SAR Categories in Support of SNURs for 43 Chemical Substances

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http://www.epa.gov/oppt/newchems/tools/21ecosar.htm
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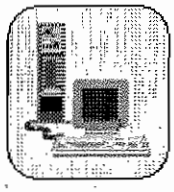
New Chemicals Program

Ecological Structure Activity Relationships (ECOSAR)



v. 1.00a, February, 2009

"You will need Adobe Reader to view some of the files on this page. See EPA's PDF page to learn more."

What is ECOSAR?

The Ecological Structure Activity Relationships (ECOSAR) Class Program is a computerized predictive system that estimates the aquatic toxicity of industrial chemicals. The program estimates a chemical's acute (short-term) toxicity and chronic (long-term or delayed) toxicity to aquatic organisms such as fish, aquatic invertebrates, and aquatic plants by using Structure Activity Relationships (SARs).

What is a Structure Activity Relationship (SAR)?

Structure Activity Relationships, or SARs, is a technique routinely used by the U.S. EPA Office of Pollution Prevention and Toxics under the New Chemicals Program to estimate the toxicity of industrial chemicals being reviewed in response to Pre-Manufacture Notices mandated under Section 5 of the Toxic Substances Control Act (TSCA). Through publication of ECOSAR, the U.S. EPA provides public access to the same methods the EPA uses for evaluating aquatic toxicity.

How Does ECOSAR Work?

ECOSAR uses SARs to predict the aquatic toxicity of untested chemicals based on their structural similarity to chemicals for which aquatic toxicity data are available. The toxicity data used to build the SARs are collected from publicly available experimental studies and confidential submissions submitted to the U.S. EPA New Chemicals Program. The SARs in ECOSAR express correlations between a compound's physicochemical properties and its aquatic toxicity within specific chemical classes.

ECOSAR contains a library of class-based SARs for predicting aquatic toxicity, overlaid with an expert decision tree based on expert rules for selecting the appropriate chemical class for the compound. ECOSAR version 1.00 is programmed to identify over 120 chemical classes and allows access to over 440 SARs. The SARs estimate acute and chronic toxicity endpoints for fish, aquatic invertebrates, and green algae (species used in standard U.S. EPA New

Chemicals Program aquatic toxicity profiles) along with limited SARs for other salt water and terrestrial species, where data were available.

Many of the SARs have been validated through studies published in the open literature or through validation activities conducted by the U.S. EPA is conjunction with other regulatory agencies. For access to some of the ECOSAR validation activities, see the publications attached below under the **ECOSAR Documentation** section, or visit the U.S. EPA's Sustainable Futures/Publications webpage.

What Information Do I Need to Use ECOSAR?

- Descriptions of Chemical Structure
  - Entered using Simplified Molecular Input Line Entry System (SMILES) notation or CAS Registry number if the CAS is available in the look-up data base within ECOSAR. ECOSAR will also accept a .mol file for single chemical entry, or .sdf file or string files to perform batch runs.
- Octanol/water Partitioning Coefficient (Kow)
  - If measured Kow values are not available, ECOSAR will estimate Kow using the EPISuite (WSKowwin) module and use the value in subsequent toxicity predictions.
- Charge density and other information may also be required for some chemical classes

With this information, ECOSAR can perform a SAR analysis and automatically estimate standard toxicity values for a chemical of interest.

How Are ECOSAR Data Used?

The U.S. EPA Office of Pollution Prevention and Toxics uses SARs to predict the aquatic toxicity of new industrial chemicals in the absence of test data. The use of SARs has been an accepted practice in the U.S. EPA New Chemicals Program for estimating the aquatic toxicity of industrial chemicals for over 25 years. Environmental assessors, chemical manufactuerers, chemical suppliers, and other regulatory agencies have used ECOSAR to develop quantitative screening level toxicity profiles for fish, aquatic invertebrates, and green algae. For more information on the use of ECOSAR in assessing aquatic toxicity of industrial chemicals when measured data are not available, please visit the U.S. EPA's Sustainable Futures webpage and review the training material developed by EPA.

The Sustainable Futures Initiative is a voluntary program that encourages chemical developers to use EPA's models and methods to screen new chemicals for potential risks early in the development process. The overall goal of the program is to provide public access to predictive tools that can assist in chemical management decisions and ultimately allow the production of safer chemicals. Sustainable Futures Partners and other interested stakeholders are free to use these materials. The Sustainable Futures site contains presentations, including an over view of ECOSAR with a discussion of what the method does, necessary model inputs, how to interpret results, and how the results are used in a U.S. EPA New Chemicals Program screening level assessment.

How can Community Groups use ECOSAR?

Community groups can use ECOSAR in ways similar to those listed above to estimate aquatic toxicity. However, technical assistance from specialists is advisable as the program was designed for use by individuals with experience and knowledge of organic chemistry, ecotoxicology, and SARs.

What Type of Computer System Do I Need?

Software Required: Microsoft Windows 95 or later (including 98, ME, NT, XP and Vista).

Hardware: IBM-compatible computer with an 80386, 80486 or more recent processor; 2 MB RAM minimum; at least 30 MB available disk space.

What Do I Need to Know to Run the Program and Model Results?

The program requires an understanding of organic chemistry, ecotoxicology, and SARs.

How Can I Obtain ECOSAR?

Download ECOSAR by selecting the following link ECOSAR EcoSarsetup.exe (19MB). ECOSAR is a self-extracting file. Once it is copied to diskette or hard drive, execute (double-click) the file to install the program.

Download the latest ECOSAR User's Guide (PDF) (39 pps, 241KB). This file also requires the Acrobat Reader which is available below.

How Can I Obtain Additional Information about ECOSAR and Structure Activity Relationships?

The U.S. EPA, in conjunction with various public partners and interested public sponsors, provides training on the use and application of models used within the New Chemicals Program including ECOSAR. For additional information about ECOSAR and other predictive tools used by the U.S. EPA Office of Pollution Preventions and Toxics, please visit the U.S. EPA's Sustainable Futures webpage for training and information on models for assessing industrial chemicals.

ECOSAR Documentation:

1. OPPT's report: U.S. EPA/EC Joint Project on the Evaluation of (Quantitative) Structure Activity Relationships: Final report (PDF) (364 pps, 16.64 MB) This file requires the Acrobat Reader which is available below. This file is very large and may take a while to download. Also, it has elements that may cause problems to those using Adobe Reader 5.0.

2. OECD's Monograph: Joint Project on the Evaluation of (Quantitative) Structure Activity Relationships (PDF) (81 pps, 159 KB) This file requires the Acrobat Reader which is available below.

Model Updates to ECOSAR for Version 1.00 Release

- Over 80 additional chemical classes were added to version 1.00; ECOSAR now contains over 120 chemical classes and over 440 SARs based on publicly available and confidential experimental data
- Updates to the ECOSAR help file system
- New technical reference sheets will be available in the help menu for all chemical classes including the non-confidential training set chemicals for each endpoint within a class.
- All octanol-water partition coefficient (Kow) values for the training set chemicals were updated to reflect the newest method from EPISuite (WSKowwin)

Additional Updates to ECOSAR Include

- The water solubility (WS) module in ECOSAR was updated to reflect the newest method available from EPISuite (WSKowwin).

Next Steps in the Future Development of ECOSAR

- Identify additional data points to increase training sets for all chemical classes and soliciting contribution of additional data from interested partners
- Refining data sets and regression analysis for neutral organics and chemical classes with excess toxicity and investigating outliers identified during statistical analysis
- Investigating predictive methods for inorganics and organometallics
- Incorporating a limited number of SARs for polymer evaluation

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1.0. ECOSAR Introduction & Overview

The structure-activity relationships (SARs) presented in this program are used to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. Most SAR calculations in the ECOSAR Class Program are based upon the octanol/water partition coefficient (Kow). Various surfactant SAR calculations are based upon the average length of carbon chains or the number of ethoxylate units.

SARs have been used by the U.S. Environmental Protection Agency since 1981 to predict the aquatic toxicity of new industrial chemicals in the absence of test data. The acute toxicity of a chemical to fish (both fresh and saltwater), water fleas (daphnids), and green algae has been the focus of the development of SARs, although for some chemical classes SARs are available for other effects (e.g, chronic toxicity and bioconcentration factor) and organisms (e.g., earthworms). SARs are developed for chemical classes based on measured test data that have been submitted by industry or they are developed by other sources for chemicals with similar structures, e.g., phenols. Using the measured aquatic toxicity values and estimated Kow values, regression equations can be developed for a class of chemicals. Toxicity values for new chemicals may then be calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound.

There are currently 130 chemical classes programmed into ECOSAR. For those 130 classes, there are a total of 440 QSARs based on publicly available experimental data and confidential studies collected under the EPA New Chemicals Program. For each class, a standard EPA New Chemicals Program aquatic toxicity profile will be created using available QSARs and/or alternate SAR approaches and professional judgment. This standard profile typically contains 3 acute values, and 3 chronic values for fish, daphnid, and green algae. In an effort to complete a profile for each class, 173 endpoints have been estimated using alternative approaches such as acute-to-chronic ratios and substitute QSARs based on scientific judgment.

ECOSAR estimates log Kow values using the US EPA's KOWWIN Program. Information about the KOWWIN Program its log Kow estimations are available in the on-line KOWWIN Help File.

The ECOSAR Class Program is a computerized version of the ECOSAR analysis procedures as currently practiced by the Office of Pollution Prevention and Toxics (OPPT). It has been developed within the regulatory constraints of the Toxic Substances Control Act (TSCA). It is a pragmatic approach to SAR as opposed to a theoretical approach.

This ECOSAR program is designed for the expert user. You are expected to have some knowledge of environmental toxicology and organic chemistry. It is menu-driven and contains various help functions to assist you. You cannot change any of the equations or data stored within the program or accidentally erase any important information. The following pages show you how to access and use the ECOSAR program. If you have any questions or comments on the ECOSAR program, or find any errors, please contact:

How can I obtain additional information about ECOSAR and Structure Activity Relationships?

