ESTIMATING TOXICITY OF INDUSTRIAL CHEMICALS

TO AQUATIC ORGANISMS USING

STRUCTURE-ACTIVITY RELATIONSHIPS

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Office of Pollution Prevention and Toxics
U.S. Environmental Protection Agency
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FORWARD to the SECOND EDITION

As discussed in the FORWARD to the first edition of **Estimating Toxicity of Industrial Chemicals to Aquatic Organisms Using Structure-Activity Relationships**, the development of predictive ecotoxicology models for industrial chemicals creates challenges that are unique compared to those faced in drug or agrichemical design. Under the requirements of the Toxic Substances Control Act there is, however, no choice but to face these challenges and provide the means to assess the ecological risks of new and existing compounds.

Since releasing their first edition in 1988, the scientists within the Environmental Effects Branch of the Office of Pollution Prevention and Toxics have continued to develop property-activity correlations that are relevant for industrial chemicals found in commerce. In publish the second edition of **Estimating Toxicity of Industrial Chemicals to Aquatic Organisms Using Structure-Activity Relationships**, the contributors have once again demonstrated their commitment to share the results of these efforts with the scientific and regulatory community. This second edition contains over 70 additional property-activity correlations and is a companion document to ECOSAR, which is a computerized version of the relationships developed by the contributors. Through this on-going contribution to the world-wide 'structure-activity relationship knowledge base', the scientist in the Environmental Effects Branch are also providing the means to identify first-order uncertainties in the development and use of these predictive models. The influence of the first and second edition on the application of structure-activity relationships and the course of future research in are of environmental toxicology can not be minimized. Of particular interest is the continuing to develop models for chronic effects and to establish objective techniques whereby compounds can be assigned to specific relationships.

Again, I congratulate the contributors to this document for their dedication in implementing structure-activity relationships in ecological risk assessments and for fostering the exchange of information that is essential for the advancement of the field.

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Duluth, Minnesota
April, 1995

FORWARD

The world of the scientist in a regulatory agency which is responsible for chemical safety is quite different from that in physical organic chemistry, toxicology, or drug design. Nothing highlights the difference quite like the scientists who implement the EPA mandate to review industrial chemicals for health and environmental effects. More conventional research scientists work in data-rich areas where chemical models are comparatively precise. Only under the Toxic Substances Control Act (TSCA), implemented by the Office of Toxic Substances, can we find the responsibility to evaluate the broad spectrum of chemical safety with little or no data on either new or existing chemicals.

These scientist responded to the EPA responsibilities by adapting approaches used in drug design and chemistry to predict the environmental behavior and toxicology of chemicals from their structure rather than extensive test data. The Office of Research and Development has enjoyed a ten-year partnership with the Office of Toxic Substances in developing quantitative structure-activity relationships to estimate the bioaccumulation potential, the persistence, and the toxicity of chemicals in the environment. Much developmental work remains to be done in efforts to more thoroughly evaluate chronic effects of long term exposure; nonetheless, many relationships are adequate to assist regulatory scientists in making judgements concerning the risks of chemicals.

As we continue to improve our understanding of relationships between chemical structure and effects, the Environmental Effects Branch realized the value of this technology to other scientists in EPA Regions and states. Their initiative to summarize the state-of-the-art in this document and make it available to others is another example of the futuristic planning of this group. The predictive power of the methods included in this document varies with the available data and complexity of the toxicity mechanisms. However, the predictive power will continue to increase over the next decade as new chemical models are formed. I congratulate the contributors to this document for the increasing effort to formulate structure-activity relationships from scant data, and for their desire to share this work with others in the scientific and regulatory community.

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Jun, 1988

INTRODUCTION

For many years, the manufacturers of pharmaceuticals, pesticides, and dyes have used the relationship between chemical structure and a specific effect to search for new chemicals. These relationships are called structure-activity relationships (SARs). Under Section 5 of the Toxic Substances Control Act of 1976, EPA must review and evaluate all new chemicals before enter they enter commerce. The Environmental Effects Branch (EEB) of OPPT has been responsible for the assessment and evaluation of these new chemicals and for identifying those chemicals of greatest concern for environmental hazard. Since 1976, of all chemicals submitted to EPA under Section 5 of TSCA, fewer than 5% of the Premanufacture Notices have contained toxicity data pertaining to terrestrial and aquatic organisms. To meet its regulatory mandate, EEB began using SARs in 1979 to estimate the toxicity of chemicals in the absence of test data.

The application of SARs in the field of environmental toxicology is relatively new. Some of the early research work began in the 1960's. During the 1970's, many investigators began examining the relationships among chemical properties and the toxicity to aquatic and terrestrial organisms. Among the leaders in this area was the U.S. EPA Environmental Research Laboratory at Duluth (ERL-Duluth) who pioneered research in the development and application of SARs to environmental toxicology. In the mid-1970's they developed and later published the SAR for predicting the bioconcentration of neutral organic compounds in fish based upon the octanol/water partition coefficient. In 1979, they initiated a long-term research program to develop SARs for industrial organic chemicals. Between 1981 and 1983, EEB staff evaluated and adopted 13 of these SARs for use in predicting toxicity to fish, aquatic invertebrates, and green algae. To date, the scientists at ERL-Duluth have measured the toxicity of over 800 compounds. From this research, they have developed SARs for at least a dozen classes of compounds to both freshwater and marine fish. Recently, emphasis at ERL-Duluth has shifted toward SARs for chronic toxicity with numerous chronic values now being published.

The octanol/water partition coefficient (K_{ow}) has been the major attribute used by most investigators to correlate structure and toxic effect. The most frequently used relationship is the logarithm of the K_{ow} versus the logarithm of the median toxicity (LC_{50} and EC_{50}) value. To date the major focus has been centered around the class of industrial organic chemicals known as neutral organics. These compounds are non-ionizable, non-reactive and neutral with respect to charge; however, SARs have been developed for other classes of chemicals and new ones continue to be derived as data become available.

This manual is intended to accompany an SAR program, called ECOSAR, that has been developed by EEB for use on a personal computer. ECOSAR is menu-driven and contains on-line help, including a User's Guide. ECOSAR includes all of the chemical classes and SARs contained in this manual. Most toxicity values (in mg/L) are based on log K_{ow} and molecular weight information supplied by the user, although as discussed below, some SARs require other physical data, such as number of ethoxylates or percent amine nitrogen. ECOSAR may be obtained from the sources listed at the end of the Introduction.

Chemical Classes

This manual presents information for deriving toxicity values for four primary classes of chemicals:

(1) Neutral organics that are nonreactive and nonionizable;
(2) Organics that are reactive and ionizable and that exhibit excess toxicity in addition to narcosis;
(3) Surface-active organic compounds such as surfactants and polycationic polymers; and
(4) Inorganic compounds including organometallics.

Neutral organic compounds that are nonelectrolytic and nonreactive act as anesthetics or narcotics. This class of compounds includes alcohols, ketones, ethers, alkyl halides, aryl halides, aromatic hydrocarbons, aliphatic hydrocarbons, many cyanates, sulfides, and disulfides.

Organic compounds with a more specific mode of toxicity may contain reactive functional groups such as electrophilic moieties. These compounds are more toxic than would be predicted by using an SAR for a narcotic compound. Chemicals which exhibit excess toxicity include acrylates, methacrylates, aldehydes, anilines, beta-diketones (linear forms), benzotriazoles, esters, phenols, aziridines, and epoxides. A separate SAR has been developed for each of these classes.

Surface-active chemicals may act on the respiratory membranes of aquatic organisms. These chemicals consist primarily of surfactants that can be absorbed through respiratory membranes and charged polymers that cannot be absorbed. SARs have been developed for anionic surfactants such as linear alkyl benzene sulfonates, nonionic surfactants such as alcohol ethoxylates and cationic surfactants, such as ethoxylated beta-amine surfactants (ethomeen) and linear N-alkyl quaternary ammonium compounds. The SARs for surfactants are parabolic, i.e., toxicity is related to the size of the hydrophobic component in a parabolic manner when the size of the hydrophilic component remains constant. The size of the hydrophobic component, usually a linear alkyl carbon chain, can be estimated by simply counting the number of carbons in the hydrophobic alkyl chain. Maximum toxicity occurs when there are approximately 16 or 17 carbons in the linear alkyl chain. Toxicity for the nonionic surfactants is also affected by the number of ethoxylate units and the size of the hydrophobe and the number of ethoxy groups must be known to use the SAR.

Polycationic polymers include those with primary, secondary, and tertiary amines and/or quaternary ammoniums, phosphoniums, and sulfoniums. The molecular descriptor used to predict toxicity for these polymers is equivalent charge density as determined from chemical structure, i.e., percent amine-nitrogen, number of cationic charges per 1000 units of molecular weight, or cation equivalent weight. These polymers must be water soluble or self-dispersing or both.

Quantitative SARs have not been developed for inorganic compounds. However, in lieu of such equations, water quality criteria values have been used to predict their toxicity. Water quality criteria have been developed for several metals. These criteria are usually indicative of the lowest concentration that is believed to be protective of aquatic life in the receiving water. Consequently, most criteria are expressed only for acute or chronic toxicity to freshwater or marine organisms in general. SAR equations will eventually be developed for organometallics based on their K_{ow} values.

Some chemical classes do not have quantitative SARs. These include polyanionic polymers, cationic dyes, and most classes of pesticides. Two classes of polyanionic polymers are known to be toxic to aquatic organisms; polyaromatic sulfonic acids are moderately toxic to aquatic organisms; and polycarboxylic acids are moderately toxic only to green algae. However, the high molecular weight of these polymers indicate that they will not be absorbed through the surface membranes of these organisms and their toxicity is the result of their surface activity and is not correlated with their anionic charge density. Cationic dyes can be absorbed and are known to be highly toxic to aquatic organisms. During acute exposure, the toxicity of these dyes is believed to be mostly the result of their activity on the surface membrane while chronic exposure also results in systemic toxicity. Dyes with delocalized cationic charges may be more toxic, followed by dyes with four localized charges, then three localized charges, etc. Most commercial dyes contain impurities which may, in part, be responsible for some of the toxic effects seen in these dyes. Acid dyes are moderately toxic only to green algae which results more from shading of the algae by the dye rather than from direct toxic effects. Data on which to validate this assumption are lacking in most PMN submissions.

How SARs Are Developed

Work sheets were developed to provide pertinent information about each SAR, especially the mathematical procedures for calculating toxicity values based on molecular weight and K_{ow}. Data to develop

new SARs are entered in a spreadsheet that allows the SAR equations to be calculated based on a measured toxicity values (in mmoles/L) and an estimated K_{ow}. Using these estimated values, regression equations can be developed for a class of chemicals, e.g, neutral organics, acrylates, anionic surfactants, etc. Toxicity values for new chemicals may then be calculated by inserting the estimated K_{ow} into the regression equation and correcting the resultant values for the molecular weight of the compound.

As discussed above, the mode of toxic action for most neutral organics appears to be narcosis; however, some organic chemicals have a more specific mode of toxicity with comparable K_{ow}s and molecular weights. For these chemicals, the toxicity is also related to the K_{ow} and as the K_{ow} decreases (i.e., as the chemicals become more water soluble), the amount of excess toxicity compared to neutral organic compounds increases. Consequently, at some higher K_{ow} the toxicity of the compound is not significantly different from the toxicity of the equivalent neutral organic. For organic chemicals which haves excess toxicity and for which are data poor, e.g., amino anilines, a neutral organic data point may be used in addition to the measured toxicity value to give a regression equation. These are the chemicals that have a N=2 entry under statistics but show only one chemical in the list of chemicals used to develop the SAR. The second point is a neutral organic K_{ow} value. In addition, for some lists of chemicals used to develop the SAR, a single chemical is listed more than once. This is because the chemical has been tested more than once. Each toxicity value is included for the chemical if it provides a reliable data point, i.e., if a second study confirmed a previously derived toxicity value.

To date, over 100 SARs have been developed for over 40 classes of organic chemicals (see Table 1). These chemical classes include neutral organics, surfactants, polymers, and other organic compounds. Most of the SARs are for acute toxicity to fish or daphnids; however, acute and chronic SARs have been developed for other organisms. Some classes, such as acid chlorides, only have one SAR (e.g., fish 96-hour LC_{50}), while for other classes such as neutral organics more than 10 SARs have been developed ranging from acute and chronic SARs for fish to a 14-day LC_{50} for earthworms in artificial soil. New SARs will be added as data become available. This manual will be periodically updated to reflect the additions.

Selecting an Appropriate SAR

Selecting the appropriate SAR for a new chemical is based on a variety of chemical-specific information. This information includes the exact chemical structure, chemical class, predicted K_{ow}, molecular weight of the compound, physical state, water solubility, number of carbons or ethoxylates or both, and percent amine nitrogen or number of cationic charges or both, per 1000 molecular weight. The most important factor for deriving a SAR is the chemical class as SARs are chemical class specific. An alphabetical listing of chemical classes and appropriate SARs to use for each is included at the conclusion of this section.

To estimate the toxicity to aquatic organisms of neutral, nonreactive, non-ionizable organics and organics that exhibit excess toxicity, the K_{ow} and molecular weight are required. The value for the K_{ow} should be obtained from estimated values using the computer program CLOGP, Version 3.3. The range of K_{ow} values are valid to estimate the toxicity is SAR specific and is given for each SAR in a chemical class. In general, when the log K_{ow} is less than or equal to 5.0, valid predictions can be obtained for estimating acute toxicity to aquatic organisms from neutral organic compounds. If the log K_{ow} is greater than 5.0, the decreased solubility of a compound will result in no effects in a saturated solution during a 96-hour test and a longer exposure duration should be used to determine the LC_{50}. For chronic exposures, the applicable log K_{ow} may be extended up to 8.0. If the log K_{ow} of the compound exceeds 8.0, no adverse effects are

Table 1. Existing SARs

SAR Class	Acute Toxicity			Chronic Toxicity			Other
	Fish	Daphnid	Algae	Fish	Daphnid	Algae	
Acid chlorides	X						
Acrylates	X	X					
Acrylates, methacrylates	X						
Alcohols, propargyl	X						
Aldehydes	X	X	X	X		X	
Amines, aliphatic	X	X	X			X	
Anilines	X	X		X	X	X	
Anilines, amino, meta or 1,3-substituted	X	X	X				
Anilines, amino, ortho or 1,2-substituted	X	X	X				
Anilines, amino, para or 1,4-substituted	X	X	X		X		
Anilines, dinitroanilines	X	X		X			
Aziridines	X	X	X				
Benzenes, dinitro	X	X		X	X		
Benzotriazoles	X	X	X				
Carbamates							X
Carbamates, dithio	See	SAR	Title	Page			
Crown Ethers	See	SAR	Title	Page			
Diazoniums, aromatic	X						
Epoxides, monoepoxides	X	X					
Epoxides, diepoxides	X	X					
Esters	X	X	X			X	
Esters, monoesters, aliphatic				X			
Esters, diesters, aliphatic				X			
Esters, phosphate	X						
Esters, phthalate	X	X			X		
Hydrazines	X	X	X				
Hydrazines, semicarbazide, alkyl substituted			X				
Hydrazines, semicarbazides, aryl, meta/para substituted			X				
Hydrazines, semicarbazides, aryl, ortho substituted			X				
Imides	X						
Ketones, diketones, aliphatic	X	X			X	X	
Malononitriles	X						

SAR Class	Acute Toxicity			Chronic Toxicity			Other
	Fish	Daphnid	Algae	Fish	Daphnid	Algae	
Neutral organics	X	X	X	X	X	X	X
Peroxy acids	X	X					
Phenols	X	X	X	X	X	X	
Phenols, dinitrophenols	X	X		X	X		
Polymers, polycationic	X	X	X				
Surfactants, anionic	X	X	X	X	X	X	
Surfactants, cationic, quaternary ammonium, monoalkyl	X	X					X
Surfactants, cationic, quaternary ammonium, dialkyl	X	X	X	X	X	X	
Surfactants, ethomeen	X	X	X				
Surfactants, nonionic	X	X					
Thiazolinones, iso	X	X	X			X	
Thiols (mercaptans)	X	X					
Triazines, substituted	X	X					
Ureas, substituted			X				

for neutral organic compounds in saturated solutions even with long-term exposures. Other chemical classes have other upper limits for $K_{ow.}$ For examples, the maximum log K_{ow} for aldehydes is 6.0 and 7.0 for phenols.

Using SARs

All SARs contain an equation that predicts the aquatic toxicity of a chemical. Most of the SARs require the user to know the predicted log of the octanol water partition coefficient (K_{ow}). When this number is entered into the equation, a toxicity values in millimoles/L (mM/L) is derived. The molecular weight of the subject compound is required to convert the SAR estimates from millimoles/L to mg/L. The ECOSAR program does this automatically, however, manual estimates require that conversions be made. For example, the equation for predicting the fish 96-hour LC_{50} values for neutral organics is:

$$\text{Log } LC_{50} = 1.75 - 0.94 \log K_{ow}$$

Using 1,1'-biphenyl (CASRN [92-52-4] as a representative chemical, the estimated log K_{ow} for this compound is 4.0, to give a log LC_{50} of -2.01. Taking the antilog of -2.01, gives an LC_{50} value of 0.009 mM/L. However, to express the toxicity of the 1,1'-biphenyl as mg/L, the toxicity must be multiplied by the molecular weight of the compound which is 154.20, to give a final toxicity value of 1.5 mg/L. Conversions from mM/L to mg/L are not necessary for compounds and equations (e.g., surfactants, polymers) that do not use K_{ow} as the input parameter for toxicity.

Molecular weight is also used to determine the absorption cutoff limit for aquatic organisms. As the molecular weight of a chemical increases above 600, passive absorption through respiratory membranes decreases significantly. Therefore, for chemicals with molecular weights above 1000, it has been assumed that such absorption is negligible. For surface active chemicals such as cationic polymers, molecular weight

is not limiting because the toxic effect is not due to absorption, for example, some polycationic polymers with molecular weights in excess of 1,000,000 are highly toxic to aquatic organisms.

An important aspect of determining the toxicity of a compound is knowing the water solubility. The water solubility of a compound can be compared with the SAR toxicity value derived for that compound. If the toxicity value is significantly greater than the measured or predicted maximum water solubility, then an effect is not expected to occur in a saturated solution. In addition, a determination of the physical state (liquid, solid, or gas) of the compound is helpful in selecting an SAR. SARs currently used by EEB were developed using toxicity data on chemicals that are liquids at room temperature (25 EC). If an organic chemical is a solid at room temperature, then the melting point should be known because of the effect it has on water solubility, i.e., assuming K_{ow} is constant, the higher the melting point of a neutral organic chemical, the lower its water solubility. For other chemicals such as surfactants, water dispersibility is used; however, for practical purposes, water solubility and dispersibility are considered to be synonymous.

To determine the toxicity of a surfactant, it is necessary to know the number of carbon atoms in the alkyl chain for anionic surfactants or the number of ethoxylate units in the compound if it is an cationic (ethomeen) or nonionic surfactant. For cationic quaternary ammonium surfactants, the toxicity is based on the average length of a linear carbon chain, if the chain length is between 10 and 24 carbons long. The surfactant SARs developed by EEB are based on surfactants where the hydrophobic component is composed of a single linear chain of carbons and/or chains of ethoxylate units. Surfactants that have complex hydrophobic components are assessed by calculating the K_{ow} of the complex hydrophobic component alone and determining which aliphatic alkyl (carbon) chain has an equivalent K_{ow}. Toxicity predictions are based on this equivalent chemical structure. See the SAR for cationic dialkyl quaternary ammonium surfactants for more details on these calculations.

For polycationic polymers, it is necessary to calculate the percent amine nitrogen and/or number of cationic charges per 1000 molecular weight.

For inorganic and organometallic compounds, only the molecular weight of the compound is used for calculating the toxicity value. Acute and/or chronic toxicity values will be expressed in mg/L, and further conversions and/or calculations are not necessary.

Reliability of SARs

As may be seen by reviewing the chemicals used to derive the individual SARs in this manual, some chemical classes have a greater number of chemicals with accompanying toxicity values than do others. For example, the neutral organic 96-hour fish LC_{50} SAR was based on toxicity values for over 60 chemicals, whereas, the fish 96-hour LC_{50} SAR for propargyl alcohols was based on only one toxicity value. In the cases where there is only one toxicity value for a chemical class, the SAR is based on the line drawn between the one toxicity value and the maximum toxicity value of a neutral organic compound. Obviously SARs developed using only one or two toxicity values taken from the literature or premanufacture notices may not have the same reliability as an SAR developed from a larger toxicity database; however, on a regulatory basis this is the best estimate that can be scientifically achieved.

To determine how reliable the SARs in this manual are, Nabholz et al. (1993) conducted a validation study which compared the predicated toxicity values of chemicals with their measured toxicity values. Several chemical classes were included in the study: neutral organics, organic chemicals which show excess toxicity compared with neutral organics of a similar structure, anionic surfactants, cationic surfactants, polycationic polymers, cationic dyes, acid dyes, polyanionic monomers which are strong chelators of nutrient elements, and compounds which undergo hydrolysis (e.g., acid chlorides and alkyloxysilanes). In all, test data from 462 chemicals were used in the validation study. SARs for acute and chronic toxicity for fish, daphnids, and green algae were reviewed. Validation was expressed as a ratio, i.e., predicted toxicity:measured toxicity. A ratio of 1.0 would indicate that the predictions were perfectly accurate, a ratio

of less than 1.0 would indicate an over-prediction of toxicity, and a ratio of more than 1.0 would indicate that SARs were under predicting the toxicity of the chemicals. The results of the study indicated that the algal chronic effect was most accurately predicted (ratio 1.07) while the fish chronic value was the least reliable (ration 0.24). The fish 96-hour LC_{50} ratio was 0.64, the daphnid 48-hour LC_{50} was 0.79, and the algae 96-hour EC_{50} was 0.81. Work on validating the SARs is continuously ongoing in EEB.

FURTHER DISCUSSION NEEDED FOR USE OF NEAREST ANALOG; WHY GASES DON'T HAVE SAR; AND RADIONUCLIDES

Sources for ECOSAR

ECOSAR: Computer Program and User's Guide for Estimating the Ecotoxicity of Industrial Chemicals Based on Structure Activity Relationships (Publication Number EPA-748-R-93-002) is available from the following sources:

- National Center for Environmental Publications and Information
  U.S. Environmental Protection Agency
  26 West Martin Luther King Drive
  Cincinnati, OH 45268
  (513) 569-7562

- National Technical Information Service
  U.S. Department of Commerce
  5285 Port Royal Road
  Springfield, VA 22161
  (703) 487-4650

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Nabholz, JV, Miller, P, Zeeman, M. 1993. Environmental Risk Assessment of New Chemicals Under the Toxic Substances Control Act (TSCA) Section Five. In: Landis, WG, Hughes, JS, and Lewis, MA, eds. Environmental Toxicology and Risk Assessment, ASTM STP 1179. Philadelphia, PA: American Society for Testing and Materials. pp. 40-55.

CHEMICAL CLASSES AND APPLICABLE SARs

Chemical Class	SAR to Use
ACETATES	Use SAR for **ESTERS**
ACETYLENIC CARBAMATES	No SAR available, excess toxicity
ACID CHLORIDES	Use SAR for **ACID CHLORIDES**
ACID DYES with ONE ACID	Some are moderately toxic to fish and daphnids, others are not; No SAR available, Use nearest analog
ACID DYES with TWO ACIDS	Some are moderately toxic to fish and daphnids, others are not; No SAR available, Use nearest analog
ACID DYES with THREE ACIDS	Only moderately toxic to green algae due to the indirect effect of shading; shading inhibits growth due to the colored water; Use nearest analog based on chemical structure, color, and intensity of color.
ACRYLAMIDES and SUBSTITUTED ACRYLAMIDES	Excess toxicity, Use toxicity data for acrylamides with MW adjustment
ACRYLATES (log Kow <5.0)	Use SAR for **ACRYLATES**
ACRYLATES (log Kow >5.0)	Use SAR for **NEUTRAL ORGANICS**
ACRYLATES, METHACRYLATES	Use SAR for **ACRYLATES, METHACRYLATES**
ACTINIUM	No SAR available
ALCOHOLS	Use SAR for **NEUTRAL ORGANICS**
ALCOHOLS, PROPARGYL	Use SAR for **ALCOHOLS PROPARGYL**
ALDEHYDES	Use SAR for **ALDEHYDES,** R-C(=O)-H,
ALDEHYDES, VINYL	No SAR available; some exhibit excess toxicity, e.g., acrolein,
ALIPHATIC AMINES	Use SAR for **AMINES, ALIPHATIC**
ALIPHATIC DIESTERS	Use SAR for **ESTERS**, **DI**, ALIPHATIC
ALIPHATIC DIKETONES, LINEAR	Use SAR for **KETONES**, **DI**, ALIPHATIC
ALIPHATIC HYDROCARBON, á-HYDROXY-ß-NITRO SUBSTITUTED or ALIPHATIC HYDROCARBON, 1-HYDROXY-2-NITRO SUBSTITUTED	Excess toxicity towards algae, e.g., tris(hydroxymethyl)nitromethane
ALIPHATIC MONOESTERS	Use SAR for **ESTERS**
ALIPHATIC HYDROCARBONS	Use SAR for **NEUTRAL ORGANICS** Straight chain or cycloalkane,
ALKANES, CYCLO	Use SAR for **NEUTRAL ORGANICS**
ALKANES, STRAIGHT & BRANCHED	Use SAR for **NEUTRAL ORGANICS**
ALKENES	Use SAR for **NEUTRAL ORGANICS**
ALKYLANILINES	Use SAR for **ANILINES**
ALKYL BENZENE SULFONATES	Use SAR for **SURFACTANTS, ANIONIC**
ALKYL ESTERS OF CARBAMIC ACID	No SAR available
ALKYL HALIDES	Use SAR for **NEUTRAL ORGANICS**
ALKYL-NITROGEN-ETHOXYLATES	Use SAR for **SURFACTANTS, ETHOMEEN**
ALKYL SULFONATES	Use SAR for **SURFACTANTS, ANIONIC**
ALKYL SULFONATES AND CARBOXYLIC ACID	
ALLYL CYANIDES	Use SAR for **MALONONITRILES**
ALLYL DIESTERS	Use SAR for **ESTERS , DI**, ALIPHATIC

ALLYL ESTER	Use SAR for **ESTERS**
ALLYL HALOGENS	No SAR available ALLYL CHLORIDES show excess toxicity, ALLYL BROMIDES are even more toxic
ALKYNES	Use SAR for **NEUTRAL ORGANICS**
ALLYL, NITRILES	
ALUMINUM	Use SAR for ALUMINUM
AMERICIUM	No SAR available
AMIDES, VINYL	No SAR available. Excess toxicity, Use toxicity data for arcylamides with MW adjustment
AMINES, ALIPHATIC, PRIMARY	Use SAR for **AMINES, ALIPHATIC** when log Kow < 7.0, Use nearest analog when log Kow > 7.0
AMINES, ALIPHATIC, SECONDARY	Use SAR for **AMINES, ALIPHATIC** when log Kow < 7.0, Use nearest analog when log Kow > 7.0
AMINES, ALIPHATIC, TERTIARY	Use SAR for **AMINES, ALIPHATIC** when log Kow < 7.0, Use nearest analog when log Kow > 7.0
AMINES, ALIPHATIC, QUATERNARY, SURFACTANT	Use SAR for **SURFACTANTS, CATIONIC**, QUATERNARY AMMONIUM, MONOALKYL
AMINES, ALIPHATIC, QUATERNARY, NOT A SURFACTANT	Calculate Kow for the tertiary amine and Use SAR for **AMINES, ALIPHATIC** when log Kow < 7.0, nearest analog when log Kow > 7.0; or Use nearest analog method.
AMINES, SCHIFF BASES	No SAR available
AMINES, AROMATIC	Use SAR for **ANILINES**
AMINO-PHENOLS	Use SAR for **ANILINES**
AMINOTRIAZOLES	
AMPHOTERIC DYES	If charges are balanced, low toxicity towards fish and daphnids, and shading only towards algae; if more cationic than anionic, see CATIONIC DYES; and if more anionic than cationic, see ACID DYES
ANILINES	Use SAR for **ANILINES**
ANILINES, ALKYL	Use SAR for **ANILINES**
ANILINES AR-NH2 with N-substitutions	Use SAR for **NEUTRAL ORGANICS**
ANILINES, AMINO, META, OR 1,3-SUBSTITUTED	Use SAR for **ANILINES**, **AMINO**, **META**, **OR 1,3-SUBSTITUTED**
ANILINES, AMINO, ORTHO, OR 1,2-SUBSTITUTED	Use SAR for **ANILINES**, **AMINO**, **ORTHO**, **OR**
1,2-SUBSTITUTED	
ANILINES, AMINO, PARA, OR 1,4-SUBSTITUTED	Use SAR for **ANILINES**, **AMINO**, **PARA OR**
1,4-SUBSTITUTED	
ANILINES, DINITRO	Use SAR for **ANILINES**, **DINITRO**
ANILINES, MONOHYDROXY	Use SAR for **ANILINES**
ANILINES, POLYNITRO	Use SAR for **ANILINES**, **DINITRO**
ANTIMONY	No SAR available; however water quality criteria may be
used	
ARGON	Gas; No SAR available
AROMATIC DIAZONIUMS	Use SAR for **DIAZONIUMS, AROMATIC**
ARSENIC(III)	Use SAR for **ARSENIC**

ARYL HALIDES	Use SAR for **NEUTRAL ORGANICS**
ASTATINE	No SAR available
AZIRIDINES	Use SAR for **AZIRIDINES**,
AZO DYES	No SAR available; see DYES
BARIUM	No SAR available
BENZENE, DINITRO	Use SAR for **BENZENES, DINITRO**
BENZENEAMINES	Use SAR for **ANILINES**
BENZOATES	Use SAR for **ESTERS**
BENZOTRIAZOLES	Use SAR for **BENZOTRIAZOLES**
BENZOTRIAZOLES with free -NH	Use SAR for **BENZOTRIAZOLES**, has excess toxicity,
BENZOTRIAZOLES with N-alkyl substitution	Use SAR for **NEUTRAL ORGANICS**
BENZOTRIAZOLES with N-thiol substitution	No SAR available
BENZOYL PEROXIDES	Use SAR for **PEROXY ACIDS**, RC(=O)OOC(=O)R, excess toxicity,
BERKELIUM	No SAR available
BERYLLIUM	Use SAR for BERYLLIUM
BIPHENYLS, POLYBROMINATED	Use SAR for **NEUTRAL ORGANICS**
BISMUTH	No SAR available
BORON	Use SAR for **BORON**
BROMINE	No SAR available
CADMIUM	Use SAR for **CADMIUM**
CALCIUM	No SAR available
CALIFORNIUM	No SAR available
CAPROLACTAMS	Use SAR for **NEUTRAL ORGANICS**
CARBAMATES	No SAR available
CARBAMATES, BIS(ETHYL)- JOINED AT -NRN- BY ALKYL OR ARYL GROUPS	No SAR available
CARBAMATES, ETHYL, N-ALKYL OR ARYL SUBSTITUTED	No SAR available
CARBAMATES, BIS OR TRIS, ESTERIFIED ON A SINGLE PHENYL RING	No SAR available
CARBAMATES, THIO	No SAR available
CARBON	No SAR available
CARBOXYLIC ACIDS	
CATIONIC DYES	No SAR available, Use nearest analog, MWs can be over 1000
CERIUM	No SAR available
CESIUM	Use SAR for CESIUM
CHLORINATED HYDROCARBONS	Use SAR for **NEUTRAL ORGANICS**
CHLORINE	Use SAR for **CHLORINE**
CHLOROANILINES	Use SAR for **ANILINES**
CHLOROFLUOROCARBONS (CFCs)	Use SAR for **NEUTRAL ORGANICS**
CHROMIUM	Use SAR for **CHROMIUM**
CHROMIUM(III)	Use SAR for **CHROMIUM**
CHROMIUM(VI)	Use SAR for **CHROMIUM**
COBALT	Use SAR for **COBALT**
COPPER	Use SAR for **COPPER**
CROWN ETHERS	See SAR for **CROWN ETHERS**

CURIUM	No SAR available
CYANIDE, VINYL	No SAR available, R-C=C-C/N, e.g., acrylonitrile, fumaronitrile, have excess toxicity,
CYANATES	No SAR available, (NCO-R) or (R-OCN),excess toxicity, Use nearest analog
CYCLIC DIKETONES	Use SAR for **NEUTRAL ORGANICS**
CYCLOALKANES	Use SAR for **NEUTRAL ORGANICS**
CYCLODIENE	Use SAR for **NEUTRAL ORGANICS**
DIAMINES, PHENYLENE (META OR 1,3 SUBSTITUTED)	Use SAR for **ANILINES**, **AMINO**, **META**, **OR 1,3-SUBSTITUTED**
DIAMINES, PHENYLENE (ORTHO OR 1,2-SUBSTITUTED)	Use SAR for **ANILINES**, **AMINO**, **ORTHO OR 1,2-SUBSTITUTED**
DIAMINES, PHENYLENE (PARA OR 1,4-SUBSTITUTED)	Use SAR for **ANILINES**, **AMINO**, **PARA OR 1,4-SUBSTITUTED**
DIAZONIUMS, ALIPHATIC	No SAR available (R-N/N-A), (very explosive and are used as synthesizing agents)
DIAZONIUMS, AROMATIC	Use SAR for **DIAZONIUM, AROMATIC**(AR-N/N-AR),
DICARBOXYLIC ALIPHATIC ESTERS	Use SAR for **ESTERS**
DIEPOXIDES	Use SAR for **EPOXIDES**, **DI**
DIESTER, ALLYL	No SAR available R-C-C=C-C-(O-C(=O)-C-R)-O-C(=O)-C-R) excess toxicity e,g., 2-propene-1,1-diol, diacetate, 1000X more toxic than an equivalent NEUTRAL ORGANIC,
DIESTERS, AROMATIC OR ALIPHATIC/AROMATIC	Use SAR for **ESTERS, PHTHALATE**
DIKETONES, á,Ã-diketone or 1,3-diketones, linear pentanediols, excess toxicity	Use SAR for **KETONES, DI**, ALIPHATIC; e.g., 2,4-
DIKETONES, 1,3-diketones, cyclic	Use SAR for **NEUTRAL ORGANICS**
DINITROANILINES	Use SAR for **ANILINES**, **DINITRO**
DINITROBENZENES	Use SAR for **BENZENES, DINITRO**
DINITROPHENOLS	Use SAR for **PHENOLS**, **DINITRO**
DIPHENOLS	Use SAR for **PHENOLS**
DISPERSE DYES	Use SAR for **NEUTRAL ORGANICS**
DISULFIDES	Use SAR for **NEUTRAL ORGANICS**
DISULFIDE, PHENYL	No SAR available, excess toxicity,
DITHIOCARBAMATES	See SAR for **CARBAMATES, DITHIO**
DITHIOCARBAMATES, POLY	No SAR available, excess toxicity,
DYES	see ACID DYES if ANIONIC DYES; see CATIONIC DYES if cationic; see NEUTRAL DYES if neutral; and see AMPHOTERIC DYES if both cationic and anionic; MWs can be over 1000 for CATIONIC DYES, AMPHOTERIC DYES, and ACID DYES; MWs of NEUTRAL DYES have to be less than 1000 for toxicity towards fish and daphnids; toxicity to green algae is based on color and intensity of color, and is an indirect effect
DYSPROSIUM	No SAR available
ERBIUM	No SAR available
EPOXIDES, AZIRIDINES	Use SAR for **AZIRIDINES**

