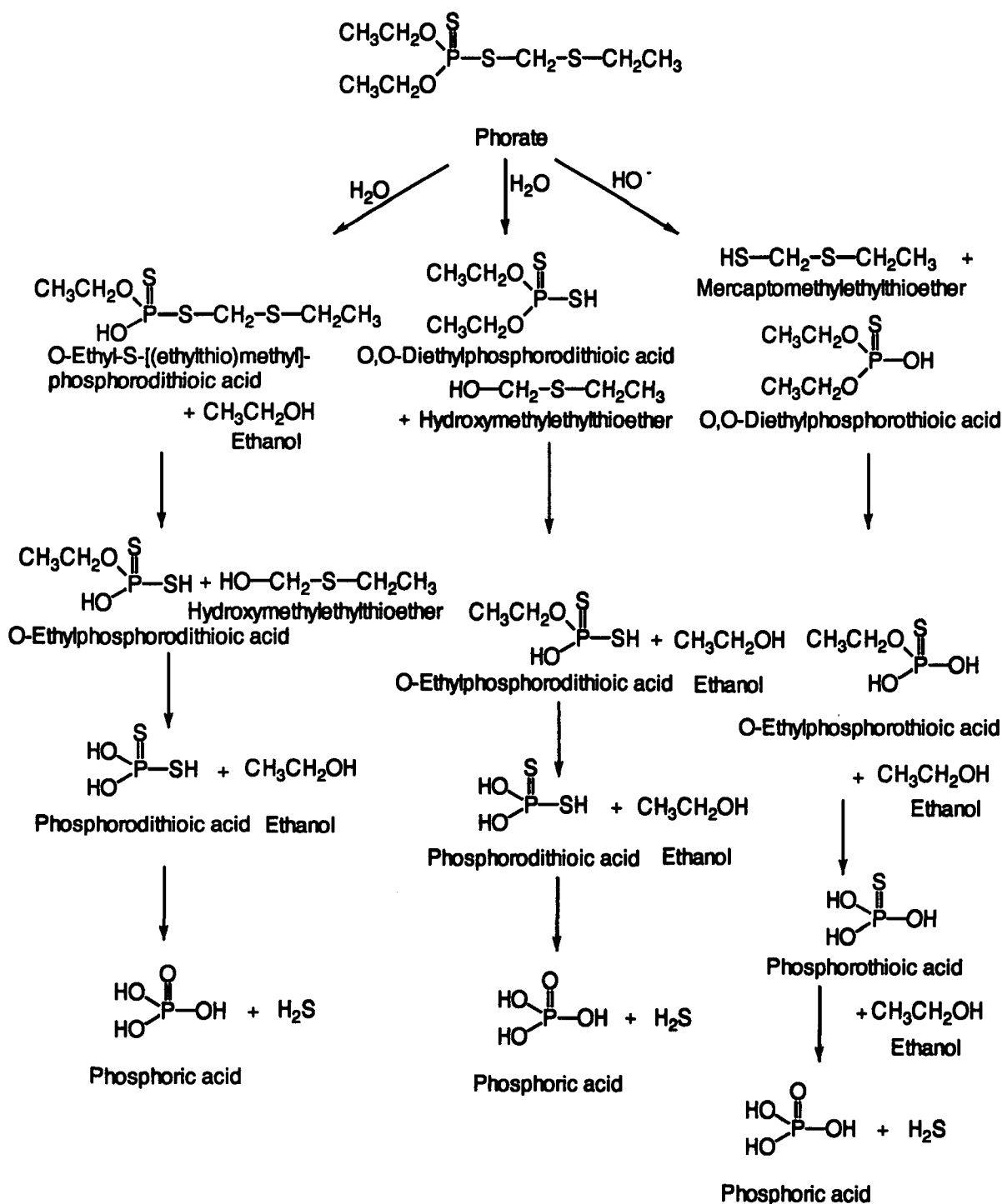


1,2-Phenylenediamine



## 162. Phorate

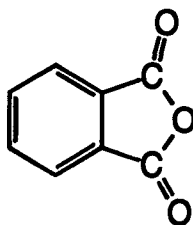
Phorate, by virtue of having one less methylene group in the sulfide side chain, is an analog of disulfoton. The products formed and mechanisms of hydrolysis parallel those of disulfoton. Phorate has a neutral hydrolysis rate of approximately 30 times that of disulfoton (#96).



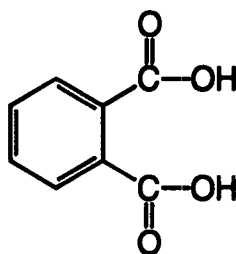
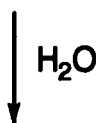
### 163. Phthalic anhydride

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Phthalic anhydride hydrolyzes to *o*-phthalic acid in water. The hydrolysis occurs through nucleophilic attack of  $\text{H}_2\text{O}$  at a carbonyl carbon. The resulting ring opening yields *o*-phthalic acid.