For additional information about ECOSAR and Structure Activity Relationships:

Documentation: The ECOSAR User Manual, ECOSAR: A Computer Program for Estimating the Ecotoxicity of Industrial Chemicals (EPA-748-R-93-002), and Estimating Toxicity of Industrial Chemicals to Aquatic Organisms Using Structure Activity Relationships (EPA-748-R-93-001) are available by calling the National Center for Environmental Publications and Information at 1-800-490-9198.

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SAR Equations

Example SAR Equations

The following are example SAR equations used by the ECOSAR Class Program to calculate ecotoxicity values. They are indicative of all SARs calculated from SMILES and log Kow values.

Acrylates:

Log 96-h LC50 (mmol/L) = -0.2427 (log Kow) - 1.3597 (FISH 96-h LC50 Mortality)
Log 48-h EC50 (mmol/L) = -0.3226 (log Kow) - 0.773 (DAPHNID 48-h EC50)
Log 96-h EC50 (mmol/L) = -0.1145 (log Kow) - 1.8295 (GREEN ALGAE 96-h EC50)
Log ChV (mmol/L) = -0.4834 (log Kow) - 2.2111 (FISH 30-d ChV)
Log ChV (mmol/L) = -0.4896 (log Kow) - 1.773 (DAPHNID ChV)
Log ChV (mmol/L) = -0.1958 (log Kow) - 2.2582 (GREEN ALGAE ChV)
(values calculated by these equations are in units of millimoles/L)

More Detailed Information:

Carbamate Esters, Oximes
Diazoniums, Aromatic
Diketones
Dinitroanilines - Dinitroaromatic Amines
Dinitrobenzenes
Dinitrophenols
Dyes, Cationic
Epoxides, Mono
Epoxides, Mono Acid Substituted
Epoxides, Poly
Epoxides, Halo
Esters
Esters, Dithiophosphates
Esters, Monothiophosphates
Esters, Phosphate
Esters, Phosphinate
Esters, Halo
Esters, Nitriles
Esters, Peroxy
Haloacetamides
Haloalcohols
Halo Benzamides
Halo Epoxides
Halo Esters
Halo Ethers
Halo Hydantoins
Halo Ketones
Halo Nitriles
Halo Pyridines
Hydrazines
Hydroquinones / Quinones
Imidazoles
Imides
Imide Acids
Isothiazolones
Ketone Alcohols
Melamines
Mercaptans
Methacrylates
Neutral Organics
Nitriles, alpha OH
Nitriles, Esters
Nitriles, Polyaliphatic
Nitro alcohols
Nitro-/Nitrosobenzamides
Oxetanes
Peroxy Acids / Peroxides
Peroxy esters
Phenols
Phenols, Amines
Phenols, Poly
Phosphine Oxide
Phthalonitriles
Propargyl Alcohols
Propargyl Alcohols (Hindered)
Propargyl Amines

Propargyl Carbamates
Propargyl Ethers
Propargyl Halides
Pyrazoles, Pyrroles
Pyrethroids
Pyridines, alpha-Acid
Pyridine Thiones
Quinones / Hydroquinones
Rosins
Schiff Bases
Silanes (alkoxy)
Sulfonyl Ureas
Thiazolidinones
Thiazolidinones, Acid
Thiocarbamates, Di (Free Acid)
Thiocarbamates, Di (Substituted)
Thiocarbamates, Di (Fe salts)
Thiocarbamates, Di (Mn salts)
Thiocarbamates, Di (Na salts)
Thiocarbamates, Di (Zn salts)
Thiocarbamates, Mono
Thiols
Thiomethacrylates
Thiophenes
Thiotetrazoles
Thioureas
Triazines
Triazole Pyrimidines
Triazoles (non-fused)
Ureas, Substituted
Vinyl / Allyl Alcohols
Vinyl / Allyl Aldehyes
Vinyl / Allyl Amines
Vinyl / Allyl Esters
Vinyl / Allyl Ethers
Vinyl / Allyl Ether Amines
Vinyl / Allyl Halides
Vinyl / Allyl Ketones
Vinyl / Allyl Nitriles
Vinyl / Allyl Sulfones
Vinyl / Allyl Thiocarbamates

FISH 96-h LC50 (Mortality)

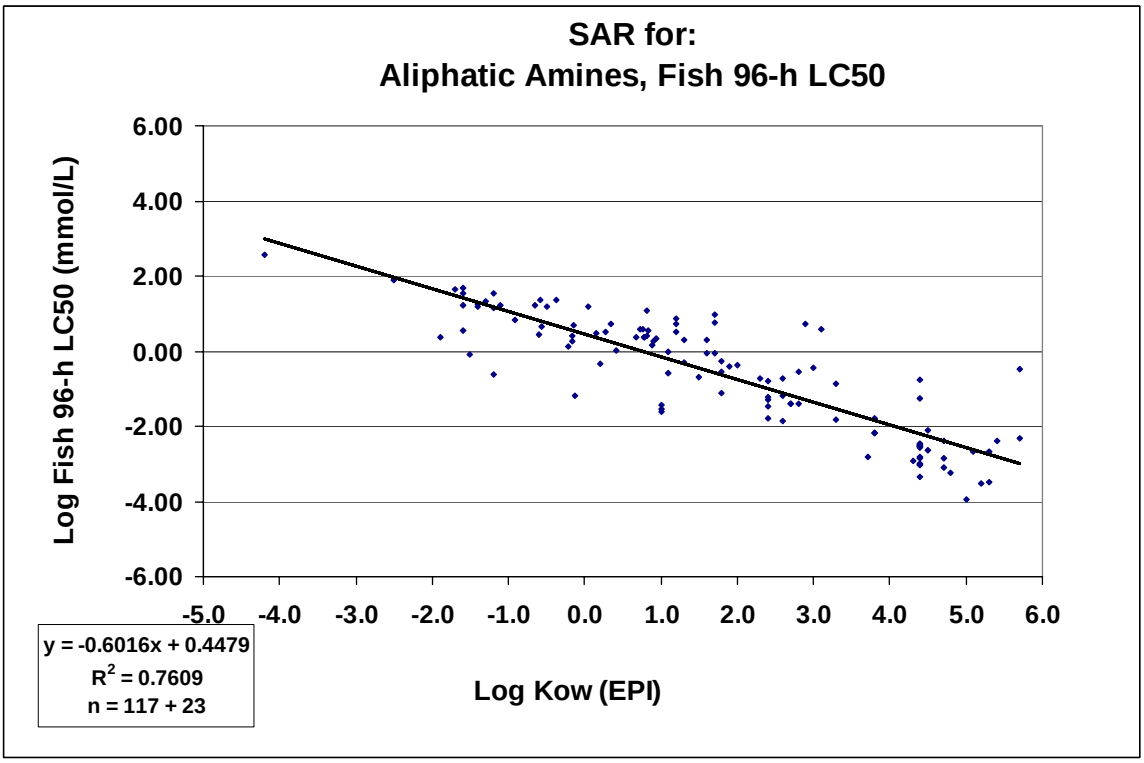
ESTIMATED TOXICITY:
The fish 96-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h LC50 (mmol/L) = -0.6016 (log Kow) + 0.4479

The LC50 is in millimoles per liter (mM/L); N = 117 + 23; and the Coefficient of Determination (R^2) = 0.7609. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 6.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for aliphatic amines.