EPOXIDES, DIEPOXIDES	Use SAR for **EPOXIDES , DI**
EPOXIDES, MONOEPOXIDES	Use SAR for **EPOXIDES , MONO**
EPOXIDES, POLYEPOXIDES	Use SAR for **EPOXIDES, DI**
ESTERS (log Kow <5.0)	Use SAR for **ESTERS**
ESTERS (log Kow >5.0)	Use SAR for **NEUTRAL ORGANICS**
ESTERS	Use SAR for **ESTERS,** RC(=O)OR,
ESTER, ALLYL	Use SAR for **ESTERS,** R-C=C-C-O-C(=O)-C-R, excess toxicity,
ESTERS, á-HALO-	No SAR available, C-O-C(=O)-C-X, excess toxicity, BROMIDES are more toxic than CHLORIDES
	Use SAR for **ESTERS**
ESTERS, DICARBOXYLIC, ALIPHATIC	Use SAR for **ESTERS , DI**,**ALIPHATIC**
ESTERS, DIESTERS, ALIPHATIC	Use SAR for **ESTERS**
ESTERS, METHANESULFONATES	Use SAR for **ESTERS, PHOSPHATE**
ESTERS, PHOSPHATE	No SAR Available, R-O-P(=S)(O-R)R, pesticide, Use nearest analog
ESTERS, PHOSPHINOTHIOIC ACID, TRISUBSTITUTED	Use SAR for **SURFACTANTS, ANIONIC** if alkyl chains are long; if alkyl chains are short, use nearest analog (R-O-P(=S)(OH)R)
ESTERS, PHOSPHINOTHIOIC ACID, DISUBSTITUTED-FREE ACID	Use SAR for **SURFACTANTS, ANIONIC** if alkyl chains are long; if alkyl chains are short, Use nearest analog (HO-P(=S)(OH)R)
ESTERS, PHOSPHINOTHIOIC ACID, MONOSUBSTITUTED-FREE DIACID	**WE NEED A DESCRIPTION FOR THIS; USES BOTH ANIONIC SURFACTANT AND DIESTER SARS**
ESTERS, PHOSPHOROTHIOIC, MONOESTER	Use SAR for **SURFACTANTS, ANIONIC** if alkyl chain is long; if alkyl chain is short, Use nearest analog (R-O-P(=S)(OH)OH)
ESTERS, PHOSPHOROTHIOIC, MONOSUBSTITUTED ESTER	Use SAR for **SURFACTANTS, ANIONIC**, if alkyl chain is long, if alkyl chain is short, Use nearest analog
ESTERS, PHOSPHOROTHIOIC, DISUBSTITUTED ESTER	Use SAR for **ESTERS**, **PHOSPHATE**
ESTERS, PHOSPHOROTHIOIC, TRIESTER	Use SAR for **ESTERS**, **PHOSPHATE**
ESTERS, PHOSPHOROTHIOIC, TRISUBSTITUTED	Use SAR for **ESTERS, PHTHALATE**
ESTERS, PHTHALATE	Use SAR for **ESTERS**
ESTERS, POLY	No SAR available, have excess toxicity
ESTERS, PROPARGYLIC	Use SAR for **ESTERS**
ESTERS, SULFONATE	Use SAR for **ESTERS**, **PHOSPHATE**
ESTERS, TRIALKYL PHOSPHATE	No SAR available, excess toxicity
ESTERS, VINYL	No SAR available
EINSTEINIUM	Use SAR for **NEUTRAL ORGANICS**
ETHERS	Use SAR for **SURFACTANTS, NONIONIC**
ETHOXYLATES, ALKYL	No SAR available
EUROPIUM	Use SAR for **SURFACTANTS, ANIONIC**
FATTY ACIDS	No SAR available
FERMIUM	No SAR available
FLUORINE	No SAR available
FRANCIUM	

GADOLINIUM	No SAR available
GALLIUM	No SAR available
GERMANIUM	Use SAR for **GERMANIUM**
GOLD	Use SAR for **GOLD**
GUANIDINE	Use SAR for **AMINES, ALIPHATIC**
HAFNIUM	No SAR available
HALIDES, ALKYL	Use SAR for **NEUTRAL ORGANICS**
HALIDES, ARYL	Use SAR for **NEUTRAL ORGANICS**
HALOGENATED FLUOROCARBONS	Use SAR for **NEUTRAL ORGANICS**
HELIUM	No SAR available
HFCs	Use SAR for **NEUTRAL ORGANICS**
HOLMIUM	No SAR available
HYDRAZIDES	Use SAR for **HYDRAZINES**
HYDRAZINES	Use SAR for **HYDRAZINES**
HYDRAZINES, CARBOXYLIC (FREE) ACID SUBSTITUTION	No SAR available, about 10 times less toxic than HYDRAZINES
HYDRAZINES, SEMICARBAZIDES, ARYL, META/PARA SUBSTITUTED	Use SAR for **SEMICARBAZIDES**, **ARYL**, **META/PARA SUBSTITUTED**
HYDRAZINES, SEMICARBAZIDES, ARYL, ORTHO SUBSTITUTED	Use SAR for **SEMICARBAZIDES, ARYL, ORTHO SUBSTITUTED**
HYDRAZONES	Use SAR for **HYDRAZINES**
HYDROCARBONS, AROMATIC	Use SAR for **NEUTRAL ORGANICS**
HYDROCARBONS, AROMATIC, HALOGENATED	Use SAR for **NEUTRAL ORGANICS**
HYDROCARBONS, ALIPHATIC, HALOGENATED	Use SAR for **NEUTRAL ORGANICS**
HYDROGEN	No SAR available; toxicity is based on pH *********
HYDROQUINONES or PARA-HYDROXY PHENOL	No SAR available, excess toxicity
IMIDES	Use SAR for **IMIDES**
INDIUM	No SAR available
INDOLES, HALOGENATED	Use SAR for **NEUTRAL ORGANICS**
IODINE	No SAR available
IRIDIUM	No SAR available
IRON	Use SAR for **IRON**
ISOCYANATES, MONO- AND DI- ISOCYANATES (R-NCO) and ISOTHIOCYANATES	No SAR available, excess toxicity if very water soluble. Use nearest analog
ISOTHIAZOLINONES	Use SAR for **THIAZOLINOES, ISO**
KETONES, á-HALO-	No SAR available, excess toxicity
KETONES, MONO	Use SAR for **NEUTRAL ORGANICS**
KETONES, DIKETONES, ALIPHATIC	Use SAR for **KETONES, DI** Aliphatic
KRYPTON	No SAR available
LANTHANUM	Use SAR for **LANTHANUM**
LAWRENCIUM	No SAR available
LEAD	Use SAR for **LEAD**
LINALOOLS	Use SAR for **NEUTRAL ORGANICS**
LINEAR ALKYL BENZENES	Use SAR for **SURFACTANTS, ANIONIC**
LINEAR ALKYL BENZENE	

SULFONATES	Use SAR for **SURFACTANTS, ANIONIC**
LINEAR ALKYL SULFONATES	Use SAR for **SURFACTANTS, ANIONIC**
LITHIUM	No SAR available
LUTETIUM	No SAR available
MAGNESIUM	No SAR available
MALEIMIDES	Use SAR for **IMIDES**
MALONONITRILES	Use SAR for **MALONONITRILES**
MANGANESE	No SAR available
MENDELEVIUM	No SAR available
MERCAPTANS/THIOLS	Use SAR for **THIOLS**; (R-SH)
MERCAPTOBENZOTRIAZOLES:	No SAR available , excess toxicity
MERCURY	Use SAR for **MERCURY**
METHACRYLAMIDES SUBSTITUTED ACRYLAMIDES	No SAR available, less toxic than ACRYLAMIDES and
METHACRYLATES (log Kow <5.0)	Use SAR for **METHACRYLATES**
METHACRYLATES (log Kow >5.0)	Use SAR for **NEUTRAL ORGANICS**
METHANESULFONATES	Use SAR for **ESTERS**
MOLYBDENUM	Use SAR for **MOLYBDENUM**
MONOEPOXIDES	Use SAR for **EPOXIDES**, **MONO**
NEON	No SAR available
NEUTRAL DYES	Use SAR for **NEUTRAL ORGANICS**
NEUTRAL ORGANICS	Use SAR for **NEUTRAL ORGANICS**
NEODYMIUM	No SAR available
NEPTUNIUM	No SAR available
NICKEL	Use SAR for **NICKEL**
NIOBIUM	No SAR available
NITRILES	Use SAR for **NEUTRAL ORGANICS**
NITRILES, ALLYL	Use SAR for **MALONONITRILES**
NITRILES, VINYL	Use SAR for **MALONONITRILES**
NITROBENZENES, DINITROBENZENES	Use SAR for **BENZENES, DINITRO**
NITROGEN	No SAR available
NITROSO COMPOUNDS	No SAR available, excess toxicity
NOBELIUM	No SAR available
OSMIUM	No SAR available
OXYGEN	No SAR available
PALLADIUM	No SAR available
PEROXY ACIDS	Use SAR for **PEROXY ACIDS**
PHENOLS	Use SAR for **PHENOLS**
PHENOLS, AMINO	Use SAR for **ANILINES**
PHENOLS, DI	Use SAR for **PHENOLS**
PHENOLS, DINITRO	Use SAR for **PHENOLS**, **DINITRO**
PHENOLS, HALOGENATED	Use SAR for **PHENOLS**
PHENOL, META-HYDROXY	Use SAR for **PHENOLS**
PHENOL, ORTHO-HYDROXY	No SAR available, CATECHOL, 16 times excess fish acute toxicity
PHENOL, PARA-HYDROXY or HYDROQUINONE	No SAR available, 1400 times excess fish acute toxicity
PHENOLS, POLY	Use SAR for **PHENOLS**
PHENOLS, SUBSTITUTED	Use SAR for **PHENOLS**
PHENYLENEDIAMINES	Use SAR for **ANILINES**, AMINO ********
PHOSPHINOTHIOIC ACID ESTERS, DISUBSTITUTED FREE ACID	Use SAR for **SURFACTANTS, ANIONIC**

PHOSPHINOTHIOIC ACID ESTERS, MONOSUBSTITUTED FREE ACID	Use SAR for **SURFACTANTS, ANIONIC**
PHOSPHITES	No SAR available, excess toxicity
PHOSPHONIUM	Use SAR for **SURFACTANTS, CATIONIC**, QUATERNARY AMMONIUM if a surfactant; if not a surfactant use nearest analog: SULFONIUM or QUATERNARY AMMONIUM analogs are acceptable
PHOSPHOROTHIOIC ESTERS, DIESTER	Use SAR for **SURFACTANTS, ANIONIC**
PHOSPHOROTHIOIC ESTERS, MONOESTER	Use SAR for **SURFACTANTS, ANIONIC**
PHOSPHORUS	Use SAR for **PHOSPHORUS**
PLATINUM	Use SAR for **PLATINUM**
PLUTONIUM	No SAR available
POLONIUM	No SAR available
POLYANIONIC MONOMERS	No SAR available, monomers with two or more acid groups and which act like organic acid chelators, Use nearest analog
POLYAROMATIC HYDROCARBONS	Use SAR for **NEUTRAL ORGANICS**
POLYBROMINATED BIPHENYLS	Use SAR for **NEUTRAL ORGANICS**
POLYCATIONIC POLYMERS	Use SAR for **POLYMERS, POLYCATIONIC**
POLYEPOXIDES	Use SAR for **EPOXIDES, DI**,
POLYISOCYANATES	No SAR available, if water solubility is 13 mg/L or less, then no effects at saturation; these chemicals will polymerize: one NCO will hydrolyze to the amine and the amine will react with another NCO to form a urethane; a crosslinked polymer will be formed
POLYMERS, POLYNONIONIC	No SAR available, low environmental hazard.
POLYMERS, POLYANIONIC, POLY(CARBOXYLIC ACID)	No SAR available, Use nearest analog
POLYMERS, POLYANIONIC, POLY(ACRYLIC ACID)	No SAR available, Use nearest analog
POLYMERS, POLYANIONIC, POLY(METHACRYLIC ACID)	No SAR available, Use nearest analog
POLYMERS, POLYANIONIC, POLY(AROMATIC SULFONIC ACID)	No SAR available, Use nearest analog
POLYMERS, POLYANIONIC, POLY(ALIPHATIC SULFONIC ACID)	No SAR available, Use nearest analog
POLYMERS, POLYCATIONIC	Use SAR for **POLYMERS, POLYCATIONIC**
POLYMERS, POLYAMINE	Use SAR for **POLYMERS, POLYCATIONIC**
POLYMERS, POLYQUATERNARY AMMONIUM	Use SAR for **POLYMERS, POLYCATIONIC**
POLYMERS, POLYPHOSPHONIUM	Use SAR for **POLYMERS, POLYCATIONIC**
POLYMERS, POLYSULFONIUM	Use SAR for **POLYMERS, POLYCATIONIC**
POLYNUCLEAR AROMATICS	Use SAR for **NEUTRAL ORGANICS**
POLYSULFIDES	Use SAR for **NEUTRAL ORGANICS**
POTASSIUM	No SAR available
PRASEODYMIUM	No SAR available
PROMETHIUM	No SAR available
PROPARGYL ALCOHOLS	Use SAR for **ALCOHOLS**, **PROPARGYL**
PROPARGYL CARBAMATES	No SAR available, excess toxicity

PROPARGYLIC ESTERS	No SAR available, excess toxicity
PROPARGYL HALIDE	No SAR available, excess toxicity, PROPARGYL BROMIDE more toxic than PROPARGYL CHLORIDE
PROTACTINIUM	No SAR available
QUATERNARY AMMONIUM SURFACTANTS, DIALKYL QUATERNARY AMMONIUM, DIALKYL	Use SAR for **SURFACTANTS, CATIONIC**,
QUATERNARY AMMONIUM SURFACTANTS, MONOALKYL QUATERNARY AMMONIUM, MONOALKYL	Use SAR for **SURFACTANTS, CATIONIC**,
QUINONES	No SAR available, para-benzoquinone, 5500X excess toxicity to fish
RADIUM	No SAR available
RADON	No SAR available
RHENIUM	No SAR available
RHODIUM	No SAR available
RUBIDIUM	No SAR available
RUTHENIUM	No SAR available
SAMARIUM	No SAR available
SCANDIUM	No SAR available
SCHIFF BASES	Use SAR for SCHIFF BASES, a subclass of AMINES with excess toxicity; (R-N=C-R)
SELENIUM	Use SAR for SELENIUM
SEMICARBAZIDES, ALKYL SUBSTITUTED	Use SAR for **SEMICARBAZIDES**, ALKYL SUBSTITUTED
SEMICARBAZIDES, ARYL META/PARA SUBSTITUTED	Use SAR for **SEMICARBAZIDES**, ARYL, META/PARA SUBSTITUTED
SEMICARBAZIDES ARYL ORTHO SUBSTITUTED	Use SAR for **SEMICARBAZIDES**, ARYL, ORTHO SUBSTITUTED
SEMICARBAZIDES	Use SAR for **HYDRAZINES**
SEMICARBAZONES	Use SAR for **HYDRAZINES**
SILANES, ALKOXY RSi(OR)(OR)(OR) and CHLOROSILANES	reactive with water (hydrolyses) and generally shows low toxicity towards fish, moderate toxicity towards daphnids, and high toxicity towards green algae; the hydrolysis products (silic acids and silanols) probably overchelate nutrient elements and inhibit the growth of algae; all SARs for silanes have to be based on Kows which have C substituted for Si.
SILICON	No SAR available
SILVER	Use SAR for **SILVER**
SODIUM	No SAR available
STRONTIUM	No SAR available
SULFIDES	Use SAR for **NEUTRAL ORGANICS**
SULFIDES (C-S-C), DISULFIDES (C-S-S-C), and POLYSULFIDES	Use SAR for **NEUTRAL ORGANICS**
SULFONATES, ALKYL BENZENE	Use SAR for **SURFACTANTS, ANIONIC**
SULFONATES, ALKYL	Use SAR for **SURFACTANTS, ANIONIC**

SULFONATES, METHANE	Use SAR for **ESTERS**
SULFONIUM	Use SAR for **SURFACTANTS, CATIONIC**, QUATERNARY AMMONIUM, if a surfactant; if not a surfactant, Use nearest analog: PHOSPHONIUM or QUATERNARY AMMONIUM analogs are acceptable.
SULFUR	No SAR available
SULFONATES, LINEAR ALKYL	Use SAR for **SURFACTANTS, ANIONIC**
SULFONYL CHLORIDES	No SAR available, excess toxicity (RS(=O)(=O)Cl)
SURFACTANTS, ALCOHOL ETHOXYLATE	Use SAR for **SURFACTANTS, NONIONIC**
SURFACTANTS, ALKYL ETHOXYLATE	Use SAR for **SURFACTANTS, NONIONIC**
SURFACTANTS, AMPHOTERIC	Use SAR for **SURFACTANTS, ANIONIC**
SURFACTANTS, ANIONIC	Use SAR for **SURFACTANTS, ANIONIC**
SURFACTANTS, ANIONIC, CARBOXYLIC ACID	No SAR available
SURFACTANTS, ANIONIC, ALKYL-BENZENE-SULFONATE	Use SAR for **SURFACTANTS, ANIONIC**
SURFACTANTS, ANIONIC, ALKYL-SULFONATE	Use SAR for **SURFACTANTS, ANIONIC** ,calculate Kow of alkyl, convert to equivalent alkyl-benzene based on equivalent Kow and use SAR for **SURFACTANTS, ANIONIC**
SURFACTANTS, ANIONIC, PHOSPHATE	Use SAR for **SURFACTANTS, ANIONIC**
SURFACTANTS, ANIONIC, ALKYL-ETHOXYLATE-SULFONATE	Use SAR for **SURFACTANTS, ANIONIC** to predict toxicity of alkyl-sulfonate and then adjust toxicity depending on number of ethoxylates
SURFACTANTS, ANIONIC, ALKYL-(SULFONATE and CARBOXYLIC ACID)	No SAR available; predict toxicity of alkyl-sulfonate and divide effective concentration by 10 times
SURFACTANTS, ANIONIC, TWEEN-TYPE	No SAR available, Use nearest analog
SURFACTANTS, CATIONIC, ALKYL-NITROGEN-ETHOXYLATES	Use SAR for **SURFACTANTS, ETHOMEEN**
ETHOMEEN	Use SAR for **SURFACTANTS, ETHOMEEN**
SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM DIALKYL	Use SAR for **SURFACTANTS, CATIONIC**, QUATERNARY AMMONIUM, DIALKYL, with two large alkyl chains
SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, MONOALKYL	Use SAR for **SURFACTANTS, CATIONIC**, QUATERNARY AMMONIUM, MONOALKYL, with one large alkyl chain
SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, N-ETHOXYLATED	Use SAR for **SURFACTANTS, CATIONIC** QUATERNARY AMMONIUM, MONOALKYL, if ethoxy

	groups are less than five. If ethoxylates are greater than five, Use SAR for **SURFACTANTS, CATIONIC**, QUATERNARY AMMONIUM MONOALKYL and then reduce toxicity due to the presence of the ethoxylates through the use of the SAR for **SURFACTANTS, NONIONIC**.
SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM TRIALKYL	Use SAR for **SURFACTANTS, CATIONIC**, QUATERNARY AMMONIUM, MONOALKYL, three large alkyls,
SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, TETRAALKYL	Use SAR for **SURFACTANTS, CATIONIC**, QUATERNARY AMMONIUM, MONOALKYL, four large alkyls
SURFACTANTS, NONIONIC	
SURFACTANTS, ETHOMEEN	Use SAR for **SURFACTANTS, ETHOMEEN**
SURFACTANTS, LINEAR ALKYL BENZENE SULFONATES	Use SAR for **SURFACTANTS, ANIONIC**
SURFACTANTS, NONIONIC	Use SAR for **SURFACTANTS, NONIONIC**
SURFACTANT, NONIONIC, ALKYL-ETHOXYLATES	Use SAR for **SURFACTANTS, NONIONIC**
SURFACTANT, NONIONIC, ALKYL-ETHOXYLATE-ALKYL	No SAR available, use nearest analog
SURFACTANT, NONIONIC, TWEEN-TYPE	No SAR available, Use nearest analog
SULFONATES, LINEAR ALKYL BENZENE	Use SAR for **SURFACTANTS, ANIONIC**
TANTALUM	No SAR available
TECHNIUM	No SAR available
TELLURIUM	No SAR available
TERBIUM	No SAR available
TERPENES	Use SAR for **NEUTRAL ORGANICS**
THALLIUM	Use SAR for **THALLIUM**
THIAZOLINONES, ISO	Use SAR for **THIAZOLINONES, ISO**
THIOLS (MERCAPTANS)	Use SAR for **THIOLS**
THIOHYDRAZIDES	Use SAR for **HYDRAZINES**
THIOSEMICARBAZIDES	Use SAR for **HYDRAZINES**
THIOSEMICARBAZONES	Use SAR for **HYDRAZINES**
THORIUM	No SAR available
THULIUM	No SAR available
TIN	No SAR available for inorganic tins or organotins, Use nearest analog
TITANIUM	Use SAR for **TITANIUM**
TRIAZIDES, BENZO, N-ALKYL SUBSTITUTED	Use SAR for **NEUTRAL ORGANICS**
TRIAZINES, SUBSTITUTED	See SAR for **TRIAZINES, SUBSTITUTED**
TRIAZOLES	No SAR available, excess toxicity, Use nearest analogs
TRIAZOLES, AMINO	Use SAR for **NEUTRAL ORGANICS,** herbicide, excess toxicity,
TRIAZOLES, BENZO	Use SAR for BENZOTRIAZOLES
TUNGSTEN	Use SAR for TUNGSTEN

VANADIUM	Use SAR for VANADIUM
URANIUM	No SAR available
UREAS, CYCLIC	Use SAR for **NEUTRAL ORGANICS**
UREAS, SUBSTITUTED	Use SAR for UREAS, SUBSTITUTED for green algae; to predict toxicity to fish and aquatic invertebrates, Use SAR for **NEUTRAL ORGANICS**
VINYL AMIDES	No SAR available
VINYL ESTERS	No SAR available
VINYL NITROS	No SAR available, á-nitro-styrene, excess toxicity, (R-C=C=N(=O)(=O))
VINYL SULFONE	No SAR available, e.g., divinyl sulfone, excess toxicity, (C=C-S(=O)(=O)-R)
XENON	No SAR available
YTTERBIUM	No SAR available
YTTRIUM	No SAR available
ZINC	Use SAR for **ZINC**
ZIRONIUM	Use SAR for **ZIRCONIUM**

CHEMICAL CLASSES

AND THEIR

STRUCTURE ACTIVITY RELATIONSHIPS

SAR **ACID CHLORIDES**

Organism: Fish
Duration: 96-h
Endpoint: LC50 (Mortality)

Equation: Log LC50 (mM/L) = 0.565 - 0.613 log K_{ow}

Statistics: N = 3; R^2 = 1.0

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate the toxicity of acid chlorides.

Limitations: If the log K_{ow} value is greater than 8.0, or if the compound is solid and the LC50 exceeds the water solubility.

References:

Curtis MW, Copeland TL, and Ward CH. 1978. Aquatic toxicity of substances proposed for spill prevention regulation. Proc. Natl. Conf. Control of Hazardous Material Spills, Miami Beach, FL. p. 93-103.

Curtis MW and Ward CH. 1981. Aquatic toxicity of forty industrial chemicals: testing in support of hazardous substance spill prevention regulation. J. Hydrol. 51:359-367.

LIST OF ACID CHLORIDES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Benzoyl chloride	34.7	1.9	C1
Benzoyl chloride	34.1	1.9	C2

C1 = Curtis et al (1978)
C2 = Curtis et al (1981)

ACID CHLORIDES
9/1993

SAR	**ALCOHOLS, PROPARGYL**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log 96-h LC50 (mM/L) = 0.056 - 0.511 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for propargyl alcohols.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, use SAR with longer duration.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

LIST OF PROPARGYL ALCOHOLS USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Chemical identity CBI	310.0	-0.4	EPA

EPA = USEPA (1991); chemical identity is Confidential Business Information under TSCA.

ALCOHOL, PROPARGYL
9/1993

SAR	**ACRYLATES**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log LC50 (mM/L) = -1.46 - 0.18 log K_{ow}
Statistics:	N = 10; R^2 = 0.627
Maximum K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate the toxicity of acrylates and polyacrylates. Allyl acrylate is expected to be about 30 times more toxic than predicted by this SAR.
Limitations:	
References:	Nabholz JV and Platz RD. 1987. Environmental effects of acrylates and methacrylates. I. Category Program Support Document - Generic SNUR and II. Generic Environmental Hazard Assessment (Addendum to Standard Review of PMN 87-930/931). Washington, DC: Environmental Effects Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency 20460-0001. United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

ACRYLATES
7/1988

LIST OF ACRYLATES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
2-Hydroxyethyl acrylate	4.8	-0.058	EPA
2-Hydroxypropyl acrylate	3.61	0.251	EPA
2-Hydroxypropyl acrylate	3.26	0.251	EPA
2-Hydroxypropyl acrylate	3.10	0.251	EPA
Chemical identity CBI	13.0	1.6	EPA
Isobutyl acrylate	2.110	2.204	EPA
Isobutyl acrylate	2.090	2.204	EPA
Cyclohexyl acrylate	1.48	2.778	EPA
Hexyl acrylate	1.14	3.392	EPA
Hexyl acrylate	1.09	3.392	EPA
Lauryl acrylate	*	6.566	EPA

* No mortalities within 96 hours at saturation.

EPA = USEPA (1991); chemical identity is Confidential Business Information under TSCA.

SAR **ACRYLATES**

Organism: Daphnid
Duration: 48-h
Endpoint: LC50

Equation: Log LC50 (mM/L) = 0.009 - 0.511 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum K_{ow}: 5.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for acrylates.

Limitations:

References:

Beach SA. 1990. Acute toxicity of isooctyl acrylate to Daphnia magna. St Paul, MN: 3M Environmental Laboratory, 3M Company; Toxicity Test Report.

United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF ACRYLATES USED TO DEVELOP THE DAPHNID LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)		Log K_{ow}	Ref.
Chemical identity CBI	59.0		0.78	EPA
Isooctyl acrylate	1.2	4.3		B

B = Beach (1990)
EPA = USEPA (1991); Chemical identity is Confidential Business Information under TSCA.

ACRYLATES
7/1988

SAR **ACRYLATES**

Organism: Green Algae
Duration: 96-h
Endpoint: EC50 (Growth)

Equation: Log EC50 (mM/L) = -1.02 - 0.49 log K_{ow}

Statistics: N = 3; R^2 = 0.91

Maximum log K_{ow}: 6.4
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for acrylates.

Limitations: If the log K_{ow} value is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility, use SAR with longer exposure.

References: United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF ACRYLATES USED TO DEVELOP THE SAR.

CHEMICAL	96-h EC50 (mg/L)	Log K_{ow}	Ref.
Chemical identity CBI	2.2	0.78	EPA
Chemical identity CBI	18.5	1.6	EPA

EPA = U.S. EPA (1991); Chemical identities are Confidential Business Information under TSCA.

ACRYLATES
7/1988

SAR	**ACRYLATES**
Organism:	Fish
Duration:	32-d
Endpoint:	Chronic Value (Survival/Growth)
Equation:	Log ChV (mM/L) = -1.99 - 0.526 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for acrylates.
Limitations:	If the ChV is greater than water solubility or the log K_{ow} is greater than 8.0, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. Fish Chronic Toxicity Data Base. Duluth, MN: Environmental Research Laboratory (ERL), Office of Research and Development, USEPA, 6201 Congdon Boulevard, 55804; contact C.L. Russom (218) 720-5500.

LIST OF ACRYLATES USED TO DEVELOP THE FISH CHRONIC VALUE (ChV) SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
2-Hydroxyethyl acrylate	1.33	-0.1	D

D = USEPA (1991)

ACRYLATES
7/1988

SAR	**ACRYLATES, METHACRYLATES**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log LC50 (mM/L) = 0.552 - 0.715 log K_{ow}
Statistics:	N = 19; R^2 = 0.774
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate the toxicity of methacrylates and polyacrylates. Allyl methacrylate is about 35 times more toxic than predicted by this SAR.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	Nabholz JV and Platz RD. 1987. Environmental effects of acrylates and methacrylates. I. Category Program Support Document - Generic SNUR and II. Generic Environmental Hazard Assessment (Addendum to Standard Review of PMN 87-930/931). Washington, DC: Environmental Effects Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency 20460-0001. United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

LIST OF METHACRYLATES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Methylene chloride	322.895	1.25	Z
2-Hydroxyethyl methacrylate	227.0	0.251	EPA
Methylmethacrylate	151.0	1.056	EPA
Tetrahydrofurfuryl	34.7	1.297	EPA
2-Ethoxyethyl methacrylate	27.7	1.402	EPA
3-(Trimethoxysilyl)propyl	175.0	1.464	EPA
Allyl methacrylate	0.99	1.570	EPA
Chemical identity CBI	34.0	1.774	EPA
Chemical identity CBI	32.0	1.774	EPA
Isopropyl methacrylate	38.0	1.894	EPA
Benzyl methacrylate	4.67	2.824	EPA

EPA = USEPA (1991); chemical identity is Confidential Business Information under TSCA.

SAR	**ALDEHYDES**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log LC50 (mM/L) = -0.449 log K_{ow} - 0.314
Statistics:	N = 54; R^2 = 0.527
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate the toxicity of aldehydes. Acrolein is about 1400 times more toxic than predicted by this SAR.
Limitations:	
References:	Brooke LT, Call DJ, Geiger DL, and Northcott CE. 1984. Acute toxicity of organic chemicals to fathead minnows (Pimephales promelas). Volume I. Center for Lake Superior Environmental Studies, University of Wisconsin - Superior. Superior, Wisconsin. Geiger DL, Northcott CE, Call DJ, and Brooke LT. 1985. Acute toxicity of organic chemicals to fathead minnows (Pimephales promelas). Volume II. Center for Lake Superior Environmental Studies, University of Wisconsin - Superior. Superior, Wisconsin. Geiger DL, Poirier SH, Brooke LT, and Call DJ. 1986. Acute toxicity of organic chemicals to fathead minnows (Pimephales promelas). Volume III Center for Lake Superior Environmental Studies, University of Wisconsin - Superior. Superior, Wisconsin. United States Environmental Protection Agency (USEPA). 1991. Fish acute toxicity databae. Duluth, MN: Environmental Research Laboratory (ERL), Office of Research and Development, USEPA. 6201 congdon Blvd, 55804; contact C.L. Russom (218) 720-5500.

ALDEHYDES
7/1988

LIST OF ALDEHYDES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Ethanal	30.800	-0.22	EPA
Butanal #1	19.000	0.88	EPA
Butanal #2	16.000	0.88	EPA
Butanal #3	13.400	0.88	EPA
2-Methylbutyraldehyde	9.970	1.14	EPA
Vanillin #2	123.000	1.21	EPA
Vanillin #1	57.000	1.21	EPA
Isovaleraldehyde	3.250	1.23	EPA
Valeraldehyde #1	12.400	1.36	EPA
Valeraldehyde #2	13.400	1.37	EPA
o-Vanillin #1	2.600	1.37	EPA
o-Vanillin #2	2.200	1.37	EPA
2,4,5-Trimethoxybenzaldehyde	49.500	1.38	EPA
Benzaldehyde #2	12.800	1.48	EPA
Benzaldehyde #1	7.610	1.48	EPA
4-Nitrobenzaldehyde	10.100	1.50	EPA
5-Hydroxy-2-nitrobenzaldehyde	41.900	1.65	EPA
2-Methylvaleraldehyde	18.800	1.67	EPA
2,4-Dihydroxybenzaldehyde	13.100	1.71	EPA
o-Nitrobenzaldehyde #1	12.500	1.74	EPA
o-Nitrobenzaldehyde #2	16.600	1.74	EPA
o-Fluorobenzaldehyde	1.350	1.76	EPA
Hexanal #1	22.000	1.78	EPA
Hexanal #2	14.000	1.78	EPA
p-Dimethylaminobenzaldehyde	45.700	1.81	EPA
Salicylaldehyde	2.300	1.81	EPA
3-Ethoxy-4-hydroxybenzaldehyde	87.600	1.88	EPA
5-Bromo-2-nitrovanillin	73.300	1.88	EPA
2,4-Dimethoxybenzaldehyde	20.100	1.91	EPA
2,3-Dimethylvaleraldehyde	16.000	2.07	EPA
5-Bromovanillin	59.700	2.09	EPA
4-Chlorobenzaldehyde	2.200	2.10	EPA
o-Tolualdehyde	52.900	2.26	EPA
2-Chloro-5-nitrobenzaldehyde #1	3.800	2.28	EPA
2-Chloro-5-nitrobenzaldehyde #2	3.950	2.28	EPA
p-Ethoxybenzaldehyde	28.100	2.31	EPA
4,6-Dimethoxy-2-hydroxy-benzaldehyde	2.680	2.33	EPA
Pentafluorobenzaldehyde	1.100	2.45	EPA
á,á,á-Trifluoro-m-tolualdehyde #3	1.130	2.47	EPA
á,á,á-Trifluoro-m-tolualdehyde #2	0.760	2.47	EPA
á,á,á-Trifluoro-m-tolualdehyde #1	0.920	2.47	EPA

Continued.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
2-Chloro-6-fluorobenzaldehyde	9.410	2.54	EPA
4-(Diethylamino)benzaldehyde	23.900	2.94	EPA
5-Chlorosalicylaldehyde	0.770	3.00	EPA
p-Isopropyl benzaldehyde	6.620	3.07	EPA
2,4-Dichlorobenzaldehyde	1.800	3.11	EPA
5-Bromosalicylaldehyde	1.300	3.15	EPA
4-(Diethylamino)salicylaldehyde	5.360	3.34	EPA
3,5-Dibromosalicylaldehyde	0.850	3.83	EPA
p-Phenoxybenzaldehyde	4.600	3.96	EPA
4-(Hexyloxy)-m-anisaldehyde	2.670	3.99	EPA
3-(3,4-Dichlorophenoxy) benzaldehyde	0.300	5.49	EPA
3-(4-Tert-butylphenoxy) benzaldehyde	0.370	5.93	EPA
Tetradecanal	*	6.12	EPA

* No effects at saturation.

EPA = USEPA (1991)

ALDEHYDES
7/1988

SAR **ALDEHYDES**

Organism: Daphnid
Duration: 48-h
Endpoint: LC50 (Mortality)

Equation: Log 48-h LC50 (mM/L) = -0.059 - 0.607 log K_{ow}

Statistics: N = 4; R^2 = 1.0

Maximum log K_{ow}: 6.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for aldehydes.

Limitations:

References:
Sloof W, Canton JH, and Hermens JLM. 1983. Comparison of the susceptibility of 22 freshwater species to 15 chemical compounds. I. (Sub)Acute toxicity tests. Aquatic Toxicology 4:113-128.

LIST OF ALDEHYDES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
Salicylaldehyde	5.4	2.1	S
Salicylaldehyde	5.5	2.1	S
Salicylaldehyde	5.8	2.1	S

S = Sloof et al (1983)

ALDEHYDES
9/1993

SAR	**ALDEHYDES**
Organism:	Green Algae
Duration:	96-h
Endpoint:	EC50 (Growth)
Equation:	Use green algae 96-h EC50 SAR developed for neutral organics.
Maximum log K_{ow}:	6.4
Maximum MW:	1000.0
Application:	The green algae 96-h SAR for neutral organics may be used to estimate toxicity for aldehydes.
Limitations:	
References:	See references for neutral organics.

ALDEHYDES
9/1993

SAR **ALDEHYDES**

Organism: Fish
Duration: 32-d
Endpoint: Chronic Value (Survival/Growth)

Equation: Log ChV = -0.81 - 0.68 log K_{ow}

Statistics: N = 3; R^2 = 0.97

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for aldehydes.

Limitations: If the log Kow is greater than 8.0, or if the ChV exceeds the water solubility, no effects expected at saturation.

References: United States Environmental Protection Agency (USEPA). 1991. Fish Chronic Toxicity Data Base. Duluth, MN: Environmental Research Laboratory (ERL), Office of Research and Development, USEPA, 6201 Congdon Boulevard, 55804; contact C.L. Russom (218) 720-5500.

LIST OF ALDEHYDES USED TO DEVELOP THE FISH 32-d Chronic Value (Survival/Growth) SAR.

CHEMICAL	32-d ChV (mg/L)	Log K_{ow}	Ref.
o-Tolualdehyde	1.61	2.1	D
á,á,á-Trifluoro-m-tolualdehyde	0.19	2.6	D

D = USEPA (1991)

ALDEHYDES
9/1993

SAR	**ALDEHYDES**
Organism:	Green Algae
Duration:	96-h
Endpoint:	Chronic Value (Growth)
Equation:	Use the equation for the green algae chronic value SAR developed for neutral organics.
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	The green algae chronic value SAR for neutral organics may be used to estimate toxicity for aldehydes.
Limitations:	If the log K_{ow} is greater than 8.0, or if the ChV exceeds the water solubility, no effects expected at saturation.
References:	Sloof W, Canton JH, and Hermens JLM. 1983. Comparison of the susceptibility of 22 freshwater species to 15 chemical compounds. I. (Sub)Acute toxicity tests. Aquatic Toxicology 4:113-128.

