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TECHNICAL REPORT 88-10

OCTANOL WATER PARTITION COEFFICIENTS OF
SURFACE AND GROUND WATER CONTAMINANTS FOUND AT MILITARY INSTALLATIONS

MICHAEL A. MAJOR, Ph.D.

NOVEMBER 1989

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U S ARMY BIOMEDICAL RESEARCH & DEVELOPMENT LABORATORY
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<p>An octanol/water partition coefficient (K_{ow}) is the ratio of the concentrations of a solute in the two phases that are created when water containing the solute is extracted with octanol. K_{ow} values are of considerable use in an estimating other equilibrium constants needed for predicting the fate of chemicals in the environment. This paper reports K_{ow} values for a number of compounds, some of which are unique to the military. The values have been selected from government reports and the open literature or determined in the U.S. Army Biomedical Research and Development Laboratory.</p>					
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TABLE OF CONTENTS

	<u>Page</u>
EXECUTIVE SUMMARY.....	1
INTRODUCTION.....	1
DERIVATIVES OF METHYLPHOSPHONIC ACID.....	2
METHYLMERCURIES AND DIMETHYLMERCURY.....	4
COMPOUNDS OF ARSENIC.....	5
ELEMENTAL METALS.....	5
OTHER COMPOUNDS FOR WHICH K_{OW} IS NOT APPLICABLE.....	6
TABLE OF $LOGK_{OW}$ VALUES.....	6
REFERENCES.....	13
APPENDIX A.....	16
DISTRIBUTION LIST.....	17

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EXECUTIVE SUMMARY

This report summarizes the octanol/water partition coefficients (K_{ow}) for a variety of substances frequently encountered as environmental pollutants that are unique to or of particular interest to the military. Sources of the data are experimental values published in the open literature or in government reports, and values determined experimentally in this Laboratory. The purpose of the report is to contribute to the establishment of a K_{ow} data base to be used in predictive models of transport and transformation in the environment; it will aid in the assessment of possible ecological and health impacts due to past or present military activities.

INTRODUCTION

The ecological and health effects of chemical pollutants disseminated in association with the production and use of munitions and chemical agents are an important concern of the U.S. Army Medical Research and Development Command. The problem is complex from a chemical standpoint because of the large variety of toxic chemicals associated with their manufacture. The situation is further complicated by the physical and chemical transformations these compounds undergo in storage, during use and in the environment. Moreover, much of the current contamination was generated by a succession of government and corporate laboratories; proper containment procedures were yet to be developed and records were sometimes inadequate.

Octanol/water partition coefficients (K_{ows}) are of considerable use for deriving other equilibrium constants needed to predict the fate of chemicals in the environment¹. Values of K_{ow} can be estimated by a variety of calculations² but are more accurately derived experimentally. The earliest experimental method relied on establishing an equilibrium of solute between the immiscible distribution solvents octanol and water. In this "shake flask" method, octanol and water containing the solute are vigorously shaken until equilibrium is achieved and the two phases allowed to separate; the concentration of the solute in the octanol divided by that in water is the K_{ow} . This method, although still the standard, is time-consuming and presents problems whenever very large or very small K_{ows} are encountered. A more convenient method³ has been developed that relies on the relationship between a compound's octanol/water partition coefficient and its retention time in reverse phase high-performance liquid chromatography (HPLC). In this method the known $\log K_{ow}$ values for a series of standards are plotted against the logarithms of their corrected HPLC retention times, and the slopes of such relationships are determined by linear regression. K_{ow} values for compounds similar to the standards can then be accurately estimated from their retention times by interpolation. While this solves many of the problems associated with the shake flask method, it is only accurate when the compounds used as standards and the unknowns contain similar functional groups and have similar

polarity. Compounds with very high K_{ow} values require a special modification of the shake flask method. In this technique the combined octanol/water phases are carefully layered to avoid emulsion, the solute added and the mixture slowly stirred for several days to achieve equilibrium. The phases are then analyzed and the K_{ow} determined as in the shake flask procedure.