LIMITATIONS:
For aliphatic amines with log Kow values greater than 7.0, 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.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish 96-h LC50 (mg/L)	Log Fish 96-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Fish 96-h LC50)
100-97-0	Hexamethylenetetramine	140	2.5	-4.2		49800	2.55		DUL
102-71-6	Triethanolamine	149	-1.5	-2.5	-1	11800	1.90	Hansch et al., 1995	DUL
CBI	CBI	252	-0.9	-1.9		585	0.37		P91-___
111-42-2	Diethanolamine	105	-1.5	-1.7	-1.43	4710	1.65	Hansch & Leo, 1985	DUL
107-15-3	Ethylenediamine	60	-1.2	-1.6	-2.04	220	0.56	Hansch et al., 1995	DUL
141-43-5	2-Aminoethanol	61	-1.3	-1.6	-1.31	2070	1.53	Hansch & Leo, 1985	DUL
140-31-8	1-(2-Aminoethyl)piperazine	129	-0.6	-1.6		2190	1.23		DUL
103-76-4	1-(2-Hydroxyethyl) piperazine	130	-0.68	-1.6		6410	1.69		DUL
5407-04-5	3-Dimethylaminopropyl chloride hydrochloride	158	3.1	-1.5		133	-0.07		DUL
7209-38-3	1,4-Bis (3-aminopropyl) piperazine	200	-1.4	-1.4	-1.43	3100	1.19		DUL
CBI	CBI	208	0.09	-1.4		3900	1.27		P00-___
622-40-2	4-(2-Hydroxyethyl) morpholine	131	-0.45	-1.3		2710	1.32		DUL
78-90-0	1,2-Propane diamine	74	-0.91	-1.2		1010	1.14		DUL
78-96-6	Isopropanol amine	75	-0.99	-1.2	-0.96	2520	1.53	Hansch & Leo, 1985	DUL
CBI	CBI	317	-3.2	-1.2		75	-0.63		P95-___
109-76-2	1,3-Propane diamine	74	-1.5	-1.1	-1.43	1190	1.21	Hansch et al., 1995	DUL
109-85-3	2-Methoxyethylamine	75	-0.67	-0.91		524	0.84		DUL
110-73-6	2-(Ethylamino) ethanol	89	-0.46	-0.66		1480	1.22		DUL
CBI	CBI	249	-0.25	-0.6		677	0.43		P95-___
109-01-3	1-Methylpiperazine	100	-0.099	-0.59		2300	1.36		DUL
110-91-8	Morpholine	87	-0.72	-0.56	-0.86	380	0.64	Hansch & Leo, 1985	Calamari et al., 1980
280-57-9	1,4-Diazabicyclo (2,2,2) octane	112	0.69	-0.49		1730	1.19		DUL
109-07-9	2-Methylpiperazine	100	-0.44	-0.38		2240	1.35		DUL
107-29-9	Acetaldoxime	59	-0.14	-0.21	-0.13	76	0.11	Hansch et al., 1995	DUL
124-40-3	Dimethylamine	45	-0.51	-0.17	-0.38	118	0.42	Hansch & Leo, 1985	Calamari et al., 1980
59-97-2	Tolazoline hydrochloride	197	MF	-0.16		354	0.25		DUL
75-04-7	Ethylamine	45	-0.14	-0.15	-0.13	227	0.70	Hansch & Leo, 1985	U.S. EPA, 1990 (ERL-D)
22104-62-7	4-Dimethylamino-3-methyl-2-butanone	129	0.34	-0.12		8.5	-1.18		DUL
100-37-8	N,N-Diethylethanolamine	117	0.48	0.05		1780	1.18		DUL
CBI	CBI	135	0.2	0.15		390	0.46		P91-___
107-11-9	Allylamine	57	-0.09	0.21	0.03	27	-0.32	Hansch & Leo, 1985	Bridie et al., 1979
141-91-3	2,6-Dimethylmorpholine	115	0.73	0.28		387	0.53		DUL
107-10-8	Propylamine	59	0.39	0.34	0.48	308	0.72	Hansch & Leo, 1985	DUL
CBI	CBI	238	0	0.41		250	0.02		P91-___
6921-29-5	Tripropargylamine	131	0.19	0.67	1.27	296	0.35	Hansch et al., 1995	DUL
75-64-9	tert-Butylamine	73	0.57	0.72	0.4	270	0.57	Hansch & Leo, 1985	Calamari et al., 1980
13952-84-6	(+-)-sec-Butylamine	73	0.74	0.76	0.74	275	0.58	Hansch & Leo, 1985	DUL
6948-86-3	N,N-Bis(2,2-diethoxyethyl) methylamine	263	1.4	0.78		637	0.38		DUL
6948-86-3	N,N-Bis(2,2-diethoxyethyl) methylamine	263	1.4	0.78		634	0.38		DUL
109-89-7	Diethylamine	73	0.54	0.81	0.58	855	1.07	Hansch & Leo, 1985	DUL
109-89-7	Diethylamine	73	0.54	0.81	0.58	182	0.40	Hansch & Leo, 1985	Calamari et al., 1980
109-73-9	Butylamine	73	0.92	0.83	0.97	268	0.56	Hansch & Leo, 1985	DUL
96-80-0	2-(Diisopropylamino) ethanol	145	1.1	0.88		201	0.14		DUL
100-64-1	Cyclohexanone oxime	113	1.2	0.91	0.84	208	0.26	TSCATS	DUL
105-14-6	5-Diethylamino-2-pentanone	157	0.57	0.94		336	0.33		DUL
54-11-5	(s)-3-Methyl-2-pyrrolidinyl pyridine nicotine	162	1.3	1	1.17	4	-1.61	Hansch & Leo, 1985	Edsall, 1991
65-30-5	Nicotine sulfate	419	MF	1	1.17	12.2	-1.54	Hansch & Leo, 1985	DUL
65-30-5	Nicotine sulfate	419	MF	1	1.17	15.6	-1.43	Hansch & Leo, 1985	DUL
100-46-9	Benzylamine	107	1.1	1.1	1.09	102	-0.02	Hansch & Leo, 1985	U.S. EPA, 1990 (ERL-D)
2759-28-6	1-Benzylpiperazine	176	1.8	1.1		47.4	-0.57		DUL
127-06-0	Acetone oxime	73	0.12	1.2	0.12	558	0.88	Pomona, 1987	DUL
598-74-3	(+-)-1,2-Dimethylpropylamine	87	1.1	1.2		284	0.51		DUL
5813-64-9	2,2-Dimethyl-1-propylamine	87	1.2	1.2		475	0.74		DUL
110-58-7	Amylamine	87	1.5	1.3	1.49	177	0.31	Hansch & Leo, 1985	DUL
34274-04-9	N-(3-Methoxypropyl)-3,4,5-trimethoxybenzylamine	269	0.05	1.3		136	-0.30		DUL
124-02-7	Diallylamine	97	0.63	1.5	1.11	20	-0.69	Hansch & Leo, 1985	Bridie et al., 1979
108-91-8	Cyclohexylamine	99	1.4	1.6	1.49	90	-0.04	Hansch & Leo, 1985	Calamari et al., 1980
108-18-9	Diisopropylamine	101	1.1	1.6	1.4	196	0.29	Hansch & Leo, 1985	Calamari et al., 1980
96-29-7	2-Butanone oxime	87	0.36	1.7	0.63	843	0.99	Chem Inspect Test Inst, 1992	DUL
15673-00-4	3,3-Dimethylbutylamine	101	1.7	1.7		602	0.78		DUL
7250-67-1	1-(2-Chloroethyl) pyrrolidine Hydrochloride	170	1.4	1.7		153	-0.05		DUL
111-26-2	Hexylamine	101	2	1.8	2.06	56.6	-0.25	Hansch & Leo, 1985	DUL
103-83-3	N,N-Dimethylbenzylamine	135	2	1.8	1.98	37.8	-0.55	Hansch & Leo, 1985	DUL
60-13-9	Amphetamine sulfate	369	1.8	1.8	1.76	28.8	-1.11	Hansch & Leo, 1985; Sangster	DUL
80-52-4	1,8-Diamino-p-menthane	170	1.2	1.9		65.3	-0.42		DUL
14321-27-8	N-Ethylbenzylamine	135	2	2	1.8	57.1	-0.37	Sangster, 1993	DUL
111-68-2	n-Heptylamine	115	2.5	2.3	2.57	21.8	-0.72	Hansch & Leo, 1985	DUL
768-94-5	1-Adamantanamine	151	2	2.4	2.44	25	-0.78	Hansch & Leo, 1985	DUL
CBI	CBI	198	2.7	2.4		3.23	-1.79		P85-___

CBI	CBI	198	2.7	2.4		6.8	-1.46		P85-____
CBI	CBI	198	2.7	2.4		12	-1.22		P85-____
CBI	CBI	198	2.7	2.4		10.2	-1.29		P85-____
107-45-9	tert-Octylamine	129	2.4	2.6		24.6	-0.72		DUL
CBI	CBI	238	MF	2.6		3.4	-1.85		P__-____
CBI	CBI	494	1.2	2.6	5.8	33	-1.18	HPLC	P92-____
693-16-3	1-Methylheptylamine	129	2.8	2.7		5.11	-1.40		DUL
693-16-3	1-Methylheptylamine	129	2.8	2.7		5.28	-1.39		DUL
111-86-4	Octylamine	129	3	2.8	2.9	5.19	-1.40	Sangster, 1993	DUL
111-92-2	Dibutylamine	129	2.7	2.8	2.83	37	-0.54	Hansch & Leo, 1985	Calamari et al., 1980
CBI	CBI	212	2.4	2.9		1100	0.72		P93-____
102-69-2	Tripropylamine	143	2.8	3	2.79	50.9	-0.45	Hansch & Leo, 1985	DUL
CBI	CBI	200	1.9	3.1		778	0.59		P89-____
112-20-9	Nonylamine	143	3.6	3.3		2.16	-1.82		DUL
91-65-6	N,N-Diethylcyclohexylamine	155	3	3.3		21.4	-0.86		DUL
CBI	CBI	392	MF	3.71		0.59	-2.82		P87-____
2016-57-1	n-Decylamine	157	4.1	3.8		1.03	-2.18		U.S. EPA, 1990 (ERL-D)
2016-57-1	n-Decylamine	157	4.1	3.8		1.04	-2.18		DUL
CBI	CBI	278	4.3	3.8	3.17	4.6	-1.78	Unknown	P00-____
7307-55-3	Undecylamine	171	4.6	4.3		0.21	-2.91		DUL
CBI	CBI	217	4.9	4.4		0.21	-3.01		P85-____
CBI	CBI	217	4.9	4.4		0.66	-2.52		P85-____
CBI	CBI	217	4.9	4.4		0.72	-2.48		P85-____
CBI	CBI	217	4.9	4.4	3.7	0.65	-2.52	Unknown	P96-____
CBI	CBI	217	4.9	4.4	3.7	0.6	-2.56	Unknown	P96-____
CBI	CBI	217	4.9	4.4	3.7	0.2	-3.04	Unknown	P96-____
29873-30-1	N-Decylthioamine	217	4.9	4.4		0.22	-2.99		8(e)-3587
29873-30-1	N-Decylthioamine	217	4.9	4.4		0.7	-2.49		8(e)-3587
29873-30-1	N-Decylthioamine	217	4.9	4.4		0.77	-2.45		8(e)-3587
CBI	CBI	228	4.9	4.4		13	-1.24		P94-____
CBI	CBI	228	4.9	4.4		39	-0.77		P94-____
CBI	CBI	253	4.9	4.4		0.11	-3.36		P85-____
CBI	CBI	253	4.9	4.4		0.345	-2.87		P96-____
CBI	CBI	253	4.9	4.4		0.38	-2.82		P96-____
CBI	CBI	300	3.8	4.5		0.71	-2.63		P91-____
CBI	CBI	367	4.1	4.5		2.8	-2.12		P90-____
143-16-8	Di-n-hexylamine	185	4.8	4.7		0.78	-2.38		DUL
56296-78-7	Fluoxetin hydrochloride	346	4.1	4.7	3.82; 4.05	0.49	-2.85	Unknown; Adlard, M et al., 1995	8(e)-15316
CBI	CBI	411	6.8	4.7		0.33	-3.10		P02-____
124-22-1	Dodecyamine	185	5.2	4.8		0.103	-3.25		DUL
52898-18-7	1,3-Propanediamine, N- 3-(dodecyloxy)propyl -	301	4.1	5		0.033	-3.96		8(e)-14601
NK	Hydrogenated cocoamidopropyldiethylamine-N-oxide	343	3	5.1		0.75	-2.66		8(e)-14655
CBI	CBI	940	2.4	5.2		0.28	-3.53		P05-____
2869-34-3	Tridecylamine	199	5.7	5.3		0.0654	-3.48		DUL
CBI	CBI	259	5.7	5.3		0.55	-2.67		T94-____
112-18-5	Dimethyl dodecyl amine	213	5.5	5.4		0.84	-2.40		SIDS, 1998
CBI	CBI	295	MF	5.7	3.8	100	-0.47	HPLC	P00-____
CBI	CBI	316	5.7	5.7	4.9	1.466	-2.33	PMN est.	P91-____
SAR Data Not Included in Regression Equation:									
2706-56-1	2-(2-Aminoethyl) pyridine	122	-0.21	0.02	0.08	*		Hansch & Leo, 1985	DUL
CBI	CBI	341	3.7	4.4	4.4	*		Unknown	P03-____
CBI	CBI	481	5.5	6.5		*4.4	*-2.04		CBI
CBI	CBI	481	5.5	6.5		*13	*-1.57		CBI
CBI	CBI	1527	7.1	6.7		*2.5	*-2.79		P98-____
CBI	CBI	1527	7.1	6.7		*2.9	*-2.72		P98-____
CBI	CBI	509	7.1	6.9		*1	*-2.71		CBI
CBI	CBI	509	7.1	6.9		*7.9	*-1.81		CBI
CBI	CBI	377	8.4	7.1		*2.3	*-2.21		P00-____
CBI	CBI	501	7.1	7.1		*0.13	*-3.59		P98-____
CBI	CBI	501	7.1	7.1		*0.28	*-3.25		P98-____
95-38-5	2-(8-Heptadecenyl)-4,5-dihydro-1H-imidazole-1-ethanol	351	7.9	7.5		*0.3	*-3.07		8(e)-4252
CBI	CBI	439	5.7	7.5		*0.13	*-3.53		P97-____
CBI	CBI	469	7.9	7.5		*0.45	*-3.02		P90-____
CBI	CBI	494	8.6	8.1		0.82	-2.78		P05-____
CBI	CBI	284	8.6	8.1		*0.44	*-2.81		P92-____
CBI	CBI	582	MF	8.2		*			P90-____
CBI	CBI	423	8.7	9.1		*0.43	*-2.99		P00-____
CBI	CBI	961	14.8	9.6		*			P89-____
CBI	CBI	565	14	13		*2.3	*-2.39		P91-____
CBI	CBI	676	11	13		*0.525	*-3.11		P91-____
CBI	CBI	1066	16	14		*			P98-____
CBI	CBI	1066	16	14		*4.4	*-2.38		P98-____