ALDEHYDES
9/1993

SAR	**AMINES, ALIPHATIC**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log 96-h LC50 (mM/L) = 0.72 - 0.64 log K_{ow}
Statistics:	N = 55; R^2 = 0.82
Maximum log K_{ow}:	6.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate the toxicity of aliphatic amines.
Limitations:	If the log K_{ow} value is greater than 6.0, no effects expected in a saturated solution.
References:	Bridie AL, Wolff CJM, and Winter M. 1979. The acute toxicity of some petrochemicals to goldfish. Water Research 13:623-626.
	Brooke LT, Call DJ, Geiger DL, and Northcott CE (eds). 1984. Acute toxicities of organic chemicals to fathead minnows (Pimephales promelas). Superior, WI: Center for Lake Superior Environmental Studies, University of Wisconsin-Superior. Volume I.
	Calamari D, DaGasso R, Galassi S, Provini A, and Vighi M. 1980. Biodegradation and toxicity of selected amines on aquatic organisms. Chemosphere 9:753-762.
	Geiger DL, Piorier SH, Brooke LT, and Call DJ (eds). 1986. Acute toxicities of organic chemicals to fathead minnows (Pimephales promelas). Superior, WI: Center for Lake Superior Environmental Studies, University of Wisconsin-Superior. Volume III.
	Geiger DL, Call DJ, and Brooke LT (eds). 1988. Acute toxicities of organic chemicals to fathead minnows (Pimephales promelas). Superior, WI: Center for Lake Superior Environmental Studies, University of Wisconsin-Superior. Volume IV.
	Platz RD and Nabholz JV. 1990. Generic environmental hazard assessment of aliphatic amines. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency. Unpublished manuscript.

United States Environmental Protection Agency (USEPA). 1990. Summary of structure-activity data files: University of Wisconsin - Superior (UWS) and Environmental Research Laboratory, Duluth, MN (ERL-D) research team. Computer printout from Environmental Effects Branch, HERD, USEPA, Washington, DC.

United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, United States Environmental Protection Agency.

LIST OF ALIPHATIC AMINES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Triethanolamine	1180.000	-1.59	EPA1
1,3-Diaminopropane	1190.000	-1.49	BR
Diethanolamine	47100.000	-1.46	EPA1
Ethanolamine	2070.000	-1.30	EPA1
Ethylenediamine	220.000	-1.22	EPA1
1,2-Diaminopropane	1010.000	-0.91	BR
Morpholine	380.000	-0.72	C
2-Methoxyethylamine	524.000	-0.67	BR
Dimethylamine	118.000	-0.52	C
2-(Ethylamino)ethanol	1480.000	-0.46	BR
Allylamine	27.000	-0.15	B
Ethylamine	227.000	-0.14	EPA1
N-(3-Methoxypropyl)-3,4,5-trimethoxybenzylamine	136.000	0.09	EPA1
5-Diethylamino-2-pentanone	336.000	0.35	G1
Propylamine	308.000	0.39	BR
N,N-Diethylethanolamine	1780.000	0.40	G1
Diallylamine	20.000	0.51	B
Diethylamine	855.000	0.54	BR
Diethylamine	182.000	0.54	C
tert-Butylamine	270.000	0.57	C
3-Dimethylaminopropyl chloride hydrochloride	133.000	0.66	G1
sec-Butylamine	275.000	0.70	EPA1
2-(Diisopropylamino)ethanol	201.000	0.86	G2
n-Butylamine	268.000	0.92	G1
Benzylamine	102.000	1.09	EPA1
1,2-Dimethylpropylamine	284.000	1.10	G1
Diisopropylamine	196.000	1.16	C
2,2-Dimethyl-1-propylamine	475.000	1.19	G1
1,8-Diamino-p-menthane	65.300	1.23	G2
Tripropargylamine	296.000	1.26	G1
Cyclohexylamine	90.000	1.37	C
N,N-bis(2,2-Diethoxyethyl) methylamine	634.000	1.39	G1
N,N-bis(2,2-Diethoxyethyl) methylamine	637.000	1.39	G1
Amylamine	177.000	1.45	G1
3,3-Dimethylbutylamine	602.000	1.72	G2
Chemical Identity CBI	778.000	1.93	EPA
N,N-Dimethylbenzylamine	37.800	1.98	EPA1
Hexylamine	56.600	1.98	G1

Continued.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
1-Adamantylamine	25.000	2.00	G1
N-Ethylbenzylamine	57.100	2.04	EPA1
tert-Octylamine	24.600	2.43	G2
Heptylamine	21.800	2.51	BR
Dibutylamine	37.000	2.66	C
Tripropylamine	50.900	2.82	G1
1-Methylheptylamine	5.110	2.82	BR
1-Methylheptylamine	5.280	2.82	BR
N,N-Diethylcyclohexylamine	21.400	2.98	G2
Octylamine	5.190	3.04	G2
Nonylamine	2.160	3.57	EPA1
Chemical identity CBI	2.800	4.10	EPA
Decylamine	1.030	4.10	EPA1
Undecylamine	0.210	4.63	EPA1
Dihexylamine	0.780	4.77	BR
Dodecylamine	0.103	5.16	EPA1
Tridecylamine	0.065	5.68	EPA1

EPA = USEPA (1991); Chemical identity is Confidential Business Information under TSCA.
EPA1 = USEPA (1990)
BR = Brooke et al (1984)
B = Bridie et al (1979)
C = Calamari et al (1980)
G1 = Geiger et al (1986)
G2 = Geiger et al (1988)

SAR	**AMINES, ALIPHATIC**
Organism:	Daphnids
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Log 48-h LC50 (mM/L) = -0.524 - 0.584 log K_{ow}
Statistics:	N = 10; R^2 = 0.78
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate the toxicity of aliphatic amines.
Limitations:	If the log K_{ow} value is greater than 5.0, no effects expected in a saturated solution.
References:	Cowgill UM, Takahashi IT, and Applegath SL. 1985. A comparison of the effect of four benchmark chemicals on Daphnia magna and Ceriodaphnia dubia/affinis tested at two different temperatures.
	Gersich FM, Milazzo DP, and Voos-Esquivel C. 1988. An invertebrate life-cycle study of the toxicity of Daphnia magna Straus. Mammalian and Environmental Toxicology Research Laboratory. Dow Chemical Company. Study ID: ES-DR-0065-5425-6.
	LeBlanc GA. 1980. Acute toxicity of priority pollutants to water flea (Daphnia magna). Bulletin of Environmental Contamination and Toxicology 24:684-691.
	Platz RD and Nabholz JV. 1990. Generic environmental hazard assessment of aliphatic amines. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency. Unpublished manuscript.
	United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, United States Environmental Protection Agency.
	Van Leeuwen CJ, Maas-Diepeveen JL, Niebeek G, Vergouw WHA, Griffioen PS, and Luijken MW. 1985. Aquatic toxicological aspects of dithiocarbamates and related compounds. I. Short-term toxicity tests. Aquatic Toxicology 7:145-164.

LIST OF ALIPHATIC AMINES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
Diethanolamine	131.000	-1.46	C
Diethanolamine	55.000	-1.46	L
Ethylenediamine	26.500	-1.22	VL
Chemical identity CBI	1760.000	-0.90	EPA
Dimethylamine	50.000	-0.52	VL
Chemical identity CBI	4.300	0.44	EPA
Diethylamine	56.000	0.54	VL
Chemical identity CBI	15.000	1.03	EPA
Chemical identity CBI	3.800	2.74	EPA
2-(Decylthio)ethylamine hydrochloride	0.033	4.85	G

C = Cowgill et al (1985)
EPA = USEPA (1991); Chemical identity is Confidential Business Information under TSCA.
G = Gersich et al (1988)
L = LeBlanc (1980)
VL = Van Leeuwen et al (1985)

SAR	**AMINES, ALIPHATIC**
Organism:	Green Algae
Duration:	96-h
Endpoint:	EC50 (Growth)
Equation:	Log 96-h EC50 (mM/L) = -0.548 - 0.434 log K_{ow}
Statistics:	N = 14; R^2 = 0.74
Maximum log K_{ow}:	7.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for aliphatic amines.
Limitations:	If the log K_{ow} value is greater than 7.0, no effects expected in a saturated solution.
References:	Calamari D, DaGasso R, Galassi S, Provini A, and Vighi M. 1980. Biodegradation and toxicity of selected amines on aquatic organisms. Chemosphere 9:753-762. Platz RD and Nabholz JV. 1990. Generic environmental hazard assessment of aliphatic amines. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency. Unpublished manuscript. United States Environmental Protection Agency (USEPA). 1990. Summary of structure-activity data files: University of Wisconsin - Superior (UWS) and Environmental Research Laboratory, Duluth, MN (ERL-D) research team. Computer printout from Environmental Effects Branch, HERD, USEPA, Washington, DC. United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, United States Environmental Protection Agency. Van Leeuwen CJ, Maas-Diepeveen JL, Niebeek G, Vergouw WHA, Griffioen PS, and Luijken MW. 1985. Aquatic toxicological aspects of dithiocarbamates and related compounds. I. Short-term toxicity tests. Aquatic Toxicology 7:145-164.

AMINES, ALIPHATIC

LIST OF ALIPHATIC AMINES USED TO DEVELOP THE ALGAL 96-h EC50 SAR.

CHEMICAL	96-h EC50 (mg/L)	Log K_{ow}	Ref.
Ethylenediamine	61.000	-1.22	VL
Morpholine	28.000	-0.72	C
Dimethylamine	30.000	-0.52	VL
Dimethylamine	9.000	-0.52	C
Diethylamine	20.000	0.54	C
Diethylamine	56.000	0.54	VL
tert-Butylamine	16.000	0.57	C
Chemical identity CBI	1.800	1.03	EPA
Diisopropylamine	20.000	1.16	C
Cyclohexylamine	20.000	1.37	C
Dibutylamine	19.000	2.66	C
Chemical identity CBI	1.040	2.74	EPA
Octylamine	0.220	3.04	EPA1
Chemical identity CBI	0.130	6.85	EPA

C = Calamari et al (1980)
EPA1 = USEPA (1990)
EPA = USEPA (1991); Chemical identity is Confidential Business Information under TSCA.
VL = Van Leeuwen et al (1985)

SAR	**AMINES, ALIPHATIC**
Organism:	Green Algae
Duration:	
Endpoint:	Chronic Value (Growth)
Equation:	Log ChV (mM/L) = -1.399 - 0.334 log K_{ow}
Statistics:	N = 11; R^2 = 0.61
Maximum log K_{ow}:	7.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for aliphatic amines.
Limitations:	If the log K_{ow} value is greater than 7.0, no effects expected at saturation.
References:	Calamari D, DaGasso R, Galassi S, Provini A, and Vighi M. 1980. Biodegradation and toxicity of selected amines on aquatic organisms. Chemosphere 9:753-762. Platz RD and Nabholz JV. 1990. Generic environmental hazard assessment of aliphatic amines. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency. Unpublished manuscript. United States Environmental Protection Agency (USEPA). 1989. Report on alga toxicity tests on selected OTS chemicals. Unpublished preliminary draft. Corvallis Environmental Research Laboratory. Corvallis, OR: United States Environmental Protection Agency. United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, United States Environmental Protection Agency.

AMINES, ALIPHATIC

LIST OF ALIPHATIC AMINES USED TO DEVELOP THE ALGAL ChV SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
Morpholine	1.000	-0.72	C
Dimethylamine	2.000	-0.52	C
Diethylamine	2.000	0.54	C
tert-Butylamine	2.000	0.57	C
Chemical identity CBI	0.110	1.03	EPA2
Diisopropylamine	5.000	1.16	C
Cyclohexylamine	5.000	1.37	C
Dibutylamine	2.500	2.66	C
Chemical identity CBI	0.410	2.74	EPA2
Octylamine	0.650	3.04	EPA1
Chemical identity CBI	0.050	6.85	EPA2

C = Calamari et al (1980)
EPA1 = USEPA (1989)
EPA2 = USEPA (1991); Chemical identity is Confidential Business Information under TSCA.

SAR	**ANILINES**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log 96-h LC50 (mM/L) = 0.956 - 0.739 log K_{ow}
Statistics:	N = 20; R^2 = 0.882
Maximum log K_{ow}:	7.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for anilines.
Limitations:	Di- and tri-nitroanilines are more toxic than predicted; a fish 96-h LC50 SAR has been developed for dinitroanilines. 2,3,5,6-Tetrachloroaniline is 19 times more toxic than predicted by this SAR. Tetrabromoaniline may be more toxic than predicted by this SAR as well. N-substituted anilines are less toxic than predicted by this SAR; for these compounds use the neutral organics fish 96-h LC50 SAR. If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	Veith GD and Broderius SJ. 1987. Structure-toxicity relationships for industrial chemicals causing type (II) narcosis syndrome. In: Kaiser KLE (ed.). QSAR in Environmental Toxicology-II. Boston, MA: D. Reidel Pub. Co., pp. 385-391.

ANILINES
7/1988

LIST OF ANILINES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
ANILINES USED IN CALCULATION OF THIS SAR			
aniline	134.0	0.9	VB
4-nitroaniline	125.0	1.3	VB
4-toluidine	149.0	1.4	VB
4-chloroaniline	32.5	1.8	VB
4-ethylaniline	73.0	2.0	VB
pentafluoroaniline	37.1	2.2	VB
2-chloro-4-nitroaniline	20.2	2.2	VB
4-bromoaniline	47.5	2.3	VB
4-ethoxy-2-nitroaniline	26.0	2.5	VB
á,á,á-4-tetrafluoro-2-toluidine	29.6	2.6	VB
á,á,á-4-tetrafluoro-3-toluidine	30.1	2.6	VB
3,4-dichloroaniline	7.6	2.7	VB
3-benzyloxyaniline	9.14	2.8	VB
4-butylaniline	10.2	3.2	VB
2,3,6-trichloroaniline	3.64	3.3	VB
4-hexyloxyaniline	3.2	3.7	VB
2,6-diisopropylaniline	15.3	4.1	VB
4-octylaniline	0.120	5.3	VB
4-decylaniline	0.062	6.3	VB
4-dodecyl aniline	.*	7.4	VB
ANILINES WITH EXCESS TOXICITY			
2,3,5,6-tetrachloroaniline	0.270	4.1	VB

* No fish mortality in saturated solutions.

VB = Veith and Broderius (1987)

SAR	**ANILINES**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Log 48-h LC50 (mM/L) = -1.623 - 0.271 log K_{ow}
Statistics:	N = 24; R^2 = 0.24
Maximum log K_{ow}:	7.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for anilines.
Limitations:	Di- and tri-nitroanilines are more toxic than predicted by this SAR; a daphnid 48-h LC50 SAR has been developed for dinitroanilines. Tetrachloro- and tetrabromo-aniline may be 20 times more toxic than predicted by this SAR. N-substituted anilines are less toxic than predicted by this SAR; for these compounds use the neutral organics daphnid 48-h LC50 SAR. If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	Canton JH and Adema DMM. 1978. Reproducibility of short-term and reproduction toxicity experiments with Daphnia magna and comparison of the sensitivity of Daphnia magna with Daphnia pulex and Daphnia cucullata in short-term experiments. Hydrobiologia 2:135-140. Kuhn R, Pattard M, Pernak K-D and Winter A. 1989. Results of the harmful effects of selected water pollutants (anilines, phenols, aliphatic compounds) to Daphnia magna. Water Research 23:495-499. Sloof W, Canton JH, and Hermens JLM. 1983. Comparison of the susceptibility of 22 freshwater species to 15 chemical compounds. I. (Sub)Acute toxicity tests. Aquatic Toxicology 4:113-128.

ANILINES
9/1993

LIST OF ANILINES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
p-aminophenol	0.240	0.2	K
m-aminophenol	1.1	0.2	K
aniline	0.640	0.6	S
benzidine (dianiline)	0.600	1.6	K
4-aminoacetophenone	5.0	0.9	K
aniline	0.300	0.9	K
aniline	0.100	0.9	CA
aniline	0.680	0.9	CA
p-methoxyaniline	1.9	1.0	K
2-amino-4-methoxyphenol	3.0	1.3	K
5-chloro-2,4-dimethoxyaniline	1.62	1.8	K
p-chloroaniline	0.310	1.9	K
m-chloroaniline	0.350	1.9	K
o-chloroaniline	1.8	1.9	K
p-ethylaniline	2.0	2.1	K
o-bromoaniline	3.0	2.1	K
o-ethylaniline	14.0	2.1	K
2,4-dimethylaniline	9.9	2.2	K
3-trifluoromethylaniline	2.7	2.3	K
4-chloro-2-nitroaniline	3.2	2.6	K
3-chloro-4-methylaniline	0.620	2.6	K
2,6-dichloroaniline	1.4	2.8	K
2,4-dichloroaniline	2.7	2.8	K

K = Kuhn et al (1989)
S = Sloof et al (1983)
CA = Canton and Adema (1978)

SAR	**ANILINES**
Organism:	Fish
Duration:	32-d
Endpoint:	Chronic Value (Survival/Growth)
Equation:	Log ChV (mM/L) = -1.516 - 0.625 log K_{ow}
Statistics:	N = 11; R^2 = 0.66
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for anilines.
Limitations:	N-substituted anilines are less toxic than predicted by this SAR; for these compounds use the neutral organics fish ChV SAR. If the log K_{ow} is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.
References:	Bresch H, Beck H, Ehlermann D, Schlaszus H and Urbanek M. 1990. A long-term toxicity test comprising reproduction and growth of zebrafish with 4-chloroaniline. Archives of Environmental Contamination and Chemistry 19:419-427. Call DJ, Poirier SH, Knuth ML, Harting SL and Lindbery CA. 1987. Toxicity of 3,4-dichloroaniline to fathead minnow, Pimephales promelas, in acute and early life-stage exposures. Bulletin of Environmental Contamination and Toxicology 38:352-358. United States Environmental Protection Agency (USEPA). 1990. Rainbow trout early life stage toxicity test with 2,6-dichloro-4-nitrobenzeneamine. TSCA Section 4 Test Report. Washington, DC: Office of Toxic Substances, USEPA. United States Environmental Protection Agency (USEPA). 1991. Fish Chronic Toxicity Data Base. Duluth, MN: Environmental Research Laboratory (ERL), Office of Research and Development, USEPA, 6201 Congdon Boulevard, 55804; contact C.L. Russom (218) 720-5500. Van Leeuwen CJ, Adema DMM and Hermens J. 1990. Quantitative structure-activity relationships for fish early life stage toxicity. Aquatic Toxicology 16:321-334.

ANILINES
9/1993

LIST OF ANILINES USED TO DEVELOP THE FISH CHRONIC VALUE (ChV) SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
aniline	1.8	0.9	VL
aniline	0.569	0.9	D
4-chloroaniline	0.400	1.8	B
3-chloroaniline	1.0	1.9	VL
3,4-dichloroaniline	0.020	2.7	C
3,4-dichloroaniline	0.006	2.7	C
3,5-dichloroaniline	0.320	2.9	VL
2,6-dichloro-4-nitroaniline	0.016	3.0	EPA
2,4,5-trichloroaniline	0.056	3.7	VL
2,3,4,5-tetrachloroaniline	0.032	4.6	VL
pentachloroaniline	0.010	5.1	VL

EPA = USEPA (1990)
C = Call et al (1987)
D = USEPA (1991)
VL = Van Leeuwen et al (1990)
B = Bresch et al (1990)

SAR **ANILINES**

Organism: Daphnid
Duration: 16-d
Endpoint: Chronic Value (Survival/Reproduction)

Equation: Log ChV (mM/L) = -3.12 - 0.36 log Kow

Statistics: N = 3;; R^2 = 0.98

Maximum log K_{ow}: 9.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for anilines.

Limitations: N-substituted anilines are less toxic than predicted by this SAR; for these compounds use the daphnid ChV SAR for neutral organics.

If the log Kow value is greater than 9.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.

References: United States Environmental Protection Agency (USEPA). 1990. Daphnid Chronic Toxicity Tests with aniline and 2-chloroaniline. TSCA Sec. 4 Test Reports. Washington, DC: U.S. Environmental Protection Agency, Office of Toxic Substances.

LIST OF ANILINES USED TO DEVELOP THE DAPHNID CHRONIC VALUE (ChV) SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
aniline	0.021	0.9	EPA
2-chloroaniline	0.034	1.9	EPA

EPA = USEPA (1990)

ANILINES
9/1993

SAR **ANILINES**

Organism: Green Algae
Duration:
Endpoint: Chronic Value (Growth)

Equation: Log ChV (mM/L) = -0.411 - 0.588 log K_{ow}

Statistics: N = 5; R^2 = 1.0

Maximum log K_{ow}: 9.0
Maximum MW: 1000.0

Application: This equation may be used to estimate toxicity for anilines.

Limitations: N-substituted anilines are less toxic than predicted by this SAR; for these compounds use the neutral organics green algae ChV SAR.

If the log Kow value is greater than 9.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.

References: Sloof W, Canton JH, and Hermens JLM. 1983. Comparison of the susceptibility of 22 freshwater species to 15 chemical compounds. I. (Sub)Acute toxicity tests. Aquatic Toxicology 4:113-128.

LIST OF ANILINES USED TO DEVELOP THE GREEN ALGAE CHRONIC VALUE (ChV) SAR.

CHEMICAL	Log ChV (mg/L)	Log K_{ow}	Ref.
aniline	11.0	0.9	S
aniline	8.0	0.9	S
aniline	16.0	0.9	S
aniline	10.0	0.9	S

S = Slooff et al (1987)

ANILINES
9/1993

SAR	**ANILINES**
Organism:	Fish
Duration:	14-d
Endpoint:	LC50 (Mortality)
Equation:	Log LC50 (mM/L) = 1.02 - 0.988 log K_{ow}
Statistics:	N = 17; R^2 = 0.783
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for the following classes of compounds: 1. Anilines 2. Chloroanilines 3. Alkylanilines
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	Hermans J, Leeuwangh P, and Musch A. 1984. Quantitative structure-activity relationships and mixture toxicity studies of chloro- and alkylanilines at an acute lethal toxicity level to the guppy, Poecilia reticulata. Ecotoxicology and Environmental Safety 8:388-394.

ANILINES
9/1993

LIST OF ANILINES USED TO DEVELOP THE FISH 14-d LC50 SAR.

CHEMICAL	Log LC50 (mg/L)	Log K_{ow}	Ref.
Aniline	125.0	1.03	H
2-Methylaniline	81.3	1.54	H
3-Methylaniline	36.3	1.54	H
4-Methylaniline	10.7	1.54	H
2-Chloroaniline	6.2	1.76	H
3-Chloroaniline	13.4	1.76	H
4-Chloroaniline	26.0	1.76	H
2-Ethylaniline	74.7	2.07	H
3-Ethylaniline	27.1	2.07	H
4-Ethylaniline	29.1	2.07	H
2,5-Dichloroaniline	1.65	2.42	H
2,4-Dichloroaniline	6.3	2.42	H
3,5-Dichloroaniline	3.9	2.42	H
3,4-Dichloroaniline	6.3	2.42	H
2,3,4-Trichloroaniline	1.4	3.17	H
2,4,5-Trichloroaniline	2.0	3.17	H
2,3,4,5-Tetrachloroaniline	0.36	3.92	H

H = Hermans et al (1984)

SAR **ANILINES, AMINO, META OR 1,3-SUBSTITUTED**

Organism: Fish
Duration: 96-h
Endpoint: LC50 (Mortality)

Equation: Log 96-h LC50 (mM/L) = 0.978 - 0.740 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum log K_{ow}: 7.0
Maximum MW: 1000.0

Application: This equation may be used to estimate toxicity for meta or 1,3 substituted amino anilines.

Limitations: If the log K_{ow} value is greater than 7.0, no effects expected at saturation. duration.

References: United States Environmental Protection Agency (USEPA). 1991. OTS TSCA Section 4 database. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF META SUBSTITUTED AMINO ANILINES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
m-Phenylenediamine	1618	-0.3	EPA

EPA = USEPA (1991)

ANILINES, AMINO, META OR 1,3-SUBSTITUTED

SAR	**ANILINES, AMINO, META OR 1,3-SUBSTITUTED**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Log 48-h LC50 (mM/L) = -1.44 - 0.466 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	7.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for meta or 1,3 substituted amino anilines.
Limitations:	If the log K_{ow} value is greater than 7.0, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS TSCA Section 4 database. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF META SUBSTITUTED AMINO ANILINES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
m-Phenylenediamine	5.9	-0.3	EPA

EPA = USEPA (1991)

ANILINES, AMINO, META OR 1,3-SUBSTITUTED

SAR	**ANILINES, AMINO, META OR 1,3-SUBSTITUTED**
Organism:	Green Algae
Duration:	96-h
Endpoint:	EC50
Equation:	Log 96-h EC50 (mM/L) = -1.8 - 0.333 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	6.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for meta or 1,3 substituted amino anilines.
Limitations:	If the log K_{ow} value is greater than 6.0, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS TSCA Section 4 database. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF META SUBSTITUTED AMINO ANILINES USED TO DEVELOP THE GREEN ALGAE 96-h EC50 SAR.

CHEMICAL	96-h EC50 (mg/L)	Log K_{ow}	Ref.
m-Phenylenediamine	2.4	-0.3	EPA

EPA = USEPA (1991)

ANILINES, AMINO, META OR 1,3-SUBSTITUTED
9/1993

SAR	**ANILINES, AMINO, META OR 1,3-SUBSTITUTED**
Organism:	Daphnid
Duration:	16-d
Endpoint:	Chronic Value
Equation:	Log ChV (mM/L) = -3.29 - 0.301 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for meta or 1,3 substituted amino anilines.
Limitations:	If the log K_{ow} value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS TSCA Section 4 database. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF META SUBSTITUTED AMINO ANILINES USED TO DEVELOP THE DAPHNID ChV SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
m-Phenylenediamine	0.070	-0.3	EPA

EPA = USEPA (1991)

ANILINES, AMINO, ORTHO OR 1,2-SUBSTITUTED
9/1993

SAR	**ANILINES, AMINO, ORTHO OR 1,2-SUBSTITUTED**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log 96-h LC50 (mM/L) = -0.547 - 0.522 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	7.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for ortho or 1,2 substituted amino anilines.
Limitations:	If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS TSCA Section 4 database. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF ORTHO SUBSTITUTED AMINO ANILINES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
o-Phenylenediamine	44	-0.3	EPA

EPA = USEPA (1991)

ANILINES, AMINO, ORTHO OR 1,2-SUBSTITUTED
9/1993

SAR	**ANILINES, AMINO, ORTHO OR 1,2-SUBSTITUTED**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Log 48-h LC50 (mM/L) = -2.21 - 0.356 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	7.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for ortho or 1,2 substituted amino anilines.
Limitations:	If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS TSCA Section 4 database. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF ORTHO SUBSTITUTED AMINO ANILINES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
o-Phenylenediamine	0.880	-0.3	EPA

EPA = USEPA (1991)

ANILINES, AMINO, ORTHO OR 1,2-SUBSTITUTED
9/1993

SAR	**ANILINES, AMINO, ORTHO OR 1,2-SUBSTITUTED**
Organism:	Green Algae
Duration:	96-h
Endpoint:	EC50
Equation:	Log 96-h EC50 (mM/L) = -2.848 - 0.159 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	6.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for ortho or 1,2 substituted amino anilines.
Limitations:	If the log K_{ow} value is greater than 6.0, or if the compound is solid and the EC50 exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS TSCA Section 4 database. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF ORTHO SUBSTITUTED AMINO ANILINES USED TO DEVELOP THE GREEN ALGAE 96-h EC50 SAR.

CHEMICAL	96-h EC50 (mg/L)	Log K_{ow}	Ref.
o-Phenylenediamine	0.160	-0.3	EPA

EPA = USEPA (1991)

ANILINES, AMINO, PARA OR 1,4-SUBSTITUTED
9/1993

SAR	**ANILINES, AMINO, PARA OR 1,4-SUBSTITUTED**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log 96-h LC50 (mM/L) = -3.337 - 0.123 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	7.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for para or 1,4 substituted amino anilines.
Limitations:	If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS TSCA Section 4 database. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF PARA SUBSTITUTED AMINO ANILINES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
p-Phenylenediamine	0.060	-0.3	EPA

EPA = USEPA (1991)

ANILINES, AMINO, PARA OR 1,4-SUBSTITUTED
9/1993

SAR	**ANILINES, AMINO, PARA OR 1,4-SUBSTITUTED**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Log 48-h LC50 (mM/L) = -2.686 - 0.288 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	7.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for para or 1,4 substituted amino anilines.
Limitations:	If the log K_{ow} is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS TSCA Section 4 database. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF PARA SUBSTITUTED AMINO ANILINES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
p-Phenylenediamine	0.280	-0.3	EPA

EPA = USEPA (1991)

ANILINES, AMINO, PARA OR 1,4-SUBSTITUTED
9/1993

SAR	**ANILINES, AMINO, PARA OR 1,4-SUBSTITUTED**
Organism:	Green Algae
Duration:	96-h
Endpoint:	EC50
Equation:	Log 96-h EC50 (mM/L) = -2.657 - 0.190 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	6.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for para or 1,4 substituted amino anilines.
Limitations:	If the log K_{ow} value is greater than 6.0, or if the compound is solid and the EC50 exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS TSCA Section 4 database. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF PARA SUBSTITUTED AMINO ANILINES USED TO DEVELOP THE GREEN ALGAE 96-h EC50 SAR.

CHEMICAL	96-h EC50 (mg/L)	Log K_{ow}	Ref.
p-Phenylenediamine	0.28	-0.3	EPA

EPA = USEPA (1991)

SAR **ANILINES, DINITRO**

Organism: Fish
Duration: 96-h
Endpoint: LC50 (Mortality)

Equation: Log 96-h LC50 (mM/L) = -0.027 - 0.596 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum log K_{ow}: 7.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for dinitroanilines and other polynitroanilines.

Limitations: If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.

References: Veith GD and Broderius SJ. 1987. Structure-toxicity relationships for industrial chemicals causing type (II) narcosis syndrome. In: Kaiser KLE (ed.). QSAR in Environmental Toxicology-II. Boston, MA: D. Reidel Pub. Co., pp. 385-391.

LIST OF DINITROANILINES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-hour LC50 (mg/L)	Log K_{ow}	Ref.
2,4-dinitroaniline	15.5	1.8	VB

VB = Veith and Broderius (1987)

ANILINES, DINITRO
9/1993

SAR **ANILINES, DINITRO**

Organism: Daphnid
Duration: 48-h
Endpoint: LC50 (Mortality)

Equation: log 48-h LC50 (mM/L) = -0.296 - 0.558 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum log K_{ow}: 7.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for dinitroanilines and other polynitroanilines.

Limitations: If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.

References: Kuhn R, Pattard M, Pernak K-D, and Winter A. 1989. Results of the harmful effects of selected water pollutants (anilines, phenols, aliphatic compounds) to Daphnia magna. Water Research 23:495-499.

LIST OF DINITROANILINES USED TO DEVELOP THE DAPHNID 48-h LC50.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
2,4-dinitroaniline	9.6	1.8	K

Kuhn = Kuhn et al (1989)

ANILINES, DINITRO
9/1993

SAR **ANILINES, DINITRO**

Organism: Fish
Duration: 32-d
Endpoint: Chronic Value (Survival/Growth)

Equation: Log ChV (mM/L) = -0.91 - 0.661 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for dinitroanilines and other polynitroanilines.

Limitations: If the log K_{ow} value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.

References: United States Environmental Protection Agency (USEPA). 1991. Fish Chronic Toxicity Data Base. Duluth, MN: Environmental Research Laboratory (ERL), Office of Research and Development, USEPA, 6201 Congdon Boulevard, 55804; contact C.L. Russom (218) 720-5500.

LIST OF DINITROANILINES USED TO DEVELOP THE FISH CHRONIC (ChV) SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
2,4-dinitroaniline	1.41	1.8	D

D = USEPA (1991)

ANILINES, DINITRO
9/1993

SAR **AZIRIDINES**

Organism: Fish
Duration: Acute
Endpoint: LC50 (Mortality)

Equation: Log LC50 (mM/L) = -1.65 - 0.364 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum log K_{ow}: 7.0
Maximum MW: 1000.0

Application: This equation may be used to estimate toxicity for aziridines.

Limitations: If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.

References: Juhnke I and Luedemann D. 1978. Results of the investigation of 200 chemical compounds for acute toxicity with the Golden Orfe test. Z.F. Wasser-Und Abwasser-Forschung 11:161-164. Translation by SCITRAN (Scientific Translation Service), Santa Barbara, CA 93108.

LIST OF AZIRIDINES USED TO DEVELOP THE FISH ACUTE LC50 SAR.

CHEMICAL	LC50 (mg/L)	Log K_{ow}	Ref.
Aziridine	2.4	-1.1	J

J = Juhnke and Luedemann (1978)

AZIRIDINES
9/1993

SAR **AZIRIDINES**

Organism: Daphnid
Duration: 48-h
Endpoint: LC50 (Mortality)

Equation: Log 48-h LC50 (mM/L) = -1.062 - 0.52 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum log K_{ow}: 7.0
Maximum MW: 1000.0

Application: This equation may be used to estimate toxicity for aziridines.

Limitations: If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.

References: Bringmann G and Kuhn R. 1977. Results of the damaging effect of water pollutants on Daphnia magna. Z. Wasser Abwasser Forsch. 10(5):161-166.

LIST OF AZIRIDINES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	LC50 (mg/L)	Log K_{ow}	Ref.
Aziridine	14.0	-1.1	B

B = Bringmann and Kuhn (1977)

AZIRIDINES
9/1993

SAR	**AZIRIDINES**
Organism:	Green Algae
Duration:	7-d
Endpoint:	Chronic Value
Equation:	Log ChV (mM/L) = -2.4 - 0.33 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for aziridines.
Limitations:	If the log K_{ow} value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.
References:	Bringmann G and Kuhn R. 1980. Comparison of the toxicity thresholds of water pollutants to bacteria, algae, and protozoa in the cell multiplication inhibition test. Water Research 14(3):231-241.

LIST OF AZIRIDINES USED TO DEVELOP THE GREEN ALGAE CHV SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
Aziridine	0.370	-1.1	B

B = Bringmann and Kuhn (1980)

AZIRIDINES
9/1993

SAR **BENZENES, DINITRO**

Organism: Fish
Duration: 96-h
Endpoint: LC50 (Mortality)

Equation: Log 96-h LC50 (mM/L) = -1.867 - 0.333 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum log K_{ow}: 7.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for dinitrobenzenes and other polynitrobenzenes.

Limitations: If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.

References:

Veith GD and Broderius SJ. 1987. Structure-toxicity relationships for industrial chemicals causing type (II) narcosis syndrome. In: Kaiser KLE (ed.). QSAR in Environmental Toxicology-II. Boston, MA: D. Reidel Pub. Co., pp. 385-391.

United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF DINITROBENZENES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
1,3-dinitrobenzene	0.71	1.5	VB
Chemical identity CBI	0.013	3.2	EPA

VB = Veith and Broderius (1987)
EPA = USEPA (1991); chemical identity is Confidential Business Information under TSCA.

BENZENES, DINITRO
9/1993

SAR **BENZENES, DINITRO**

Organism: Daphnid
Duration: 48-h
Endpoint: LC50 (Mortality)

Equation: Log 48-h LC50 (mM/L) = -0.325 - 0.634 log K_{ow}

Statistics: N = 3; R^2 = 0.86

Maximum log K_{ow}: 7.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for dinitrobenzenes or other polynitrobenzenes.

Limitations: If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.

References:

Hermens J, Canton J, Janssen P, and DeJong R. 1984. Quantitative structure-activity relationships and toxicity studies of mixtures of chemicals with anaesthetic potency: Acute lethal and sublethal toxicity to Daphnia magna. Aquatic Toxicology 5:143-154.

LeBlanc. 1980. Acute toxicity of priority pollutants to water flea (Daphnia magna). Bulletin of Environmental Contamination and Toxicology. 24: 684-691.

United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF DINITROBENZENES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
1,3-dinitrobenzene	43.0	1.6	H
2,3-dinitrotoluene	0.66	2.0	LB
Chemical identity CBI	0.012	3.2	EPA

LB = LeBlanc (1987)

BENZENES, DINITRO
9/1993

H = Hermens et al (1984)
EPA = USEPA (1991); chemical identities are Confidential Business Information under TSCA.

SAR **BENZENES, DINITRO**

Organism: Fish
Duration: 32-d
Endpoint: Chronic Value (Survival/Growth)

Equation: Log ChV (mM/L) = -3.0 - 0.40 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for dinitrobenzenes or other polynitrobenzenes.

Limitations: If the log K_{ow} value is greater than 8.0, or is the compound is solid and the ChV exceeds the water solubility, no effects are expected at saturation.

References: United States Environmental Protection Agency (USEPA). 1991. Fish Chronic Toxicity Data Base. Duluth, MN: Environmental Research Laboratory (ERL), Office of Research and Development, USEPA, 6201 Congdon Boulevard, 55804; contact C.L. Russom (218) 720-5500.