Phthalic anhydride

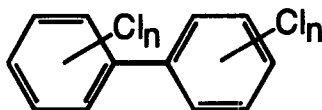


*o*-Phthalic acid

### 164. Polychlorinated biphenyls

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Polychlorinated biphenyls will not hydrolyze to any reasonable extent.

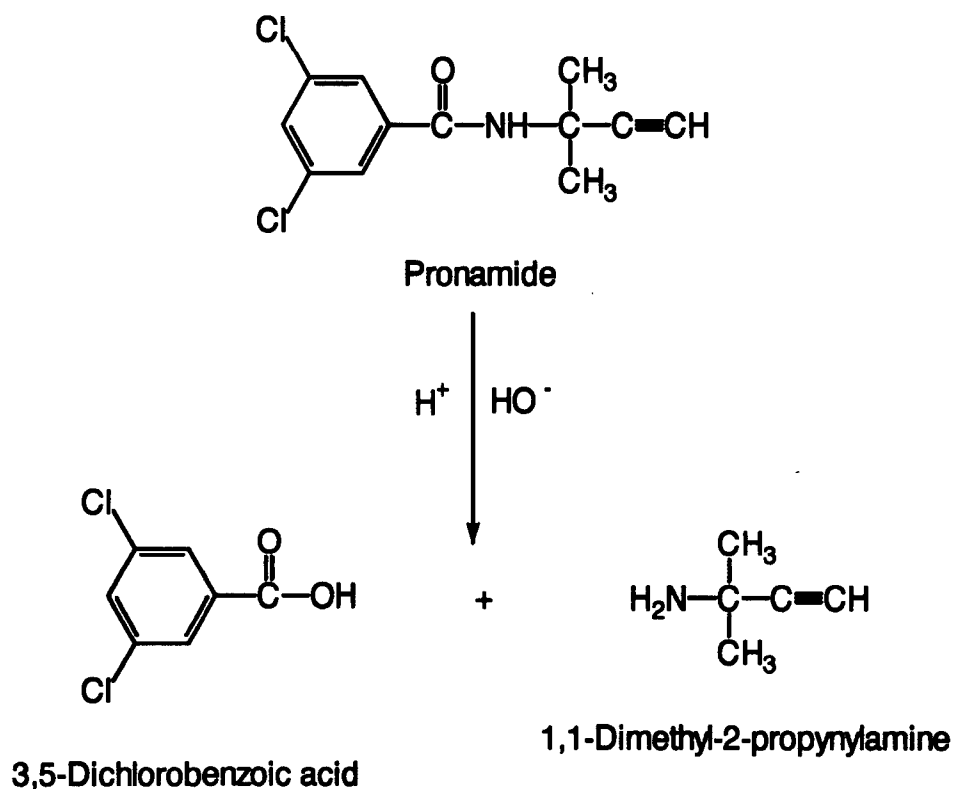


$$n = 1 - 5$$

Polychlorinated biphenyls

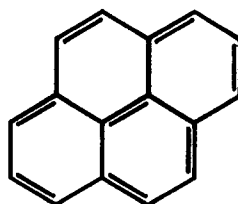
## 165. Pronamide

The *N*-substituted amide bond in pronamide, formed by reaction of a carboxylic acid and primary amine, is more resistant to hydrolysis than similar bonds formed with carboxylic acids and alcohols such as the previously discussed acrylate and phthalate esters.



## 166. Pyrene

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

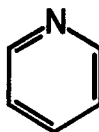


Pyrene

## 167. Pyridine

---

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

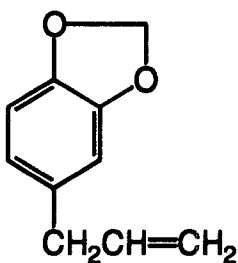


Pyridine

## 168. Safrole

---

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

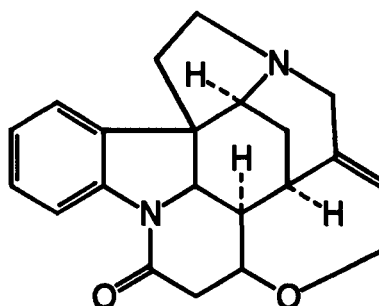


Safrole

### 171. Strychnine

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Strychnine will not hydrolyze to any reasonable extent.

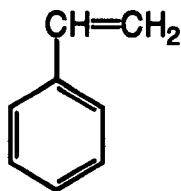


Strychnine

### 172. Styrene

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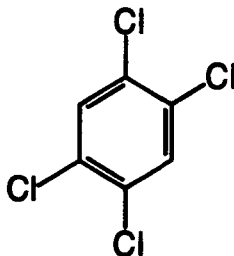
Styrene will not hydrolyze; however, it may undergo other abiotic transformation processes.