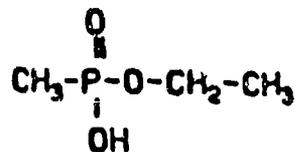
Regressions have been established between K_{ow} and solubility, adsorption on soil and uptake by aqueous organisms¹. Due to the utility of K_{ow} as a predictive tool, values for many compounds have been determined, and a convenient listing of these was provided a decade ago by Hansch and Leo². In addition, relatively accurate estimates of K_{ow} can often be obtained by calculations that utilize fragment analyses and by regression equations that relate K_{ow} to the partition coefficient of solutes between water and other solvents².

The listing we provide here is in response to a U.S. Army Toxic and Hazardous Materials Agency (USATHAMA) request for K_{ow} values for the compounds found in Appendix A. The reported values are experimentally derived but estimation methods have been used to pick best values among widely differing published K_{ows} . Laboratory determinations of K_{ow} were performed in-house by the HPLC retention time method of Harnisch³ when literature results were not available. K_{ow} determinations for compounds with known values were also performed for standardization, and as a check on the accuracy of the laboratory procedures.

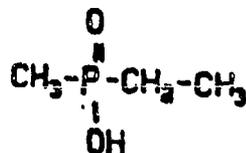
To assist the reader in identifying the compounds of interest, chemical structures are provided and related compounds are handled as subgroups. Compounds not found in water in the form listed, such as lewisite, and compounds that are ions under normal conditions (pH values between 5 and 9) do not have meaningful K_{ow} values. These compounds are identified in the text.

DERIVATIVES OF METHYLPHOSPHONIC ACID

Owing to changes in the rules of nomenclature one may experience some ambiguity as to the structure of these compounds. Under older rules of nomenclature⁴, ethyl methylphosphonate and ethyl methylphosphonic acid would denote the monoethyl ester and the "secondary phosphonic" (really a phosphinic) acid shown here.

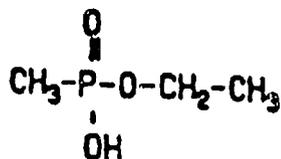


Ethyl half ester



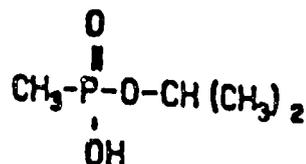
Secondary phosphonic acid

Under current rules⁵ the latter compounds are named phosphinic acids, and the terms ethyl methylphosphonate and ethyl methylphosphonic acid now designate the same compound.



Ethyl methylphosphonate/Ethyl methylphosphonic acid

Similar nomenclature applies to isopropyl methylphosphonate (isopropyl methylphosphonic acid).

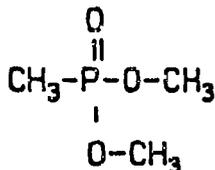


Isopropyl methylphosphonate/Isopropyl methylphosphonic acid

Apparently USATHAMA (Appendix A) used the suffix "ate" to indicate the salt form and the "acid" ending to indicate an undisassociated Lowry-Bronsted acid. The question of whether these compounds exist in the ionized or un-ionized form is important, for if they are ionized they will remain almost exclusively in the aqueous phase and will not have a demonstrable K_{ow} . Acid strength of organic acids decreases with increasing length of the attached hydrocarbon chains. Therefore, since the pK_a of the largest phosphonic acid on our list (isopropyl methylphosphonic acid) is lower than 5, it follows that it and the other phosphonic acids would be almost completely ionized under normal environmental conditions.

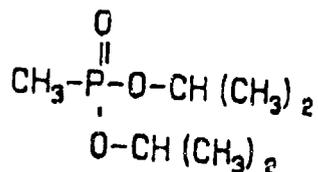
Experiments in our laboratory⁶ using the titration method of Rosenblatt and Davis⁷ have demonstrated a pK_a for isopropyl methylphosphonate of 2.41. Kosolapoff⁴ reports a pK_{a1} for methylphosphonic acid of 2.35. We therefore consider both ethyl methylphosphonate and isopropyl methylphosphonate to have vanishingly small K_{ow} s at ambient pH.