LIST OF DINITROBENZENES USED TO DEVELOP THE FISH CHRONIC VALUE (ChV) SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
1,3-dichloro-4,6-dinitro benzene	0.023	2.5	D

D = USEPA (1991)

BENZENES, DINITRO
9/1993

SAR **BENZENES, DINITRO**

Organism: Daphnid
Duration: 16-d
Endpoint: Chronic Value (Survival/Reproduction)

Equation: Log ChV (mM/L) = -0.7 - 0.625 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for dinitrobenzenes or other polynitrobenzenes.

Limitations: If the log K_{ow} value is greater than 8.0, or is the compound is solid and the ChV exceeds the water solubility, no effects are expected at saturation.

References: Hermens J, Canton H, Janssen P, and DeJong R. 1984. Quantitative structure-activity relationships and toxicity studies of mixtures of chemicals with anaesthetic potency: Acute lethal and sublethal toxicity to Daphnia magna. Aquatic Toxicology 5:143-154.

LIST OF DINITROBENZENES USED TO DEVELOP THE DAPHNID CHRONIC VALUE (ChV) SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
1,3-dinitrotoluene	3.2	1.6	H

H = Hermens et al (1984)

BENZENES, DINITRO
9/1993

SAR **BENZOTRIZOLES**

Organism: Fish
Duration: 96-h
Endpoint: LC50 (Mortality)

Equation: Log LC50 (mM/L) = 0.366 - 0.587 log K_{ow}

Statistics: N = 2; R^2 = 1.00

Maximum log K_{ow}: 5.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate the toxicity of substituted benzotriazoles with substitution on the 5th position. Toxicity estimates for substituted benzotriazoles with substitutions on the triazole ring may not be valid with this SAR.

This SAR may be used for substituted benzotriazoles with substitutions on the 3rd, 4th or 6th positions (other benzo positions).

Limitations: If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.

References: Nabholz JV. 1987. Generic review of various benzotriazoles. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency.

LIST OF BENZOTRIAZOLES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	LC50 (mg/L)	Log K_{ow}	Ref.
Benzotriazole	39.0	1.45	N
5-Butylbenzotriazole	2.8	3.68	N

N = Nabholz (1987).

BENZOTRIAZOLES
7/1988

SAR **BENZOTRIAZOLES**

Organism: Daphnid
Duration: 48-h
Endpoint: LC50 (Mortality)

Equation: To determine the acute toxicity of benzotriazoles to daphnids use the neutral organic daphnid 48-h LC50 SAR.

Statistics:

Maximum log K_{ow}: 5.0
Maximum MW: 1000.0

Application: The neutral organic SAR may be used to estimate the toxicity of substituted benzotriazoles with substitution on the 5th position, log K_{ow} values of less than 5.0, and molecular weights less than 1000. Toxicity estimates for substituted benzotriazoles with substitutions on the triazole ring may not be valid with this SAR.

This SAR may be used for substituted benzotriazoles with substitutions on the 3rd, 4th or 6th positions (other benzo positions).

Limitations: If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.

References: Nabholz JV. 1987. Generic review of various benzotriazoles. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency.

LIST OF BENZOTRIAZOLES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	LC50 (mg/L)	Log K_{ow}	Ref.
Benzotriazole	141.6	1.45	N
5-Butylbenzotriazole	10.7	3.68	N

N = Nabholz (1987).

BENZOTRIAZOLES
7/1988

SAR **BENZOTRIAZOLES**

Organism: Green Algae
Duration: 96-h
Endpoint: EC50 and EC10 (Growth)

Equation: Log EC50 (mM/L) = 0.061 - 0.573 log K_{ow}

The 96-h EC10 may be determined by:

EC10 = EC50/8

Statistics: N = 2; R^2 = 1.00

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate the toxicity of substituted benzotriazoles with substitution on the 5th position. Toxicity estimates for substituted benzotriazoles with substitutions on the triazole ring may not be valid with this SAR.

This SAR may be used for substituted benzotriazoles with substitutions on the 3rd, 4th or 6th positions (other benzo positions).

Limitations: If the log K_{ow} value is greater than 8.0, or if the compound is solid and the EC50 or EC10 exceeds the water solubility, no effects expected at saturation.

References: Nabholz JV. 1987. Generic review of various benzotriazoles. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency.

LIST OF BENZOTRIAZOLES USED TO DEVELOP THE GREEN ALGAE 96-h EC50 AND EC10 SARs.

CHEMICAL	EC50 (mg/L)	EC10 (mg/L)	Log K_{ow}	Ref.
Benzotriazole	15.4	1.75	1.45	N
5-Butylbenzotriazole	1.18	0.16	3.68	N

N = Nabholz (1987)

BENZOTRIAZOLES
7/1988

CARBAMATES
7/1988

SAR	**CARBAMATES**
Organism:	Sea Urchin
Duration:	48-h
Endpoint:	NEC (Early Development)
Equation:	Log NEC (mM/L) = 0.51 - 0.72 log K_{ow}
Statistics:	N = 35; R^2 = 0.62
Maximum log K_{ow}:	4.5
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for carbamates and the following classes of carbamates: 1. Alkyl esters of carbamic acid 2. N-alkyl or aryl substitutes on ethyl carbamate 3. Bis(ethylcarbamates) joined at -NRN- by alkyl or aryl groups 4. Bis- and tris- carbamates esterified on a single phenyl ring 5. Thiocarbamates This SAR may be used for other similar substituted carbamates with log K_{ow} values less than 4.5 and molecular weights less than 1000.
Limitations:	The following classes of carbamates are more toxic than predicted by this SAR: 1. Meta-phenylene bis(ethyl carbamates) - 200 X 2. N-methyl-ortho phenyl biscarbamates - 1000 X 3. N-methyl-para phenyl biscarbamates - 400 X 4. N,N-dimethyl-1,2,3-phenyl triscarbamates - 400 X If the log K_{ow} value is greater than 4.5, or if the compound is solid and the NEC exceeds the water solubility, no effects expected at saturation.
References:	Cornman I. 1950. Inhibition of sea-urchin egg cleavage by a series of substituted carbamates. Journal of the National Cancer Institute 50:1123-1138.

LIST OF CARBAMATES USED TO DEVELOP THE SEA URCHIN 48-h NEC SAR.

CHEMICAL	48-h NEC (mg/L)	Log K_{ow}	Ref.
CARBAMATES USED FOR THIS SAR			
Methyl carbamate	2000.0	-0.70	C
Ethyl carbamate	999.0	-0.18	C
1,2-Hydrazine di(ethylcarboxylate)	2000.0	-0.11	C
1,2-Hydrazine di(ethylcarboxylate)	1000.0	-0.11	C
N-methyl-ethylcarbamate	10.3	0.37	C
N,N-dimethyl-ethylcarbamate	994.0	0.42	C
Propylene bis(ethylcarbamate)	998.0	0.58	C
1,4-Phenylene bis(N,N-dimethyl carbamate	501.0	0.88	C
1,4-Phenylene bis(N,N-dimethyl carbamate	101.0	0.88	C
N-ethyl-ethylcarbamate	99.0	0.90	C
Ethylidene bis(ethylcarbamate)	100.0	0.97	C
Ethylene bis(ethylcarbamate)	100.0	0.98	C
Tetramethylene bis(ethylcarbamate)	998.0	0.58	C
N-isopropyl-ethylcarbamate	9.2	1.21	C
3-Methylbutyl carbamate	10.5	1.28	C
Cyclohexyl carbamate	1.43	1.33	C
N,N-propyl-ethylcarbamate	97.0	1.43	C
N,N-diethyl-ethylcarbamate	95.7	1.48	C
N,N-cyclopentamethylene-ethylcarbamate	39.1	1.61	C
N,N-diethyl ethylcarbamodithioate	<41.0	1.68	C
N,N-butyl-ethylcarbamate	8.7	1.96	C
1,3-Phenylene bis(N,N-dimethyl carbamate	<39.0	2.09	C
N,N-di-isopropyl-ethylcarbamate	92.0	2.09	C
N-ethyl ethylcarbamothioate	<39.0	2.09	C
Para-xylylene bis(ethylcarbamate)	19.6	2.14	C
Hexamethylene bis(ethylcarbamate)	502.0	2.16	C
Hexamethylene bis(ethylcarbamate)	99.0	2.16	C
N-phenyl-ethylcarbamate	1.0	2.29	C
N-cyclohexyl-ethylcarbamate	1.7	2.40	C
Ortho-phenylene bis (ethylcarbamate)	20.2	2.44	C
N,N-di-n-propyl-ethylcarbamate	9.4	2.53	C
N,N-di-n-butyl-ethylcarbamate	10.0	3.59	C
N,N-diphenyl-ethylcarbamate	9.6	NC	C
N-decyl carbamate	1.0	4.06	C
N-n-octyl-ethylcarbamate	1.0	4.07	C
N-2-fluorene-ethylcarbamate	<0.10	4.34	C
2,7-fluorene-bis(ethylcarbamate)	*	4.52	C

CARBAMATES
7/1988

CONTINUED.

CHEMICAL	48-h NEC (mg/L)	Log K_{ow}	Ref.
CARBAMATES USED FOR THIS SAR			
n-Dodecyl carbamate	*	5.12	C
N-n-decyl-ethylcarbamate	*	5.13	C
CARBAMATES WITH EXCESSIVE TOXICITY			
1,2-Phenylene bis(N-methyl carbamate	0.9	-0.11	C
1,3-Phenylene bis(N-methyl carbamate	0.9	-0.11	C
1,4-Phenylene bis(n-methyl carbamate	0.9	0.45	C
1,2,3-Phenylene tris(N,N-dimethyl carbamate	10.2	2.44	C

* No effects in a saturated solution.

C = Cornman (1950)

CARBAMATES, DITHIO
9/1993

SAR **CARBAMATES, DIOTHIO**

Includes N,N-dialkyldithiocarbamates and ethylenebisdithiocarbamates and their metal salts which include but are not limited to Zn, Na, Fe, Mn, Cu, Pb, Hg, Ag, and Se. The SARs for the dithiocarbamates and their degradation products are sigmoidal with acute and chronic toxicity increasing with increasing Kow. The sigmoidal relationship between Kow and toxicity is very poor statistically. Consequently, toxicity predictions must be made using either the closest analog or averaging data for the two closest analogs which bracket the dithiocarbamate under question.

CROWN ETHERS
9/1993

SAR **CROWN ETHERS**

Use SAR for **NEUTRAL ORGANICS** for fish and daphnids; some should show excess toxicity toward green algae due to over chelation of nutrient elements; each crown ether chelates a different element; the type of element chelated by a crown ether has to be matched up with a nutrient element needed by algae, e.g, Fe, Ca, Mg. There are no test data to show that crown ethers do in fact overchelate nutrient elements in the algal toxicity test. Conclusions about crown ethers are based on extrapolations of theory.

DIAZONIUMS, AROMATIC
9/1993

SAR	**DIAZONIUMS, AROMATIC**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log 96-h LC50 (mM/L) = -2.456 - 0.331 log K_{ow}
Statistics:	N = 3; R^2 = 0.98
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for aromatic diazoniums.
Limitations:	If the log K_{ow} value is greater than 8.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS TSCA 8(e) database. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF AROMATIC DIAZONIUMS USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
4-Dimethylamino benzene diazonium	0.150	2.1	EPA
4-Dimethylamino benzene diazonium	0.330	2.1	EPA

EPA = USEPA (1991).

EPOXIDES, MONO
9/1993

SAR	**EPOXIDES, MONO**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log 96-h LC50 (mM/L) = -0.290 - 0.382 log K_{ow}
Statistics:	N = 4; R^2 = 0.92
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for monoepoxides.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation. Monoepoxides which are significantly more toxic than predicted by this SAR, based on the fish 14-d LC50 SAR, are: epichlorohydrin, and epibromohydrin. Endrin has an excess toxicity of over 33,000 times the value predicted by this SAR. Diepoxides are significantly more toxic than predicted by this SAR and a SAR for diepoxides has been developed.
References:	Bridie AL, Wolff CJM, and Winter M. 1979. The acute toxicity of some petrochemicals to goldfish. Water Research, 13: 623-626. Conway RA, Waggy GT, Speigel MH, and Berglund RL. 1983. Environmental fate and effects of ethylene oxide. Environmental Science and Technology 17:107-112. Leach JM and Thakore AN. 1975. Isolation and identification of constituents toxic to juvenile rainbow trout (Salmo gairdneri) in caustic extraction effluents from kraft pulpmill bleach plants. Journal of the Fisheries Research Board of Canada, 32: 1249. United States Environmental Protection Agency (USEPA). 1986. Water Quality Criteria for 1986. Washington, DC: USEPA.

LIST OF MONOEPOXIDES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
MONOEPOXIDES USED IN CALCULATION OF THE SAR			
Ethylene oxide	84.0	-0.8	C
Allyl glycidyl ether	30.0	-0.33	B
Phenyl glycidyl ether	43.0	1.12	B
9,10-Epoxystearic acid	1.5	5.14	LT
MONOEPOXIDES HAVING EXCESS TOXICITY			
Endrin	0.000410	2.9	W

B = Bridie et al. (1979)
C = Conway et al (1983)
LT = Leach and Thakore (1975)
W = USEPA (1986); water quality criteria document

EPOXIDES, MONO
9/1993

SAR	**EPOXIDES, MONO**
Organism:	Fish
Duration:	14-d
Endpoint:	LC50 (Mortality)
Equation:	Log 14-d LC50 (mM/L) = -0.49506 - 0.34618 log K_{ow}
Statistics:	N = 9; R^2 = 0.87
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for monoepoxides.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation. Monoepoxides which are significantly more toxic than predicted by this SAR are: epichlorohydrin, 53 X excess toxicity; and epibromohydrin, 57 X excess toxicity. Diepoxides are significantly more toxic than predicted by this SAR and a SAR for diepoxides has been developed.
References:	Deneer JW, Sinnige TL, Seinen W, and Hermens JLM. 1988. A quantitative structure-activity relationship for the acute toxicity of some epoxy compounds to the guppy. Aquatic Toxicology 13:195-204.

LIST OF MONOEPOXIDES USED TO DEVELOP THE FISH 14-d LC50 SAR.

CHEMICAL	14-d LC50 (mg/L)	Log K_{ow}	Ref.
MONOEPOXIDES USED IN CALCULATION OF THE SAR			
Glycidol	50.0	-1.46	D
Propylene oxide	31.9	-0.27	D
1,2-Epoxybutane	32.9	0.26	D
Styrene oxide	7.07	0.73	D
1,2-Epoxyhexane	18.6	1.31	D
1,2-Epoxyoctane	10.4	2.37	D
1,2-Epoxydecane	3.26	3.43	D
1,2-Epoxydodecane	1.11	4.49	D
1,2-Epoxyhexadecane	*	6.60	D
MONOEPOXIDES HAVING EXCESS TOXICITY			
Epichlorohydrin	0.651	-0.21	D
Epibromohydrin	0.807	-0.07	D

* No fish mortality in saturated solutions.

D = Deneer et al (1988)

EPOXIDES, MONO
9/1993

SAR	**EPOXIDES, MONO**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Log 48-h LC50 (mM/L) = 0.036 - 0.567 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for monoepoxides.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	Conway RA, Waggy GT, Speigel MH, and Berglund RL. 1983. Environmental fate and effects of ethylene oxide. Environmental Science and Technology 17:107-112.

LIST OF MONOEPOXIDES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
Ethylene oxide	137.0	-0.8	C

C = Conway et al. (1983)

EPOXIDES, DI
9/1993

SAR	**EPOXIDES, DI**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log 96-h LC50 (mM/L) = -1.184 - 0.263 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for diepoxides and other polyepoxides.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	Bailey RE and Rhinehart WL. 1976. Evaluation of D.E.R. 331, diglycidyl ether of bisphenol-A, in the aquatic environment. R&D Report D0004653. Midland, MI: The Dow Chemical Company. United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: USEPA, Office of Toxic Substances.

LIST OF DIEPOXIDES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Diglycidyl ether of bisphenol A	3.1	3.1	B
Chemical identity CBI	*	7.1	EPA

* No fish mortality in saturated solutions.

B = Bailey and Rhinehart (1976)
EPA = USEPA (1991); chemical identity is Confidential Business Information under TSCA.

EPOXIDES, DI
9/1993

SAR	**EPOXIDES, DI**
Organism:	Fish
Duration:	14-d
Endpoint:	LC50 (Mortality)
Equation:	Log 14-d LC50 (mM/L) = -1.5692 - 0.1216 log K_{ow}
Statistics:	N = 3; R^2 = 0.83
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for diepoxides and other polyepoxides.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	Deneer JW, Sinnige TL, Seinen W and Hermens JLM. 1988. A quantitative structure-activity relationship for the acute toxicity of some epoxy compounds to the guppy. Aquatic Toxicology 13:195-204.

LIST OF DIEPOXIDES USED TO DEVELOP THE FISH 14-d LC50 SAR.

CHEMICAL	14-d LC50 (mg/L)	Log K_{ow}	Ref.
1,3-Butadiene diepoxide	2.66	-1.84	D
1,2,7,8-Diepoxyoctane	6.64	-0.18	D

D= Deneer et al (1988)

EPOXIDES, DI
9/1993

SAR	**EPOXIDES, DI**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Log 48-h LC50 (mM/L) = -2.093 - 0.1474 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for diepoxides and other polyepoxides.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	Bailey RE and Rhinehart WL. 1976. Evaluation of D.E.R. 331, diglycidyl ether of bisphenol-A, in the aquatic environment. R&D Report D0004653. Midland, MI: The Dow Chemical Company.

LIST OF DIEPOXIDES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
Diglycidyl ether of bisphenol A	0.95	3.1	B

B = Bailey and Rhinehart (1976)

ESTERS
9/1993

SAR	**ESTERS**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log LC50 (mM/L) = -0.535 log K_{ow} + 0.25
Statistics:	N = 29; R^2 = 0.828
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for the following esters: 1. Acetates 2. Benzoates 3. Dicarboxylic aliphatics 4. Phthalates derived from aliphatic alcohols and phenol.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	Veith GD, DeFoe D, and Knuth M. 1984. Structure-activity relationships for screening organic chemicals for potential ecotoxicity effects. Drug Metabolism Reviews 15(7):1295-1303.

LIST OF ESTERS USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Methylene chloride	322.895	1.25	Z
Methyl acetate	320.0	0.18	V
Ethyl acetate	230.0	0.69	V
2-Ethoxyethyl acetate	42.2	0.71	V
Diethyl malonate	14.9	1.19	V
Ethyl-p-aminobenzoate	35.2	1.22	V
Propyl acetate	60.0	1.25	V
Methyl-2,4-dihydroxybenzoate	38.5	1.59	V
Butyl acetate	18.0	1.79	V
Diethyl adipate	19.3	1.80	V
Methyl-p-nitrobenzoate	23.6	2.10	V
Dimethyl-2-nitro-p-phthalate	6.52	2.28	V
Methyl-4-chloro-2-nitrobenzoate	27.2	2.35	V
Dimethyl-2-amino-p-phthalate	8.94	2.65	V
Diethyl-o-phthalate	30.0	2.69	V
Hexyl acetate	4.40	2.87	V
Ethyl hexanoate	8.90	2.87	V
Methyl-p-chlorobenzoate	10.9	3.15	V
Methyl-2,5-dichlorobenzoate	13.8	3.45	V
Ethyl salicylate	19.6	3.45	V
Dibutyl succinate	4.45	3.65	V
Dibutyl adipate	3.66	3.96	V
Diethyl sebacate	2.75	3.96	V
Di-n-butyl-o-phthalate	1.10	4.74	V
Di-n-butyl-m-phthalate	0.90	5.07	V
Diphenyl-1-phthalate	0.80	7.06	V
Di-2-ethylhexyl-o-phthalate	*	7.06	V
Di-n-octyl-o-phthalate	*	7.06	V
Di-n-octyl-m-phthalate	*	7.06	V
Di-n-octyl-p-phthalate	*	7.06	V

* = No fish mortality in saturated solutions.

V = Veith et al (1984)

ESTERS
7/1988

SAR	**ESTERS**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	To find the estimated acute toxicity of an ester, use the neutral organics daphnid 48-h LC50 SAR.
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	The daphnid 48-h LC50 SAR for neutral organics may be used to estimate acute toxicity for esters. The neutral organic 48-h LC50 SAR for daphnids may be used for other esters; however, a separate SAR has been developed for phthalate esters.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	Kuhn R, Pattard M, Pernack K-D, and Winter A. 1989. Results of the harmful effects of selected water pollutants (anilines, phenols, aliphatic compounds) to Daphnia magna. Water Research 23:495-499. United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

LIST OF ESTERS USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL		48-h LC50 (mg/L)		Log K_{ow}		Ref.
Methylene chloride		322.895		1.25		Z
Chloroacetic ethyl ester	1.6		?		K	
Chemical identity CBI		3.32		3.7		EPA
Chemical identity CBI		*		4.4		EPA

* = No daphnid mortality in saturated solutions.

EPA = USEPA (1991); chemical identities are Confidential Business Information under TSCA.
K = Kuhn et al (1989)

ESTERS
7/1988

SAR	**ESTERS**
Organism:	Green Algae
Duration:	96-h
Endpoint:	EC50 (Growth)
Equation:	Log EC50 (mM/L) = -0.881 - 0.519 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	6.4
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for esters.
Limitations:	If the log K_{ow} value is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

LIST OF ESTERS USED TO DEVELOP THE GREEN ALGAE 96-h EC50 SAR.

CHEMICAL	96-h EC50 (mg/L)	Log K_{ow}	Ref.
Chemical identity CBI	0.410	3.7	EPA

EPA = USEPA (1991); chemical identities are Confidential Business Information under TSCA.

ESTERS
7/1988

SAR	**ESTERS**
Organism:	Green Algae
Duration:	16-d
Endpoint:	Chronic Value (Growth)
Equation:	Log ChV (mM/L) = -1.01 - 0.51 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for esters.
Limitations:	If the log K_{ow} value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

LIST OF ESTERS USED TO DEVELOP THE GREEN ALGAE CHRONIC VALUE (ChV) SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
Chemical identity CBI	0.390	3.7	EPA

EPA = USEPA (1991); chemical identities are Confidential Business Information under TSCA.

ESTERS
7/1988

SAR **ESTERS, MONO**

Organism: Fish
Duration: 32-d
Endpoint: Chronic Value (Survival/Growth)

Equation: Log ChV (mM/L) = 0.421 - 0.828 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for aliphatic monoesters.

Limitations: If the log K_{ow} value is greater than 8.0, no effects expected at saturation.

References: United States Environmental Protection Agency (USEPA). 1991. Fish Chronic Toxicity Data Base. Duluth, MN: Environmental Research Laboratory (ERL), Office of Research and Development, USEPA, 6201 Congdon Boulevard, 55804; contact C.L. Russom (218) 720-5500.

LIST OF ALIPHATIC MONOESTERS USED TO DEVELOP THE FISH CHRONIC VALUE (ChV) SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
Methyl acetate	133.0	0.2	D

D = USEPA (1991)

ESTERS, MONO, ALIPHATIC
9/1993

SAR **ESTERS, DI**

Organism: Fish
Duration: 32-d
Endpoint: Chronic Value (Survival/Growth)

Equation: Log ChV (mM/L) = -1.677 - 0.565 log K_{ow}

Statistics: N = 3; R^2 = 1.0

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for aliphatic diesters.

Limitations: If the log K_{ow} value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.

References: United States Environmental Protection Agency (USEPA). 1991. Fish Chronic Toxicity Data Base. Duluth, MN: Environmental Research Laboratory (ERL), Office of Research and Development, USEPA, 6201 Congdon Boulevard, 55804; contact C.L. Russom (218) 720-5500.

LIST OF ALIPHATIC DIESTERS USED TO DEVELOP THE FISH CHRONIC VALUE (ChV) SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
Diethyl malonate	0.759	1.1	D
Dibutyl fumerate	0.030	3.9	D

D = USEPA (1991)

ESTERS, DI, ALIPHATIC
9/1993

SAR **ESTERS, PHOSPHATE**

Organism: Fish
Duration: 96-h
Endpoint: LC50 (Mortality)

Equation: Log LC50 (mM/L) = -0.0695 - 0.5178 log K_{ow}

Statistics: N = 16; R^2 = 0.595

Maximum log K_{ow}: 5.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate the toxicity of phosphate esters and other tri-alkyl-phenyl phosphate esters. This SAR may be used to estimate toxicity for the following classes of phosphate esters all of which are weak acetylcholinesterase inhibitors:

1. Tri-alkyl phosphate esters
2. Tri-phenyl phosphate esters
3. Halogenated tri-alkyl phosphate esters
4. Halogenated tri-phenyl phosphate esters

Some halogenated tri-alkylphosphate esters are significantly more toxic than predicted by this SAR as a result of their strong acetylcholinesterase and cholinesterase inhibition. These include:

1. 1,2-dibromoethyldiethyl phosphate ester - 400 X
2. 1,2-dichloroethyldiethyl phosphate ester - .30 X

Limitations: If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.

References: United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

LIST OF PHOSPHATE ESTERS USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Tris(betachloroethyl)	210.0	0.92	EPA
Tris(betachloroethyl)	90.0	0.92	EPA
Chemical identity CBI	21.0	1.80	EPA
Tris(dichloropropyl)	3.6	2.67	EPA
Tris(dichloropropyl)	5.1	2.67	EPA
Tris(2,3-dibromopropyl)	1.33	3.51	EPA
Tris(2,3-dibromopropyl)	1.45	3.51	EPA
Tributyl	11.0	3.53	EPA
Tributyl	8.18	3.53	EPA
Tributyl	8.8	3.53	EPA
Tributyl	9.6	3.53	EPA
Tributyl	11.8	3.53	EPA
Tributyl	11.4	3.53	EPA
Triphenyl	0.87	4.63	EPA
Triphenyl	0.70	4.63	EPA
Triphenyl	1.2	4.63	EPA

EPA = USEPA (1991)

SAR **ESTERS, PHTHALATE**
Organism: Fish
Duration: 96-h
Endpoint: LC50 (Mortality)

Equation: Use the ester fish 96-h SAR to determine the acute toxicity of a phthalate ester.

Maximum log K_{ow}: 5.0
Maximum MW: 1000.0

Application: The ester SAR may be used to estimate the toxicity of phthalate esters. The ester SAR is applicable for the following phthalate esters:

1. Aliphatic diesters
2. Aromatic diesters
3. Aliphatic-aromatic diesters
4. Phthalates, derived from aliphatic alcohols and phenol.

Limitations: If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturationse SAR with longer exposure.

References: Veith GD, DeFoe D, and Knuth M. 1984. Structure-activity relationships for screening organic chemicals for potential ecotoxicity effects. Drug Metabolism Reviews 15(7):1295-1303.

LIST OF PHTHALATE ESTERS USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Dimethyl-2-nitro-p-phthalate	6.52	2.28	V
Dimethyl-2-amino-p-phthalate	8.94	2.65	V
Diethyl-o-phthalate	30.0	2.69	V
Di-n-butyl-o-phthalate	1.10	4.74	V
Di-n-butyl-m-phthalate	0.90	4.74	V
Diphenyl-i-phthalate	0.80	5.07	V
Di-2-ethylhexyl-o-phthalate	*	7.06	V
Di-n-octyl-o-phthalate	*	7.06	V
Di-n-octyl-m-phthalate	*	7.06	V
Di-n-octyl-p-phthalate	*	7.06	V

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* No fish mortality in saturated solutions.

V = Veith et al (1984).

SAR	**ESTERS, PHTHALATE**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Use the neutral organic daphnid 48-h SAR to determine the acute toxicity of a phthalate ester.
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	The neutral organic SAR may be used to estimate the toxicity of phthalate esters. The neutral organic SAR is applicable for the following phthalate esters: 1. Aliphatic diesters 2. Aromatic diesters 3. Aliphatic-aromatic diesters 4. Phthalates, derived from aliphatic alcohols and phenol.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, use SAR with longer exposure.
References:	Nabholz JV. 1987. The acute and chronic toxicity of dialkyl phthalate esters to daphnids. Interagency memorandum to "Whom It May Concern." Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Toxic Substances, United States Environmental Protection Agency.

LIST OF PHTHALATE ESTERS USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
Methylene chloride	322.895	1.25	Z
Dimethyl	>52.0	1.52	N
Diethyl	90.0	2.57	N
Di-n-butyl-ortho	3.4	4.69	N
Di-n-butyl-ortho	5.2	4.69	N
Butyl-benzyl	1.83	4.87	N
Butyl-benzyl	3.7	4.87	N
Butyl-benzyl	1.6	4.87	N
Butyl-benzyl	1.0	4.87	N
Butyl-benzyl	2.4	4.87	N
Butyl-benzyl	1.7	4.87	N
Dihexyl	*	6.80	N
Butyl-2-ethylhexyl	*	7.93	N
Di-(n-hexyl, n-octyl, n-decyl)	*	8.57	N
Di-(2-ethylhexyl)	*	8.66	N
Di-(2-ethylhexyl)	*	8.66	N
Diisooctyl	*	8.66	N
Di-(n-octyl)	*	8.92	N
Di-(heptyl, nonyl, undecyl)	*	9.59	N
Diisononyl	*	9.72	N
Diisodecyl	*	10.78	N
Diisodecyl	*	10.78	N
Diundecyl	*	12.10	N
Ditridecyl	*	14.21	N

* No daphnid mortality in saturated solutions.

N = Nabholz (1987).

SAR	**ESTERS, PHTHALATE**
Organism:	Daphnid
Duration:	21-d
Endpoint:	No Effect Concentration (NEC) (Reproduction)
Equation:	Log 21-d NEC (mM/L) = 0.05 - 0.72 log K_{ow}
Statistics:	;
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	The neutral organic 16-d NEC SAR may be used to estimate the toxicity of phthalate esters. The neutral organic SAR is applicable for the following phthalate esters: 1. Aliphatic diesters 2. Aromatic diesters 3. Aliphatic-aromatic diesters 4. Phthalates, derived from aliphatic alcohols and phenol.
Limitations:	If the log K_{ow} value is greater than 8.0, or if the compound is solid and the NEC exceeds the water solubility, no effects expected at saturation.
References:	Nabholz JV. 1987. The acute and chronic toxicity of dialkyl phthalate esters to daphnids. Interagency memorandum to "Whom It May Concern." Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Toxic Substances, United States Environmental Protection Agency.

ESTERS, PHTHALATE
9/1993

LIST OF PHTHALATE ESTERS USED TO DEVELOP THE DAPHNID 21-d NEC SAR.

CHEMICAL	21-d NEC (mg/L)	Log K_{ow}	Ref.
Methylene chloride	322.895	1.25	Z
Dimethyl	15.0	1.52	N
Diethyl	38.0	2.57	N
Di-n-butyl-ortho	1.0	4.69	N
Di-n-butyl-ortho	1.4	4.69	N
Di-n-butyl-ortho	1.5	4.69	N
Butyl-benzyl	0.63	4.87	N
Butyl-benzyl	0.44	4.87	N
Di-n-butyl-iso	0.15	5.53	N
Di-n-butyl-tere	0.32	5.53	N
Dihexyl	*	6.80	N
Butyl-2-ethylhexyl	*	7.93	N
Di-(n-hexyl, n-octyl, n-decyl)	*	8.57	N
Di-(2-ethylhexyl)	*	8.66	N
Di-(2-ethylhexyl)	*	8.66	N
Diisooctyl	*	8.66	N
Di-(n-octyl)	*	8.92	N
Di-(heptyl, nonyl, undecyl)	*	9.59	N
Diisononyl	*	9.72	N
Diisodecyl	*	10.78	N
Diisodecyl	*	10.78	N
Diundecyl	*	12.10	N
Ditridecyl	*	14.21	N

* No daphnid systemic effects in saturated solutions.

N = Nabholz (1987).

SAR **HYDRAZINES**

Organism: Fish
Duration: 96-h
Endpoint: LC50 (Mortality)

Equation: Log 96-h LC50 (mM/L) = -1.53 - 0.438 log K_{ow}

Statistics: N = 9; R^2 = 0.91

Maximum log K_{ow}: 5.0
Maximum MW: 1000.0

Application: This equation may be used to estimate toxicity for:

hydrazines
hydrazones
hydrazides
thiohydrazides
semicarbazides
thiosemicarbazides
semicarbazones
thiosemicarbazones

For hydrazines with missing fragment constants in CLOGP the following constants may be used:

1. missing fragment (-C(=S)-): -0.24
2. missing fragment (-NC(=O)N-N): -3.13
3. missing fragment (C=NNC(=O)N): -3.39.

Limitations: Hydrazines which are 10 times less toxic than predicted by this SAR are those hydrazines which have a carboxylic acid substitution:

butanedioic acid mono-(2,2'-dimethylhydrazide).

If the log K_{ow} value is greater than 5.0 and less than 6.6, use the neutral organics fish 14-d LC50 SAR; and if the log K_{ow} value is equal to or greater than 6.6, use the neutral organics fish ChV SAR.

References:

Buccafusco RJ, Ells SJ, and LeBlanc GA. 1981. Acute toxicity of priority pollutants to bluegill (Lepomis macrochirus). Bulletin of Environmental Contamination and Toxicology 26:446-452.

Hammermeister D, Kahl M, and Broderius S. 1990. EEB/ERL-Duluth interaction on various join projects. Duluth, MN: Environmental

Research Laboratory-Duluth, United States Environmental Protection Agency, 6201 Congdon Blvd., 55804, Unpublished memorandum to V. Nabolz.

Odenkirchen EW and Nabholz JV. 1989. Generic environmental hazard assessment of hydrazines and related compounds. Rockville, Maryland: Dynamac Corporation, 11140 Rockville Pike, 20852.

LIST OF HYDRAZINES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
HYDRAZINES USED IN CALCULATION OF THE SAR			
Hydrazine	2.81	-1.37	H
Hydrazine	3.4	-1.37	ON
Monomethyl hydrazine	3.26	-1.06	ON
Monomethyl hydrazine	2.58	-1.06	ON
1,1-Dimethyl hydrazine	7.75	-1.50	H
1,1-Dimethyl hydrazine	10.0	-1.50	ON
1,1-Dimethyl hydrazine	26.5	-1.50	ON
Thiosemicarbazide	20.8	-2.4	ON
1,2-Diphenyl hydrazine	0.27	2.97	B
HYDRAZINES LESS TOXIC THAN PREDICTED			
Butanedioic acid mono-(2,2'-dimethylhydrazide)	423.0	-0.619	ON
Butanedioic acid mono-(2,2'-dimethylhydrazide)	149.0	-0.619	ON
HYDRAZINES NOT ACUTELY TOXIC AT SATURATION			
N-Acetyl-1,2-diphenylhydrazine	* (mp 164EC)	2.2	H

H = Hammermeister et al (1990)
ON = Odenkirchen and Nabholz (1989)
B = Buccafusco et al (1981)

SAR **HYDRAZINES**

Organism: Daphnid
Duration: 48-h
Endpoint: LC50 (Mortality)

Equation: Log 48-h LC50 (mM/L) = -1.2941 - 0.256 log K_{ow}

Statistics: N = 4; R^2 = 0.46

Maximum log K_{ow}: 5.0
Maximum MW: 1000.0

Application: This equation may be used to estimate toxicity for:

hydrazines
hydrazones
hydrazides
thiohydrazides
semicarbazides
thiosemicarbazides
semicarbazones
thiosemicarbazones

For hydrazines with missing fragment constants in CLOGP the following constants may be used:

1. missing fragment (-C(=S)-): -0.24
2. missing fragment (-NC(=O)N-N): -3.13
3. missing fragment (C=NNC(=O)N): -3.39

Limitations: Hydrazines which are significantly less toxic than predicted by this SAR are those hydrazines which have a carboxylic acid substitution:

butanedioic acid mono-(2,2'-dimethylhydrazide).

If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.

References:

LeBlanc. 1980. Acute toxicity of priority pollutants to water flea (Daphnia magna). Bulletin of Environmental Contamination and Toxicology. 24: 684-691.

Hammermeister D, Kahl M, and Broderius S. 1990. EEB/ERL-Duluth interaction on various join projects. Duluth, MN: Environmental Research Laboratory-Duluth, United States Environmental Protection Agency, 6201 Congdon Blvd., 55804, Unpublished memorandum to V. Nabolz.