Styrene

### 173. 1,2,4,5-Tetrachlorobenzene

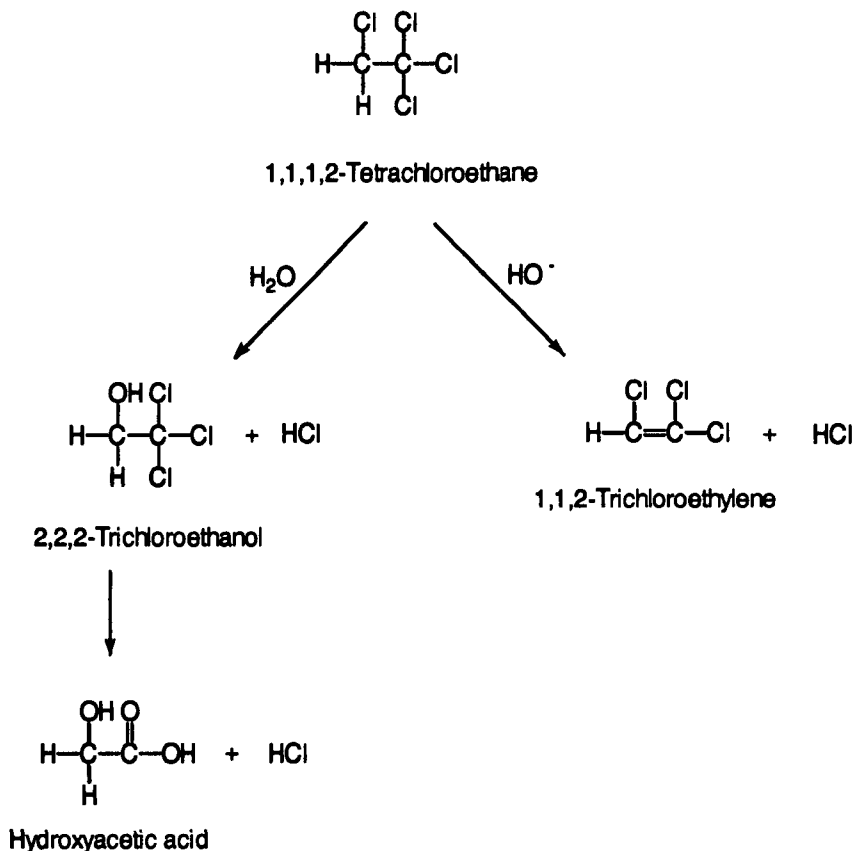
1,2,4,5-Tetrachlorobenzene will not hydrolyze to any reasonable extent.



1,2,4,5-Tetrachlorobenzene

### 174. 1,1,1,2-Tetrachloroethane

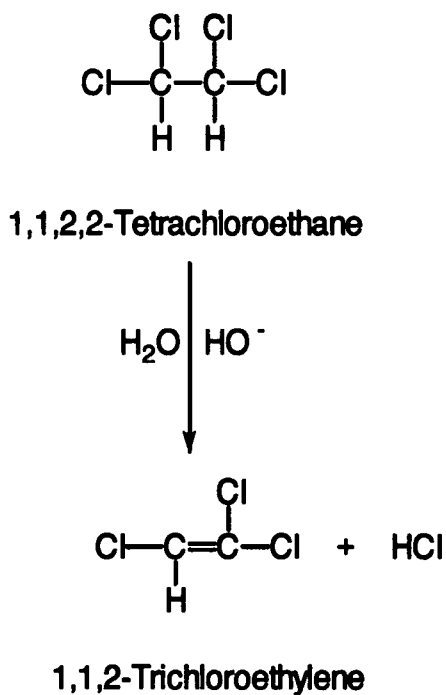
The hydrolysis pathway for 1,1,1,2-tetrachloroethane will proceed through competing pathways (nucleophilic substitution and dehydrohalogenation). Nucleophilic substitution will occur at the monochlorinated carbon with formation of trichloroethanol. Degradation of trichloroethanol will continue to yield glycolic acid (hydroxyacetic acid). Base-mediated elimination of chlorine from 1,1,1,2-tetrachloroethane will result in formation of 1,1,2-trichloroethylene.



### 175. 1,1,2,2-Tetrachloroethane

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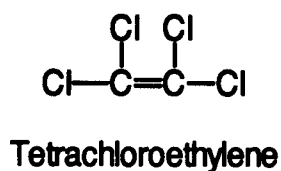
1,1,2,2-Tetrachloroethane hydrolyzes by the base-mediated elimination of chlorine to 1,1,2-trichloroethylene. This quantitative conversion occurs in the pH range of 5-9.



### 176. Tetrachloroethylene

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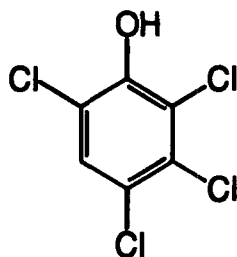
Tetrachloroethylene will not hydrolyze to any reasonable extent.