Dimethyl methylphosphonate has a $\log K_{ow}$ of -0.61 according to Krikorian⁸.

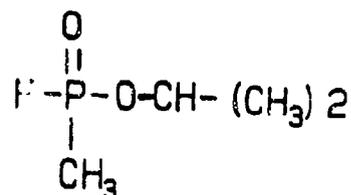


Dimethyl methylphosphonate

Diisopropyl methylphosphonate (DIMP) has $\log K_{ow}$ values reported as 1.03 by Krikorian and Chorn⁸ and 1.35 by Brueggemann⁹. The relationship between the $\log K_{ow}$ values reported by Krikorian and Chorn for a series of phosphonates and the number of carbon atoms in these molecules, appears to be linear⁶. Regression of the data indicates an anomaly in the fit of DIMP, such that Krikorian and Chorn's value for $\log K_{ow}$ is probably too low. Inclusion of Brueggemann's result in this relationship yields a much better fit and is therefore considered the more accurate value.



Diisopropyl methylphosphonate



GB

GB (isopropyl methylphosphonofluoridate) is a quick-acting nerve agent. It could not be tested in our laboratory, and K_{ow} values were not available in the literature. Rosenthal et al. reported chloroform/water, benzene/water, carbon tetrachloride/water and hexane/water partition coefficients of 31.2, 2.08, 0.84 and 0.20 respectively¹⁰. Such values can sometimes be used to estimate K_{ow} through solvent regression equations¹. However, the results of such calculations were so divergent in the present instance that a credible value for K_{ow} could not be determined. It is known, however, that GB is volatile and hydrolyzes in water¹¹ and should therefore not pose a long-term environmental hazard.

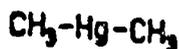
METHYLMERCURIES AND DIMETHYLMERCURY

Determination of the K_{ow} for metallic mercury and for methylmercury compounds presents several interesting problems. Mercury may be found in oxidation states 0, +1 and +2. Mercury metal (oxidation state 0) has limited solubility in water¹² and high volatility¹³. Shoichi and Sokichi¹⁴ report K_{ow} values for metallic mercury of from 3.80 to 4.80, with values decreasing as a function of temperature in the range of 278 to 308 K. Mercury +1 and +2 salts may be methylated abiotically or microbially. In the methylated molecules the covalent bond between carbon and mercury resists hydrolytic cleavage¹⁵. K_{ow} values for mixed methylmercuric hydroxide and methylmercuric chloride are a result of equilibrium between the two species. The K_{ow} of the mixture in an aqueous medium appears to depend on salinity (chloride concentration) and pH¹⁶.

Dimethylmercury is a product of a microbial disproportionation reaction in which two methylmercury cations condense to yield un-ionized dimethylmercury and ionized mercury +2¹⁵.



Dimethylmercury is nearly insoluble in water and it has a high vapor pressure. These properties combine to give the compound a short residence time in aqueous systems and tend to make accurate determination of K_{ow} by conventional methods difficult. Wasik¹⁷ was able to overcome these problems with an elegant method that determined the octanol/water partition coefficient and the Henry's law constant simultaneously. This system yielded the log K_{ow} value for dimethylmercury of 2.26 at 20° C.

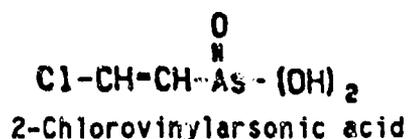
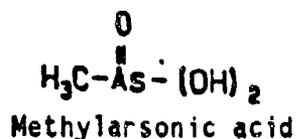


Dimethylmercury

COMPOUNDS OF ARSENIC

The compounds of arsenic for which K_{ow} values were requested are 2-chlorovinylarsonic acid, 2-chlorovinylarsonous acid, dimethylarsenic acid, lewisite, lewisite oxide and methylarsonic acid.