HYDRAZINES
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LIST OF HYDRAZINES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
HYDRAZINES USED IN CALCULATION OF THE SAR			
Hydrazine	0.280	-1.37	H
1,1-Dimethyl hydrazine	68.2	-1.50	H
1,2-Diphenyl hydrazine	4.1	2.97	L
HYDRAZINES NOT ACUTELY TOXIC AT SATURATION			
N-Acetyl-1,2-diphenylhydrazine	* (mp 164EC)	2.2	H

H = Hammermeister et al (1990)
L = LeBlanc (1980)

SAR **HYDRAZINES**

Organism: Green Algae
Duration: 144-h
Endpoint: EC50 (Growth)

Equation: Log 144-h EC50 (mM/L) = -5.1725 - 0.0999 Log K_{ow}

Statistics: N = 3; R^2 = 0.3

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This equation may be used to estimate toxicity for hydrazines. SAR equations for other subclasses of hydrazines, i.e., alkylsemicarbazides and arylsemicarbazides, may be found elsewhere in this volume.

Limitations: Hydrazines which are significantly less toxic than predicted by this SAR are those hydrazines which have a carboxylic acid substitution:

butanedioic acid mono-(2,2'-dimethylhydrazide).

References: Odenkirchen EW and Nabholz JV. 1989. Generic environmental hazard assessment of hydrazines and related compounds. Rockville, Maryland: Dynamac Corporation, 11140 Rockville Pike, 20852.

LIST OF HYDRAZINES USED TO DEVELOP THE GREEN ALGAE 144-h EC50 SAR.

CHEMICAL	144-h EC50 (mg/L)	Log K_{ow}	Ref.
1,1-Dimethyl hydrazine	0.004100	-1.50	ON
Hydrazine	0.000041	-1.37	ON

ON = Odenkirchen and Nabholz (1989)

HYDRAZINES
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SAR **HYDRAZINES, SEMICARBAZIDE, ALKYL SUBSTITUTED**

Organism: Green Algae
Duration: 6-h
Endpoint: EC50 (Growth)

Equation: (1) For log K_{ow} less than -1.02:

Log 6-h EC50 (mM/L) = -2.1 - 0.521 log K_{ow}

(2) For log K_{ow} greater than -1.02:

Log 6-h EC50 (mM/L) = -0.89 + 0.625 log K_{ow}

Statistics: (1) For log K_{ow} less than -1.02: N = 6, R^2 = 0.75;
(2) For log K_{ow} greater than -1.02: N = 7, R^2 = 0.86

Maximum log K_{ow}: 1.5
Maximum MW: 1000.0

Application: This equation may be used to estimate toxicity for the following hydrazine classes with alkyl substitutions:

semicarbazides
thiosemicarbazides
semicarbazones
thiosemicarbazones
hydrazides
thiohydrazides
hydrazones

SAR equations for aryl substituted semicarbazides and hydrazines may be found elsewhere in this volume.

For semicarbazides with missing fragment constants in CLOGP the following constants may be used:

1. missing fragment (-C(=S)-): -0.24
2. missing fragment (-NC(=O)N-N): -3.13
3. missing fragment (C=NNC(=O)N): -3.39.

Limitations: If the log K_{ow} value is greater than 1.5, no effects expected at saturation.

References: Odenkirchen EW and Nabholz JV. 1989. Generic environmental hazard assessment of hydrazines and related compounds. Rockville, Maryland: Dynamac Corporation, 11140 Rockville Pike, 20852.

HYDRAZINES, SEMICARBAZIDES, ALKYL SUBSTITUTED
9/1993

LIST OF ALKYL SUBSTITUTED SEMICARBAZIDES USED TO DEVELOP THE GREEN ALGAE 6-h EC50 SAR.

CHEMICAL	6-h EC50 (mg/L)	Log K_{ow}	Ref.
4-Methyl	9.9	-2.25	ON
4-Allyl	3.8	-1.74	ON
4-Ethyl	5.1	-1.73	ON
4,4-Dimethyl	4.2	-1.50	ON
4-Isopropyl	2.7	-1.42	ON
4-n-Propyl	2.5	-1.20	ON
4-t-Butyl	4.1	-1.02	ON
4-Isobutyl	3.9	-0.80	ON
4-Benzyl	12.8	-0.69	ON
4-n-Butyl	5.9	-0.67	ON
4,4-Diethyl	6.1	-0.44	ON
4-n-Pentyl	12.6	-0.14	ON
4-n-Hexyl	38.2	0.39	ON

ON = Odenkirchen and Nabholz (1989)

SAR **HYDRAZINES, SEMICARBAZIDES, ARYL, ORTHO SUBSTITUTED**

Organism: Green Algae
Duration: 6-h
Endpoint: EC50 (Growth)

Equation: Log 6-h EC50 (mM/L) = -0.88 - 0.563 log K_{ow}

Statistics: N = 7; R^2 = 0.98

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This equation may be used to estimate toxicity for the following arylsemicarbazides with ortho substituents on the aryl group:

thiosemicarbazides
semicarbazones
thiosemicarbazones
hydrazides
thiohydrazides
hydrazones

SAR equations for arylsemicarbazides with meta and para substituents, alkylsemicarbazides, and hydrazines may be found elsewhere in this volume.

For semicarbazides with missing fragment constants in CLOGP the following constants may be used:

1. missing fragment (-C(=S)-): -0.24
2. missing fragment (-NC(=O)N-N): -3.13
3. missing fragment (C=NNC(=O)N): -3.39.

Limitations: Arylsemicarbazides which are significantly more toxic than predicted by this SAR are:

4-(o-hydroxyphenyl)semicarbazide, 30X excess toxicity.

If the log K_{ow} is greater than 5.0, or if the compound is solid and the EC50 exceeds the water solubility, no effects expected at saturation.

References: Odenkirchen EW and Nabholz JV. 1989. Generic environmental hazard assessment of hydrazines and related compounds. Rockville, Maryland: Dynamac Corporation, 11140 Rockville Pike, 20852.

HYDRAZINES, SEMICARBAZIDE, ARYL, ORTHO SUBSTITUTED
9/1993

LIST OF ARYLSEMICARBAZIDES WITH ORTHO SUBSTITUENTS ON THE ARYL GROUP USED TO DEVELOP THE GREEN ALGAE 6-h EC50 SAR.

CHEMICAL	6-h EC50 (mg/L)	Log K_{ow}	Ref.
ARYLSEMICARBAZIDES USED IN CALCULATION OF THE SAR			
4-[o-Nitrophenyl]	194.6	-1.47	ON
4-[o-Carboxyphenyl]	176.6	-1.47	ON
4-[o-Methoxyphenyl]	116.2	-1.30	ON
4-[o-Methylphenyl]	52.0	-0.57	ON
4-[o-Chlorophenyl]	39.4	-0.50	ON
4-[m-Bromophenyl]	26.2	-0.35	ON
4-[o-Bromophenyl]	53.4	-0.35	ON
4-[2,5-Dichlorophenyl]	22.3	0.21	ON
ARYLSEMICARBAZIDES HAVING EXCESS TOXICITY			
4-[o-Hydroxyphenyl]	6.0	-1.88	ON

ON = Odenkirchen and Nabholz (1989)

SAR	**HYDRAZINES, SEMICARBAZIDES, ARYL, META/PARA SUBSTITUTED**
Organism:	Green Algae
Duration:	6-h
Endpoint:	EC50 (Growth)
Equation:	Log 6-h EC50 (mM/L) = -1.13 - 0.461 log K_{ow}
Statistics:	N = 19; R^2 = 0.98
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for the following arylsemicarbazides with meta or para substituents on the aryl group: thiosemicarbazides semicarbazones thiosemicarbazones hydrazides thiohydrazides hydrazones For semicarbazides with missing fragment constants in CLOGP the following constants may be used: 1. missing fragment (-C(=S)-): -0.24 2. missing fragment (-NC(=O)N-N): -3.13 3. missing fragment (C=NNC(=O)N): -3.39.
Limitations:	SAR equations for arylsemicarbazides with ortho substituents, alkylsemicarbazides, and hydrazines may be found elsewhere in this volume. If the log K_{ow} value is greater than 8.0, or if the compound is solid and the EC50 exceeds the water solubility, no effects expected at saturation.
References:	Odenkirchen EW and Nabholz JV. 1989. Generic environmental hazard assessment of hydrazines and related compounds. Rockville, Maryland: Dynamac Corporation, 11140 Rockville Pike, 20852.

HYDRAZINES, SEMICARBAZIDE, ARYL, META/PARA SUBSTITUTED
9/1993

LIST OF ARYLSEMICARBAZIDES WITH META AND PARA SUBSTITUENTS ON THE ARYL GROUP USED TO DEVELOP THE GREEN ALGAE 6-h EC50 SAR.

CHEMICAL	6-h EC50 (mg/L)	Log K_{ow}	Ref.
4-[m-Hydroxyphenyl]	144.8	-1.88	ON
4-[p-Hydroxyphenyl]	170.0	-1.88	ON
4-[m-Nitrophenyl]	109.5	-1.47	ON
4-[p-Nitrophenyl]	98.0	-1.47	ON
4-[m-Carboxyphenyl]	104.0	-1.47	ON
4-[p-Carboxyphenyl]	92.7	-1.47	ON
4-[m-Methoxyphenyl]	71.7	-1.30	ON
4-[p-Methoxyphenyl]	70.0	-1.30	ON
4-Phenyl	42.5	-1.22	ON
4-[p-Ethoxyphenyl]	38.7	-0.77	ON
4-[m-Methylphenyl]	26.7	-0.57	ON
4-[p-Methylphenyl]	24.9	-0.57	ON
4-[m-Chlorophenyl]	22.7	-0.50	ON
4-[p-Chlorophenyl]	22.2	-0.50	ON
4-[m-Bromophenyl]	26.2	-0.35	ON
4-[p-Bromophenyl]	22.3	-0.35	ON
4-[p-Iodophenyl]	17.7	-0.09	ON
4-[3,4-Dichlorophenyl]	9.3	0.21	ON
4-[2,5-Dichlorophenyl]	22.3	0.21	ON

ON = Odenkirchen and Nabholz (1989)

SAR **IMIDES**

Organism: Fish
Duration: 96-h
Endpoint: LC50 (Mortality)

Equation: Log 96-h LC50 (mM/L) = 1.256 - 0.76 log K_{ow}

Statistics: N = 4; R^2 = 0.98

Maximum log K_{ow}: 5.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for imides.

Limitations: For imides with log K_{ow} values greater than 5.0, a test duration of greater than 96 hours may be required for proper expression of toxicity. Also, if the toxicity value obtained by the use of this equation exceeds the water solubility of the compound (measured or estimated), mortalities greater than 50% would not be expected in a saturated solution during an exposure period of 96 hours.

References:

Fukunaga K (ed). 1987. Japanese Pesticides Guide. Tokyo, Japan: Japan Plant Protection Association.

Worthing CR (ed). 1983. The Pesticide Manual. A World Compendium. 7th Ed. Croydon, Great Britain: British Crop Protection Council.

LIST OF IMIDES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Methylene chloride	322.895	1.25	Z
Sumilex	*	2.2	F
Vinclozolin	32.5	2.8	W
Vinclozolin	52.5	2.8	W
Spartcide	5.5	3.7	F

* = No fish mortality in saturated solutions.

IMIDES
9/1993

F = Fukunaga (1987)
W = Worthing (1983)

SAR	**KETONES, DI, ALIPHATIC**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log 96-h LC50 (mM/L) = -0.151 - 0.433 log K_{ow}
Statistics:	N = 22; R^2 = 0.87
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for aliphatic diketones.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.

References:

Brooke LT, Call DJ, Geiger DL, and Northcott CE. 1984. Acute toxicities of organic chemicals to fathead minnows (Pimephales promelas). Volume 1. Superior, WI: University of Wisconsin, Center for Lake Superior Environmental Studies. pp. 414.

Geiger DL, Northcott EC, Call DJ, and Brooke LT. 1985. Acute toxicities of organic chemicals to fathead minnows (Pimephales promelas). Volume 2. Superior, WI: University of Wisconsin, Center for Lake Superior Environmental Studies. pp. 326.

Juhnke I and Luedemann D. 1978. Results of the investigation of 200 chemical compounds for acute fish toxicity with the golden orfe test. Z. F. Wasser-Und-Abwasser-Forschung 11(5):161-164.

Nacci D, et al. 1986. Comparative evaluation of three rapid marine toxicity tests: sea urchin early embryo growth test, sea urchin sperm cell toxicity test and microtox. Environmental Toxicology and Chemistry. 5:521-525.

Phipps GL and Holcombe GW. 1985. A method for aquatic multiple species toxicant testing: Acute toxicity of 10 chemicals to 5 vertebrates and 2 invertebrates. Environ. Pollut. Ser. A Ecol. Biol. 38(2):141-157.

Thurston RV, Gilfoil TA, Meyn EL, Zajdel RK, Aoki, TL, and Veith GD. 1985. Comparative toxicity of ten organic chemicals to ten common aquatic species. Water Res. 19(9):1145-1155.
United States Environmental Protection Agency (USEPA). 1991. Fish Chronic Toxicity Data Base. Duluth, MN: Environmental Research Laboratory (ERL), Office of Research and Development, USEPA, 6201 Congdon Boulevard, 55804; contact C.L. Russom (218) 720-5500.

KETONES, DI, ALIPHATIC
9/1993

LIST OF ALIPHATIC DIKETONES USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Methylene chloride	322.895	1.25	Z
2,4-pentanedione	116.0	-0.5	J
2,4-pentanedione	104.0	-0.5	N
5,5-dimethyl-1,3-cyclohexanedione	11,500.0	0.5	EPA
2,4-pentanedione	175.0	-0.5	G
1-benzoyl acetone	1.1	1.0	EPA
2,4-pentanedione	104.0	-0.5	B
2,4-pentanedione	146.0	-0.5	J
2,4-pentanedione	155.0	-0.5	P
2,4-pentanedione	71.6	-0.5	P
2,4-pentanedione	107.0	-0.5	P
2,4-pentanedione	83.6	-0.5	P
2,4-pentanedione	74.3	-0.5	P
2,4-pentanedione	92.4	-0.5	T
2,4-pentanedione	71.7	-0.5	T
2,4-pentanedione	66.9	-0.5	T
2,4-pentanedione	60.1	-0.5	T
2,4-pentanedione	204.0	-0.5	T
2,4-pentanedione	151.0	-0.5	T
2,4-pentanedione	106.0	-0.5	T
2,4-pentanedione	121.0	-0.5	T
2,4-pentanedione	143.0	-0.5	T
2,4-pentanedione	141.0	-0.5	T

B = Brooke et al (1984)
EPA = USEPA (1991)
G = Geiger et al (1985)
J = Juhnke and Luedemann (1978)
N = Nacci et al (1986)
P = Phipps and Holcombe (1985)
T = Thurston et al (1985)

SAR **KETONES, DI, ALIPHATIC**

Organism: Daphnid
Duration: 48-h
Endpoint: LC50

Equation: Log 48-h LC50 (mM/L) = -0.466 - 0.467 log K_{ow}

Statistics: N = 6; R^2 = 0.98

Maximum log K_{ow}: 5.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for aliphatic diketones.

Limitations: If the K_{ow} value is greater than 5.0, a or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.

References:

Elnabarawy MT, Welter AN, and Robideau RR. 1986. Relative sensitivity of three daphnid species to selected organic and inorganic chemicals. Environ. Toxicol. Chem. 5(4):393-398.

Mount DI and Norberg TJ. 1984. A seven-day life-cycle cladoceran toxicity test. Environ. Toxicol. Chem. 3(3):425-434.

Nacci D, et al. 1986. Comparative evaluation of three rapid marine toxicity tests: sea urchin early embryo growth test, sea urchin sperm cell toxicity test and microtox. Environmental Toxicology and Chemistry. 5:521-525.

LIST OF ALIPHATIC DIKETONES USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}		Ref.
Methylene chloride	322.895	1.25		Z
2,4-pentanedione	47.6	-0.5		N
2,4-pentanedione	75.0	-0.5		E
2,4-pentanedione	75.0	-0.5		E
2,4-pentanedione	75.0	-0.5	E	
2,4-pentanedione	35.4	-0.5	M	

KETONES, DI, ALIPHATIC
9/1993

E = Elnabarawy et al (1986)
M = Mount and Norberg (1984)
N = Nacci et al (1986)

SAR **KETONES, DI, ALIPHATIC**

Organism: Daphnid
Duration: 16-d
Endpoint: ChV

Equation: Log ChV (mM/L) = -1.841 - 0.482 log K_{ow}

Statistics: N = 4; R^2 = 0.98

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for aliphatic diketones.

Limitations: If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.

References: Elnabarawy MT, Welter AN, and Robideau RR. 1986. Relative sensitivity of three daphnid species to selected organic and inorganic chemicals. Environ. Toxicol. Chem. 5(4):393-398.

LIST OF ALIPHATIC DIKETONES USED TO DEVELOP THE DAPHNID ChV SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
Methylene chloride	322.895	1.25	Z
2,4-pentanedione	6.5	-0.5	E
2,4-pentanedione	2.6	-0.5	E
2,4-pentanedione	1.0	-0.5	E

E = Elnabarawy et al. (1986)

KETONES, DI, ALIPHATIC
9/1993

SAR **KETONES, DI, ALIPHATIC**

Organism: Green Algae
Duration:
Endpoint: ChV

Equation: Log ChV (mM/L) = -1.806 - 0.412 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for aliphatic diketones.

Limitations: If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.

References: Bringmann G and Kuhn R. 1980. Comparison of the toxicity thresholds of water pollutants to bacteria, algae, and protozoa in the cell multiplication inhibition test. Water Res. 14(3):231-241.

LIST OF ALIPHATIC DIKETONES USED TO DEVELOP THE GREEN ALGAE ChV SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
2,4-pentanedione	2.7	-0.5	BK

BK = Bringmann and Kuhn (1980)

KETONES, DI, ALIPHATIC
9/1993

SAR **MALONONITRILES**

Organism: Fish
Duration: 96-h
Endpoint: LC50 (Mortality)

Equation: Log 96-h LC50 (mM/L) = -2.079 - 0.139 log K_{ow}

Statistics: N = 3; R^2 = 0.40

Maximum log K_{ow}: 5.0
Maximum MW: 1000.0

Application: This SAR may be used to estimate toxicity for malononitriles.

Limitations: For malononitriles with log K_{ow} values greater than 5.0, a test duration of greater than 96 hours may be required for proper expression of toxicity. Also, if the acute toxicity value obtained by the use of this equation exceeds the water solubility of the compound (measured or estimated), significant mortalities would not be expected in a saturated solution during an exposure period of 96 hours.

References: Abram FSH and Wilson P. 1979. The acute toxicity of CS to rainbow trout. Water Research 13:631-635.

LIST OF MALONONITRILES USED TO DEVELOP THE FISH 96-H LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Malononitrile	1.6	-1.2	A
o-Chlorobenzylidene malononitrile	0.22	1.8	A

A = Abram and Wilson (1979)

MALONONITRILES
9/1993

SAR	**NEUTRAL ORGANICS**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log LC50 (mM/L) = 1.75 - 0.94 log K_{ow}
Statistics:	N = 60; R^2 = 0.942
Maximum K_{ow}:	5.0
Maximum MW:	1000.0
Application:	Solvents, non-reactive, non-ionizable neutral organic compounds

1. Alcohols
2. Acetals
3. Ketones
4. Ethers
5. Alkyl halides
6. Aryl halides
7. Aromatic hydrocarbons
8. Halogenated aromatic hydrocarbons
9. Halogenated aliphatic hydrocarbons
10. Sulfides and di-sulfides

Limitations: Use the fish 14-day LC50 for neutral organics with log K_{ow} greater than 5 and less than 7. If the compound is and the LC50 is exceeds the water solubility, use SAR with longer exposure.

References:

Veith GD, Call DJ, and Brooke LT. 1983. Structure-toxicity relationships for the fathead minnow, Pimephales promelas: narcotic industrial chemicals. Canadian Journal of Fisheries and Aquatic Sciences 40:743-748.

NEUTRAL ORGANICS
7/1988

LIST OF NEUTRAL ORGANICS USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Triethylene glycol	69800	-1.17	V
2-Methyl-2,4-pentandiol	10700	-0.70	V
Methanol	28100	-0.66	V
Acetone	8120	-0.24	V
Ethanol	14200	-0.16	V
2-(2-Ethoxyethoxy)ethanol	26400	-0.08	V
2-Propanol	10400	0.14	V
2-Butanone	3200	0.28	V
3-Furanmethanol (static)	508	0.32	V
Tetrahydrofuran	2160	0.46	V
3-Methyl-2-butanone	864	0.62	V
2-Methyl-1-propanol	1430	0.74	V
Cyclohexanone	527	0.81	V
3-Pentanone	1540	0.84	V
1-Butanol	1730	0.88	V
3,3-Dimethyl-2-butanone	87	0.94	V
2',3',4'-Trimethoxyacetophenone	172	1.12	V
2-Phenoxyethanol	344	1.16	V
Cyclohexanol	704	1.23	V
4-Methyl-2-pentanone	505	1.25	V
t-Butylmethyl ether	706	1.30	V
Furan	61	1.34	V
2,2,2-Trichloroethanol	299	1.38	V
Diisopropyl ether	91.7	1.56	V
Acetophenone	162	1.66	V
5-Methyl-2-hexanone	159	1.79	V
1,3-Dichloroethane	118	1.79	V
p-Dimethoxybenzene	117	2.00	V
1-Fluoro-4-nitrobenzene	28.4	2.02	V
1-Hexanol	97.5	2.03	V
1,1,2-Trichloroethane	81.7	2.07	V
6-Methyl-5-heptene-2-one	85.7	2.13	V
2'-Hydroxy-4'-methoxyacetophenone	54.9	2.14	V
1,1,2,2-Tetrachloroethane	20.3	2.39	V
1,1,2-Trichloroethylene	44.1	2.42	V
2-Octanone	36	2.46	V
Tetrachloroethane	13.5	2.53	V
2,6-Dimethoxytoluene	20.5	2.67	V
5-Nonanone	31	3.00	V
2',4'-Dichloroacetophenone	11.7	3.02	V
1-Octanol	13.5	3.03	V
Di-n-butyl ether	32.5	3.08	V

Continued.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
1,4-Dichlorobenzene	4.0	3.37	V
Benzophenone	15.3	3.38	V
1,3-Dichlorobenzene	7.8	3.38	V
1-Nonanol	5.7	3.53	V
2-Decanone	5.7	3.54	V
Pentachloroethane	7.3	3.64	V
2',3',4'-Trichloroacetophenone	2.0	3.73	V
p-Nitrophenyl phenyl ether	2.7	3.97	V
1-Decanol	2.4	4.03	V
Dipentyl ether	3.2	4.16	V
3,4-Dichlorotoluene	2.91	4.22	V
á,á-2,6-Tetrachlorotoluene	0.97	4.24	V
Diphenyl ether	4.0	4.26	V
1,2,4-Trichlorobenzene	2.9	4.28	V
1-Undecanol	1.04	4.53	V
Hexachloroethane	1.5	4.62	V
1-Dodecanol	1.01	5.00	V
7-Tridecanone	*	5.16	V
1-Tridecanol	*	5.51	V
Pentachlorobenzene	*	5.71	V
1,2,3,4-Tetrachlorobenzene	1.1	5.71	V
Hexachlorobenzene	*	5.71	V
Dioctyl ether	*	6.42	V

* = No fish mortality in saturated solutions.

V = Veith et al. (1983)

NEUTRAL ORGANICS
7/1988

SAR **NEUTRAL ORGANICS**

Organism: Fish, Sheepshead Minnow (marine)
Duration: 96-h
Endpoint: LC50 (Mortality)

Endpoint: Log LC50 (mM/L) = 0.69 - 0.73 log K_{ow}

Statistics: N = 37; R^2 = 0.656

Maximum K_{ow}: 5.0
Maximum MW: 1000.0

Application: Solvents, non-reactive, non-ionizable neutral organic compounds:

1. Alcohols
2. Acetals
3. Ketones
4. Ethers
5. Alkyl halides
6. Aryl halides
7. Aromatic hydrocarbons
8. Halogenated aromatic hydrocarbons
9. Halogenated aliphatic hydrocarbons
10. Sulfides and di-sulfides

Limitations: If the log K_{ow} is greater than 5, or if the compound is solid and the LC50 is exceeds the water solubility, use SAR with longer exposure.

References: Zaroogian G, Heltshe JF, and Johnson M. 1985. Estimation of toxicity to marine species with structure activity models developed to estimate toxicity to freshwater fish. Aquatic Toxicology 6:251-270.

NEUTRAL ORGANICS
7/1988

LIST OF NEUTRAL ORGANICS USED TO DEVELOP THE SHEEPSHEAD MINNOW 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Methylene chloride	322.895	1.25	Z
Diethyl phthalate	29.979	1.40	Z
1,1-Dichloroethylene	249.174	1.48	Z
2,4-Dinitrophenol	28.515	1.53	Z
Dimethyl phthalate	57.310	1.61	Z
Nitrobenzene	58.924	1.83	Z
1,1,1,2,2,2,-Hexachloroethane	1.380	1.91	Z
4-Nitrophenol	26.507	1.91	Z
1,3-Dichloropropene	1.759	1.98	Z
2,3-Dinitrotoluene	2.293	1.98	Z
2,4,6-Trinitrophenol	128.838	2.03	Z
Bromoform	17.893	2.30	Z
4-Chlorophenol	5.359	2.35	Z
1,1,2,2-Tetrachloroethane	11.883	2.39	Z
1,1,1-Trichloroethane	70.015	2.47	Z
1,1,1,2,2-Pentachloroethane	113.762	2.89	Z
Diazinon	1.457	3.14	Z
1,4-Dichlorobenzene	7.200	3.38	Z
1,2-Dichlorobenzene	9.491	3.40	Z
1,3-Dichlorobenzene	7.715	3.44	Z
2,4,5-Trichlorophenol	1.681	3.72	Z
Hexachlorobutadiene	0.545	3.74	Z
Chlorobenzene	9.804	3.79	Z
Disulfoton	0.739	3.81	Z
Lindane	0.801	3.89	Z
Dibenzofuran	1.761	4.10	Z
Diphenyl ether	2.350	4.21	Z
Dieldrin	0.010	4.31	Z
1,2,4-Trichlorobenzene	20.833	4.32	Z
1,2,3,5-Tetrachlorobenzene	3.666	4.46	Z
1,2,4,5-Tetrachlorobenzene	0.784	4.67	Z
Methoxychlor	0.049	4.68	Z
Chloropyrifos	0.881	4.82	Z
Heptachlor	0.004	5.44	Z
Kepone	0.693	6.08	Z
Fenvalerate	0.004	6.20	Z
Parmethrin	0.068	6.50	Z

Z = Zaroogian et al. (1985)

SAR **NEUTRAL ORGANICS**

Organism: Fish
Duration: 14-day
Endpoint: LC50 (Mortality)

Equation: Log LC50 (mM/L) = 1.87 - 0.871 log K_{ow}

Statistics: N = 50; R^2 = 0.976

Maximum K_{ow}: 8.0
Maximum MW: 1000.0

Application: Solvents, non-reactive, non-ionizable neutral organic compounds:

1. Aromatic hydrocarbons
2. Halogenated aromatic hydrocarbons
3. Halogenated aliphatic hydrocarbons
4. Alcohols
5. Ketones
6. Acetals
7. Ethers
8. Alkyl halides
9. Aryl halides
10. Sulfides and di-sulfides

Also applicable to reactive compounds (i.e., compounds which show excess toxicity) whose log K_{ow} is greater than 5.0, such as:

1. Esters
2. Acrylates
3. Methacrylates
4. Substituted benzotriazoles

Limitations: If the log K_{ow} is greater than 8.0, or if the compound is solid and the LC50 exceeds the water solubility, use SAR with longer exposure.

References: Konemann H. 1981. Quantitative structure-activity relationships in fish toxicity studies. Part 1: Relationship for 50 industrial pollutants. Toxicology 19(3):209-221.

NEUTRAL ORGANICS
7/1988

LIST OF NEUTRAL ORGANICS USED TO DEVELOP THE FISH 14-d LC50 SAR.

CHEMICAL	14-d LC50 (mg/L)	Log K_{ow}	Ref.
Ethanediol (ethyleneglycol)	49303.00	-1.35	K
Digol (diethyleneglycol)	61065.00	-1.30	K
Trigol (triethyleneglycol)	62601.00	-1.24	K
2-Methoxyethanol	17433.00	-0.74	K
Acetone	6368.00	-0.30	K
Ethanol	11051.00	-0.26	K
2-Ethoxyethanol	16399.00	-0.21	K
Propanol-2	7061.00	0.15	K
2-Isopropoxyethanol	5467.00	0.20	K
2-Methylpropanol-2	3547.00	0.77	K
2-Butoxyethanol	983.00	0.86	K
Diethylether	2137.00	0.88	K
Butyldigol	1148.00	0.91	K
Butyltrigol	197.00	0.97	K
Pentanol-3	989.00	1.21	K
Dichloromethane	294.00	1.61	K
1,3-Dichloropropane	83.80	1.71	K
1,2-Dichloroethane	106.00	1.76	K
2,2'-Dichlorodiethylether	54.40	1.81	K
1,1-Dichloroethane	202.00	1.92	K
Chloroform	102.00	2.02	K
Trans-1,4-dichloro-2-butene	39.50	2.11	K
Benzene	63.50	2.13	K
1,2-Dichloropropane	115.00	2.16	K
Trichloroethane	55.60	2.20	K
1-Chlorobutane	96.90	2.35	K
1,1,2-Trichloroethane	94.40	2.38	K
2,4-Dichloroaniline	11.70	2.42	K
1,1,1-Trichloroethane	133.00	2.49	K
Toluene	68.30	2.59	K
2,3-Dichloro-1-propane	11.10	2.60	K
1,2,3-Trichloropropane	41.60	2.63	K
1,5-Dichloropentane	11.20	2.77	K
Tetrachloromethane	67.10	2.79	K
Monochlorobenzene	19.10	2.81	K
á,á'-Dichloro-m-xylene	0.12	2.87	K
Tetrachloroethane	18.00	2.95	K
1,1,2,2-Tetrachloroethane	36.70	3.01	K
o-Xylene	35.20	3.09	K
m-Xylene	37.70	3.09	K
p-Xylene	35.20	3.09	K
Cyclohexane	84.20	3.18	K

Continued.

CHEMICAL	14-d LC50 (mg/L)	Log K_{ow}	Ref.
4-Chlorotoluene	5.90	3.31	K
3-Chlorotoluene	18.30	3.31	K
1,2-Dichlorobenzene	5.80	3.53	K
1,3-Dichlorobenzene	7.40	3.53	K
1,4-Dichlorobenzene	4.00	3.53	K
Pentachloroethane	15.00	3.58	K
2,4,á-Trichlorotoluene	0.24	3.87	K
2,4-Dichlorotoluene	4.60	3.98	K
3,4-Dichlorotoluene	5.10	3.98	K
1,2,3-Trichlorobenzene	2.30	4.20	K
1,2,4-Trichlorobenzene	2.40	4.20	K
1,3,5-Trichlorobenzene	3.30	4.20	K
Hexachlorobutadiene	0.39	4.63	K
2,4,5-Trichlorotoluene	1.70	4.72	K
1,2,4,5-Tetrachlorobenzene	0.30	4.94	K
1,2,3,5-Tetrachlorobenzene	0.80	4.94	K
1,2,3,4-Tetrachlorobenzene	0.80	4.94	K
Pentachlorobenzene	0.18	5.69	K
Hexachlorobenzene	0.32	6.44	K

K = Konemann (1981)

NEUTRAL ORGANICS
7/1988

SAR **NEUTRAL ORGANICS**

Organism: Fish
Duration: > 30 days
Endpoint: Chronic Value (Survival/Growth; Early Life Stage)

Equation: Log ChV (mM/L) = 0.72 - 0.87 log K_{ow}

Statistics: N = 20; R^2 = 0.91

Maximum K_{ow}: 7.9
Maximum MW: 1000.0

Application: Solvents, non-reactive, non-ionizable neutral organic compounds:

1. Alcohols
2. Acetals
3. Ketones
4. Ethers
5. Alkyl halides
6. Aryl halides
7. Aromatic hydrocarbons
8. Halogenated aromatic hydrocarbons
9. Halogenated aliphatic hydrocarbons
10. Sulfides and di-sulfides

Limitations: If the log K_{ow} is greater than 7.9 or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.

References: United States Environmental Protection Agency (USEPA). 1991. Fish chronic toxicity data base. Duluth, MN: Environmental Research Laboratory (ERL), Office of Research and Development, USEPA, 6201 Congdon Blvd., 55804; contact C.L. Russom (218) 720-5500.

NEUTRAL ORGANICS
7/1988

SAR **NEUTRAL ORGANICS**

Organism: Fish, Fathead minnow
Duration: 28-d
Endpoint: BCF (Bioconcentration Factor)

Equation: Log BCF = 0.79 log K_{ow} - 0.40 (the BCF is without units)

Statistics: N = 122; R_2 = 0.927

Maximum K_{ow}: 8.0
Maximum MW: 1000.0

Application: Solvents, non-reactive, non-ionizable compounds:

1. Aromatic amines
2. Acetals
3. Cyclodiene
4. Ethers
5. Halogenated alkyl
6. Halogenated aromatic
7. Halogenated indoles
8. Halogenated phenols
9. Phosphate esters

Limitations: If log K_{ow} is greater than 8.0, no significant BCF unless analog data can be found, e.g., PCBs.

Reference: Veith, GD, and Kosian, P. 1982. Estimating bioconcentration potential from octanol/water partition coefficients. IN: Physical Behavior of PCB's in the Great Lakes. MacKay, Paterson, Eisenreich, and Simmons, eds. Ann Arbor, MI: Ann Arbor Science.

NEUTRAL ORGANICS
7/1988

LIST OF CHEMICALS USED TO DEVELOP THE FISH BIOCONCENTRATION SAR.

CHEMICAL	BCF	Log K_{ow}	Ref.
____Lindane	2.67	3.85	VK
Atrazine	0.90	2.63	VK
Heptachlor	4.30	5.44	VK
2-Ethylhexiphthalate	2.93	4.20	VK
DASC-3	0.32	1.00	VK
DASC-4	0.32	1.00	VK
NTS-1	0.66	1.00	VK
BSB	0.32	1.00	VK
FWA-2-A	0.32	1.80	VK
FWA-3-A	0.32	1.48	VK
FWA-4-A	0.32	1.20	VK
Nitrobenzene	1.18	2.93	VK
p-Nitrophenol	1.88	1.91	VK
Naphthalene	2.63	3.59	VK
Chlorobenzene	2.65	3.79	VK
2,4,5-Trichlorophenol	3.28	3.72	VK
Endrin	3.66	4.56	VK
1,1,2,2-Tetrachloroethylene	2.06	2.88	VK
Hexachlorobenzene	4.37	6.18	VK
p-Biphenylphenyl ether	3.22	5.55	VK
Carbon tetrachloride	2.77	4.21	VK
p-Dichlorobenzene	1.72	2.64	VK
Biphenyl	2.81	3.38	VK
Chloropyrifos	2.67	4.82	VK
Endrin	3.17	4.56	VK
2,5,6-Trichloropyridinol	0.49	1.35	VK
Fluorene	3.11	4.38	VK
Dibenzofuran	3.13	4.12	VK
2-Chlorophenanthrene	3.63	5.16	VK
Phenanthrene	3.42	4.46	VK
2-Methylphenanthrene	3.48	4.86	VK
Heptachlor	3.98	5.44	VK
Heptachloroepoxide	4.16	5.40	VK
p,p'-DDE	4.71	5.69	VK
Pentachlorophenol	2.89	2.97	VK
Hexabromobiphenyl	6.39	4.26	VK
Methoxychlor	3.92	4.30	VK
Mirex	4.26	6.89	VK
Hexabromocyclododecane	4.26	5.81	VK
Heptachloronorborene	4.05	5.28	VK
Hexachloronorbornadiene	3.81	5.28	VK
1,2-Dichlorobenzene	1.95	3.40	VK
1,3-Dichlorobenzene	1.82	3.44	VK

Continued.