Data Not Included in SAR:									
333-18-6	Ethylenediamine dihydrochloride	133	MF	-3.4		>100	>-0.12		Ewell et al., 1986
CBI	CBI	503	3.3	-0.47	0.2	>2400	>0.68	CBI	CBI
CBI	CBI	503	3.3	-0.47	0.2	>2100	>0.62	CBI	CBI
CBI	CBI	262	0.1	0.35		>500	>0.28		P91-___
CBI	CBI	189	0.52	0.86		>100	>-0.39		P05-___
CBI	CBI	489	3.3	1.9		>101	>-0.68		P02-___
CBI	CBI	451	2	3.8		>99	>-0.66		P93-___
CBI	CBI	428		5.6		<0.1	<-3.63		8(e)-_____
27136-73-8	2-(Heptadecenyl)-4,5-dihydro-1H-imidazole-1-ethanol	351	7.8	7.5		0.22 to 0.5	-3.2 to -2.85		
CBI	CBI	284	8.6	8.1		0.56 to 0.75	-2.71 to -2.58		P92-___
						* indicates no effects at saturation			

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DAPHNID 48-h LC50

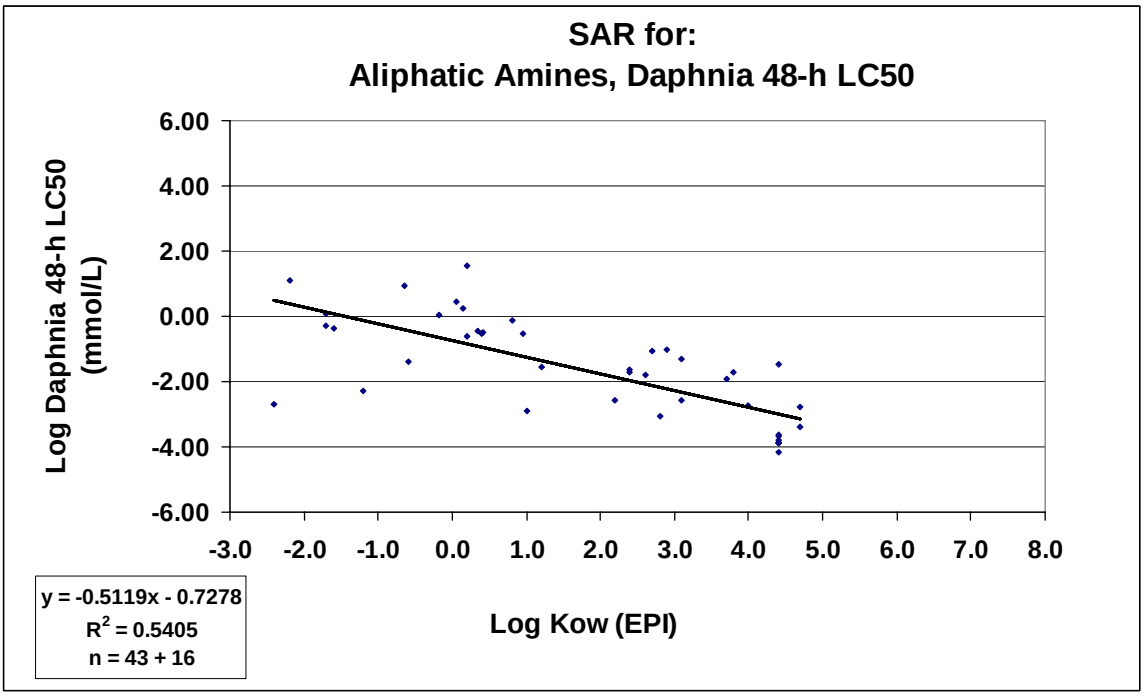
ESTIMATED TOXICITY:
The daphnid 48-h LC50 values used to develop this SAR were measured, and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 48-h LC50 (mmol/L) = -0.5119 (log Kow) - 0.7278

The LC50 is in millimoles per liter (mM/L); N = 44 + 15; and the Coefficient of Determination (R^2) = 0.554. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 5.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for aliphatic amines.

LIMITATIONS:
For aliphatic amines with log Kow values greater than 5.0, a test duration of greater than 48 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 48 hours.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Daphnia 48-h LC50 (mg/L)	Log Daphnia 48-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Daphnia 48-h LC50)
CBI	CBI	773	-7.6	-2.4		1.6	-2.68		P95-____
CBI	CBI	144	-0.8	-2.2		1760	1.09		P90-____
111-42-2	Diethanolamine	105	-1.5	-1.7	-1.43	55	-0.28	Hansch & Leo, 1985	Le Blanc, 1980
111-42-2	Diethanolamine	105	-1.5	-1.7	-1.43	131	0.10	Hansch & Leo, 1985	Cowgill et al., 1985
107-15-3	Ethylenediamine	60	-1.2	-1.6	-2.04	26.5	-0.35	Hansch et al., 1995	Van Leeuwen et al., 1985
CBI	CBI	317	-3.2	-1.2		1.7	-2.27		P95-____
74-89-5	Methylamine	31	-0.7	-0.64	-0.57	280	0.96	Hansch & Leo, 1985	Kuhn et al., 1989
CBI	CBI	249	-0.25	-0.6		10.5	-1.38		P95-____
124-40-3	Dimethylamine	45	-0.51	-0.17	-0.38	50	0.05	Hansch & Leo, 1985	Van Leeuwen et al., 1985
CBI	CBI	163	0.4	0.05		450	0.44		P03-____
CBI	CBI	135	0.2	0.15		230	0.23		P91-____
CBI	CBI	3.3	-0.47	0.2		117	1.55	Unknown	CBI
CBI	CBI	205	MF	0.2		51	-0.60		P96-____
CBI	CBI	262	0.1	0.35		90	-0.46		P91-____
CBI	CBI	143	1.1	0.4		42	-0.53		P91-____
CBI	CBI	238	0	0.41		77	-0.49		P91-____
109-89-7	Diethylamine	73	0.54	0.81	0.58	56	-0.12	Hansch & Leo, 1985	Van Leeuwen et al., 1985
CBI	CBI	154	0.37	0.95		46	-0.52		P94-____
54-11-5	(s)-3-Methyl-2-pyrrolidinyl pyridine nicotine	162	1.3	1	1.17	0.2	-2.91	Hansch & Leo, 1985	Smith, 1988
CBI	CBI	157	1	1.2		4.3	-1.56		P83-____
CBI	CBI	438	MF	2.2		1.18	-2.57		P87-____
CBI	CBI	198	2.7	2.4		3.8	-1.72		P85-____
CBI	CBI	198	2.7	2.4		4.51	-1.64		P85-____
CBI	CBI	494	1.2	2.6	5.8	7.72	-1.81	HPLC	P92-____
CBI	CBI	173	1.3	2.7		15	-1.06		P88-____
CBI	CBI	360		2.8		0.3	-3.08		8(e)-____
CBI	CBI	212	2.4	2.9		21	-1.00		P93-____
CBI	CBI	200	1.9	3.1		10	-1.30		P89-____
54739-18-3	Fluvoxamine	318		3.1		0.84	-2.58		Henry et al., 2004
59729-33-8	Citalopram	324		3.7		3.9	-1.92		Henry et al., 2004
CBI	CBI	278	4.3	3.8	3.17	5.2	-1.73		P00-____
54739-18-3	Paroxetine	329		4		0.58	-2.75		Henry et al., 2004
29873-30-1	N-Decylthioethylamine	217	4.9	4.4		0.045	-3.68		8(e)-3588
29873-30-1	N-Decylthioethylamine	217	4.9	4.4		0.034	-3.80		8(e)-3587
CBI	CBI	217	4.9	4.4	3.7	0.03	-3.86	Unknown	P85-____
CBI	CBI	217	4.9	4.4	3.7	0.05	-3.64	Unknown	P85-____
CBI	CBI	217	4.9	4.4	3.7	0.03	-3.86	Unknown	P96-____
CBI	CBI	228	4.9	4.4		7.5	-1.48		P94-____
CBI	CBI	253	4.9	4.4		0.033	-3.88		P85-____
CBI	CBI	253	4.9	4.4		0.018	-4.15		P96-____
36362-09-1	2-(Decyl thio)-ethanamine hydrochloride	254	4.9	4.4		0.033	-3.89		8(e)-3307
54910-89-3	Fluoxetine	309		4.7		0.51	-2.78		Henry et al., 2004
CBI	CBI	411	6.8	4.7		0.17	-3.38		P02-____
SAR Data Not Included in Regression Equation:									
CBI	CBI	341	3.7	4.4	4.4	*	*	Unknown	P03-____
NK	Hydrogenated cocoamidopropyldiethylamine-N-oxide	343	3	5.1		*0.96	*-2.55		8(e)-14655
79617-96-2	Sertraline	306		5.3		*0.12	*-3.41		Henry et al., 2004
112-18-5	Dimethyl dodecyl amine	213	5.5	5.4		*0.083	*-3.41		SIDS, 1998
CBI	CBI	295	MF	5.7	3.8	*0.012	*-4.39	HPLC	P00-____
CBI	CBI	295	MF	5.7	3.8	*0.51	*-2.76	HPLC	P00-____
CBI	CBI	316	5.7	5.7	4.9	*8.88	*-1.55	PMN est.	P91-____
CBI	CBI	323	5.6	5.7		*27	*-1.08		P95-____
CBI	CBI	377	8.4	7.1		*0.065	*-3.76		P00-____
CBI	CBI	439	5.7	7.5		*0.032	*-4.14		P97-____
CBI	CBI	469	7.9	7.5		*0.23	*-3.31		P90-____
CBI	CBI	614	11	7.5		*0.13	*-3.67		P90-____
CBI	CBI	494	8.6	8.1		0.79	*-2.80		P05-____
CBI	CBI	423	8.7	9.1		*0.04	*-4.02		P00-____
CBI	CBI	565	14	13		*0.97	*-2.77		P91-____
CBI	CBI	676	11	13		*0.55	*-3.09		P91-____
Data Not Included in SAR:									
CBI	CBI	189	0.52	0.86		270	0.15		P-05-____
						* indicates no effects at saturation			