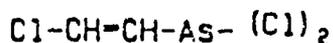
Methylarsonic acid should have an extremely low K_{ow} at pH 7 because it has a pK_a of only 4.1¹⁸. The similar compound, 2-chlorovinylarsonic acid, should hence have a low K_{ow} , as its chlorovinyl group is electron withdrawing,² making it an even stronger acid than methylarsonic acid.



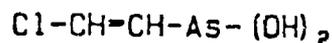
The K_{ow} of lewisite cannot be determined since this compound is not stable in water. ARMY FM 3-9¹¹ reports that "The rate of hydrolysis is rapid for both vapor and dissolved lewisite and when the humidity is high lewisite hydrolyzes so rapidly that it is difficult to maintain a concentration sufficient to blister even unprotected skin." Lewisite oxide is the species formed when lewisite is hydrolyzed and then dried. It, in turn, is converted quantitatively to 2-chlorovinylarsonous acid when dissolved in water¹⁹. The latter compound represents the lewisite species actually found in water; it has a $\log K_{ow}$ of -0.07 as determined in this Laboratory⁹.



Lewisite oxide

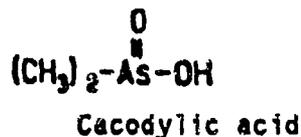
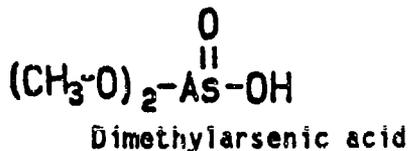


Lewisite



2-Chlorovinylarsonous acid

Dimethylarsenic acid correctly denotes the diester of arsenic acid. However esters of this compound are highly unstable in water and diesters have never been reported¹⁸. This terminology has however, been used incorrectly to denote dimethylarsinic acid (cacodylic acid). Our experiments⁶ have determined the latter compound to have a $\log K_{ow}$ of -1.18.

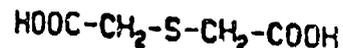
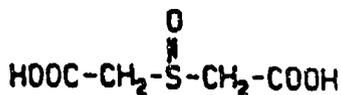
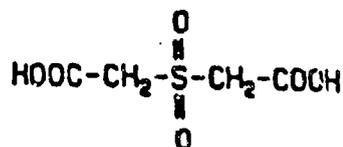


ELEMENTAL METALS

With the exception of mercury, all the native metals listed are medium to high melting solids. Melting point has a substantial effect on aqueous solubility, and, as expected, the solubility of these elements is low. K_{ow} values are not available for any metal except mercury and their determination is not within the current capability of this laboratory.

OTHER COMPOUNDS FOR WHICH K_{OW} IS NOT APPLICABLE

Biscarboxymethyl sulfone, biscarboxymethyl sulfoxide and thiodiglycolic acid are putative or known environmental breakdown products of sulfur mustard; they differ only in the oxidation state of their sulfur atoms and are all in the form of anionic salts at $pH > 5$. They are not susceptible to facile K_{OW} measurement.

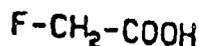
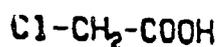


Biscarboxymethyl sulfone

Biscarboxymethyl sulfoxide

Thiodiglycolic acid

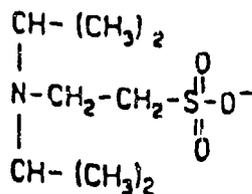
Bromide and chloride, being anions, are not susceptible to K_{OW} determination. Chloroacetic acid and fluoroacetic acid have pK_a values of 2.87 and 2.57²⁰, so that they occur as anions at ambient pH.



Chloroacetic acid

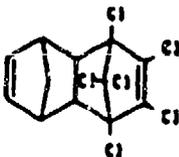
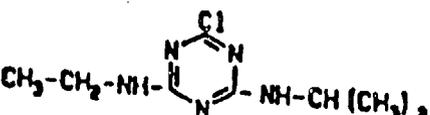
Fluoroacetic acid

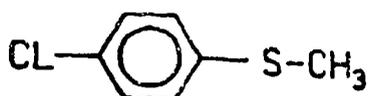
2-Diisopropylaminoethylsulfonate denotes the salt form of a sulfonic acid. Sulfonic acids as a class do not have determinable K_{OW} values because they are very strong acids. They are reported to be the most water-soluble organic compounds known²¹.