**177. 2,3,4,6-Tetrachlorophenol**

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

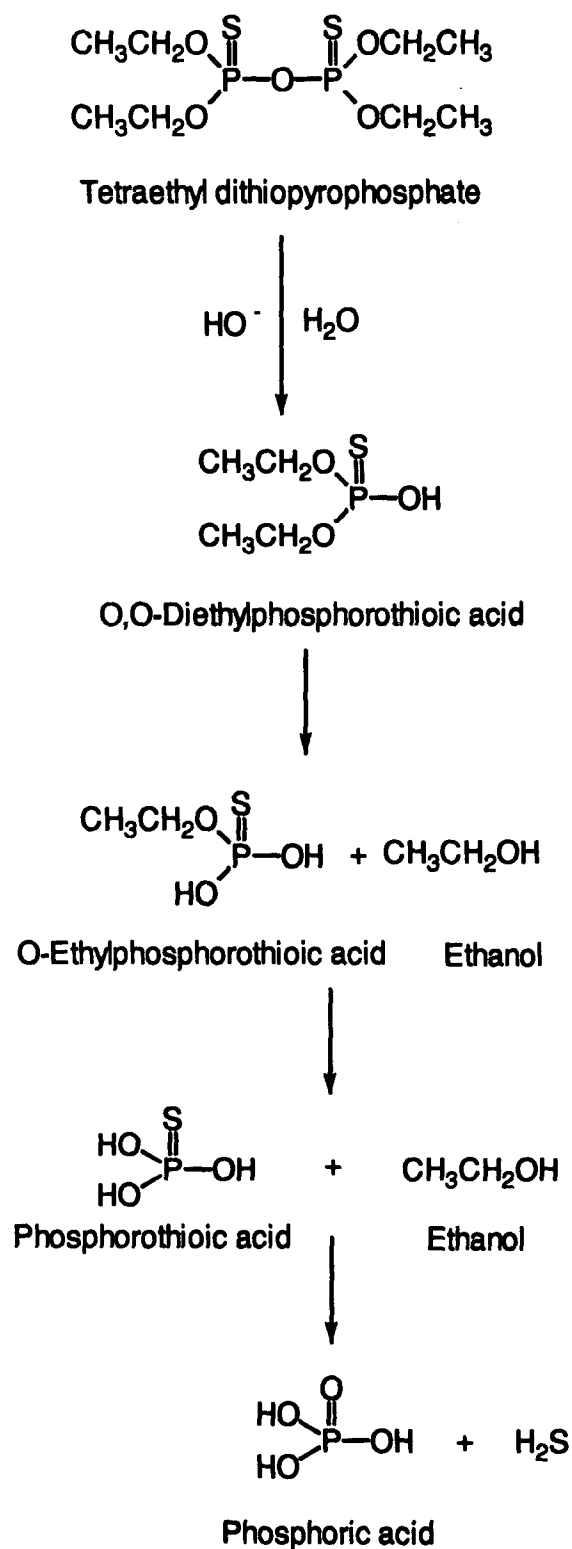


2,3,4,6-Tetrachlorophenol



## 178. Tetraethyl dithiopyrophosphate

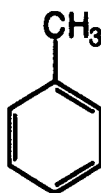
The P-O-P bond of tetraethyl dithiopyrophosphate is very labile to attack by hydroxide, even at concentrations of hydroxide present below pH 7. The resulting *O,O*-diethylphosphorothioic acid is hydrolyzed to the final products phosphoric acid and ethanol by the mechanisms discussed in the section on hydrolysis of phosphates.



## 180. Toluene

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

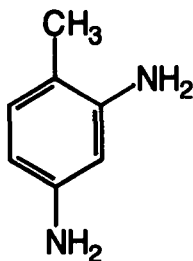


Toluene

## 181. 2,4-Toluenediamine

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2,4-Toluenediamine will not hydrolyze; however, it may undergo other abiotic transformation processes.

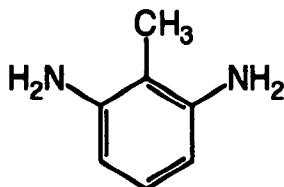


2,4-Toluenediamine

## 182. 2,6-Toluenediamine

---

2,6-Toluenediamine will not hydrolyze; however, it may undergo other abiotic transformation processes.

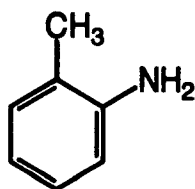


2,6-Toluenediamine

## 183. o-Toluidine

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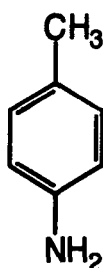
o-Toluidine will not hydrolyze; however, it may undergo other abiotic transformation processes.



o-Toluidine

## 184. *p*-Toluidine

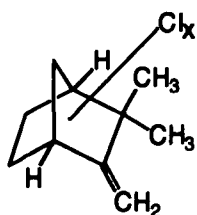
*p*-Toluidine will not hydrolyze; however, it may undergo other abiotic transformation processes.