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Van Leeuwen CJ, MASS-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. [A summary of studies also listed in the 'Reference' section.]

GREEN ALGAE 96-h EC50

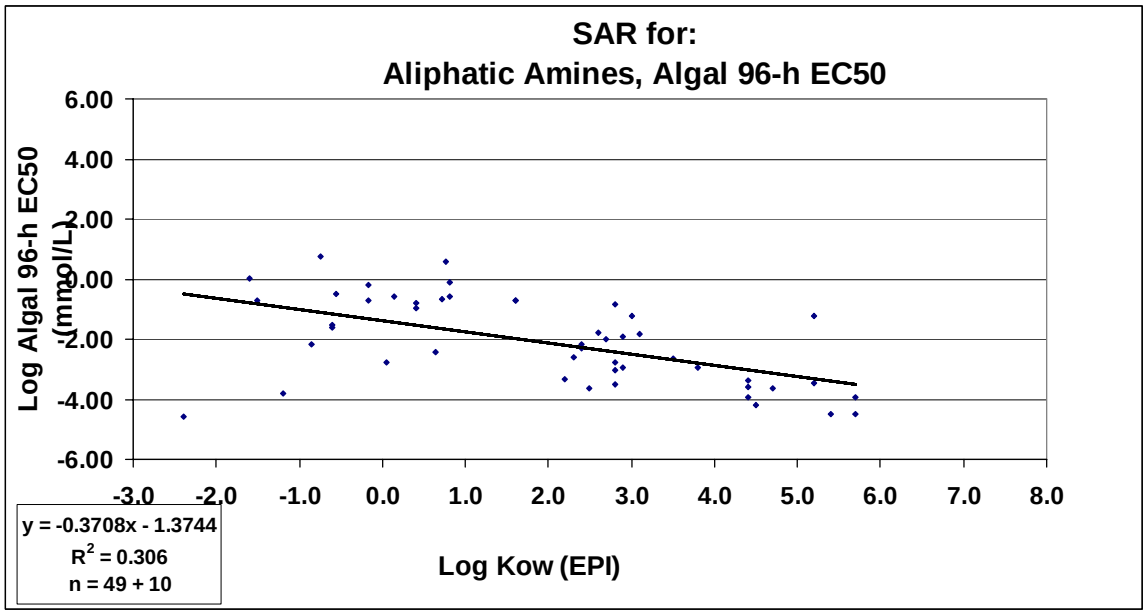
ESTIMATED TOXICITY:
The green algae 96-h EC50 values used to develop this SAR were measured, and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h EC50 (mmol/L) = -0.3708 (log Kow) -1.3744

The EC50 is in millimoles per liter (mM/L); N = 49 + 10; and the Coefficient of Determination (R^2) = 0.306. To convert the EC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 7.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for aliphatic amines.

LIMITATIONS:
If the log Kow value is greater than 7, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Algal 96-h EC50 (mg/L)	Log Algal 96-h EC50 (mmol/L)	Reference (Meas. Kow)	Reference (Algal 96-h EC50)
CBI	CBI	773	-7.6	-2.4		0.02	-4.59		P95-____
107-15-3	Ethylenediamine	60	-1.2	-1.6	-2.04	61	0.01	Hansch et al., 1995	Van Leeuwen et al., 1985
CBI	CBI	132	-0.7	-1.5		27	-0.69		P94-____
CBI	CBI	317	-3.2	-1.2		0.05	-3.80		P95-____
CBI	CBI	329		-0.85		2.2	-2.17		P94-____
CBI	CBI	89	-0.6	-0.74		480	0.73		P91-____
CBI	CBI	249	-0.25	-0.6		6.2	-1.60		P95-____
CBI	CBI	249	-0.25	-0.6		7.3	-1.53		P95-____
110-91-8	Morpholine	87	-0.72	-0.56	-0.86	28	-0.49	Hansch & Leo, 1985	Calamari et al., 1980
124-40-3	Dimethylamine	45	-0.52	-0.17	-0.38	30	-0.18	Hansch & Leo, 1985	Van Leeuwen et al., 1985
124-40-3	Dimethylamine	45	-0.52	-0.17	-0.38	9	-0.70	Hansch & Leo, 1985	Calamari et al., 1980
CBI	CBI	163	0.4	0.05		0.27	-2.78		P03-____
CBI	CBI	135	0.2	0.15		36	-0.57		P91-____
CBI	CBI	143	1.1	0.4		16	-0.95		P91-____
CBI	CBI	238	0	0.41		38	-0.80		P91-____
CBI	CBI	185		0.64		0.71	-2.42		8(e)-____
75-64-9	tert-Butylamine	73	0.57	0.72	0.4	16	-0.66	Hansch & Leo, 1985	Calamari et al., 1980
13952-84-6	(+-)-sec-Butylamine	73	0.74	0.76	0.74	275	0.58	Hansch & Leo, 1985	8(e)-14540
109-89-7	Diethylamine	73	0.54	0.81	0.58	56	-0.12	Hansch & Leo, 1985	Van Leeuwen et al., 1985
109-89-7	Diethylamine	73	0.54	0.81	0.58	20	-0.56	Hansch & Leo, 1985	Calamari et al., 1980
108-91-8	Cyclohexylamine	99	1.4	1.6	1.49	20	-0.69	Hansch et al., 1995	Calamari et al., 1980
108-18-9	Diisopropylamine	101	1.1	1.6	1.4	20	-0.70	Hansch et al., 1995	Calamari et al., 1980
CBI	CBI	438	MF	2.2		0.21	-3.32		P87-____
98-94-2	Dimethylcyclohexylamine	127	2.1	2.3		0.31	-2.61		8(e)-14542
CBI	CBI	161	2.7	2.4		1.04	-2.19		P85-____
CBI	CBI	198	2.7	2.4		1	-2.30		P85-____
CBI	CBI	592	6.5	2.5		0.14	-3.63		P88-____
CBI	CBI	238	MF	2.6		4	-1.77		P91-____
CBI	CBI	173	1.3	2.7		1.8	-1.98		P88-____
111-86-4	Octylamine	129	3	2.8	2.9	0.12	-3.03	Sangster, 1993	8(e)-14541
111-86-4	Octylamine	129	3	2.8	2.9	0.22	-2.77	Sangster, 1993	U.S.EPA, 1990 (ERL-D)
111-92-2	Dibutylamine	129	2.7	2.8	2.8	19	-0.83	Hansch & Leo, 1985	Calamari et al., 1980
CBI	CBI	360		2.8		0.114	-3.50		8(e)-____
102-06-7	N,N'-Diphenyl-guanidine	211	MF	2.9		2.6	-1.91		8(e)-13109
CBI	CBI	212	2.4	2.9		0.25	-2.93		P93-____
CBI	CBI	487	3.4	3		28	-1.24		P02-____
CBI	CBI	200	1.9	3.1		2.9	-1.84		P89-____
49745-95-1	Dobutamine hydrochloride	338	2.5	3.5		0.76	-2.65		8(e)-15346
CBI	CBI	278	4.3	3.8	3.17	0.3	-2.97	Unknown	P00-____
CBI	CBI	228	4.9	4.4		0.06	-3.58		P94-____
CBI	CBI	253	4.9	4.4		0.03	-3.93		P85-____
CBI	CBI	341	3.7	4.4	4.4	0.14	-3.39	Unknown	P03-____
CBI	CBI	300	3.8	4.5		0.02	-4.18		P91-____
CBI	CBI	411	6.8	4.7		0.1	-3.61		P02-____
CBI	CBI	639	3.5	5.2		37	-1.24		P96-____
CBI	CBI	940	2.4	5.2		0.33	-3.45		P05-____
112-18-5	Dimethyl dodecyl amine	213	5.5	5.4		0.007	-4.48		SIDS, 1998
CBI	CBI	316	5.7	5.7	4.9	0.038	-3.92	PMN est.	P91-____
CBI	CBI	323	5.6	5.7		0.01	-4.51		P95-____
SAR Data Not Included in Regression Equation:									
CBI	CBI	377	8.4	7.1		*0.091	*-3.62		P00-____
CBI	CBI	439	5.7	7.5		*0.052	*-3.93		P97-____
CBI	CBI	469	7.9	7.5		*0.006	*-4.89		P90-____
CBI	CBI	614	11	7.5		*0.23	*-3.43		P90-____
CBI	CBI	328	7.1	8.1		*0.13	*-3.4		P86-____
CBI	CBI	582	`	8.2		*			P90-____
CBI	CBI	423	8.7	9.1		*0.035	*-4.08		P00-____
CBI	CBI	676	11	13		*1.7	*-2.6		P91-____
CBI	CBI	737	MF	14		*			P89-____
CBI	CBI	1066	16	14		*0.66	*-3.21		P98-____
Data Not Included in SAR:									
CBI	CBI	189	0.52	0.86		18	-1.02		P05-____
CBI	CBI	737	MF	14		>10	>-1.87		CBI
	* indicates no effects 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. [A summary of studies also listed in the 'Reference' section.]