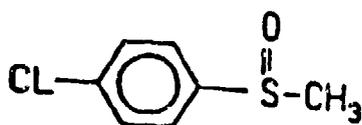
2-Diisopropylaminoethylsulfonate.

LOG K_{OW} FOR COMPOUNDS FOR WHICH K_{OW} VALUES ARE APPLICABLE (value listed first is considered most accurate)

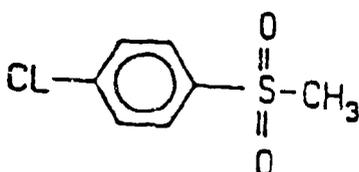
COMPOUND	Log K_{OW}	REFERENCE
	6.50	22 De Bruijn et al. 1989
	5.66	23 Geyer et al. 1984
	5.66	24 Kenaga 1980a
	5.3	25 USEPA 1986m
Aldrin		
	2.32	26 Rao and Davidson 1983
	2.64	23 Geyer et al. 1984
Atrazine		



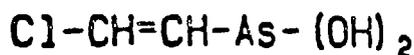
3.22 ⁹ Brueggemann 1979
 p-Chlorophenyl methyl sulfide _____



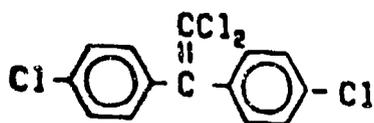
1.33 ⁹ Brueggemann 1979
 p-Chlorophenyl methyl sulfoxide _____



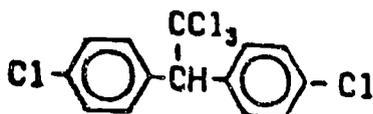
1.20 ⁹ Brueggemann 1979
 p-Chlorophenyl methyl sulfone _____



-0.07 ⁶ Major 1988
 2,Chlorovinylarsonous Acid _____



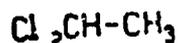
6.96 ²² De Bruijn et al. 1989
 5.69 ²⁶ Rao and Davidson 1983
 5.60 (Mean value) ³³ Kadek et al. 1986
 Dichlorodiphenyldichloroethylene (DDE) _____



6.91 ²² De Bruijn et al. 1989
 6.19 ²⁶ Rao and Davidson 1983
 5.89 ¹ Lyman et al. 1982
 Dichlorodiphenyltrichloroethane (DDT) _____

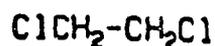


2.29 ²⁵ USEPA 1986
 2.43 ³⁴ USEPA 1985
 1,2-Dibromo-3-chloropropane _____



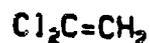
1.8 ²⁵ USEPA 1986

1,1-Dichloroethane_____



1.79 ³⁵ Veith et al. 1983
1.45 ²⁹ Davies and Dobbs 1984
1.48 ² Hansch and Leo 1979

1,2-Dichloroethane_____



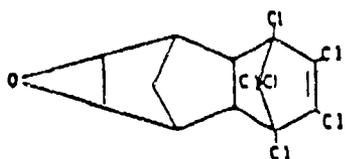
1.84 ³⁶ Mabey et al. 1981

1,1-Dichloroethylene_____



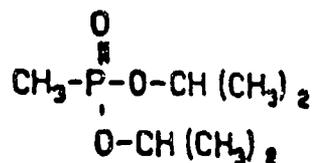
1.98 ³⁷ Gossett et al. 1983

trans-1,2-Dichloroethylene_____



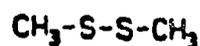
5.40 ²² De Bruijn et al. 1989
4.32 ²⁹ Davies and Dobbs 1984
6.20 ³⁸ Briggs 1981
3.69 ²⁶ Rao and Davidson 1983
5.48 ²⁴ Kenaga 1980
3.50 ²⁵ USEPA 1986