CHEMICAL	Log BCF	Log K_{ow}	Ref.
1,4-Dichlorobenzene	1.78	3.37	VK
1,2,3,5-Tetrachlorobenzene	3.26	4.46	VK
Pentachlorobenzene	3.53	4.94	VK
Carbon tetrachloride	1.48	2.73	VK
Chloroform	0.78	1.90	VK
1,2-Dichloroethane	0.30	1.45	VK
1,1,1-Trichloroethane	0.95	2.47	VK
1,1,2,2-Tetrachloroethane	0.90	2.39	VK
Pentachloroethane	1.83	3.21	VK
Hexachloroethane	2.14	3.93	VK
Bis(2-chloroethyl) ether	1.04	1.12	VK
1,1,2-Trichloroethylene	1.23	2.42	VK
Tetrachloroethylene	1.69	2.53	VK
Isophorone	0.84	1.67	VK
N-Nitrosophenylamine	2.34	3.13	VK
2-Chlorophenol	2.33	2.16	VK
2,4-Dimethylphenol	2.33	2.16	VK
Butylbenylphthalate	2.89	4.05	VK
Dimethylphthalate	1.76	1.61	VK
Alkyl benzene sulfonate	2.02	1.59	VK
Alkyl benzene sulfonate	1.56	1.59	VK
Naphthalene	1.90	3.59	VK
2-Methylnaphthalene	2.28	3.84	VK
1-Methylnaphthalene	2.11	3.84	VK
Hexachlorocyclohexane	2.15	3.85	VK
Hexachlorocyclohexane	2.70	3.85	VK
Endrin	4.02	4.56	VK
Endrin	4.18	4.56	VK
Endrin	3.85	4.56	VK
Al254	4.60	6.47	VK
Al254	4.43	6.47	VK
1,4-Dichlorobenzene	1.96	3.37	VK
1,2,3-Trichlorobenzene	2.81	4.20	VK
1,3,5-Trichlorobenzene	2.85	4.20	VK
1,2,3,5-Tetrachlorobenzene	3.56	4.46	VK
Pentachlorobenzene	4.11	4.94	VK
Hexachlorobenzene	4.16	6.18	VK
Aroclor 1016	4.63	5.86	VK
Aroclor 1248	4.85	6.11	VK
Aroclor 1254	5.00	6.47	VK
Aroclor 1260	5.29	6.91	VK
Chlordane	4.58	6.00	VK
Octachlorostyrene	4.52	6.29	VK
p,p-DDT	4.47	5.75	VK

Continued.

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CHEMICAL	BCF	Log K_{ow}	Ref.
o,p-DDT	4.57	5.75	VK
Hexachlorobenzene	4.27	6.18	VK
1,2,4-Trichlorobenzene	3.32	4.23	VK
Lindane	2.26	3.85	VK
5-Bromoindole	1.15	2.97	VK
2,4,6-Tribromoanisol	2.94	4.48	VK
N-Phenyl-2-naphylamine	2.17	4.38	VK
Tricresyl phosphate	2.22	3.42	VK
Diphenyl amine	1.48	3.42	VK
Toluene	1.96	3.16	VK
1,1,2,2-Tetrachloroethylene	0.91	2.39	VK
Pentachloroethane	1.78	3.21	VK
Hexachloroethane	2.85	3.93	VK
1,3-Dichlorobenzene	1.99	3.44	VK
1,4-Dichlorobenzene	2.05	3.37	VK
1,2,4-Trichlorobenzene	2.60	4.52	VK
1,2,3,4-Tetrachlorobenzene	3.41	4.46	VK
Hexachlorobenzene	4.37	6.18	VK
Hexachloro-1,3-butadiene	3.84	5.10	VK
Acridine	2.10	3.30	VK
Toxaphene	3.64	5.28	VK
Toxaphene	3.59	5.28	VK
Pentachlorophenol	1.11	2.97	VK
Imidan	0.90	2.83	VK
Imidan	1.04	2.83	VK
Imidan	0.90	2.83	VK
Diazinon	1.56	1.92	VK
Diazinon	1.81	1.92	VK
Diazinon	1.24	1.92	VK
Endrin	3.21	4.56	VK
Acenaphthene	2.59	3.92	VK

VK = Veith and Kosian (1982)

SAR **NEUTRAL ORGANICS**

Organism: Daphnid
Duration: 48-h
Endpoint: LC50 (Mortality)

Equation: Log LC50 (mM/L) = 1.72 - 0.91 log K_{ow}

Statistics: N = 19; R^2 = 0.992

Maximum K_{ow}: 5.0
Maximum MW: 1000.0

Application: Solvents, non-reactive, non-ionizable compounds:

1. Aromatic hydrocarbons
2. Halogenated aromatic hydrocarbons
3. Halogenated aliphatic hydrocarbons
4. Alcohols
5. Ketones
6. Acetals
7. Ethers
8. Alkyl halides
9. Aryl halides
10. Sulfides and di-sulfides

Also be applied to some classes of reactive organic compounds which show excess toxicity to fish, such as:

1. Benzotriazoles
2. Phthalate esters
3. Esters

LIMITATIONS: If the log K_{ow} is greater than 5.0 and less than 8.0, or if the compound is solid and the LC50 exceeds the water solubility, use SAR with longer exposure.

References: Hermans J, Canton H, Janssen P, and De Jong R. 1984. Quantitative structure-activity relationships and toxicity studies of mixtures of chemicals with anaesthetic potency: Acute lethal and sublethal toxicity to Daphnia magna. Aquatic Toxicology 5:143-154.

LIST OF NEUTRAL ORGANICS USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
Ethanediol	50452	-1.35	H
Acetone	6081	-0.30	H
Ethanol	5413	-0.26	H
2-Ethoxyethanol	7670	-0.21	H
Diethylether	1380	0.88	H
Benzene	56.6	2.13	H
1,2-Dichloropropane	45.0	2.16	H
1,1,2-Trichloroethene	20.8	2.20	H
Toluene	14.9	2.59	H
1,2,3-Trichloropropane	35.4	2.63	H
Monochlorobenzene	25.8	2.81	H
m-Xylene	14.3	3.09	H
4-Chlorotoluene	3.6	3.31	H
1,2-Dichlorobenzene	3.8	3.53	H
2,4-Dichlorotoluene	0.62	3.98	H
1,2,4-Trichlorobenzene	2.7	4.20	H
2,4,5-Trichlorobenzene	0.55	4.72	H
1,2,3,4-Tetrachlorobenzene	0.54	4.94	H
Pentachlorobenzene	0.12	5.69	H

H = Hermans et al. (1984)

SAR **NEUTRAL ORGANICS**

Organism: Mysid shrimp
Duration: 96-h
Endpoint: LC50 (Mortality)

Equation: Log LC50 (mM/L) = 1.83 - 1.25 log K_{ow}

Statistics: N = 17; R^2 = 0.706

Maximum K_{ow}: 5.0
Maximum MW: 1000.0

Application: Solvents, non-reactive, non-ionizable compounds:

1. Alcohols
2. Acetals
3. Ketones
4. Ethers
5. Alkyl halides
6. Aryl halides
7. Aromatic hydrocarbons
8. Halogenated aromatic hydrocarbons
9. Halogenated aliphatic hydrocarbons
10. Sulfides and di-sulfides

Limitations: If the log K_{ow} is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, use SAR with longer exposure.

References: Zaroogian G, Heltshe JF, and Johnson M. 1985. Estimation of toxicity to marine species with structure activity models developed to estimate toxicity to freshwater fish. Aquatic Toxicology 6:251-270.

NEUTRAL ORGANICS
7/1988

LIST OF NEUTRAL ORGANICS USED TO DEVELOP THE MYSID SHRIMP 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Toluene	55.5198	2.21	Z
1,3-Dichloropropane	10.0702	2.28	Z
Tetrachloroethylene	9.9922	2.60	Z
Benthiocarb	0.3235	3.40	Z
Hexachlorobutadiene	0.0611	3.74	Z
Chlorobenzene	16.2699	3.79	Z
EPN	0.0032	3.85	Z
Lindane	0.0059	3.89	Z
Dieldrin	0.0050	4.31	Z
1,2,4-Trichlorobenzene	0.4454	4.32	Z
1,2,3,5-Tetrachlorobenzene	0.3344	4.46	Z
Acenaphthene	0.0250	4.49	Z
1,2,4,5-Tetrachlorobenzene	1.4596	4.67	Z
Pentachlorobenzene	0.1616	4.94	Z
Heptachlor	0.0030	5.44	Z
Leptophos	0.0033	6.08	Z
Fenvalerate	0.0001	6.20	Z

Z = Zaroogian et al. (1985)

SAR **NEUTRAL ORGANICS**

Organism: Daphnid
Duration: 16-d
Endpoint: Chronic Value (EC50 Reproduction)

Equation: Log ChV (mM/L) = -0.72 log K_{ow} + 0.05

Statistics: N = 5; R^2 = 0.990

Maximum K_{ow}: 8.0
Maximum MW: 1000.0

Application: Solvents, non-reactive, non-ionizable compounds:

1. Aromatic hydrocarbons
2. Halogenated aromatic hydrocarbons
3. Halogenated aliphatic hydrocarbons
4. Alcohols
5. Ketones
6. Acetals
7. Ethers
8. Alkyl halides
9. Aryl halides
10. Sulfides and di-sulfides

This SAR can also be applied to some classes of reactive organic compounds which show excess toxicity to fish, such as:

1. Benzotriazoles
2. Phthalate esters
3. Esters

Limitations: If the log K_{ow} is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.

References: Hermans J, Canton H, Janssen P, and De Jong R. 1984. Quantitative structure-activity relationships and toxicity studies of mixtures of chemicals with anaesthetic potency: Acute lethal and sublethal toxicity to Daphnia magna. Aquatic Toxicology 5:143-154.

LIST OF NEUTRAL ORGANICS USED TO DEVELOP THE DAPHNID 16-d EC50 SAR.

CHEMICAL	16-d EC50 (mg/L)	Log K_{ow}	Ref.
Monochlorobenzene	25.8	2.81	H
4-Chlorotoluene	3.6	3.31	H
1,2,4-Trichlorobenzene	2.7	4.20	H
1,2,3,4-Tetrachlorobenzene	0.54	4.94	H
Pentachlorobenzene	0.23	5.96	H

H = Hermans et al. (1984)

SAR **NEUTRAL ORGANICS**

Organism: Green algae
Duration: 96-h
Endpoint: EC50 (Growth)

Equation: Log 96-h EC50 (mM/L) = 1.466 - 0.885 log K_{ow}

Statistics: N = 7; R^2 = 0.91

Maximum K_{ow}: 6.4
Maximum MW: 1000.0

Application:

Limitations: If the log K_{ow} is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility, use SAR with longer exposure.

References:

Calamari D, Galassi S, Setti F, and Vighi M. 1983. Toxicity of selected chlorobenzenes to aquatic organisms. Chemosphere 12:253-262.

Galassi S and Vighi M. 1981. Testing toxicity of volatile substances with algae. Chemosphere 10:1123-1126.

United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: USEPA, Office of Toxic Substances.

United States Environmental Protection Agency (USEPA). 1992. Aquatic toxicity database. Duluth, MN: USEPA, ERL - Duluth.

NEUTRAL ORGANICS
7/1988

LIST OF NEUTRAL ORGANICS USED TO DEVELOP THE GREEN ALGAE 96-h EC50 SAR.

CHEMICAL	96-h EC50 (mg/L)	Log K_{ow}	Ref.
Polyether	315	1.9	EPA
Benzene	29	2.1	G
Isolinalool	14	2.4	EPA
Toluene	12.5	2.8	G
Chlorobenzene	12.5	2.9	C
trans-Anethole	4.24	3.3	D
Ethylbenzene	4.6	3.3	G
o-Xylene	4.7	3.4	G
m-Xylene	4.9	3.4	G
p-Xylene	3.2	3.4	G
1,2-Dichlorobenzene	2.2	3.6	C
1,4-Dichlorobenzene	0.57	3.6	C
Isopropylbenzene	2.6	3.7	G
n-Propylbenzene	1.8	3.8	G
1,2,3-Trichlrorbenzene	0.22	4.3	C
1,2,4-Trichlorobenzene	0.37	4.3	C
Hexachlorobenzene	*	6.4	C

* = No effects in saturated solutions.

C = Calamari et al. (1983)
D = USEPA (1992).
EPA = USEPA (1991); chemical identity is Confidential Business Information under TSCA
G = Galassi and Vighi (1988)

SAR **NEUTRAL ORGANICS**

Organism: Green algae
Duration:
Endpoint: Chronic Value (Growth)

Equation: Log ChV (mM/L) = -0.036 - 0.634 log K_{ow}

Statistics: N = 7; R^2 = 0.99

Maximum K_{ow}: 8.0
Maximum MW: 1000.0

Applications: May be applied to other neutral organics including aldehydes.

Limitations: If the log K_{ow} is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.

References:

Calamari D, Galassi S, Setti F, and Vighi M. 1983. Toxicity of selected chlorobenzenes to aquatic organisms. Chemosphere 12:253-262.

Galassi S and Vighi M. 1981. Testing toxicity of volatile substances with algae. Chemosphere 10:1123-1126.

United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: USEPA, Office of Toxic Substances.

United States Environmental Protection Agency (USEPA). 1992. Aquatic toxicity database. Duluth, MN: USEPA, ERL - Duluth.

LIST OF NEUTRAL ORGANICS USED TO DEVELOP THE GREEN ALGAE ChV SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
Polyether	15.9	1.9	EPA
Isolinalool	4.8	2.4	EPA
trans-Anethole	3.09	3.3	D
1,4-Dichlorobenzene	0.57	3.6	C
1,2,3-Trichlrorbenzene	0.22	4.3	C
1,2,4-Trichlorobenzene	0.37	4.3	C
Hexachlorobenzene	0.027	6.4	C

C = Calamari et al. (1983)
D = USEPA (1992)
EPA = USEPA (1991)

SAR **NEUTRAL ORGANICS**

Organism: Earthworm
Duration: 14-d
Endpoint: LC50 (Mortality)

Equation: Log 14-d LC50 (mM/L) = 1.405 - 0.308 log K_{ow}

Statistics: N = 5; R^2 = 0.48

Maximum K_{ow}: 5.0
Maximum MW: 1000.0

Applications: Neutral organics

Limitations: None

References:

Neuhauser EF, Durkin PR, Malecki MR, and Anatra M. 1986. Comparative toxicity of ten organic chemicals to four earthworm species. Comp. Biochem. Physiol. 83C:197-200.

Neuhauser EF, Loehr RC, Malecki MR, Milligan DL, and Durkin PR. 1985. The toxicity of selected organic chemicals to the earthworm Eisenia fetida. Journal of Environmental Quality 14:383-388.

LIST OF NEUTRAL ORGANIC CHEMICALS USED TO DEVELOP THE EARTHWORM 14-d LC50 SAR.

CHEMICAL	14-d LC50 (mg/L)	Log K_{ow}	Ref.
2-chloroethylvinylether	740.0	1.0	N
nitrobenzene	319.0	1.9	N
1,2-dichloropropane	4240.0	2.0	N
fluorene	173.0	4.2	N
1,2,4-trichlorobenzene	197.0	4.3	N

N = Neuhauser et al. (1985, 1986)

NEUTRAL ORGANICS
7/1988

SAR	**PEROXY ACIDS**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	log 96-h LC50 (mM/L) = -2.6 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for peroxy acids.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, use SAR with longer exposure.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

LIST OF PEROXY ACIDS USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
Chemical identity CBI	0.750	2.6	EPA

EPA = USEPA (1991); chemical identity is Confidential Business Information under TSCA.

PEROXY ACIDS
9/1993

SAR	**PEROXY ACIDS**
Organism:	Daphnids
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Log 48-h LC50 (mM/L) = -0.717 -0.417 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for peroxy acids.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, use SAR with longer exposure.
References:	United States Environmental Protection Agency (USEPA). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

LIST OF PEROXY ACIDS USED TO DEVELOP THE DAPHNID 48-H SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
Chemical identity CBI	4.6	2.6	EPA

EPA = USEPA (1991); chemical identity is Confidential Business Information under TSCA.

PEROXY ACIDS
9/1993

SAR	**PHENOLS**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log 96-h LC50 (mM/L) = 0.399 - 0.616 log K_{ow}
Statistics:	N = 78; R^2 = 0.86
Maximum log K_{ow}:	7.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for phenols.
Limitations:	Phenols which are significantly more toxic than predicted by this SAR are: catechol with 16 x excess toxicity; hydroquinone with 1400 x excess toxicity; and p-benzoquinone with 5500 x excess toxicity. If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, use SAR with longer exposure.
References:	Alexander HC, Dill, DC, Smith LW, Guiney PD, and Dorn P. 1988. Bisphenol A: Acute aquatic toxicity. Environ. Toxicol. Chem. 7:19-26. Curtis MW and Ward CH. 1981. Aquatic toxicity of forty industrial chemicals: Testing in support of hazardous substance spill prevention regulation. Journal of Hydrology 51:359-367. DeGraeve GM, Geiger DL, Meyer JS, Bergman HL. 1980. Acute and embryo-larval toxicity of phenolic compounds to aquatic biota. Arch. Environ. Contam. Toxicol. 9:557-568. Holcombe GW, Phipps GL, Knuth M, and Felhaber T. 1984. The acute toxicity of selected substituted phenols, benzenes, and benzioic acid esters to fathead minnows, Pimephales promelas. Environ. Pollution, Ser. A, 35:367-381. Holcombe GW, Phipps GL, and Fiandt JT. 1982. Effects of phenol, 2,4-dimethylphenol, 2,4-dichlorophenol, and pentachlorophenol on embryo, larval, and early-juvenile fathead minnows (Pimephales promelas). Arch. Environ. Contam. Toxicol. 11:73-78. Konemann H, and Musch A. 1981. Quantitative structure-activity relationships in fish toxicity studies. Part 2: The influence of pH on the SAR of chlorophenols. Toxicology 19:223-228.

Marking LL, Howe GE, and Bills TD. 1991. Temperature and pH effects on acute and chronic toxicity of four chemicals to amphipods (Gammarus pseudolimnaeus) and rainbow trout (Oncorhynchus mykiss). EPA/600/X-90/286. Gulf Breeze, FL: Environmental Research Laboratory, Office of Research and Development, United States Environmental Protection Agency. August.

Saarikoski J and Viluksela M. 1982. Relation between physicochemical properties of phenols and their toxicity and accumulation in fish. Ecotoxicology and Environmental Safety 6:501-512.

United States Environmental Protection Agency (USEPA1). 1980. Ambient Water Quality Criteria for Phenol. EPA-440-5-80-066. Washington, DC: Criteria and Standards Division, Office of Water Regulations and Standards, USEPA.

United States Environmental Protection Agency (USEPA2). 1984. Dynamic 14-day acute toxicity of octylphenol to rainbow trout (Salmo gairdneri). TSCA Section 4(d). Document No. 40-8462075. Washington, DC: OTS Public Files, USEPA. Fiche No. 0507489 (2).

United States Environmental Protection Agency (USEPA3). 1990. Section 8(e)908.

United States Environmental Protection Agency (USEPA4). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

Veith GD and Broderius SJ. 1987. Structure-toxicity relationships for industrial chemicals causing type (II) narcosis syndrome. IN: Kaiser KLE (ed.). QSAR in Environmental Toxicology - II. New York: D. Reidel Publishing Company. pp. 385-391.

LIST OF PHENOLS USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
PHENOLS USED IN THE CALCULATION OF THIS SAR			
Resorcinol	60.0	0.8	C
Resorcinol	100.0	0.81	D
Phenol	44.5	1.5	EPA1
Phenol	36.3	1.5	EPA1
Phenol	36.0	1.5	EPA1
Phenol	34.9	1.5	EPA1
Phenol	26.0	1.5	EPA1
Phenol	19.0	1.5	EPA1
Phenol	16.7	1.5	EPA1
Phenol	16.4	1.5	EPA1
Phenol	10.2	1.5	EPA1
Phenol	8.9	1.5	D
Phenol	67.5	1.5	D
Phenol	29.8	1.5	K
Phenol	43.0	1.5	S
Phenol	37.0	1.5	V
3-Methoxyphenol	74.0	1.6	V
4-Methoxyphenol	110.0	1.6	V
4-Nitrophenol	14.2	1.9	S
3-Nitrophenol	11.8	1.9	S
4-Nitrophenol	41.0	1.9	H
4-Nitrophenol	6.9	1.9	M
3-Methylphenol	23.1	2.1	S
4-Methylphenol	16.5	2.1	V
p-Cresol	7.9	2.1	D
p-Cresol	28.6	2.1	D
o-Cresol	8.4	2.1	D
o-Cresol	18.2	2.1	D
m-Cresol	8.9	2.1	D
m-Cresol	55.9	2.1	D
2-Chlorophenol	11.2	2.2	K
2-Chlorophenol	13.8	2.2	S
2-Chlorophenol	9.4	2.2	V
2-Allylphenol	15.0	2.2	V
4-Chlorphenol	8.5	2.5	S
3-Chlorophenol	6.4	2.5	K
1-Naphthol	4.6	2.6	V
4-Ethylphenol	10.4	2.7	V
2,6-Dichlorophenol	7.8	2.8	S
2,4-Dimethylphenol	16.6	2.8	H
2-Chloro-4-methylphenol	35.9	2.9	V
2,4-Dichlorophenol	5.5	3.1	S

CONTINUED.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
PHENOLS USED IN CALCULATION OF THE SAR			
4,5-Dichloro-2-methoxy phenol	4.8	3.1	S
2,4-Dichlorophenol	4.2	3.1	K
3,4,5-Trichloro-2,6-dimethoxyphenol	3.4	3.1	S
2,4-Dichlorophenol	7.75	3.1	H
4-Chloro-3-methylphenol	5.72	3.1	V
2,4-Dichlorophenol	7.75	3.1	V
4-Propylphenol	11.0	3.2	V
4-Phenylazophenol	1.17	3.2	V
3,5-Dichlorophenol	2.7	3.3	K
Bis(thiophenol)	1.5	3.4	EPA3
2,3,6-Trimethylphenol	0.390	3.4	S
2-Phenylphenol	6.15	3.4	V
4,4'-[oxybis(2,1-ethane diylthio)]bisphenol	1.5	3.4	EPA4
4-Tert-butylphenol	5.15	3.5	V
3,4,5-Trichloro-2-methoxyphenol	2.1	3.6	S
2,4,6-Trichlorophenol	4.55	3.6	V
2,4,6-Trichlorophenol	2.3	3.6	S
2,3,6-Trichlorophenol	5.1	3.8	K
4-chloro-3,5-dimethyl phenol	3.4	3.8	S
4-Phenoxyphenol	4.96	3.8	V
Bisphenol A	4.6	3.8	A
2,3,5-Trichlorphenol	1.6	3.9	K
2,4,5-Trichlorophenol	1.2	3.9	S
3,4,5,6-Tetrachloro-2-hydroxyphenol	2.5	3.9	S
4-Tert-pentylphenol	2.59	4.0	V
2-Tert-butyl-4-methylphenol	2.1	4.1	S
2,3,5,6-Tetrachlorophenol	1.4	4.3	K
2,3,4,6-Tetrachlorophenol	1.1	4.3	S
2,3,4,5-Tetrachlorophenol	0.770	4.6	K
Pentachlorophenol	0.380	5.1	K
Pentachlorophenol	0.24	5.1	V
Pentachlorophenol	0.440	5.1	S
4-(Tert-octyl)phenol	0.250	5.3	EPA2
4-(Tert-octyl)phenol	0.210	5.3	EPA2

4-Nonylphenol	0.140	6.4	V

CONTINUED.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
PHENOLS USED IN CALCULATION OF THE SAR			
Substituted benzophenone glyceride	*	8.0	EPA4
Hindered phenol	*	11.0	EPA4
PHENOLS HAVING EXCESS TOXICITY			
p-Benzoquinone	0.125	-0.3	D
p-Benzoquinone	0.045	-0.3	D
Hydroquinone	0.097	0.8	D
Hydroquinone	0.044	0.8	D
Catechol	8.9	0.81	D
Catechol	3.5	0.81	D

* = No fish mortality in saturated solutions.

A = Alexander et al (1988)
C = Curtis and Ward (1981)
D = DeGraeve et al (1980)
H = Holcombe et al (1984, 1982)
K = Konemann and Musch (1981)
M = Marking et al (1991)
S = Saarikoski and Viluksela (1982)
EPA1 = USEPA (1980)
EPA2 = USEPA (1984)
EPA3 = USEPA (1990)
EPA4 = USEPA (1991)
V = Veith and Broderius (1987)

PHENOLS
9/1993

SAR	**PHENOLS**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Log 48-h LC50 (mM/L) = -0.451 - 0.409 log K_{ow}
Statistics:	N = 48; R^2 = 0.6
Maximum log K_{ow}:	5.5
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for phenols.
Limitations:	Phenols which contain the following groups may have excess toxicity compared with the values predicted by this SAR: 1,2-di(OH) groups (e.g., catechol); 1,4-di(OH) groups (e.g., hydroquinone); or 1,4-di(=O) groups (e.g., benzoquinone). If the log K_{ow} value is greater than 5.5, or if the compound is solid and the LC50 exceeds the water solubility, use SAR with longer duration. For aminophenols, use the daphnid 48-h LC50 SAR for anilines.
References:	Alexander HC, Dill, DC, Smith LW, Guiney PD, and Dorn P. 1988. Bisphenol A: Acute aquatic toxicity. Environ. Toxicol. Chem. 7:19-26. Kuhn R, Pattard M, Pernak, K-D, and Winter A. 1989. Results of the harmful effects of water pollutants to Daphnia magna in the 21 day reproduction test. Water Res. 23:501-510. LeBlanc G. 1980. Acute toxicity of priority pollutants to water flea (Daphnia magna). Bull. Environm. Contam. Toxicol. 24:684-691. United States Environmental Protection Agency (USEPA1). 1984. Dynamic 14-day acute toxicity of octylphenol to rainbow trout (Salmo gairdneri). TSCA Section 4(d). Document No. 40-8462075. Washington, DC: OTS Public Files, USEPA. Fiche No. 0507489 (2). United States Environmental Protection Agency (USEPA2). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

LIST OF PHENOLS USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
PHENOLS USED IN CALCULATION OF THE SAR			
3-Hydroxyphenylurea	93.0	0.2	K
4-Acetamidophenol	9.2	0.5	K
4-Hydroxybenzonitrile	15.0	1.6	K
4-Nitrophenol	22.0	1.9	L
2-Chlorophenol	2.6	2.2	L
4-Chlorophenol	4.1	2.5	L
2,4-Dimethylphenol	2.1	2.8	L
3-(Trifluoromethyl)phenol	11.0	2.9	K
2,4-Dichlorophenol	2.6	3.1	L
4-Chloro-6-methylphenol	0.290	3.1	L
o-Phenylphenol	1.5	3.4	K
2,4,6-Trichlorophenol	6.0	3.6	L
2,4-Dichloro-6-methyl phenol	0.430	3.7	L
4-Chloro-3,5-dimethyl phenol	4.5	3.8	K
Bisphenol A	10.2	3.8	A
2,4,5-Trichlorophenol	2.7	3.9	L
2,3,4,6-Tetrachlorophenol	0.290	4.3	L
2,3,5,6-Tetrachlorophenol	0.570	4.3	L
Pentachlorophenol	0.680	5.1	L
4-(Tert-octyl)phenol	0.270	5.3	EPA1
3,5-Di-tert-butylphenol	1.7	5.4	K
Substituted benzophenone glyceride	*	8.0	EPA2

* = No daphnid mortalities in saturated solutions.

A = Alexander et al (1988)
EPA1 = USEPA1 (1984)
EPA2 = USEPA2 (1991)
K = Kuhn et al (1989)
L = LeBlanc (1980)

SAR	**PHENOLS**
Organism:	Green Algae
Duration:	96-h
Endpoint:	EC50 (Growth)
Equation:	To find the estimated acute toxicity of a phenol, use the neutral organic green algae 96-h EC50 SAR.
Maximum log K_{ow}:	6.4
Maximum MW:	1000.0
Application:	The neutral organic green algae 96-h EC50 SAR may be used to estimate toxicity for phenols.
Limitations:	Phenols which contain the following groups may have excess toxicity compared with the values predicted by this SAR: 1,2-di(OH) groups (e.g., catechol); 1,4-di(OH) groups (e.g., hydroquinone); or 1,4-di(=O) groups (e.g., benzoquinone). If the log K_{ow} value is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility, use SAR with longer exposure. For aminophenols, use the green algae chronic value SAR for anilines.
References:	Alexander HC, Dill, DC, Smith LW, Guiney PD, and Dorn P. 1988. Bisphenol A: Acute aquatic toxicity. Environ. Toxicol. Chem. 7:19-26. Kuhn R and Pattard M. 1990. Results of the harmful effects of water pollutants to green algae (Scenedesmus subspicatus) in the cell multiplication inhibition test. Water Res. 24:31-38. United States Environmental Protection Agency (USEPA1). 1984. Dynamic 14-day acute toxicity of octylphenol to rainbow trout (Salmo gairdneri). TSCA Section 4(d). Document No. 40-8462075. Washington, DC: OTS Public Files, USEPA. Fiche No. 0507489 (2). United States Environmental Protection Agency (USEPA2). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

LIST OF PHENOLS USED TO DEVELOP THE GREEN ALGAE 96-h EC50 SAR.

CHEMICAL	96-h EC50 (mg/L)	Log K_{ow}	Ref.
PHENOLS USED IN CALCULATION OF THE SAR			
3,5-Dimethoxyphenol	110.0	1.4	K
4-Nitrophenol	26.0	1.9	K
p-Cresol	7.8	2.1	K
2-Chlorophenol	50.0	2.2	K
2-Bromophenol	60.0	2.4	K
2-Nitro-para-cresol	12.0	2.5	K
4-Chlorophenol	8.0	2.5	K
2,4-Dichlorophenol	11.5	3.1	K
4-Chloro-3-methylphenol	>10.0	3.1	K
2,4,6-Trimethylphenol	17.0	3.4	K
Bis(thiophenol)	0.740	3.4	EPA2
Bisphenol A	2.7	3.8	A
4-(Tert-octyl)phenol	1.6	5.3	EPA1
PHENOLS HAVING EXCESS TOXICITY			
2-Amino-4-methylphenol	4.6	1.3	K

A = Alexander et al (1988)
EPA1 = USEPA1 (1984)
EPA2 = USEPA2 (1991)
K = Kuhn and Pattard (1990)

SAR	**PHENOLS**
Organism:	Fish
Duration:	30-d
Endpoint:	Chronic Value
Equation:	Log ChV (mM/L) = -0.401 - 0.652 log K_{ow}
Statistics:	N = 20; R^2 = 0.94
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for phenols.
Limitations:	Phenols which contain the following groups may have excess toxicity compared with the values predicted by this SAR: 1,2-di(OH) groups (e.g., catechol); 1,4-di(OH) groups (e.g., hydroquinone); or 1,4-di(=O) groups (e.g., benzoquinone). If the log K_{ow} value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, use SAR with longer exposure. A test duration of more than 30 days may result in a lower chronic toxicity; at 60 days the toxicity will be 20 x lower than predicted by this SAR for phenols with a log K_{ow} of 1.5 and 4 x lower for phenols with a log K_{ow} of 5.3. For an exposure period of 60 days, a separate SAR has been developed. For aminophenols, use the fish ChV SAR for anilines.
References:	DeGraeve GM, Geiger DL, Meyer JS, and Bergman HL. 1980. Acute and embryo-larval toxicity of phenolic compounds to aquatic biota. Arch. Environ. Contam. Toxicol. 9:557-568. Hedtke SF, West CW, Allen KN, Norberg-King TJ, and Mount DI. 1986. Toxicity of pentachlorophenol to aquatic organisms under naturally varying and controlled conditions. Environ. Toxicol. Chem. 5:531-542. Holcombe GW, Phipps GL, and Fiandt JT. 1982. Effects of phenol, 2,4-dimethylphenol, 2,4-dichlorophenol, and pentachlorophenol on embryo, larval, and early-juvenile fathead minnows (Pimephales promelas). Arch. Environ. Contam. Toxicol. 11:73-78. Marking LL, Howe GE, and Bills TD. 1991. Temperature and pH effects on acute and chronic toxicity of four chemicals to amphipods (Gammarus pseudolimnaeus) and rainbow trout (Oncorhynchus mykiss). EPA/600/X-90/286. Gulf Breeze, FL: Envrionmental Research

Laboratory, Office of Research and Development, United States Environmental Protection Agency. August.

Spehar RL, Nelson HP, Swanson MJ, and Renos JW. 1985. Pentachlorophenol toxicity to amphipods and fathead minnows at different test pH values. Environ. Toxicol. Chem. 4:389-397.

United States Environmental Protection Agency (USEPA1). 1980. Ambient Water Quality Criteria for Phenol. EPA-440-5-80-066. Washington, DC: Criteria and Standards Division, Office of Water Regulations and Standards, USEPA.

United States Environmental Protection Agency (USEPA2). 1984. Dynamic 14-day acute toxicity of octylphenol to rainbow trout (Salmo gairdneri). TSCA Section 4(d). Document No. 40-8462075. Washington, DC: OTS Public Files, USEPA. Fiche No. 0507489 (2).

United States Environmental Protection Agency (USEPA3). 1991. Fish Chronic Toxicity Data Base. Duluth, MN: Environmental Research Laboratory (ERL), Office of Research and Development, USEPA, 6201 Congdon Boulevard, 55804; contact C.L. Russom (218) 720-5500.

LIST OF PHENOLS USED TO DEVELOP THE FISH 30-d ChV SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
PHENOLS USED IN CALCULATION OF THE SAR			
2,2'-Methylene bis (4-chlorophenol)	0.122	5.0	EPA3
4-Nitrophenol	3.38	1.9	M
Phenol	1.4	1.5	D
Phenol	2.56	1.5	EPA1
o-Cresol	1.8	2.1	EPA3
4-Nitrophenol	2.65	1.9	EPA3
2,4-Dimethylphenol	2.48	2.8	HO
2,4-Dimethylphenol	0.763	2.8	EPA3
p-Cresol	1.86	2.1	EPA3
Phenol	2.56	1.5	HO
2-Phenylphenol	1.22	3.4	EPA3
Pentachlorophenol	0.089	5.1	S
Pentachlorophenol	0.057	5.1	HO
Pentachlorophenol	0.040	5.1	S
Pentachlorophenol	0.144	5.1	HE
Pentachlorophenol	0.049	5.1	S
Pentachlorophenol	0.024	5.1	S
2,4,5-Trichlorophenol	0.232	3.9	EPA3
2,4-Dichlorophenol	0.365	3.1	HO
PHENOLS HAVING EXCESS TOXICITY			
Phenol	<0.200	1.5	D
4-(Tert-octyl)phenol	0.008	5.3	EPA2

D = DeGraeve et al (1980)
EPA1 = USEPA (1980)
EPA2 = USEPA (1984)
EPA3 = USEPA (1991)
HE = Hedtke et al (1986)
HO = Holcombe et al (1982)
M = Marking et al (1991)
S = Spehar et al (1985)

PHENOLS
9/1993

SAR **PHENOLS**

Organism: Fish
Duration: 60-d
Endpoint: Chronic Value

Equation: Log ChV (mM/L) = -2.029 - 0.447 log K_{ow}

Statistics: N = 2; R^2 = 1.0

Maximum log K_{ow}: 8.0
Maximum MW: 1000.0

Application: This equation may be used to estimate toxicity for phenols.

Limitations: If the log K_{ow} value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.

For aminophenols, use the fish ChV SAR for anilines.

References:

DeGraeve GM, Geiger DL, Meyer JS, and Bergman HL. 1980. Acute and embryo-larval toxicity of phenolic compounds to aquatic biota. Arch. Environ. Contam. Toxicol. 9:557-568.

United States Environmental Protection Agency (USEPA). 1984. Dynamic 14-day acute toxicity of octylphenol to rainbow trout (Salmo gairdneri). TSCA Section 4(d). Document No. 40-8462075. Washington, DC: OTS Public Files, USEPA. Fiche No. 0507489 (2).

LIST OF PHENOLS USED TO DEVELOP THE FISH 60-d ChV SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
PHENOLS USED IN CALCULATION OF THE SAR			
Phenol	<0.200	1.5	D
4-(Tert-octyl)phenol	0.008	5.3	EPA

D = DeGraeve et al (1980)
EPA = USEPA (1984)

PHENOLS
9/1993

PHENOLS
9/1993

SAR	**PHENOLS**
Organism:	Daphnid
Duration:	
Endpoint:	Chronic Value
Equation:	Log ChV (mM/L) = -0.573 - 0.614 log K_{ow}
Statistics:	N = 12; R^2 = 0.92
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate toxicity for phenols.
Limitations:	Phenols which contain the following groups may have excess toxicity compared with the values predicted by this SAR: 1,2-di(OH) groups (e.g., catechol); 1,4-di(OH) groups (e.g., hydroquinone); or 1,4-di(=O) groups (e.g., benzoquinone). 3,5-Dimethoxyphenol has an excess toxicity of 18 x that predicted by this SAR. If the log K_{ow} value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation. For aminophenols, use the daphnid ChV SAR for anilines.
References:	Kuhn R, Pattard M, Pernak, K-D, and Winter A. 1989. Results of the harmful effects of water pollutants to Daphnia magna in the 21 day reproduction test. Water Res. 23:501-510. Oris JT, Winner RW, and Moore MV. 1991. A four-day survival and reproduction toxicity test for Ceriodaphnia dubia. Environ. Toxicol. Chem. 10:217-224. United States Environmental Protection Agency (USEPA). 1984. Dynamic 14-day acute toxicity of octylphenol to rainbow trout (Salmo gairdneri). TSCA Section 4(d). Document No. 40-8462075. Washington, DC: OTS Public Files, USEPA. Fiche No. 0507489 (2).