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.

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

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

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. [A summary of studies also listed in the ‘Reference’ section.]

FISH ChV

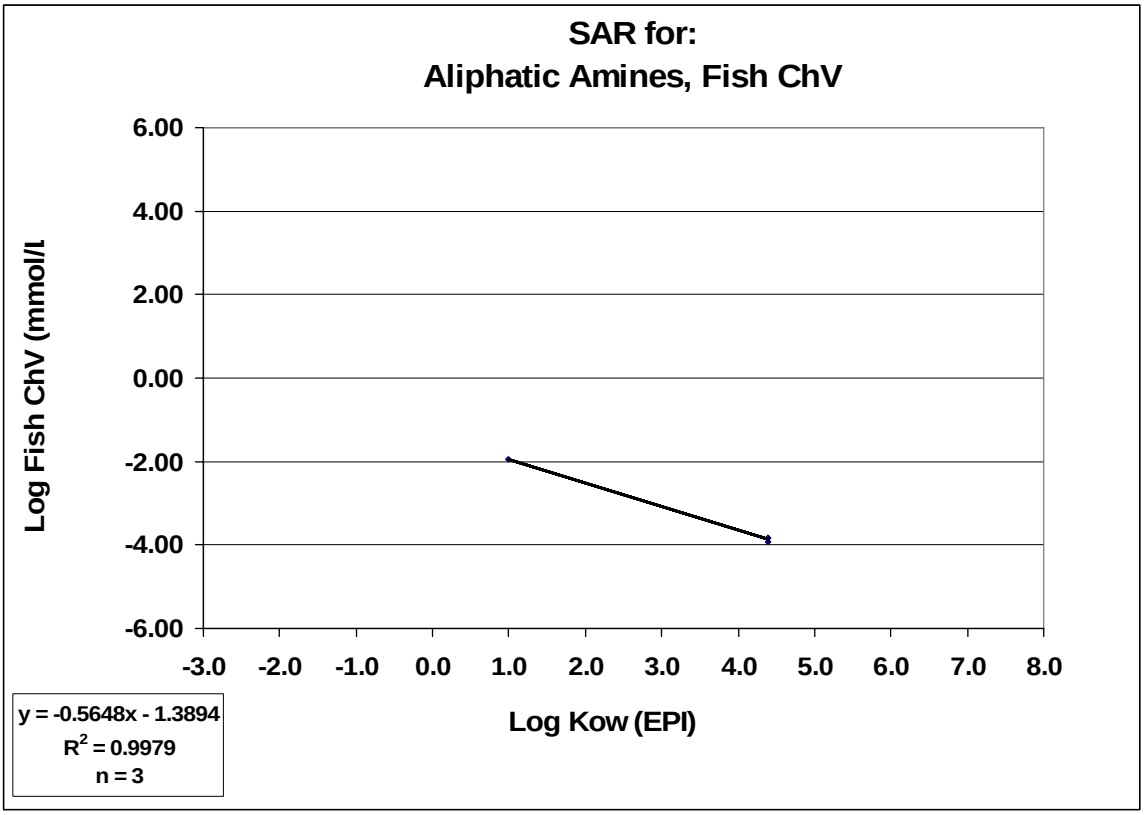
ESTIMATED TOXICITY:
The fish chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.5648 (log Kow) - 1.3894

The ChV is in millimoles per liter (mM/L); N = 3; and the Coefficient of Determination (R^2) = 0.9979. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for aliphatic amines.

LIMITATIONS:
If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish ChV (mg/L)	Log Fish ChV (mmol/L)	Reference (Meas. Kow)	Reference (Fish ChV)
54-11-5	(s)-3-Methyl-2-pyrrolidinyl pyridine nicotine	162	1.3	1	1.17	1.8	-1.95	Hansch & Leo, 1985	Passino-Reader, 1995
CBI	CBI	253	4.9	4.4		0.03	-3.93		P85-___(Analogue),P96-___
36362-09-1	2-(Decyl thiol) ethyl amine hydrochloride	253	4.9	4.4		0.038	-3.82		8(e)-3305
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
						* indicates no effects at saturation			

REFERENCES:

Passino-Reader DR, Berlin WH, and Hickey JP. 1995. Chronic bioassays of Rainbow trout fry with compounds representative of contaminants in Great Lakes fish. J. Great Lakes Res. 21:373-383.

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

DAPHNID ChV

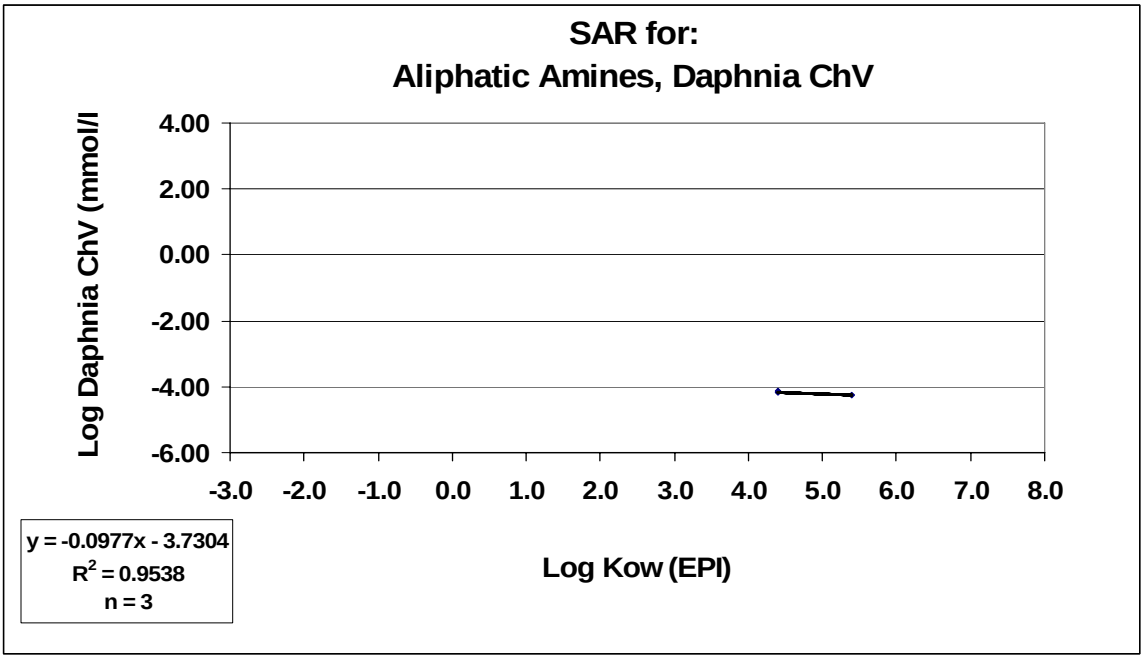
ESTIMATED TOXICITY:
The daphnid chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.0977 (log Kow) - 3.7304

The ChV is in millimoles per liter (mM/L); N =3; and the Coefficient of Determination (R^2) = 0.9538. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for aliphatic amines.

LIMITATIONS:
If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Daphnia ChV (mg/L)	Log Daphnia ChV (mmol/L)	Reference (Meas. Kow)	Reference (Daphnia ChV)
CBI	CBI	326	MF	5.4		0.018	-4.26		8(e)-___
CBI	CBI	253	4.9	4.4		0.018	-4.15		P85-___
CBI	CBI	253	4.9	4.4		0.017	-4.17		P96-___
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
36362-09-1	2-(Decyl thiol) ethyl amine hydrochloride	253	4.9	4.4		0.013-0.0248	-4.29 to -4.01		8(e)-3307
						* indicates no effects at saturation			

REFERENCES:

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. [A summary of studies also listed in the 'Reference' section.]