Dieldrin_____



1.35 ⁹ Brueggemann 1979

Diisopropyl methylphosphonate_____



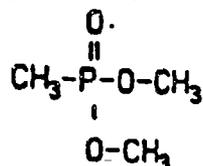
1.77 ² Hansch and Leo 1979

Dimethyl disulfide_____



2.26 ¹⁷ Wasik 1978

Dimethylmercury_____

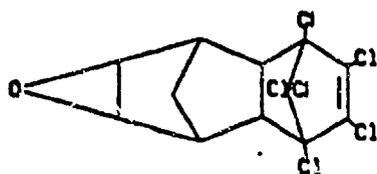


-0.61 ⁸ Krikorian 1987

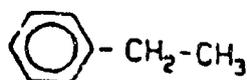
Dimethyl methylphosphonate_____



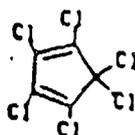
Dithiane (1,4 isomer) 1.85 ⁶ Major 1988



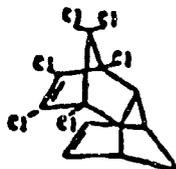
Endrin 5.20 ²² De Bruijn et al. 1969
6.34 ²⁴ Kenaga 1980



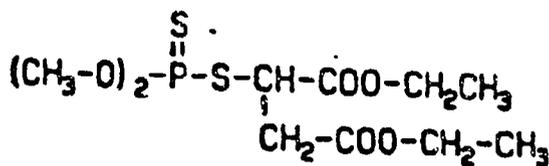
Ethylbenzene 3.15 ²⁷ Sangster 1989
3.13 ³¹ Tewari et al. 1982
3.15 ³² Moriguchi 1975



Hexachlorocyclopentadiene 5.04 ²³ Geyer et al. 1984



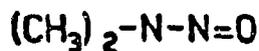
Isodrin 6.51 ¹ Lyman et al. 1982



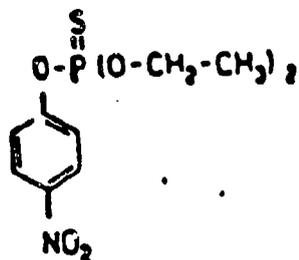
Malathion 2.89 ²⁵ USEPA 1986
2.89 ² Hansch and Leo 1979
2.89 ²⁶ Rao and Davidson 1983

Hg

Mercury 3.8 to 4.2 ¹³ Shoichi 1985

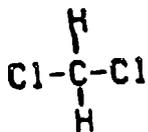


N-Nitrosodimethylamine -0.57 ² Hansch and Leo 1979



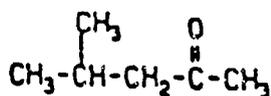
Parathion

3.9³⁸ Briggs 1981
3.8²⁶ Rao and Davidson 1983



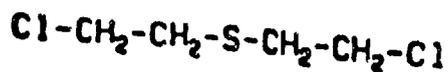
Methylene chloride

1.25³⁹ Callahan et al. 1979
1.30²⁵ USEPA 1986
1.31²⁷ Sangster 1989



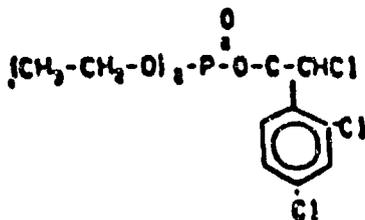
Methyl isobutyl ketone

1.53⁶ Major 1988



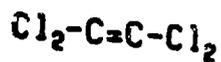
Sulfur mustard

1.37²⁵ USEPA 1986m



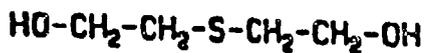
Supona

3.11³⁸ Briggs 1981



Tetrachloroethylene

2.60² Hansch and Leo 1979



Thiodiglyol

-0.08⁶ Major 1988



0.77 ⁶ Major 1988
 Thioxane (1,4 Oxathiane)