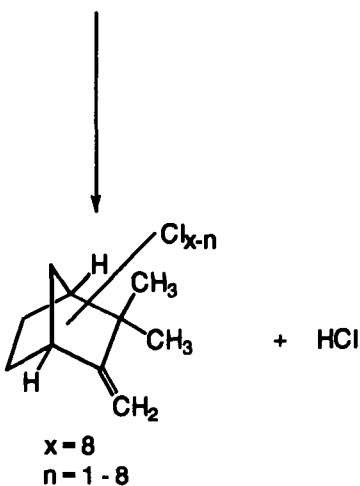
*p*-Toluidine

## 185. Toxaphene

Toxaphene is a complex but reproducible mixture of chlorinated camphene (67-69% chlorine by weight). The mixture has been shown to contain at least 177 and up to 670 components. The degradation rate was determined by monitoring the loss of chlorine with time during hydrolysis rate studies.



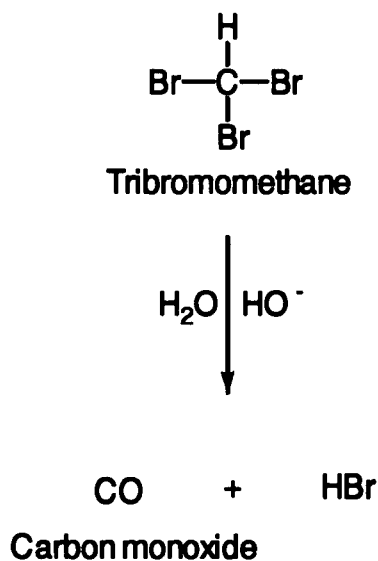
Toxaphene



## 186. Tribromomethane

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Hydrolysis of tribromomethane occurs initially by proton abstraction followed by formation of the carbene, which reacts with  $\text{HO}^-$  to form carbon monoxide and the mineral acid.



## 187. 1,2,4-Trichlorobenzene

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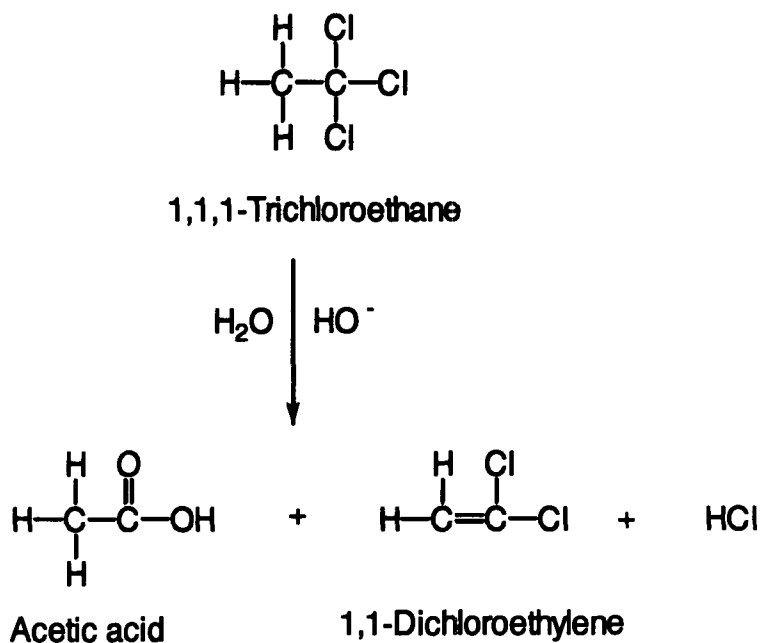
1,2,4-Trichlorobenzene will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