LIST OF PHENOLS USED TO DEVELOP THE DAPHNID ChV SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
PHENOLS USED IN CALCULATION OF THE SAR			
Phenol	4.9	1.5	O
4-Nitrophenol	1.8	1.9	K
4-Methylphenol	1.4	2.1	K
2-Chlorophenol	0.500	2.2	K
2-Bromophenol	1.5	2.4	K
4-Chlorophenol	0.840	2.5	K
2-Nitro-para-cresol	3.2	2.5	K
2,4-Dichlorophenol	0.290	3.1	K
4-Chloro-3-methylphenol	1.8	3.1	K
2,4,6-Trimethylphenol	0.160	3.4	K
4-(Tert-octyl)phenol	0.086	5.3	EPA
PHENOLS HAVING EXCESS TOXICITY			
2-Amino-4-methylphenol	0.400	1.3	K
3,5-Dimethoxyphenol	0.320	1.4	K

PHENOLS
9/1993

SAR	**PHENOLS**
Organism:	Green Algae
Duration:	
Endpoint:	Chronic Value (Growth)
Equation:	To find the estimated chronic toxicity of a phenol, use the neutral organic green algae ChV SAR.
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	The neutral organic green algae ChV SAR may be used to estimate toxicity for phenols.
Limitations:	Phenols which contain the following groups may have excess toxicity compared with the values predicted by this SAR: 1,2-di(OH) groups (e.g., catechol); 1,4-di(OH) groups (e.g., hydroquinone); or 1,4-di(=O) groups (e.g., benzoquinone). If the log K_{ow} is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation. For aminophenols, use the aniline green algae ChV SAR.
References:	Kuhn R and Pattard M. 1990. Results of the harmful effects of water pollutants to green algae (Scenedesmus subspicatus) in the cell multiplication inhibition test. Water Res. 24:31-38. Slooff W, Canton JH, and Hermens JLM. 1983. Comparison of the susceptibility of 22 freshwater species to 15 chemical compounds. I. (Sub)Acute toxicity tests. Aquatic Toxicology 4;113-128. United States Environmental Protection Agency (USEPA1). 1984. Dynamic 14-day acute toxicity of octylphenol to rainbow trout (Salmo gairdneri). TSCA Section 4(d). Document No. 40-8462075. Washington, DC: OTS Public Files, USEPA. Fiche No. 0507489 (2). United States Environmental Protection Agency (USEPA2). 1991. OTS PMN ECOTOX. Washington, DC: Office of Toxic Substances, USEPA.

LIST OF PHENOLS USED TO DEVELOP THE GREEN ALGAE ChV SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
PHENOLS USED IN CALCULATION OF THE SAR			
3,5-Dimethoxyphenol	40.0	1.4	K
4-Nitrophenol	2.1	1.9	K
o-Cresol	34.0	2.1	S
o-Cresol	11.0	2.1	S
o-Cresol	36.0	2.1	S
o-Cresol	65.0	2.1	S
p-Cresol	2.3	2.1	K
2-Chlorophenol	24.0	2.2	K
2-Bromophenol	28.0	2.4	K
2-Nitro-p-cresol	6.3	2.5	K
4-Chlorophenol	3.0	2.5	K
4-Chloro-3-methylphenol	5.2	3.1	K
2,4-Dichlorophenol	2.4	3.1	K
2,4,6-Trimethylphenol	5.8	3.4	K
Bis(thiophenol)	0.300	3.4	EPA2
4-(Tert-octyl)phenol	<0.860	5.3	EPA1
PHENOLS WITH EXCESS TOXICITY			
2-Amino-4-methylphenol	0.750	1.3	K

EPA1 = USEPA (1984)
EPA2 = USEPA (1991)
K = Kuhn and Pattard (1990)
S = Slooff et al (1983)

PHENOLS, DINITRO
9/1993

SAR	**PHENOLS, DINITRO**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log 96-h LC50 (mM/L) = -0.285 - 0.559 log K_{ow}
Statistics:	N = 4; R^2 = 0.96
Maximum log K_{ow}:	7.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for dinitrophenols and other polynitrophenols.
Limitations:	If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	Veith GD and Broderius SJ. 1987. Structure-toxicity relationships for industrial chemicals causing type (II) narcosis syndrome. In: Kaiser KLE (ed.). QSAR in Environmental Toxicology-II. Boston, MA: D. Reidel Pub. Co., pp. 385-391.

LIST OF DINITROPHENOLS USED TO DEVELOP THE FISH 96-h LC50 SAR.

CHEMICAL	96-h LC50 (mg/L)	Log K_{ow}	Ref.
2,4-dinitrophenol	11.0	1.5	VB
4,6-dinitro-o-cresol	1.54	2.6	VB
2,4-dinitro-1-naphthol sodium	4.24	3.09	VB

VB = Veith and Broderius (1987)

PHENOLS, DINITRO
9/1993

SAR	**PHENOLS, DINITRO**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Log 48-h LC50 (mM/L) = 0.083 - 0.632 log K_{ow}
Statistics:	N = 7; R^2 = 0.85
Maximum log K_{ow}:	7.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for dinitrophenols and other polynitrophenols.
Limitations:	If the log K_{ow} value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	Hermens J, Canton H, Janssen P, and DeJong R. 1984. Quantitative structure-activity relationships and toxicity studies of mixtures of chemicals with anaesthetic potency: Acute lethal and sublethal toxicity to Daphnia magna. Aquatic Toxicology 5:143-154. Kuhn R, Pattard M, Pernak K-D, and Winter A. 1989. Results of the harmful effects of selected water pollutants (anilines, phenols, aliphatic compounds) to Daphnia magna. Water Research 23:495-499. LeBlanc. 1980. Acute toxicity of priority pollutants to water flea (Daphnia magna). Bulletin of Environmental Contamination and Toxicology. 24: 684-691.

LIST OF DINITROPHENOLS USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

CHEMICAL	48-h LC50 (mg/L)	Log K_{ow}	Ref.
2,4,6-trinitrophenol	85.0	1.8	L
2,4,6-trinitrophenol	90.0	1.8	K
2,4-dinitrophenol	4.1	1.9	L
2,4-dinitro-6-methyl phenol	3.1	2.6	L
dinitro-o-cresol	3.3	2.6	H
2-methyl-4,6-dinitrophenol	2.7	2.6	K

Kuhn = Kuhn et al (1989)
H = Hermens et al (1984)
L = LeBlanc (1980)

PHENOLS, DINITRO
9/1993

SAR	**PHENOLS, DINITRO**
Organism:	Fish
Duration:	32-d
Endpoint:	Chronic Value (Survival/Growth)
Equation:	Log ChV (mM/L) = -1.78 - 0.552 log K_{ow}
Statistics:	N = 4; R^2 = 1.0
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for dinitrophenols and other polynitrophenols.
Limitations:	If the log K_{ow} is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1991. Fish Chronic Toxicity Data Base. Duluth, MN: Environmental Research Laboratory (ERL), Office of Research and Development, USEPA, 6201 Congdon Boulevard, 55804; contact C.L. Russom (218) 720-5500.

LIST OF DINITROPHENOLS USED TO DEVELOP THE FISH CHRONIC (ChV) SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
2,4-dinitrophenol	0.278	1.5	D
4,6-dinitro-o-cresol	0.171	2.3	D
2-(1-methylpropyl)-4,6-dinitrophenol	0.027	3.7	D

D = USEPA (1991)

PHENOLS, DINITRO
9/1993

SAR	**PHENOLS, DINITRO**
Organism:	Daphnid
Duration:	16-d
Endpoint:	Chronic Value (Survival/Reproduction)
Equation:	Log ChV (mM/L) = -0.465 - 0.654 log K_{ow}
Statistics:	N = 2; R^2 = 1.0
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	This SAR may be used to estimate toxicity for dinitrophenols and other polynitrophenols.
Limitations:	If the log K_{ow} is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility, no effects expected at saturation.
References:	Hermens J, Canton H, Janssen P, and DeJong R. 1984. Quantitative structure-activity relationships and toxicity studies of mixtures of chemicals with anaesthetic potency: Acute lethal and sublethal toxicity to Daphnia magna. Aquatic Toxicology 5:143-154.

LIST OF DINITROPHENOLS USED TO DEVELOP THE DAPHNID CHRONIC VALUE (ChV) SAR.

CHEMICAL	ChV (mg/L)	Log K_{ow}	Ref.
Dinitro-o-cresol	2.1	2.3	H

H = Hermens et al (1984)

POLYMERS, POLYCATIONIC
9/1993

SAR	**POLYMERS, POLYCATIONIC**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Determine either the percent amine nitrogen or the number of positive charges per 1000 units of molecular weight and use the appropriate SAR:

1. If the percent amine nitrogen is less than 3.5:

   Log LC50 (mg/L) = 1.3076 - 0.534 x (percent amine nitrogen)

If the percent amine nitrogen is greater than or equal to 3.5, then the fish 96-h LC50 is 0.27 mg/L.

2. If the number of positive charges per 1000 units of MW is less than 2.5:

   Log LC50 (mg/L) = 1.3116 - 0.7606 x (number of positive charges per 1000 MW units)

If the number of positive charges per 1000 units of molecular weight is greater than or equal to 2.5, then the fish 96-h LC50 is 0.27 mg/L.

Statistics:	For the percent amine nitrogen SAR: (less than 3.5% amine nitrogen) N = 12 and R^2 = 0.73, (greater than or equal to 3.5% amine nitrogen) N = 20 and the standard deviation is plus or minus 0.18 logarithmic units; For the number of positive charges/1000 units MW SAR: (less than 2.5 charges/100 MW) N = 12 and R^2 = 0.73
Minimum MW:	1000.0
Application:	These SARs may be used for polycationic polymers which are highly water soluble or dispersible and contain nitrogen which may be protonated and/or quaternarized. These SARs may be used for polysulfoniums and polyphosphoniums which are dispersible.
Limitations:	Polycationic polymers which contain silicon may have limited water solubility or dispersibility. Polycationic polymers which contain anionic groups may be significantly less toxic than predicted by this SAR. For example, a polycationic polymer containing 4.7 percent amine nitrogen (or 3.4 cationic charges per 1000 molecular weight) and anionic groups with a cationic:anionic molar ratio of 1:1.1, will be about 24 times less toxic than predicted, i.e., fish 96-h LC50 is 6.6 mg/L.
References:	Nabholz JV. 1988. A structure-activity relationship for polycationic polymers. Washington, DC: Environmental Effects Branch, Health and

Environmental Review Division (TS-796), Office of Toxic Substances,
United States Environmental Protection Agency 20460-0001.

LIST OF COMPOUNDS USED TO DEVELOP THE POLYCATIONIC POLYMER FISH 96-h LC50 SAR.

Percent Amine Nitrogen	Number of Positive Charges per 1000 Units of Mol. Weight	Average Molecular Weight (1000)	96-h LC50 (mg/L)	
	0.7	0.5	1.8	9.2
0.7	0.5	1.8	8.5	
0.7	0.5	1.8	3.9	
0.7	0.5	100.0	53.0	
2.0	1.4	2500.0	0.97	
2.0	1.4	2500.0	2.3	
2.0	1.4	1100.0	0.64	
2.0	1.4	1100.0	1.2	
2.1	1.5	19000.0	0.84	
3.0	2.1	100	0.94	
3.4	2.4	*	0.6	
3.4	2.4	*	0.3	
6.0	4.3	>5.0	0.15	
6.0	4.3	>5.0	0.16	
6.0	4.3	>5.0	0.29	
8.0	5.7	5.0	0.13	
8.0	5.7	5.0	0.22	
8.0	5.7	5.0	0.22	
9.2	6.6	*	0.5	
11.0	7.9	1.8	0.22	
12.0	8.6	*	1.9	
15.0	10.7	*	0.26	
15.0	10.7	*	0.24	
17.0	12.1	*	0.45	
17.2	12.3	50.0	0.45	
20.0	14.3	*	0.32	
20.0	14.3	*	0.32	
20.0	14.3	*	0.32	
20.0	14.3	*	0.32	
20.0	14.3	*	0.23	
20.0	14.3	*	0.20	

* Unavailable at present.

POLYMERS, POLYCATIONIC
0/1993

SAR POLYMERS, POLYCATIONIC

Organism: Daphnid
Duration: 48-h
Endpoint: LC50 (Mortality)

Equation: The first SAR uses percent amine nitrogen to estimate toxicity while the second SAR uses the number of positive charges per 1000 unites of molecular weight. The toxicity increases rapidly from 0.1 to 2.3 percent amine nitrogen; thereafter, toxicity increases slowing with increasing charge density. The SAR equations used to estimate the acute toxicity are:

1. Log LC50 (mg/L) = 3.41 - 1.53 x (percent amine nitrogen)

2. Log LC50 (mg/L) = 3.43 - 2.19 x (number of positive charges per 1000 MW units)

Maximum Value: percent amine nitrogen SAR: 2.3% amine nitrogen; number of positive charges/1000 MW SAR: 1.6
Minimum MW: 1000.0

Application: This SAR may be used to estimate the toxicity of polycationic polymers which are highly water soluble or dispersible and contain a nitrogen which can be protonated and/or quaternarized. This SAR may be used for polysulfoniums and polyphosphoniums which are dispersible.

Limitations: Polycationic polymers which contain silicon may have limited water solubility or dispersibility.

Polycationic polymers which contain anionic groups may be significantly less toxic than predicted by this SAR. For example, a polycationic polymer containing 4.7 percent amine nitrogen (or 3.4 cationic charges per 1000 molecular weight) and anionic groups with a cationic:anionic molar ratio of 1:1.1, will be about 31 times less toxic than predicted, i.e., daphnid 48-h LC50 is 19.8 mg/L.

References: Nabholz JV. 1988. A structure-activity relationship for polycationic polymers. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency 20460-0001.

LIST OF COMPOUNDS USED TO DEVELOP THE DAPHNID 48-h LC50 SAR.

Percent Amine Nitrogen	Number of Positive Charges per 1000 Units of Mol. Weight	Average Molecular Weight	96-h LC50 (1000) (mg/L)
0.7	0.5	*	300.0
0.7	0.5	*	310.0
2.0	1.4	*	1.7
8.0	5.7	5.0	0.34
11.0	7.9	1.8	0.58
12.0	8.6	1.2	1.2
15.0	10.7	*	0.26
20.0	14.3	*	0.17

* Unavailable at present.

POLYMERS, POLYCATIONIC
9/1993

SAR	**POLYMERS, POLYCATIONIC**
Organism:	Green Algae
Duration:	96-h
Endpoint:	EC50 (Growth)
Equation:	The algal 96-h EC50 can be estimated by dividing the equivalent fish 96-h LC50 estimate by 6. In addition, the algal 96-h no effect concentration (NEC; same as GMATC) can be estimated by dividing the algal 96-h EC50 by 2.5.
Minimum MW:	1000.0
Application:	This SAR may be used to estimate the toxicity of polycationic polymers which are highly water soluble or dispersible and contain a nitrogen which can be protonated and/or quaternarized. This SAR may be used for polysulfoniums and polyphosphoniums which are dispersible.
Limitations:	Polycationic polymers which contain silicon may have limited water solubility or dispersibility. Polycationic polymers which contain anionic groups may be significantly less toxic than predicted by this SAR. For example, a polycationic polymer containing 4.7 percent amine nitrogen (or 3.4 cationic charges per 1000 molecular weight) and anionic groups with a cationic:anionic molar ratio of 1:1.1, will be about 30 times less toxic than predicted, i.e., the algal 96-h EC50 is 1.35 mg/L.
References:	Nabholz JV. 1988. A structure-activity relationship for polycationic polymers. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency 20460-0001.

LIST OF COMPOUNDS USED TO DEVELOP THE GREEN ALGAE 96-h EC50 SAR.

Percent Amine Nitrogen	Number of Positive Charges per 1000 Units of Mol. Weight	Average Molecular Weight (1000)	96-h EC50 (mg/L)	96-h NEC (mg/L)
0.7	0.5	*	300.0	0.88
8.0	5.7	5.0	0.16	*
11.0	7.9	1.8	0.07	0.034

* Unavailable at present.

SURFACTANTS, ANIONIC
9/1993

SAR	**SURFACTANTS, ANIONIC**
Organism:	Fish
Duration:	96-h and 28-d
Endpoint:	LC50 and NEC
Equation:	Determine the average length of the carbon chain to the nearest tenth and use the SAR equation: Log LC50 (mg/L) = $[(\text{avg. no. of carbons} - 16)^2 - 10.643]/12.9346$ The fish 28-d no effect concentrations (NEC, GMATC, or chronic value) can be estimated by dividing the estimated acute value derived above by 6.5.
Statistics:	N = 14; $R^2 = 0.624$
Maximum Value:	carbon chain length of 18 carbons
Minimum Value:	carbon chain length of 10 carbons
Application:	This SAR may be used for the following classes of compounds: 1. Alkyl benzene sulfonates 2. Linear alkyl sulfonates (LAS) 3. Amphoteric surfactants with a sulfonate, phosphonate, or carboxylate terminus 4. Anionic surfactants terminated with phosphates 5. Anionic surfactants
Limitations:	If the acute or chronic toxicity of linear alkyl benzene sulfonates which vary only in carbon chain length are to be estimated, then the weighted average of carbons in the alkyl chains (excluding the aromatic benzene ring) has to be determined.
References:	Nabholz JV. 1985. Standard Environmental Hazard Assessment of PMNs 85-1156/1163. Intra-agency memorandum to O. Gutenson, Chemical Review and Evaluation Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency, Washington, DC 20460-0001. August.

LIST OF ANIONIC SURFACTANTS USED TO DEVELOP THE FISH LC50 SAR.

	Number ofFish Carbons	LC50 (mg/L)
	10	21.2 - 47.5
	11	11.6
12	1.18 - 6.5	
13	1.11	
	14	0.25 - 0.42
	16	0.087
	18	0.38

SURFACTANTS, ANIONIC
9/1993

SAR	**SURFACTANTS, ANIONIC**
Organism:	Daphnid
Duration:	48-h and 21-d NEC
Endpoint:	LC50 and NEC
Equation:	Determine the average length of the carbon chain to the nearest tenth and use the fish 96-h LC50 SAR equation: Log LC50 (mg/L) = [(ave. no. of carbons -16)^2 - 10.643]/12.9346 The daphnid 21-d no effect concentration (NEC, GMATC, or chronic value) can be estimated by dividing the estimated acute value derived above by 6.5.
Statistics:	N = 14; R^2 = 0.624
Maximum Value:	carbon chain length of 18 carbons
Minimum Value:	carbon chain length of 10 carbons
Application:	These SARs may be used for the following classes of compounds: 1. Alkyl benzene sulfonates 2. Alkyl sulfonates 3. Amphoteric surfactants with a sulfonate, phosphonate, or carboxylate terminus 4. Anionic surfactants terminated with phosphates 5. Anionic surfactants
Limitations:	If the acute or chronic toxicity of linear alkyl benzene sulfonates which vary only in carbon chain length are to be estimated, then the weighted average of carbons in the alkyl chains (excluding the aromatic benzene ring) have to be determined.
References:	Nabholz JV. 1985. Standard Environmental Hazard Assessment of PMNs 85-1156/1163. Intra-agency memorandum to O. Gutenson, Chemical Review and Evaluation Branch, Health and Environmental Review Division (TS-796), Office of Toxic Substances, United States Environmental Protection Agency, Washington, DC 20460-0001. August.

LIST OF ANIONIC SURFACTANTS USED TO DEVELOP THE DAPHNID LC50 SAR.

Number of Carbons	Daphnid LC50 (mg/L)
10	29.55
11	21.15
12	5.88
13	2.63
14	0.68
16	0.11
18	0.12

SURFACTANTS, ANIONIC
9/1993

SAR	**SURFACTANTS, ANIONIC**
Organism:	Green Algae
Duration:	96-h
Endpoint:	EC50 and NEC (Growth)
Equation:	Determine the average length of the carbon chain to the nearest tenth and use the SAR equation: Log EC50 (mg/L) = [(ave. no. of carbons - 16)^2 - 42.466]/12.368 The green algae 96-h no effect concentration (NEC, GMATC, or chronic value) can be estimated by dividing the estimated EC50 value by 1.4.
Statistics:	N = 14; R^2 = 0.89
Maximum Value:	carbon chain length of 18 carbons
Minimum Value:	carbon chain length of 10 carbons
Maximum MW:	
Application:	These SARs may be used for the following classes of compounds: 1. Alkyl benzene sulfonates 2. Alkyl sulfonates 3. Amphoteric surfactants with a sulfonate, phosphonate, or carboxylate terminus 4. Anionic surfactants terminated with phosphates 5. Anionic surfactants
Limitations:	If the toxicity of linear alkyl benzene sulfonates which vary only in carbon chain length are to be estimated, then the weighted average of carbons in the alkyl chains (excluding the aromatic benzene ring) have to be determined.
References:	Nabholz JV. 1987. Predicting the algal 96-h EC50 from the daphnid and fish SAR for LAS's. Intra-agency memorandum to "Whom It May Concern." Washington, DC: Office of Toxic Substances, United States Environmental Protection Agency, Washington, DC, 20460-0001.

DATA FOR A C8 ANIONIC SURFACTANT USED TO DEVELOP THE GREEN ALGAE SAR.

Organism	EC50 (mg/L)	EC10 (mg/L)
Algae	12	8.5
Fish	366	
Daphnid	289	

SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, MONOALKYL
9/1993

SAR	**SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, MONOALKYL**
Organism:	Fish
Duration:	Acute
Endpoint:	LC50 (Mortality)
Equation:	Determine the average number of carbons in the hydrophobic alkyl chain of the surfactant. If the average length of the carbon chain is between 16 and 24 carbons, use the SAR equation: Log LC50 (mg/L) = -0.0918 + 0.023 (average length of carbon chain) If the length of the carbon chain is at least 10 but less than 16, use the SAR equation: Log LC50 (mg/L) = 5.43 - 0.37 (average length of carbon chain)
Maximum Value:	average carbon chain length of 24 carbons
Minimum Value:	average carbon chain length of 10 carbons
Application:	This SAR may be applied to monoalkyl (trimethyl) quaternary ammonium surfactants which are dispersible in water. This SAR may be used to estimate toxicity for: 1. monoalkyl cationic surfactants 2. monoalkyl phosphonium surfactants 3. monoalkyl sulfonium surfactants
Limitations:	This SAR may be used for monoalkyl quaternary ammonium surfactants where the anionic salt has less than 8 carbons in the alkyl chain. If the alkyl chain contains 8 or more carbons, the cationic surfactant and the anionic surfactant will form a strong ion pair. This ion pair will be much less soluble in water and consequently will be less toxic to fish.
References:	Nabholz JV. 1987. The SAR for monoalkyl (trimethyl) quaternary ammonium surfactants. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Toxic Substances, United States Environmental Protection Agency. Knauf W. 1973. Summary of the toxicity of surfactants to aquatic organisms. Tenside Detergents 5:251-255.

LIST OF MONOALKYL-TRIMETHYL-AMMONIUM CHLORIDE SURFACTANTS USED TO DEVELOP THE SAR FOR QUATERNARY AMMONIUM SURFACTANTS FOR FISH

Number of Carbons	Species Tested	Acute LC50 (mg/L)
10	Golden orfe	68
12	Golden orfe	9.0
14	Golden orfe	2.1
16	Golden orfe	0.36
18	Golden orfe	0.41
21	Golden orfe	0.42

SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, MONOALKYL
9/1993

SAR	**SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, MONOAKYL**
Organism:	Daphnid
Duration:	Acute
Endpoint:	LC50 (Mortality)
Equation:	Determine the average number of carbons in the hydrophobic alkyl chain of the surfactant. If the average length of the carbon chain is between 16 and 22 carbons, use the SAR equation: Log LC50 (mg/L) = -1.64 + 0.115 (average length of carbon chain) If the length of the carbon chain is at least 10 but less than 16, use the SAR equation: Log LC50 (mg/L) = 2.07 - 0.13 (average length of carbon chain)
Maximum Value:	average carbon chain length of 22 carbons
Minimum Value:	average carbon chain length of 10 carbons
Application:	This SAR may be applied to monoalkyl (trimethyl) quaternary ammonium surfactants which are dispersible in water. This SAR may be used to estimate toxicity for: 1. monoalkyl cationic surfactants 2. monoalkyl phosphonium surfactants 3. monoalkyl sulfonium surfactants
Limitations:	This SAR may be used for monoalkyl quaternary ammonium surfactants where the anionic salt has less than 8 carbons in the alkyl chain. If the alkyl chain contains 8 or more carbons, the cationic surfactant and the anionic surfactant will form a strong ion pair. This ion pair will be much less soluble in water and consequently will be less toxic to daphnids.
References:	Nabholz JV. 1987. The SAR for monoalkyl (trimethyl) quaternary ammonium surfactants. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Toxic Substances, United States Environmental Protection Agency. Knauf W. 1973. Summary of the toxicity of surfactants to aquatic organisms. Tenside Detergents 5:251-255.

LIST OF MONOALKYL-TRIMETHYL-AMMONIUM CHLORIDE SURFACTANTS USED TO DEVELOP THE SAR FOR QUATERNARY AMMONIUM SURFACTANTS FOR DAPHNIDS

Number of Carbons	Species Tested	Acute LC50 (mg/L)
10	Daphnia magna	7.0
12	Daphnia magna	3.2
14	Daphnia magna	1.7
16	Daphnia magna	1.2
18	Daphnia magna	3.2
21	Daphnia magna	6.0

SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, MONOALKYL
9/1993

SAR	**SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, MONOALKYL**
Organism:	Snail
Duration:	Acute
Endpoint:	LC50 (Mortality)
Equation:	Determine the average number of carbons in the hydrophobic alkyl chain of the surfactant. If the average length of the carbon chain is between 16 and 22 carbons, use the SAR equation: Log LC50 (mg/L) = -1.56 + 0.087 (average length of carbon chain) If the length of the carbon chain is at least 10 but less than 16, use the SAR equation: Log LC50 (mg/L) = 5.74 - 0.37 (average length of carbon chain)
Maximum Value:	carbon chain length of 22 carbons
Minimum Value:	carbon chain length of 10 carbons
Application:	This SAR may be applied to monoalkyl (trimethyl) quaternary ammonium surfactants which are dispersible in water. This SAR may be used to estimate toxicity for: 1. monoalkyl cationic surfactants 2. monoalkyl phosphonium surfactants 3. monoalkyl sulfonium surfactants
Limitations:	This SAR may be used for monoalkyl quaternary ammonium surfactants where the anionic salt has less than 8 carbons in the alkyl chain. If the alkyl chain contains 8 or more carbons, the cationic surfactant and the anionic surfactant will form a strong ion pair. This ion pair will be much less soluble in water and consequently will be less toxic to snails.
References:	Nabholz JV. 1987. The SAR for monoalkyl (trimethyl) quaternary ammonium surfactants. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Toxic Substances, United States Environmental Protection Agency. Knauf W. 1973. Summary of the toxicity of surfactants to aquatic organisms. Tenside Detergents 5:251-255.

LIST OF MONOALKYL-TRIMETHYL-AMMONIUM CHLORIDE SURFACTANTS USED TO DEVELOP THE SAR FOR QUATERNARY AMMONIUM SURFACTANTS FOR SNAILS

Number of Carbons	Species Tested	Acute LC50 (mg/L)
10	Water snail	100
12	Water snail	23
14	Water snail	3.5
16	Water snail	0.7
18	Water snail	1.0
21	Water snail	1.9

SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, DIALKYL
9/1993

SAR	**SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, DI-ALKYL**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 and ChV (Mortality)
Equation:	Calculate the average log K_{ow} for the two alkyl groups and use the average value in the SAR equation: Log 96-h LC50 (mM/L) = 0.747 - 0.367 log K_{ow} To determine the chronic toxicity value (ChV) of a di-alkyl quaternary ammonium surfactant to fish, divide the 96-hour LC50 value by 26.
Statistics:	N = 6; R^2 = 0.9
Maximum Value:	There are no limits on the log K_{ow} values.
Maximum MW:	There are no limits on the molecular weight of the two alkyl groups of the cationic surfactant.
Application:	This SAR may be applied to cationic dialkyl (dimethyl) quaternary ammonium surfactants which are dispersible in water. This SAR may be used to estimate toxicity for: 1. dialkyl cationic surfactants 2. dialkyl phosphonium surfactants 3. dialkyl sulfonium surfactants
Limitations:	None.
References:	FDA. Unpublished data. ITC. IR-488. USEPA. ECOTOX database. P85-505 Standard Review.

SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, DIALKYL
9/1993

SAR	**SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, DI-ALKYL**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 AND ChV (Mortality)
Equation:	Calculate the average log K_{ow} for the two alkyl groups and use the average value in the SAR equation: Log 48-h LC50 (mM/L) = 0.874 - 0.462 log K_{ow} To determine the chronic toxicity value (ChV) of a di-alkyl quaternary ammonium surfactant to daphnids, divide the 48-hour LC50 value by 1.8.
Statistics:	N = 4; R^2 = 0.94
Maximum Value:	There are no limits on the log K_{ow} values of the two alkyl groups of the cationic surfactant.
Maximum MW:	There are no limits on the molecular weight of the two alkyl groups of the cationic surfactant.
Application:	This SAR may be applied to cationic dialkyl (dimethyl) quaternary ammonium surfactants which are dispersible in water. This SAR may be used to estimate toxicity for: 1. dialkyl cationic surfactants 2. dialkyl phosphonium surfactants 3. dialkyl sulfonium surfactants
Limitations:	None.
References:	FDA. Unpublished data. ITC. IR-488. EPA. ECOTOX database. P85-505 Standard Review.

SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, DIALKYL
9/1993

SAR	**SURFACTANTS, CATIONIC, QUATERNARY AMMONIUM, DI-ALKYL**
Organism:	Green Algae
Duration:	96-h
Endpoint:	EC50 and ChV
Equation:	Calculate the average log K_{ow} for the two alkyl groups and use the average value in the SAR equation: Log 96-h EC50 (mM/L) = -0.595 - 0.296 log K_{ow} To determine the chronic toxicity value (ChV) of a di-alkyl quaternary ammonium surfactant to green algae, divide the 96-hour EC50 value by 4.
Statistics:	N = 3; R^2 = 0.99
Maximum Value:	There are no limits on the log K_{ow} values of the two alkyl groups of the cationic surfactant.
Maximum MW:	There are no limits on the molecular weight of the two alkyl groups of the cationic surfactant.
Application:	This SAR may be applied to cationic dialkyl (dimethyl) quaternary ammonium surfactants which are dispersible in water. This SAR may be used to estimate toxicity for: 1. dialkyl cationic surfactants 2. dialkyl phosphonium surfactants 3. dialkyl sulfonium surfactants
Limitations:	None.
References:	FDA. Unpublished data. ITC. IR-488. EPA. ECOTOX database. P85-505 Standard Review.

SURFACTANTS, NONIONIC
9/1993

SAR	**SURFACTANTS, NONIONIC**
Organism:	Fish and Daphnid
Duration:	96-h, 48-h
Endpoint:	LC50 (Mortality) in mg/L
Equation:	Determine the number of carbons in the alkyl chains and the number of ethoxylate groups in the surfactant. Determine the toxicity using the appropriate SAR equation based on the length of the carbon chain:
	C = 8; Log LC50 = 0.952 + 0.130 (number of ethoxylates)
	C = 9; Log LC50 = 0.796 + 0.120 (number of ethoxylates)
	C = 10; Log LC50 = 0.642 + 0.112 (number of ethoxylates)
	C = 11; Log LC50 = 0.261 + 0.103 (number of ethoxylates)
	C = 12; Log LC50 = -0.204 + 0.0996 (number of ethoxylates)
	C = 13; Log LC50 = -0.388 + 0.092 (number of ethoxylates)
	C = 14; Log LC50 = -0.480 + 0.0847 (number of ethoxylates)
	C = 15; Log LC50 = -0.533 + 0.0776 (number of ethoxylates)
	C = 16; Log LC50 = -0.775 + 0.072 (number of ethoxylates)
	C = 17; Log LC50 = -1.054 + 0.0674 (number of ethoxylates)
	C = 18; Log LC50 = -1.290 + 0.063 (number of ethoxylates)
Statistics:	
Maximum Value:	Maximum carbon chain length of 18; minimum carbon chain length of 8; the maximum number of ethoxylates is 55.
Application:	This SAR may be used to estimate the toxicity for the following classes of nonionic surfactants:

1. Alcohol ethoxylate surfactants
2. Alkyl ethoxylate surfactants
3. Nonionic surfactants

Generally, this SAR is expected to be applicable to other nonionic surfactants, such as alcohol ethoxlyate-propoxylate surfactants where number of ethoxylates is greater than tje mumber of propoxylates.

Limitations:

When the number of ethoxylates is less than 5, chemicals may begin to act less like surfactants and more like neutral organic chemicals. Alcohol propoxylates and alcohol butoxylates will not act like surfactants; the propoxylate and butoxylate units are not water soluble enough. Alcohol propoxylates and alcohol butoxylates should be treated like neutral organic chemicals.

References:

Nabholz JV. 1988. The structure-activity relationships between nonionic surfactants. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Toxic Substances, United States Environmental Protection Agency.

SURFACTANTS, NONIONIC
9/1993

LIST OF NONIONIC SURFACTANTS USED TO DEVELOP FISH 96-h AND DAPHNID 48-H LC50 SARS.

Number of Carbons	Number of Ethoxylates	Species	Time (hours)	LC50 (mg/L)
8	12.0	Golden orfe	96	465.0
10	2.5	Rainbow trout	96	5-7
10	5.0	Rainbow trout	96	8-9
12	6.0	Fish spp.	96	2.8
12	9.0	Fish spp.	96	5.4
12	12.0	Fish spp.	96	4.4
12	12.0	Golden orfe	96	4.4
12	15.0	Fish spp.	96	22.0
12.5	2.0	Rainbow trout	96	1-2
12.5	5.3	Rainbow trout	96	1.0
12.5	6.5	Daphnia	24	1.05
12.5	6.5	Rainbow trout	96	2.36
12.5	6.5	Bluegill	96	0.57
12.5	6.5	Daphnia	24	0.57
12.5	6.5	Daphnia	96	1.14
13	6.3	Fathead minnow	24	1.8
13	6.3	Goldfish	24	1.4
13	6.3	Daphnia	48	2.4
13	7.4	Fathead minnow	24	1.8
13	7.4	Goldfish	24	1.4
13	7.4	Daphnia	24	2.3
13	8.0	Goldfish	48	1.4
13	8.0	Harlequin fish	48	1.2
13	8.0	Golden orfe	96	1.8
13	8.0	Rainbow trout	96	0.8
13	8.0	Golden orfe	96	2.7
13	10.5	Harlequin fish	96	1.6-2.8
13	10.5	Rainbow trout	96	1.8
13	10.5	Rainbow trout	96	0.8
13	10.5	Golden orfe	96	4.1
13	10.5	Golden orfe	96	4.1
13	10.5	Goldfish	48	3.0
13	11.0	Golden orfe	48	2.7
13	11.0	Daphnia	24	5.1
13	11.0	Rainbow trout	48	6.2
13.5	3.0	Blugill	96	1.5
13.5	3.0	Rainbow trout	96	1.3-1.7
13.5	3.0	Rainbow trout	96	3.9
13.5	7.0	Rainbow trout	96	2.7
13.5	9.0	Bluegill	96	2.1
13.5	9.0	Bluegill	96	11.0
13.5	9.0	Channel catfish	96	1.2
13.5	9.0	Daphnia	24	1.71

Continued.