2.73 ²⁷ Sangster 1989
 2.73 ²⁵ USEPA 1986
 2.58 ²⁸ Valvani et al. 1980
 2.65 ³¹ Tewari et al. 1982
 2.69 ²³ Geyer et al. 1984
 2.69 ³² Moriguchi 1975
 Toluene

$\text{Cl}_3\text{C}-\text{CH}_3$
 2.50 ²⁵ USEPA 1986
 2.47 ²⁹ Davies and Dobbs 1984
 1,1,1-Trichloroethane

$\text{Cl}_2\text{CH}-\text{CH}_2\text{Cl}$
 2.47 ²⁵ USEPA 1986
 1,1,2-Trichloroethane

$\text{Cl}_2\text{C}=\text{CHCl}$
 2.38 ²⁵ USEPA 1986
 2.29 ² Hansch and Leo 1979
 2.42 ³⁵ Veith et al. 1983
 3.3 ²⁸ Valvani et al. 1980
 3.3 ²⁹ Davies and Dobbs 1984
 3.3 ²³ Geyer et al. 1984
 2.29 ⁴⁰ Rogers et al 1980
 2.53 ²⁹ Tewari et al. 1982
 Trichloroethylene

$\text{P}(\text{O})(\text{O}-\text{CH}_3)_3$
 0.52 ² Hansch and Leo 1979
 Trimethyl phosphate

$\text{Cl}_2\text{C}=\text{CH}-\text{O}-\text{P}(\text{O})(\text{OCH}_3)_2$
 1.40 ² Hansch and Leo 1979
 Vapona

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APPENDIX A: LIST OF SUBSTANCES FOR WHICH K_{ow} VALUES WERE REQUESTED BY THE U.S. ARMY TOXIC AND HAZARDOUS MATERIALS AGENCY.

Aldrin	Dimethyl mercury (sicl)
Arsenic	Dithiane
Atrazine	Endrin
Azodrin	Ethyl benzene (sicl)
Benzene	Ethyl methyl phosphonate (sicl)
Benzothiazole	Ethyl methyl phosphonic acid (sicl)
Bicycloheptadiene	Fluoride
Bis(carboxymethyl) sulfone	Fluoroacetic acid
Bis(carboxymethyl) sulfoxide	GB; Sarin
Bromide	Hexachlorocyclopentadiene
Cadmium	Isodrin
Carbon tetrachloride	Isopropyl methyl phosphonic acid (sicl)
Chlordane	Isopropyl methyl phosphonate (sicl)
Chloride	Lead
Chloroacetic acid	Lewisite
Chlorobenzene	Lewisite oxide
Chloroform	Malathion
2-chlorovinyl arsonic acid (sicl)	Mercury
2-chlorovinyl arsonous acid (sicl)	Methylene chloride
p-Chlorophenyl methyl sulfide	Methyl arsonic acid (sicl)
p-Chlorophenyl methyl sulfoxide	Methyl isobutyl ketone
p-Chlorophenyl methyl sulfone	Methyl mercury salts (sicl)
Chromium	Methylphosphonic acid
Copper	Mustard
DDE	N-Nitrosodimethylamine
DDT	Parathion
1,2-Dibromo-3-chloropropane	Sulfur mustard
1,1-Dichloroethane	Supona
1,2-Dichloroethane	Tetrachloroethylene
1,1-Dichloroethylene	Thiodiglycol
1,2-Dichloroethylene	2,2-Thiodiglycolic acid
Dicyclopentadiene	Thioxane
Dieldrin	Toluene
2-(Diisopropylamino)-n-ethyl sulfonate (sicl)	1,1,1-Trichloroethane
2-(Diisopropylamino)-n-ethanethiol (sicl)	1,1,2-Trichloroethane
Diisopropylmethylphosphonate (sicl)	Trichloroethylene
Dimethyl disulfide	Trimethyl phosphate
Dimethyl methyl phosphonate (sicl)	Vapona
Dimethyl arsenic acid (sicl)	

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