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the "Toxic Substance Control Act" (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

GREEN ALGAE ChV

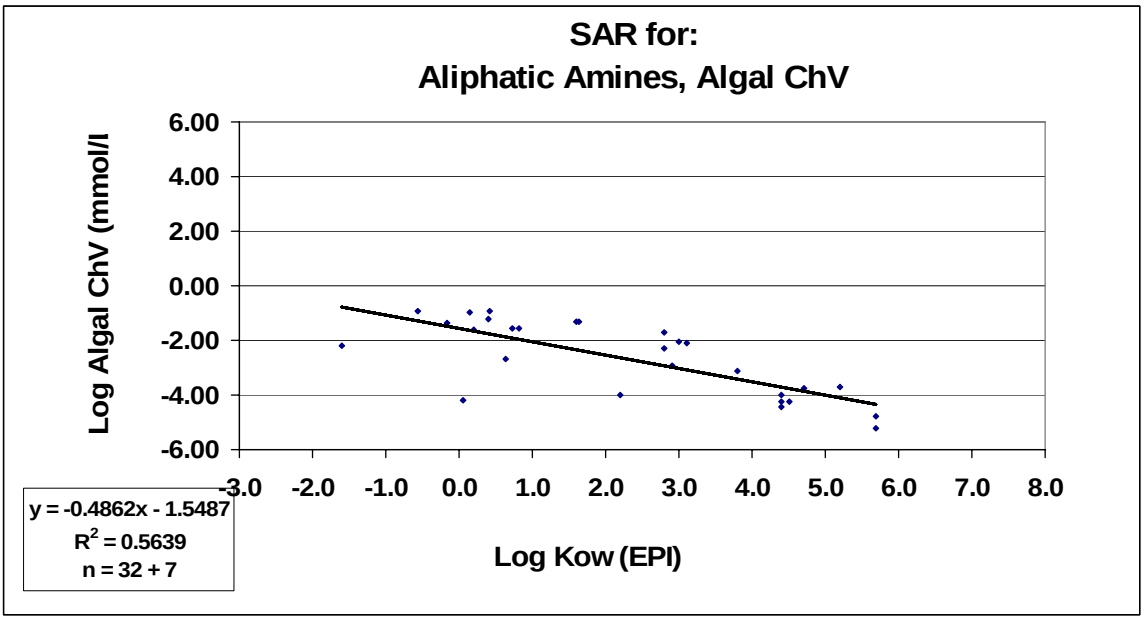
ESTIMATED TOXICITY:
The green algae chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.4862 (log Kow) - 1.5487

The ChV is in millimoles per liter (mM/L); N = 32 + 7; and the Coefficient of Determination (R^2) = 0.5639. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 7.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for aliphatic amines with log Kow values less than or equal to 7.0 and molecular weights less than 1000.

LIMITATIONS:
If the log Kow value is greater than 7.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Algal ChV (mg/L)	Log Algal ChV (mmol/L)	Reference (Meas. Kow)	Reference (Algal ChV)
CBI	CBI	132	-0.7	-1.5		16.7	-0.90		P94-___
CBI	CBI	329		-0.85		1.6	-2.31		P94-___
CBI	CBI	89	-0.6	-0.74		140	0.20		P91-___
CBI	CBI	249	-0.25	-0.6		1.8	-2.14		P95-___
110-91-8	Morpholine	87	-0.72	-0.56	-0.86	10	-0.94	Hansch & Leo, 1985	Calamari et al., 1980
124-40-3	Dimethylamine	45	-0.52	-0.17	-0.38	2	-1.35	Hansch & Leo, 1985	Calamari et al., 1980
CBI	CBI	163	0.48	0.05		0.01	-4.21		P03-___
CBI	CBI	135	0.2	0.15		15	-0.95		P91-___
CBI	CBI	205	MF	0.2		5	-1.61		P96-___
CBI	CBI	143	1.1	0.4		9	-1.20		P91-___
CBI	CBI	238	0	0.41		28	-0.93		P91-___
CBI	CBI	185		0.64		0.4	-2.67		8(e)-___
75-64-9	tert-Butylamine	73	0.57	0.72	0.4	2	-1.56	Hansch & Leo, 1985	Calamari et al., 1980
109-89-7	Diethylamine	73	0.54	0.81	0.58	2	-1.56	Hansch & Leo, 1985	Calamari et al., 1980
108-91-8	Cyclohexylamine	99	1.4	1.6	1.49	5	-1.30	Hansch & Leo, 1985	Calamari et al., 1980
108-18-9	Diisopropylamine	101	1.1	1.64	1.4	5	-1.31	Hansch et al., 1995	Calamari et al., 1980
CBI	CBI	438	MF	2.2		0.042	-4.02		P87-___
111-92-2	Dibutylamine	129	2.7	2.8	2.83	2.5	-1.71	Hansch & Leo, 1985	Calamari et al., 1980
111-86-4	Octylamine	129	3	2.8	2.9	0.65	-2.30	Sangster, 1993	Calamari et al., 1980
CBI	CBI	212	2.4	2.9		0.24	-2.95		P93-___
CBI	CBI	487	3.4	3		4.5	-2.03		P02-___
CBI	CBI	200	1.93	3.1		1.6	-2.10		P89-___
CBI	CBI	278	4.3	3.8	3.17	0.22	-3.10	Unknown	P00-___
CBI	CBI	228	4.9	4.4		0.013	-4.24		P94-___
CBI	CBI	253	4.9	4.4		0.009	-4.45		P85-___
CBI	CBI	341	3.7	4.4	4.4	0.035	-3.99	HPLC	P03-___
CBI	CBI	300	3.8	4.5		0.017	-4.25		P91-___
CBI	CBI	411	6.8	4.7		0.07	-3.77		P02-___
CBI	CBI	639	3.5	-1.6		4	-2.20		P96-___
CBI	CBI	940	2.4	5.2		0.18	-3.72		P05-___
CBI	CBI	316	5.7	5.7	4.9	0.005	-4.80	PMN est.	P91-___
CBI	CBI	323	5.6	5.7		0.002	-5.21		P95-___
SAR Data Not Included in Regression Equation:									
CBI	CBI	377	8.4	7.1		*0.054	*-3.84		P00-___
CBI	CBI	439	5.7	7.5		*0.01	*-4.64		P97-___
CBI	CBI	469	7.9	7.5		*0.002	*-5.37		P90-___
CBI	CBI	614	11	7.5		*0.1	*-3.79		P90-___
CBI	CBI	423	8.7	9.1		*0.009	*-4.67		P00-___
CBI	CBI	676	11	13		*0.44	*-3.19		P91-___
CBI	CBI	1066	16	14		*0.47	*-3.36		P98-___
Data Not Included in SAR:									
CBI	CBI	189	0.52	0.86		4.4	-1.63		P05-___
	* indicates no effects 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. [A summary of studies also listed in the 'Reference' section.]

U.S. 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.

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the "Toxic Substance Control Act" (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

FISH (SW) 96-h LC50 (Mortality)

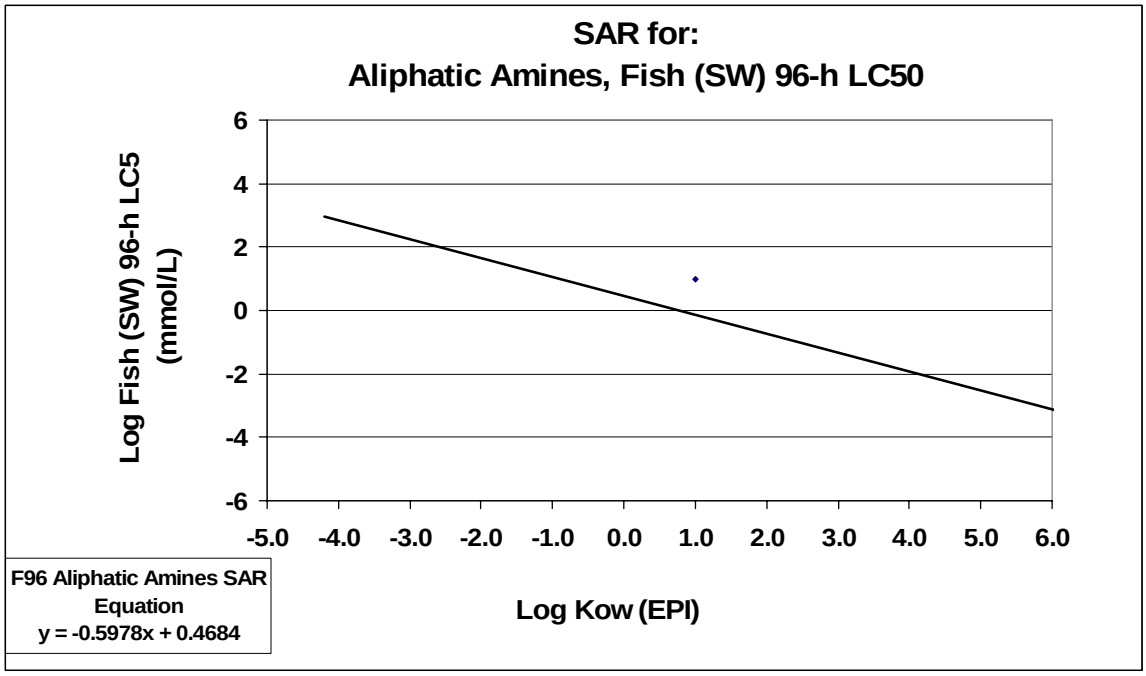
ESTIMATED TOXICITY:
No adequate data were available for the aliphatic amines SAR fish (SW) acute endpoint. Predictions for this endpoint are based on the aliphatic amines SAR for the freshwater fish 96-h LC50 endpoint. The SAR equation used to estimate toxicity is:

Log 96-h LC50 (mmol/L) = -0.5978 (log Kow) + 0.4684

The EC50 is in millimoles per liter (mM/L). To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 6.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for aliphatic amines.