## 188. 1,1,1-Trichloroethane

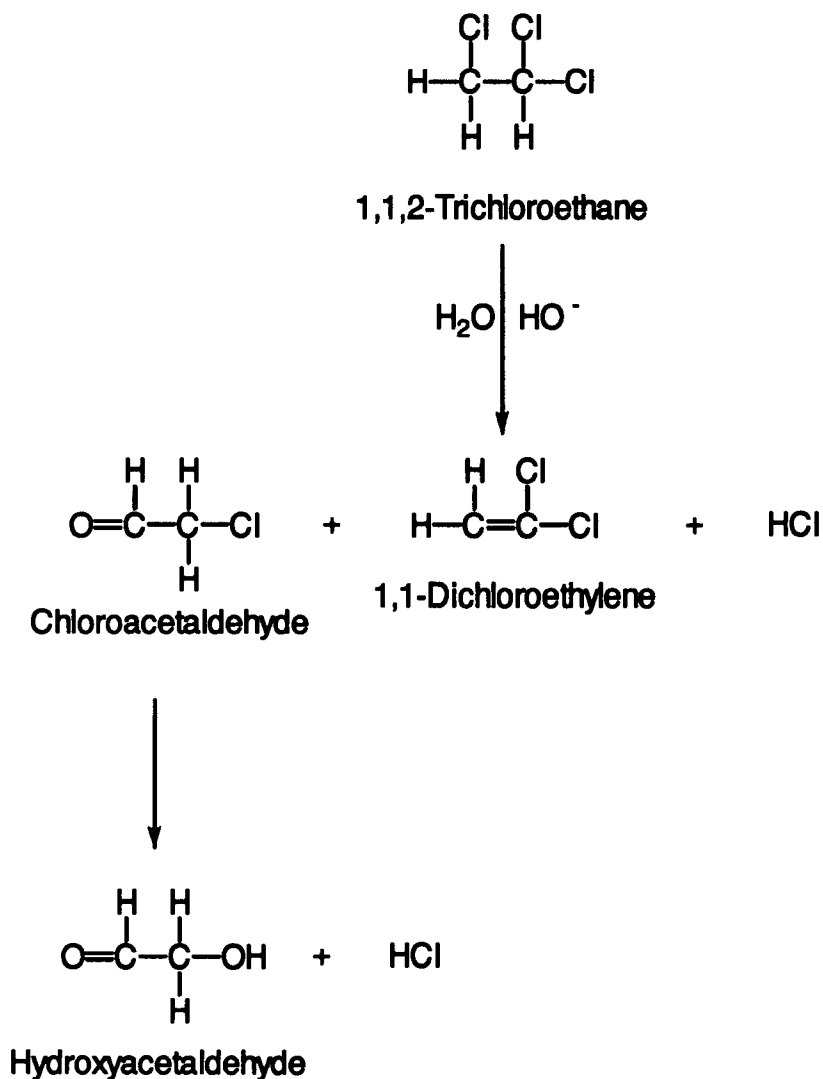
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Nucleophilic attack by  $\text{H}_2\text{O}$  on the trichloro- substituted carbon yields acetic acid, while the hydroxide-ion-mediated elimination product is 1,1-dichloroethylene. The ratio of these products is pH dependent. Acetic acid is the major product at low values of pH, while the amount of the hydroxide-ion-mediated elimination product, 1,1-dichloroethylene, increases with increasing values of pH.



### 189. 1,1,2-Trichloroethane

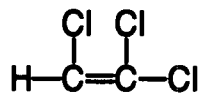
Hydrolysis of 1,1,2-trichloroethane will yield the substitution product, chloroacetaldehyde, and the base-mediated elimination product, 1,1-dichloroethylene. The most acidic hydrogen (dichloro-substituted carbon) is lost during elimination of chlorine to form 1,1-dichloroethylene rather than 1,2-dichloroethylene. The ratio of products will be determined by the pH of the system.



## 190. Trichloroethylene

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Trichloroethylene will not hydrolyze to any reasonable extent.

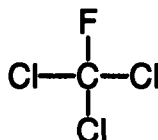


Trichloroethylene

## 191. Trichlorofluoromethane

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Trichlorofluoromethane will not hydrolyze to any reasonable extent based on other polyhalogenated methanes.



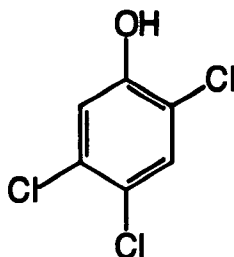
Trichlorofluoromethane



**192. 2,4,5-Trichlorophenol**

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2,4,5-Trichlorophenol will not hydrolyze to any reasonable extent.

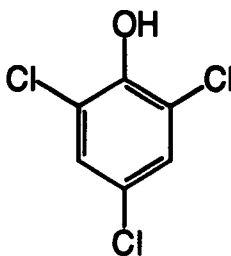


2,4,5-Trichlorophenol

**193. 2,4,6-Trichlorophenol**

---

2,4,6-Trichlorophenol will not hydrolyze to any reasonable extent.

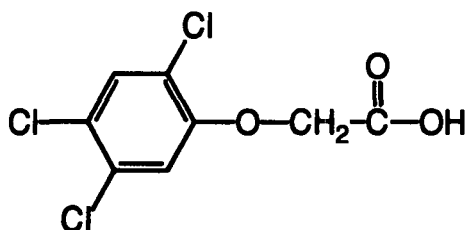


2,4,6-Trichlorophenol

**194. 2,4,5-Trichlorophenoxyacetic acid**

---

2,4,5-Trichlorophenoxyacetic acid will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.