Number of Carbons	Number of Ethoxylates	Species	Time (hours)	LC50 (mg/L)
13.5	9.0	Bluegill	96	7.8
17	14.0	Minnow	24	3.4
17	14.0	Rainbow trout	96	0.4
17	14.0	Golden orfe	96	2.3
17	14.0	Golden orge	96	2.5
17	14.0	Harlequin fish	96	0.7

SURFACTANTS, ETHOMEEN
9/1993

SAR	**SURFACTANTS, ETHOMEEN**
Organism:	Fish, Daphnid, and Algae
Duration:	96-h, 48-h, and 96-h
Endpoint:	LC50, LC50, and EC50 (Mortality) in mg/L
Equation:	Determine the number of carbons in the alkyl chains and the number of ethoxylate groups in the surfactant. Determine the toxicity using the appropriate SAR equation based on the length of the carbon chain: C = 8; Log LC50 = 1.022 + 0.122 (number of ethoxylates) C = 9; Log LC50 = 0.794 + 0.116 (number of ethoxylates) C = 10; Log LC50 = 0.553 + 0.112 (number of ethoxylates) C = 11; Log LC50 = 0.335 + 0.104 (number of ethoxylates) C = 12; Log LC50 = 0.107 + 0.098 (number of ethoxylates) C = 13; Log LC50 = -0.102 + 0.092 (number of ethoxylates) C = 14; Log LC50 = -0.348 + 0.086 (number of ethoxylates) C = 15; Log LC50 = -0.566 + 0.079 (number of ethoxylates) C = 16; Log LC50 = -0.706 + 0.074 (number of ethoxylates) C = 17; Log LC50 = -1.057 + 0.069 (number of ethoxylates) C = 18; Log LC50 = -1.316 + 0.063 (number of ethoxylates)
Maximum Value: **Maximum MW:**	18 carbons in the alkyl chain; 55 ethoxylates
Application:	This SAR may be used to estimate the toxicity of ethomeen surfactants (i.e., ethoxylated beta-amine surfactants) with a carboxylic acid terminus.
Limitations:	None.
References:	Nabholz JV. 1986. The structure-activity relationships between nonionic surfactants. Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Toxic Substances, United States Environmental Protection Agency.

THIAZOLINONES, ISO
9/1993

SAR	**THIAZOLINONES, ISO**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log LC50 (mM/L) = -2.159 - 0.068 log K_{ow}
Statistics:	N = 2; R^2 =1.0
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate the toxicity of isothiazolinones or allyl thioamides.
Limitations:	If the log K_{ow} value is greater tah 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1993. OPPT PMN ECOTOX. Washington, DC: Office of Pollution Prevention and Toxics, USEPA.

LIST OF ISOTHIAZOLINONES USED TO DEVELOP THE FISH 96-h LC50 SAR

CHEMICAL	96-H LC50 (mg/L)	Log K_{ow}	Ref.
Chemical identity CBI	0.90	0.6	EPA

EPA = USEPA (1993); chemical identity is Confidential Business Information under TSCA.

THIAZOLINONES, ISO
9/1993

SAR	**THIAZOLINONES, ISO**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Log LC50 (mM/L) = -2.0 - 0.159 log K_{ow}
Statistics:	N = 2; R^2 =1.0
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate the toxicity of isothiazolinones or allyl thioamides.
Limitations:	If the log K_{ow} value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1993. OPPT PMN ECOTOX. Washington, DC: Office of Pollution Prevention and Toxics, USEPA.

LIST OF ISOTHIAZOLINONES USED TO DEVELOP THE FISH 96-h LC50 SAR

CHEMICAL	96-H LC50 (mg/L)	Log K_{ow}	Ref.
Chemical identity CBI	1.2	0.6	EPA

EPA = USEPA (1993); chemical identity is Confidential Business Information under TSCA.

THIAZOLINONES, ISO
9/1993

SAR	**THIAZOLINONES, ISO**
Organism:	Green Algae
Duration:	96-h
Endpoint:	EC50
Equation:	Log LC50 (mM/L) = -2.555 - 0.241 log K_{ow}
Statistics:	N = 2; R^2 =1.0
Maximum log K_{ow}:	6.4
Maximum MW:	1000.0
Application:	This equation may be used to estimate the toxicity of isothiazolinones or allyl thioamides.
Limitations:	If the log K_{ow} value is greater than 6.4, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1993. OPPT PMN ECOTOX. Washington, DC: Office of Pollution Prevention and Toxics, USEPA.

LIST OF ISOTHIAZOLINONES USED TO DEVELOP THE FISH 96-h LC50 SAR

CHEMICAL	96-H LC50 (mg/L)	Log K_{ow}	Ref.
Chemical identity CBI	0.290	0.6	EPA

EPA = USEPA (1993); chemical identity is Confidential Business Information under TSCA.

THIAZOLINONES, ISO
9/1993

SAR	**THIAZOLINONES, ISO**
Organism:	Green Algae
Duration:	
Endpoint:	Chronic Value
Equation:	Log LC50 (mM/L) = -2.938 - 0.270 log K_{ow}
Statistics:	N = 2; R^2 =1.0
Maximum log K_{ow}:	8.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate the toxicity of isothiazolinones or allyl thioamides.
Limitations:	If the log K_{ow} value is greater than 8.0, or if the compound is solid and the LC50 exceeds the water solubility, no effects expected at saturation.
References:	United States Environmental Protection Agency (USEPA). 1993. OPPT PMN ECOTOX. Washington, DC: Office of Pollution Prevention and Toxics, USEPA.

LIST OF ISOTHIAZOLINONES USED TO DEVELOP THE FISH 96-h LC50 SAR

CHEMICAL	96-H LC50 (mg/L)	Log K_{ow}	Ref.
Chemical identity CBI	0.130	0.6	EPA

EPA = USEPA (1993); chemical identity is Confidential Business Information under TSCA.

THIOLS AND MERCAPTANS
9/1993

SAR	**THIOLS AND MERCAPTANS**
Organism:	Fish
Duration:	96-h
Endpoint:	LC50 (Mortality)
Equation:	Log LC50 (mM/L) = -1.022 - 0.447 log K_{ow}
Statistics:	N = 4; R^2 = 0.85
Maximum log K_{ow}:	6.5
Maximum MW:	1000.0
Application:	This equation may be used to estimate the toxicity for thiols and mercaptans. Thiols with a carboxylic acid substitution will be about 10 times less toxic than the toxicity value predicted by using this SAR with a log K_{ow} and molecular weight for the free acid. Therefore, for thiols with a carboxylic acid substitution, predict the toxicity values for the free acid and multiply by 10.
Limitations:	For thiols with log K_{ow} values greater than 4.5, the toxicity prediction may only apply to rainbow trout and other cold water fish species. While a 96-h LC50 value was measured for t-dodecane thiol (log K_{ow} = 6.2), nonylthiol (log K_{ow} = 4.9) showed no toxicity at saturation with fathead minnows. The recommended species for testing thiols with log K_{ow} values greater than 4.5 is rainbow trout using flow-through methods, measured concentrations, and treatment concentrations which do not exceed the aqueous solubility limit of the thiol being tested. If the log K_{ow} value is greater than 6.5, or if the compound is solid and the LC50 exceeds the water solubility, use SAR with longer exposure.
References:	Bender ME. 1969. The toxicity of the hydrolysis and breakdown products of malathion to the fathead minnow Pimephales promelas, Rafinesque. Water Research 3:571-582. U.S. Environmental Protection Agency. 1991. Toxicity of data gap compounds to fathead minnow (Pimephales promelas) and daphnids (Daphnia magna). Duluth, MN: Environmental Research Laboratory, Office of Research and Development, USEPA. U.S. Environmental Protection Agency. 1992. TSCA Sec. 8(e) submission number 994. Washington, DC: Office of Pollution Prevention and Toxics, USEPA. Verschueren K. 1983. Handbook of environmental data on organic chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co.

THIOLS AND MERCAPTANS
9/1993

SAR	**THIOLS AND MERCAPTANS**
Organism:	Daphnid
Duration:	48-h
Endpoint:	LC50 (Mortality)
Equation:	Log LC50 (mM/L) = -3.2 - 0.097 log K_{ow}
Statistics:	N = 3; R^2 = 0.46
Maximum log K_{ow}:	5.0
Maximum MW:	1000.0
Application:	This equation may be used to estimate the toxicity for thiols and mercaptans.
Limitations:	If the log K_{ow} is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility, use SAR with longer exposure.
References:	U.S. Environmental Protection Agency. 1991. Toxicity of data gap compounds to fathead minnows (Pimephales promelas) and daphnids (Daphnia magna). Duluth, MN: Environmental Research Laboratory, Office of Research and Development, USEPA. U.S. Environmental Protection Agency. 1992. TSCA Sec. 8(e) submission number 994. Washington, DC: Office of Pollution Prevention and Toxics, USEPA.

THIOLS AND MERCAPTANS
9/1993

SAR **TRIAZINES, SUBSTITUTED**

For fish and daphnid use SAR for **NEUTRAL ORGANICS**;

This category includes substituted triazines which can be aromatic, partially aromatic (or partially saturated), and unsaturated. The nitrogens in the triazine ring may be symmetrical or asymmetrical. Substitutions on the carbons may include but not be limited to: aliphatic alcohols; ketones; benzene and substituted benzenes; aliphatic hydrocarbons, alkyenes and alkynes; free amines and substituted amines; cyclic aliphatic hydrocarbons; halogens; amides; cyanides; ethers; methoxy groups; sulfides; azido groups; and carboxylic acid esters. Substitutions on the nitrogens may include but not be limited to: free amines and substituted amines; -N=CH; aliphatic hydrocarbons, alkyenes and alkynes; and benzene and substituted benzenes. Hazard Concerns: many members of this category are commercial herbicides which are used to control both aquatic plants and terrestrial plants. Their mode of toxic action is generally considered to be inhibition of photosynthesis. Many members of this class are toxic to algae at < 1 mg/L and toxic to terrestrial vascular plants at < 1 mg/kg. Members of this group can also be highly toxic to fish and aquatic invertebrates. Toxicity is expected to be related to the octanol/water partition coefficient with respect to fish and aquatic invertebrates, but toxicity to plants may not be related to Kow when log Kow < 5. When the log Kow is < 5, algae and terrestrial plants are expected to be the most sensitive species. As log Kow increases, species differences are expected to diminish. At this time there is no formalized SAR for this category for any species. Toxicity predictions will be made using either the closest analog or averaging data for the two closest analogs which bracket the chemical under question.

UREAS, SUBSTITUTED
9/1993

SAR	**UREAS, SUBSTITUTED**
Organism:	Algae
Duration:	4-h
Endpoint:	EC50 (Inhibition of Photosynthesis)
Equation:	Log EC50 (mM/L) = -1.29 log K_{ow} + 0.133
Statistics:	N = 12; R^2 = 0.944
Maximum log K_{ow}:	3.9
Maximum MW:	1000.0
Application:	This SAR may be used to estimate the toxicity for substituted ureas.
Limitations:	If the log K_{ow} value is greater than 3.9 and less than 7.9, use SAR with longer exposure. If the log K_{ow} value is greater than 8.0, no effects expected at saturation.
References:	Wessels JSC and Van Der Veen R. 1956. The action of some derivatives of phenylurethan and of 3-phenyl-1,1-dimethylurea on the Hill reaction. Biochem. Biophys. Acta 19. Hansch C. 1969. Theoretical considerations of the structure-activity relationship in photosynthesis inhibitors. In: Progress in Photosynthesis Research, Vol. III. Metzner H, ed. pp. 1685-1692.

LIST OF SUBSTITUTED UREAS USED TO DEVELOP THE ALGAE 4-h EC50 SAR.

CHEMICAL	4-h EC50 (mg/L)	Log K_{ow}	Ref.
Ethyl-N-phenylcarbamate (phenylurethan)	$5x10^{-4}$	*	
Ethyl-N-(3-chlorophenyl)-carbamate	10_{-4}	*	
Ethyl-N-(4-chlorophenyl)-carbamate	10^{-4}	*	
Ethyl-N-(4-nitrophenyl)-carbamate	$2x10^{-4}$	*	
Allyl-N-phenylcarbamate	$5x10^{-4}$	*	
Allyl-N-(4-chlorophenyl)-carbamate	$8x10^{-5}$	*	
Ethyl-N-(3,4-dichlorophenyl)-carbamate	$2x10^{-5}$	*	
Ethyl-N-(2,5-dichlorophenyl)-carbamate	$3x10^{-4}$	*	
Benzyl-N-phenylcarbamate	$2x10^{-4}$	*	
Ethyl-N-(4-hydroxyphenyl)-carbamate	$3x10^{-3}$	*	
Ethyl-N-(3-hydroxyphenyl)-carbamate	10^{-3}	*	
3-Phenyl-1,1-dimethylurea	$4x10^{-5}$	*	
3-(4-Chlorophenyl)-1,1-dimethylurea (CMU)	$4x10^{-6}$	*	
3-(3-Chlorophenyl)-1,1-dimethylurea	$2x10^{-6}$	*	
3-(3,4-Dichlorophenyl)-1,1-dimethylurea		$2x10^{-7}$	*
3-(3,4,5-Trichlorophenyl)-1,1-dimethylurea	$2x10^{-7}$	*	
3-(4-Nitrophenyl)-1,1-dimethylurea	$8x10^{-6}$	*	
3-(3-Nitrophenyl)-1,1-dimethylurea	1.310^{-5}	*	
3-(4-Trifluoromethylphenyl)-1,1-dimethylurea	$4x10^{-6}$	*	
3-(3-Trifluoromethylphenyl)-1,1-dimethylurea	$6x10^{-4}$	*	
4-(3,3-Dimethylureido)-S-trichloromethyl-phenyl-thiosulfonate	$4x10^{-7}$	*	
3-(4-Methylphenyl)-1,1-dimethylurea	$3x10^{-5}$	*	
3-(4-Methoxyphenyl)-1,1-dimethylurea	$3x10^{-5}$	*	
3-(4-Dimethylaminophenyl)-1,1-dimethylurea	$2x10^{-4}$	*	
3-(4-Acetylaminophenyl)-1,1-dimethylurea	$2x10^{-3}$	*	

* = Not available at this time.

INORGANICS

ALUMINUM
9/1993

Organism:	Aquatic life (freshwater)
Duration:	96-hour
Endpoint:	No Observable Effect Concentration (NOEC)
Equation:	NOEC (mg/L) = (0.087 @ MW)/26.981
Application:	This equation may be used to estimate the acute toxicity of organic and inorganic compounds containing aluminum.
Limitations:	This equation is based on the pH dependent Ambient Water Quality Criteria for aluminum. The criteria for pH values between 6.5 and 9.0 were used. If the pH of the solution is less than 6.5.
References:	United States Environmental Protection Agency (USEPA). 1980. Ambient Water Quality Criteria for Aluminum. Washington, DC: Office of Water, Criteria and Standards Division.

Organism:	Aquatic Life (freshwater)
Duration:	1-hour
Endpoint:	No Observable Effect Concentration (NOEC)
Equation:	NOEC (mg/L) = (0.750 @ MW)/26.981
Application:	This equation may be used to estimate the acute toxicity of compounds containing aluminum.
Limitations:	This equation is based on the pH dependent Ambient Water Quality Criteria for aluminum. The criteria for pH values between 6.5 and 9.0 were used.
References:	United States Environmental Protection Agency (USEPA). 1980. Ambient Water Quality Criteria for Aluminum. Washington, DC: Office of Water, Criteria and Standards Division.

ANTIMONY
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.088 @ MW)/121.75
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing antimony.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.030 @ MW)/121.75
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing antimony.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

ANTIMONY
9/1993

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (1.5 @ MW)/121.75
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing antimony.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.500 @ MW)/121.75
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing antimony.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

ARSENIC(III)
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.360 @ MW)/74.92
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing arsenic(III).
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.190 @ MW)/74.92
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing arsenic(III).
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

ARSENIC(III)
9/1993

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.069 @ MW)/74.92
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing arsenic(III).
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.036 @ MW)/74.92
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing arsenic(III).
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

BERYLLIUM
9/1993

Organism:	Aquatic life (freshwater)
Duration:	Acute
Endpoint:	Lowest Observable Effect Concentration (LOEC)
Equation:	LOEC (mg/L) = (0.130 @ MW)/9.012
Application:	This equation may be used to estimate the acute toxicity of both organic and inorganic compounds containing beryllium.
Limitations:	Hardness has a substantial effect on acute toxicity.
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Regulations and Standards. EPA 440/5-86-001.

S))Q

Organism:	Aquatic Life (freshwater)
Duration:	Chronic
Endpoint:	Lowest Observable Effect Concentration (LOEC)
Equation:	LOEC (mg/L) = (0.0053 @ MW)/9.012
Application:	This equation may be used to estimate the chronic toxicity of both organic and inorganic compounds containing beryllium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Regulations and Standards. EPA 440/5-86-001.

BORON
9/1993

Organism:	Fish (freshwater)
Duration:	48-hour
Endpoint:	LC50
Equation:	LC50 (mg/L) = (315.0 @ MW)/10.81
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing boron.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

Organism:	Daphnid
Duration:	48-hour
Endpoint:	LC50
Equation:	LC50 (mg/L) = (226.0 @ MW)/10.81
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing boron.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

BORON
9/1993

Organism:	Fish (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.05 @ MW)/10.81
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing boron.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

Organism:	Daphnid
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (8.37 @ MW)/10.81
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing boron.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

CADMIUM
9/1993

Organism: Aquatic life (freshwater)

Duration:

Endpoint: Acute Value

Equation: Acute Value (mg/L) = (0.0039 @ MW)/112.41

Application: This equation may be used to estimate the toxicity of both organic and inorganic compounds containing cadmium.

Limitations: This equation is based on the hardness dependent Water Quality Criteria for cadmium. The criterion for a hardness of 100 mg/L as $CaCO_3$ was used. For a solution with a hardness of 50 mg/L as $CaCO_3$, use the following equation:

Acute Value (mg/L) = (0.0018 @ MW)/112.41

For a solution with a hardness of 200 mg/L as $CaCO_3$, use the following equation:

Acute Value (mg/L) = (0.0086 @ MW)/112.41

References: United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

CADMIUM
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.0011 @ MW)/112.41
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing cadmium.
Limitations:	This equation is based on the hardness dependent Water Quality Criteria for cadmium. The criterion for a hardness of 100 mg/L as $CaCO_3$ was used. For solutions with a hardness of 50 mg/L as $CaCO_3$, use the following equation: ChV (mg/L) = (0.00066 @ MW)/112.41 For solutions with a hardness of 200 mg/L as $CaCO_3$, use the following equation: ChV (mg/L) = (0.002 @ MW)/112.41
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

CADMIUM
9/1993

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.043 @ MW)/112.41
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing cadmium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.0093 @ MW)/112.41
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing cadmium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

CESIUM
9/1993

Organism:	Daphnid
Duration:	48-hour
Endpoint:	LC50
Equation:	LC50 (mg/L) = (7.4 @ MW)/132.9
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing cesium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

CHLORINE
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.019 @ MW)/35.45
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing chlorine.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.011 @ MW)/35.45
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing chlorine.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

CHLORINE
9/1993

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.013 @ MW)/35.45
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing chlorine.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.0075 @ MW)/35.45
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing chlorine.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

COBALT
9/1993

Organism:	Fish (freshwater)
Duration:	96-hour
Endpoint:	LC50
Equation:	LC50 (mg/L) = (48.0 @ MW)/58.933
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing cobalt.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

Organism:	Daphnid
Duration:	48-hour
Endpoint:	LC50
Equation:	LC50 (mg/L) = (1.30 @ MW)/58.933
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing cobalt.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

COBALT
9/1993

Organism:	Fish (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.0342 @ MW)/58.933
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing cobalt.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

Organism:	Daphnid
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.012 @ MW)/58.933
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing cobalt.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

COBALT
9/1993

Organism:	Fish (marine)
Duration:	96-hour
Endpoint:	LC50
Equation:	LC50 (mg/L) = (567.0 @ MW)/58.933
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing cobalt.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

COPPER
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.018 @ MW)/63.546
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing copper.
Limitations:	This equation is based on the hardness dependent Water Quality Criteria for copper. The criterion for a hardness of 100 mg/L as $CaCO_3$ were used. For a solution with a hardness of 50 mg/L as $CaCO_3$, use the following equation: Acute Value (mg/L) = (0.0092 @ MW)/63.546 For a solution with a hardness of 200 mg/L as $CaCO_3$, use the following equation: Acute Value (mg/L) = (0.034 @ MW)/63.546
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

COPPER
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.012 @ MW)/63.546
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing copper.
Limitations:	This equation is based on the hardness dependent Water Quality Criteria for copper. The criterion for a hardness of 100 mg/L as $CaCO_3$ was used. For solutions with a hardness of 50 mg/L as $CaCO_3$, use the following equation: ChV (mg/L) = (0.0065 @ MW)/63.546 For solutions with a hardness of 200 mg/L as $CaCO_3$, use the following equation: ChV (mg/L) = (0.0.021 @ MW)/63.546
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.0029 @ MW)/63.546
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing copper.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

CHROMIUM(III)
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (1.700 @ MW)/51.996
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing chromium(III).
Limitations:	This equation is based on the hardness dependent Water Quality Criteria for chromium(III). The criterion for a hardness of 100 mg/L as $CaCO_3$ was used. For solutions with a hardness of 50 mg/L as $CaCO_3$, use the following equation: Acute Value (mg/L) = (0.980 @ MW)/51.996 For solutions with a hardness of 200 mg/L as $CaCO_3$, use the following equation: Acute Value (mg/L) = (3.100 @ MW)/51.996
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

CHROMIUM(III)
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.210 @ MW)/51.996
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing chromium(III).
Limitations:	This equation is based on the hardness dependent Water Quality Criteria for chromium(III). The criterion for a hardness of 100 mg/L as $CaCO_3$ was used. For a solution with a hardness of 50 mg/L as $CaCO_3$, use the following equation: ChV (mg/L) = (0.120 @ MW)/51.996 For a solution with a hardness of 200 mg/L as $CaCO_3$, use the following equation: ChV (mg/L) = (0.120 @ MW)/51.996
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

CHROMIUM(III)
9/1993

Organism:	Eastern Oyster embryos (marine)
Duration:	Acute
Endpoint:	EC50
Equation:	EC50 (mg/L) = (10.3 @ MW)/51.996
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing chromium(III).
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

CHROMIUM(VI)
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.016 @ MW)/51.996
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing chromium(VI).
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.011 @ MW)/51.996
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing chromium(VI).
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

CHROMIUM(VI)
9/1993

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (1.100 @ MW)/51.996
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing chromium(VI).
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.050 @ MW)/51.996
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing chromium(VI).
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

GERMANIUM
9/1993

Organism:	Fish (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.003 • MW)/72.6
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing germanium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

GOLD
9/1993

Organism:	Daphnid
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.180 @ MW)/196.967
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing gold.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

Organism:	Green Algae
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.125 @ MW)/196.967
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing gold.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

IRON
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (1.0 @ MW)/55.847
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing iron.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

LANTHANUM
9/1993

Organism:	Daphnid
Duration:	48-hour
Endpoint:	LC50
Equation:	LC50 (mg/L) = (160.0 @ MW)/138.906
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing lanthanum.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

Organism:	Fish (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.0008 @ MW)/138.906
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing lanthanum.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

LANTHANUM
9/1993

Organism:	Green Algae
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (6.4 @ MW)/138.906
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing lanthanum.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

LEAD
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.083 @ MW)/207.2
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing lead.
Limitations:	This equation is based on the hardness dependent Water Quality Criteria for lead. The criterion for a hardness of 100 mg/L as $CaCO_3$ was used.
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.0032 @ MW)/207.2
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing lead.
Limitations:	This equation is based on the hardness dependent Water Quality Criteria for lead. The criterion for a hardness of 100 mg/L as $CaCO_3$ was used.
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

LEAD
9/1993

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.220 @ MW)/207.2
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing lead.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.0085 @ MW)/207.2
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing lead.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

MERCURY
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.0024 @ MW)/200.59
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing mercury.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.00012 @ MW)/200.59
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing mercury.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

MERCURY
9/1993

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.0021 @ MW)/200.59
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing mercury.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.000025 @ MW)/200.59
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing mercury.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

MOLYBDENUM
9/1993

Organism:	Fish (freshwater)
Duration:	96-hour
Endpoint:	LC50
Equation:	LC50 (mg/L) = (553.0 @ MW)/95.94
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing molybdenum.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

Organism:	Fish (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.0223 @ MW)/95.94
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing molybdenum.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

NICKEL
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (1.400 @ MW)/58.70
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing nickel.
Limitations:	This equation is based on the hardness dependent Water Quality Criteria for nickel. The criterion for a hardness of 100 mg/L as $CaCO_3$ was used. For a solution with a hardness of 50 mg/L as $CaCO_3$, use the following equation: Acute Value (mg/L) = (0.790 @ MW)/58.70 For a solution with a hardness of 200 mg/L as $CaCO_3$, use the following equation: Acute Value (mg/L) = (2.500 @ MW)/58.70
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

NICKEL
9/1993

Organism: Aquatic life (freshwater)

Duration:

Endpoint: Chronic Value (ChV)

Equation: ChV (mg/L) = (0.160 @ MW)/58.70

Application: This equation may be used to estimate the toxicity of both organic and inorganic compounds containing nickel.

Limitations: This equation is based on the hardness dependent Water Quality Criteria for nickel. The criterion for a hardness of 100 mg/L as $CaCO_3$ was used. For solutions with a hardness of 50 mg/L as $CaCO_3$, use the following equation:

ChV (mg/L) = (0.088 @ MW)/58.70

For solutions with a hardness of 200 mg/L as $CaCO_3$, use the following equation:

ChV (mg/L) = (0.280 @ MW)/58.70

References: United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

NICKEL
9/1993

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.075 @ MW)/58.70
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing nickel.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.0083 @ MW)/58.70
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing nickel.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

PHOSPHORUS
9/1993

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.0001 @ MW)/30.974
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing phosphorus.
Limitations:	This equation is based on the Water Quality Criteria for yellow (elemental) phosphorus.
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

PLATINUM
9/1993

Organism:	Daphnid
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.082 • MW)/195.09
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing platinum.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

SELENIUM
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.020 @ MW)/78.96
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing selenium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.005 @ MW)/78.96
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing selenium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

SELENIUM
9/1993

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.300 @ MW)/78.96
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing selenium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.071 @ MW)/78.96
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing selenium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

SILVER
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.0041 @ MW)/107.868
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing silver.
Limitations:	This equation is based on the hardness dependent Water Quality Criteria for silver. The criterion for a hardness of 100 mg/L as $CaCO_3$ was used.
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.00012 @ MW)/107.868
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing silver.
Limitations:	This equation is based on the hardness dependent Water Quality Criteria for silver. The criterion for a hardness of 100 mg/L as $CaCO_3$ was used.
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

SILVER
9/1993

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.0023 @ MW)/107.868
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing silver.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1992. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division.

THALLIUM
9/1993

Organism:	Aquatic life (freshwater)
Duration:	Acute
Endpoint:	Lowest Observable Effect Concentration (LOEC)
Equation:	LOEC (mg/L) = (1.4 @ MW)/204.37
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing thallium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (freshwater)
Duration:	Chronic
Endpoint:	Lowest Observable Effect Concentration (LOEC)
Equation:	LOEC (mg/L) = (0.040 @ MW)/201.37
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing thallium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

THALLIUM
9/1993

Organism:	Aquatic life (marine)
Duration:	Acute
Endpoint:	Lowest Observed Effect Concentration (LOEC)
Equation:	LOEC (mg/L) = (2.130 @ MW)/204.37
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing thallium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

TITANIUM
9/1993

Organism:	Fish (freshwater)
Duration:	96-hour
Endpoint:	LC50
Equation:	LC50 (mg/L) = (31.0 @ MW)/47.90
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing titanium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

Organism:	Daphnid
Duration:	48-hour
Endpoint:	EC50
Equation:	EC50 (mg/L) = (4.6 @ MW)/47.90
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing titanium.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

TUNGSTEN
9/1993

Organism:	Daphnid
Duration:	48-hour
Endpoint:	EC50
Equation:	EC50 (mg/L) = (350.0 @ MW)/183.85
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing tungsten.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

Organism:	Fish (freshwater)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (15.61 @ MW)/183.85
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing tungsten.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1991. Hazard Profiles for Selected Heavy Metals. Washington, DC: Office of Pollution Prevention and Toxics, Health and Environmental Review Division, Environmental Effects Branch.

VANADIUM
9/1993

Organism:	Fish	
Duration:	96-hour	
Endpoint:	LC50	
Equation:	vanadium salts (n=4)	LC50 (mg/L) = (3.9 @ MW)/50.942
	vanadium oxides (n=13)	LC50 (mg/L) = (3.3 @ MW)/50.942
	vanadium complexed with organic acids (n=1)	LC50 (mg/L) = (26.0 @ MW)/50.942
	vanadium sulfate (n=4)	LC50 (mg/L) = (3.9 @ MW)/50.942
	sodium vanadate (VO_3) (n=4)	LC50 (mg/L) = (2.5 @ MW)/50.942
	vanadium pentoxide (n=7)	LC50 (mg/L) = (6.1 @ MW)/50.942
	ammonium vanadate (VO_3) (n=2)	LC50 (mg/L) = (2.4 @ MW)/50.942

Application: The appropriate equation may be used to estimate the toxicity of both organic and inorganic compounds containing vanadium.

Limitations: This category is not applicable to vanadium-complexed dyes. The toxicity of vanadium salts and weak organic acid complexes is expected to be related to their water solubility. Vanadium is more toxic in soft water than hard water but the relationship is not well defined. These equations are based on toxicity data measured in moderately hard water (150.0 mg/L as $CaCO_3$). Strong ion pairs with molecular weights greater than 1000 are not expected to be absorbed by aquatic organisms even if they are water soluble. The boundaries for organovanadium compounds are undefined, but the molecular weight boundary is expected to be less than 1000.

References: Nabholz JV. 1993. Vanadium compounds (Unpublished document). Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Pollution Prevention and Toxics, United States Environmental Protection Agency.

VANADIUM
9/1993

Organism:	Daphnid
Duration:	48-hour
Endpoint:	LC50
Equation:	sodium vanadate (VO_3) (n=15): LC50 (mg/L) = (4.1 * MW)/50.942
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing vanadium.
Limitations:	This category is not applicable to vanadium-complexed dyes. The toxicity of vanadium salts and weak organic acid complexes is expected to be related to their water solubility. Vanadium is more toxic in soft water than hard water but the relationship is not well defined. These equations are based on toxicity data measured in moderately hard water (150.0 mg/L as $CaCO_3$). Strong ion pairs with molecular weights greater than 1000 are not expected to be absorbed by aquatic organisms even if they are water soluble. The boundaries for organovanadium compounds are undefined, but the molecular weight boundary is expected to be less than 1000.
References:	Nabholz JV. 1993. Vanadium compounds (Unpublished document). Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Pollution Prevention and Toxics, United States Environmental Protection Agency.

VANADIUM
9/1993

Organism:	Fish
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	vanadium pentoxide (n=3)ChV (mg/L) = (0.670 ▯ MW)/50.942
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing vanadium.
Limitations:	This category is not applicable to vanadium-complexed dyes. The toxicity of vanadium salts and weak organic acid complexes is expected to be related to their water solubility. Vanadium is more toxic in soft water than hard water but the relationship is not well defined. These equations are based on toxicity data measured in moderately hard water (150.0 mg/L as $CaCO_3$). Strong ion pairs with molecular weights greater than 1000 are not expected to be absorbed by aquatic organisms even if they are water soluble. The boundaries for organovanadium compounds are undefined, but the molecular weight boundary is expected to be less than 1000.
References:	Nabholz JV. 1993. Vanadium compounds (Unpublished document). Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Pollution Prevention and Toxics, United States Environmental Protection Agency.

VANADIUM
9/1993

Organism:	Green Algae
Duration:	
Endpoint:	No Observable Effect Concentration (NOEC) (increased growth)
Equation:	ChV (mg/L) = (0.100 @ MW)/50.942
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing vanadium. This equation is based on toxicity data for vanadium sulfate and sodium vanadate.
Limitations:	This category is not applicable to vanadium-complexed dyes. The toxicity of vanadium salts and weak organic acid complexes is expected to be related to their water solubility. Vanadium is more toxic in soft water than hard water but the relationship is not well defined. These equations are based on toxicity data measured in moderately hard water (150.0 mg/L as $CaCO_3$). Strong ion pairs with molecular weights greater than 1000 are not expected to be absorbed by aquatic organisms even if they are water soluble. The boundaries for organovanadium compounds are undefined, but the molecular weight boundary is expected to be less than 1000.
References:	Nabholz JV. 1993. Vanadium compounds (Unpublished document). Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Pollution Prevention and Toxics, United States Environmental Protection Agency.

ZINC
9/1993

Organism:	Aquatic life (freshwater)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.120 @ MW)/65.38
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing zinc.
Limitations:	This equation is based on the hardness dependent Water Quality Criteria for zinc. The criterion for a hardness of 100 mg/L as $CaCO_3$ was used. For a solution with a hardness of 50 mg/L as $CaCO_3$, use the following equation: Acute Value (mg/L) = (0.065 @ MW)/65.38 For a solution with a hardness of 200 mg/L as $CaCO_3$, use the following equation: Acute Value (mg/L) = (0.210 @ MW)/65.38
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

ZINC
9/1993

Organism: Aquatic life (freshwater)

Duration:

Endpoint: Chronic Value (ChV)

Equation: ChV (mg/L) = (0.110 @ MW)/65.38

Application: This equation may be used to estimate the toxicity of both organic and inorganic compounds containing zinc.

Limitations: This equation is based on the hardness dependent Water Quality Criteria for zinc. The criterion for a hardness of 100 mg/L as $CaCO_3$ was used. For solutions with a hardness of 50 mg/L as $CaCO_3$, use the following equation:

ChV (mg/L) = (0.059 @ MW)/65.38

For solutions with a hardness of 200 mg/L as $CaCO_3$, use the following equation:

ChV (mg/L) = (0.190 @ MW)/65.38

References: United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

ZINC
9/1993

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Acute Value
Equation:	Acute Value (mg/L) = (0.095 @ MW)/65.38
Application:	This equation may be used to estimate the toxicity of both inorganic and organic compounds containing zinc.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

Organism:	Aquatic life (marine)
Duration:	
Endpoint:	Chronic Value (ChV)
Equation:	ChV (mg/L) = (0.086 @ MW)/65.38
Application:	This equation may be used to estimate the toxicity of organic and inorganic compounds containing zinc.
Limitations:	None
References:	United States Environmental Protection Agency (USEPA). 1986. Quality Criteria for Water. Washington, DC: Office of Water, Criteria and Standards Division. EPA 440/5-86-001.

ZIRCONIUM
9/1993

Organism:	Fish
Duration:	96-hour
Endpoint:	LC50
Equation:	LC50 (mg/L) = (58.0 @ MW)/91.22
Application:	This equation may be used to estimate the toxicity of both organic and inorganic compounds containing zirconium, including inorganic salts of zirconium, complexes between zirconium and organic acids, and organozirconium compounds, i.e., zirconium covalently-bonded with carbon.
Limitations:	This equation is not applicable to dyes complexed with zirconium. The equation is based on available toxicity data for solution of moderate hardness (i.e., 150 mg/L as $CaCO_3$). Zirconium is more toxic in soft water than in hard water. Acute toxicity to fish has been shown to increase 13 times as hardness decreases from 400.0 to 20 mg/L. Compounds with molecular weights greater than 1000 are not expected to be absorbed by aquatic organisms even if they are water soluble.
References:	Nabholz JV. 1993. Zirconium compounds (Unpublished internal document). Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Pollution Prevention and Toxics, United States Environmental Protection Agency.

ZIRCONIUM
9/1993

Organism:	Green Algae
Duration:	96-hour
Endpoint:	EC50
Equation:	EC50 (mg/L) = (2.6 @ MW)/91.22
Application:	This equation is not applicable to dyes complexed with zirconium. The equation is based on available toxicity data for solution of moderate hardness (i.e., 150 mg/L as $CaCO_3$). Zirconium is more toxic in soft water than in hard water.
Limitations:	This equation is not applicable to dyes complexed with zirconium. The equation is based on available toxicity data for solution of moderate hardness (i.e., 150 mg/L as $CaCO_3$). Zirconium is more toxic in soft water than in hard water. Acute toxicity to fish has been shown to increase 13 times as hardness decreases from 400.0 to 20 mg/L. Compounds with molecular weights greater than 1000 are not expected to be absorbed by aquatic organisms even if they are water soluble.
References:	Nabholz JV. 1993. Zirconium compounds (Unpublished internal document). Washington, DC: Environmental Effects Branch, Health and Environmental Review Division, Office of Pollution Prevention and Toxics, United States Environmental Protection Agency.

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