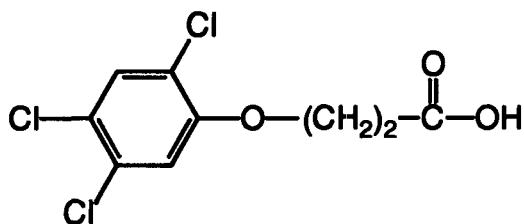


2,4,5-Trichlorophenoxyacetic acid

**195. 2-(2,4,5-Trichlorophenoxy)propionic acid (Silvex)**

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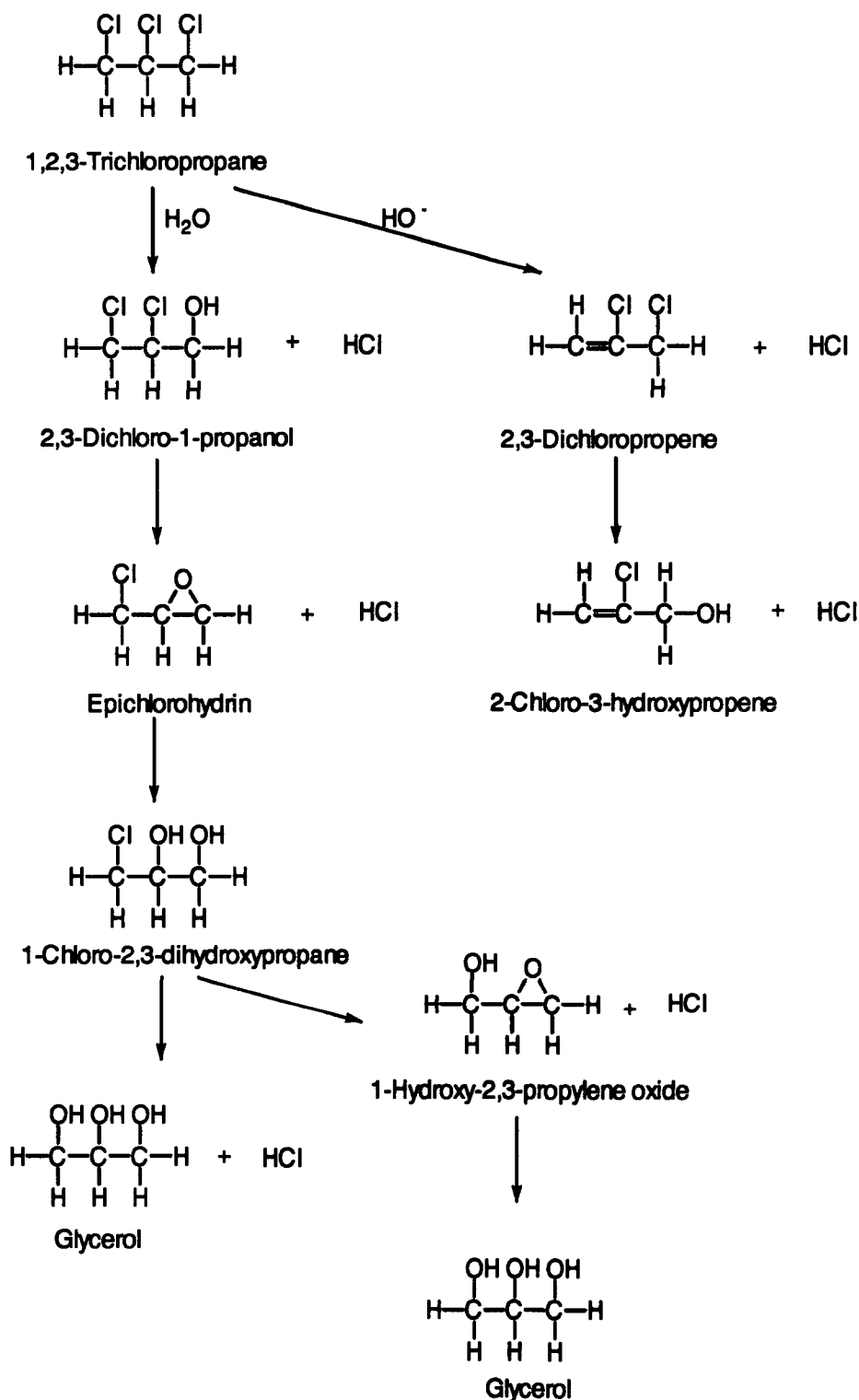
Silvex will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.



2-(2,4,5-Trichlorophenoxy)propionic acid

## 196. 1,2,3-Trichloropropane

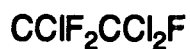
By analogy to 1,2-dibromo-3-chloropropane (#58), the ultimate products of aqueous degradation of 1,2,3-trichloropropane are 2-chloro-3-hydroxy-1-propene and glycerol. The route to the substitution product, glycerol, proceeds through intermediate haloalcohols and halohydrins. The amount of the elimination product, 2-chloro-3-hydroxy-1-propene, will increase with increase in hydroxide ion concentration.



**197. 1,1,2-Trichloro-1,2,2-trifluoroethane**

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1,1,2-Trichloro-1,2,2-trifluoroethane will not hydrolyze to any reasonable extent; however, it may undergo other abiotic transformation processes.

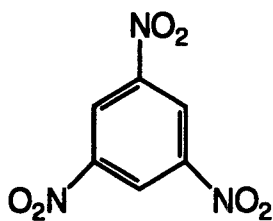


1,1,2-Trichloro-1,2,2-trifluoroethane

**198. 1,3,5-Trinitrobenzene**

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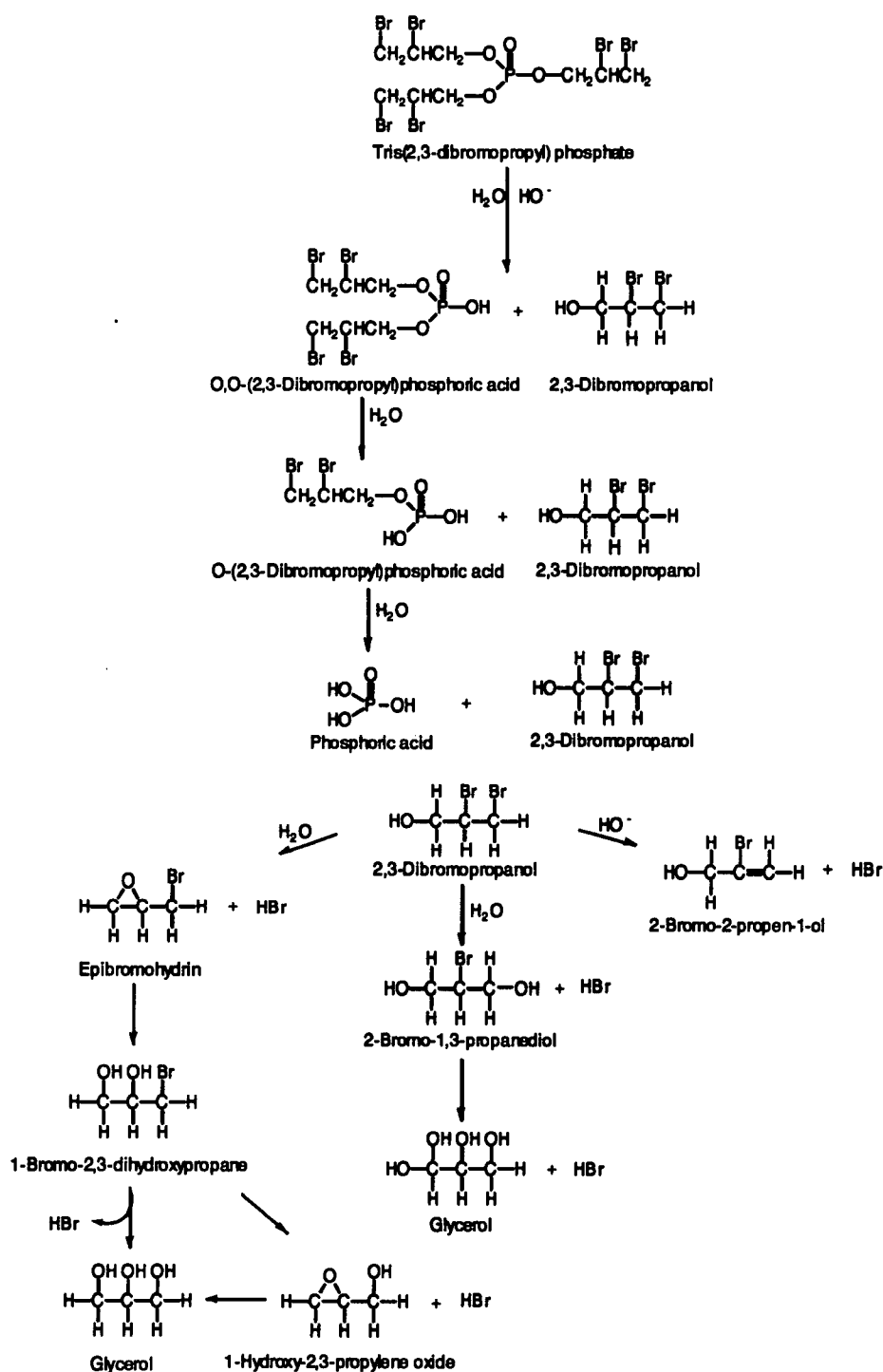
1,3,5-Trinitrobenzene will not hydrolyze; however, it may undergo other abiotic transformation processes.



sym-Trinitrobenzene

## 199. *Tris*(2,3-dibromopropyl)phosphate

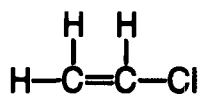
Hydrolysis of *tris*(2,3-dibromopropyl)phosphate by nucleophilic attack of  $\text{H}_2\text{O}$  on the C-O bond or hydroxide ion attack on phosphorus will yield the same products. The 2,3-dibromopropanol can undergo hydroxide-ion-mediated elimination to yield 2-bromo-2-propen-1-ol or intramolecular displacement of bromine by the adjacent hydroxyl group to form epibromohydrin. The epibromohydrin is ultimately hydrolyzed to the final product, glycerol. The *O,O*-(2,3-dibromopropyl)phosphoric acid will hydrolyze further to yield phosphoric acid and 2,3-dibromopropanol.



## 201. Vinyl chloride

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

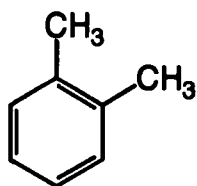


Vinyl chloride

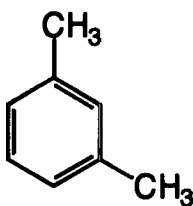
## 202. Xylenes

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The three isomers of xylene will not hydrolyze. They have no hydrolyzable functional group.



o-Xylene



m-Xylene



p-Xylene