LIMITATIONS:
If the log Kow value is greater than 6.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish (SW) 96-h LC50 (mg/L)	Log Fish (SW) 96-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Fish (SW) 96-h LC50)
CBI	CBI	455	3.4	2		17	-1.43		P93-___
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
						* indicates no effects at saturation			

REFERENCES:

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

MYSID SHRIMP (SW) 96-h LC50 (Mortality)

ESTIMATED TOXICITY:

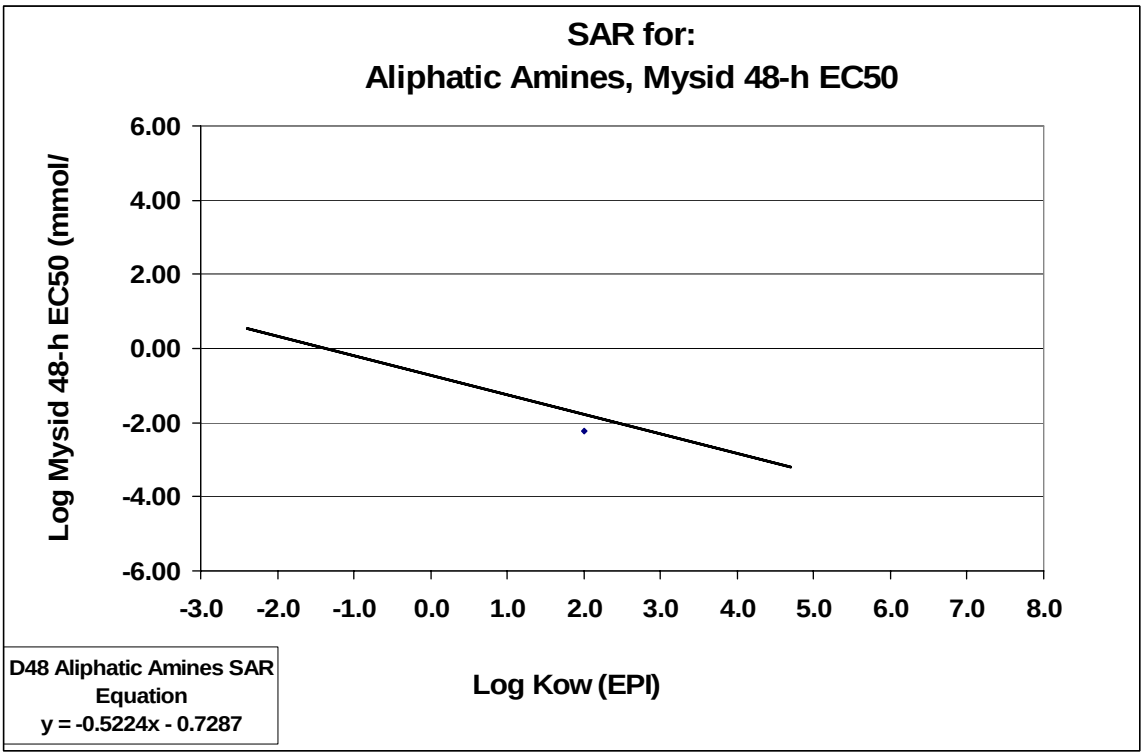
No adequate data were available for the aliphatic amines SAR mysid (SW) EC50 endpoint. Predictions for this endpoint are based on the aliphatic amines SAR for the freshwater daphnid 48-h endpoint. The SAR equation used to estimate toxicity is:

Log 96-h EC50 (mmol/L) = -0.5224 (log Kow) - 0.7287

The EC50 is in millimoles per liter (mM/L). To convert the EC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 6.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for aliphatic amines.

LIMITATIONS:
If the log Kow value is greater than 6, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Mysid 48-h LC50 (mg/L)	Log Mysid 48-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Mysid 48-h LC50)
CBI	CBI	455	3.4	2		2.6	-2.24		P93-___
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
						* indicates no effects at saturation			

REFERENCES:

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

GREEN ALGAE (SW) 96-h EC50

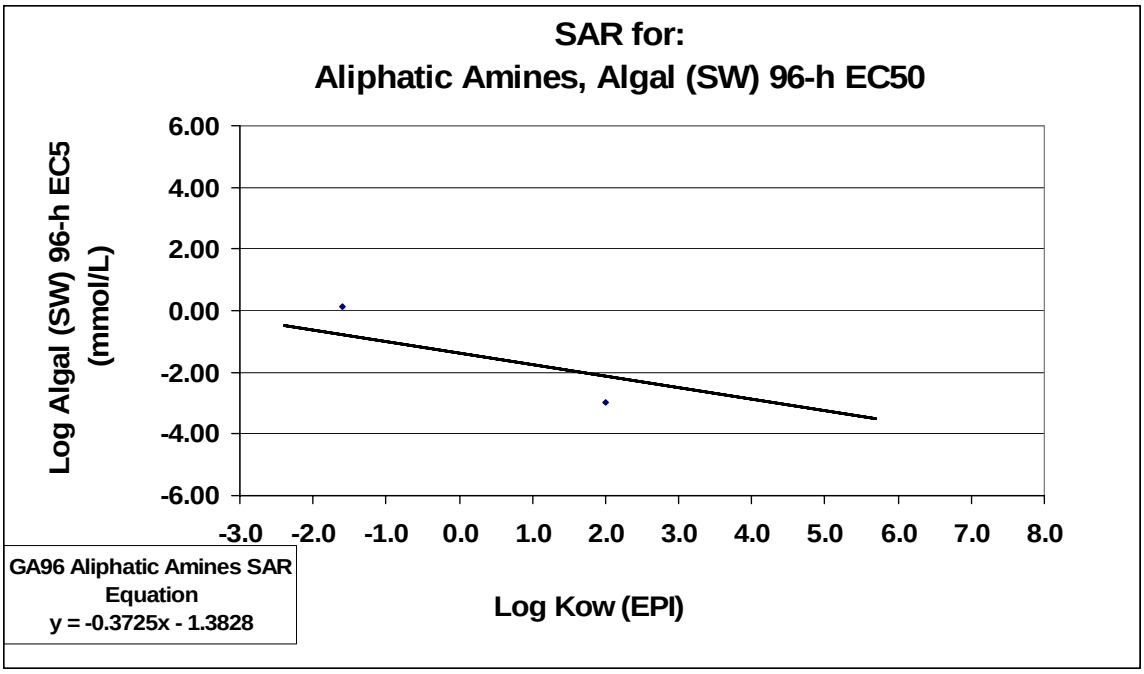
ESTIMATED TOXICITY:
No adequate data were available for the aliphatic amines SAR green algae (SW) EC50 endpoint. Predictions for this endpoint are based on the aliphatic amines SAR for the freshwater green algae 96-h endpoint. The SAR equation used to estimate toxicity is:

Log 96-h EC50 (mmol/L) = -0.3725 (log Kow) - 1.3828

The EC50 is in millimoles per liter (mM/L). To convert the EC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 7.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for aliphatic amines.

LIMITATIONS:
If the log Kow value is greater than 7.0, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Algal (SW) 96-h EC50 (mg/L)	Log Algal (SW) 96-h EC50 (mmol/L)	Reference (Meas. Kow)	Reference (Algal (SW) 96-h EC50)
CBI	CBI	455	3.4	2		0.5	-2.96		P93-___
141-43-5	Monoethanolamine	61	-1.3	-1.6	-1.31	80	0.12	Hansch C. et al., 1995	Roseth S. et al., 1996
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
						* indicates no effects at saturation			

REFERENCES:

Roseth S, Edvardsson T, Stenersen J. 1996. Comparison of acute toxicity of process chemicals used in the oil refinery. Toxicol. Chem. 15:1211.

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

FISH (SW) ChV

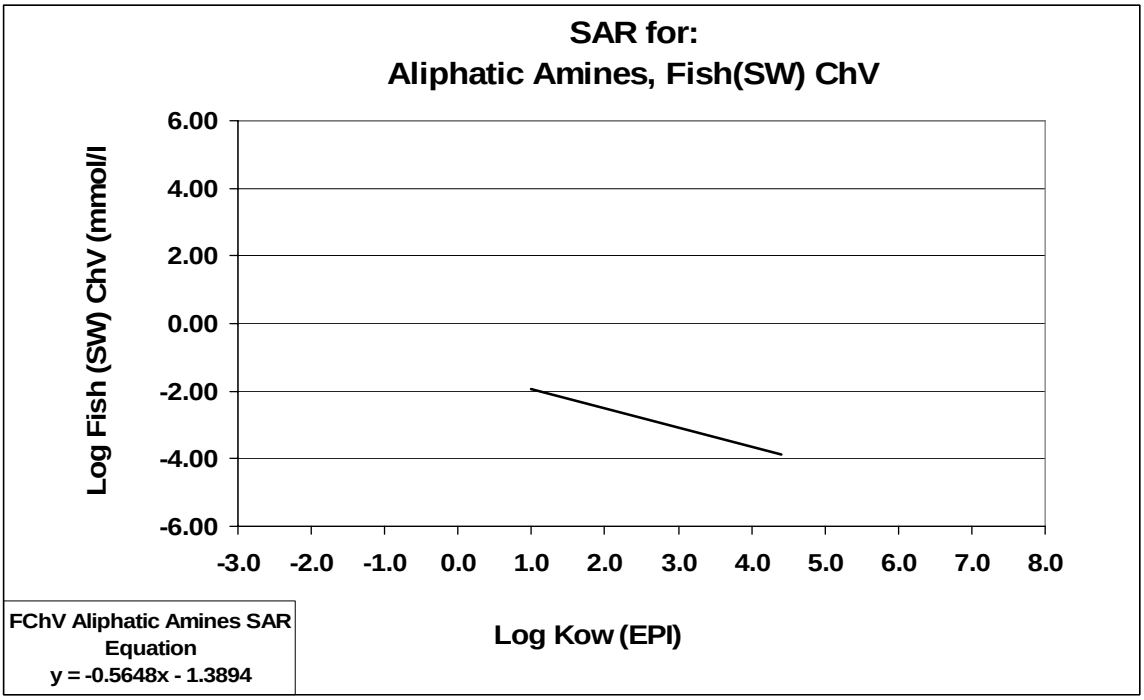
ESTIMATED TOXICITY:
No adequate data were available for the aliphatic amines SAR fish (SW) chronic value (ChV) endpoint. Predictions for this endpoint are based on the aliphatic amines SAR for the freshwater fish ChV endpoint. The SAR equation used to estimate toxicity is:

Log 96-h ChV (mmol/L) = -0.5648 (log Kow) – 1.3894

The Chv is in millimoles per liter (mM/L). To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for aliphatic amines.

LIMITATIONS:
If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

REFERENCES:

MYSID SHRIMP (SW) ChV

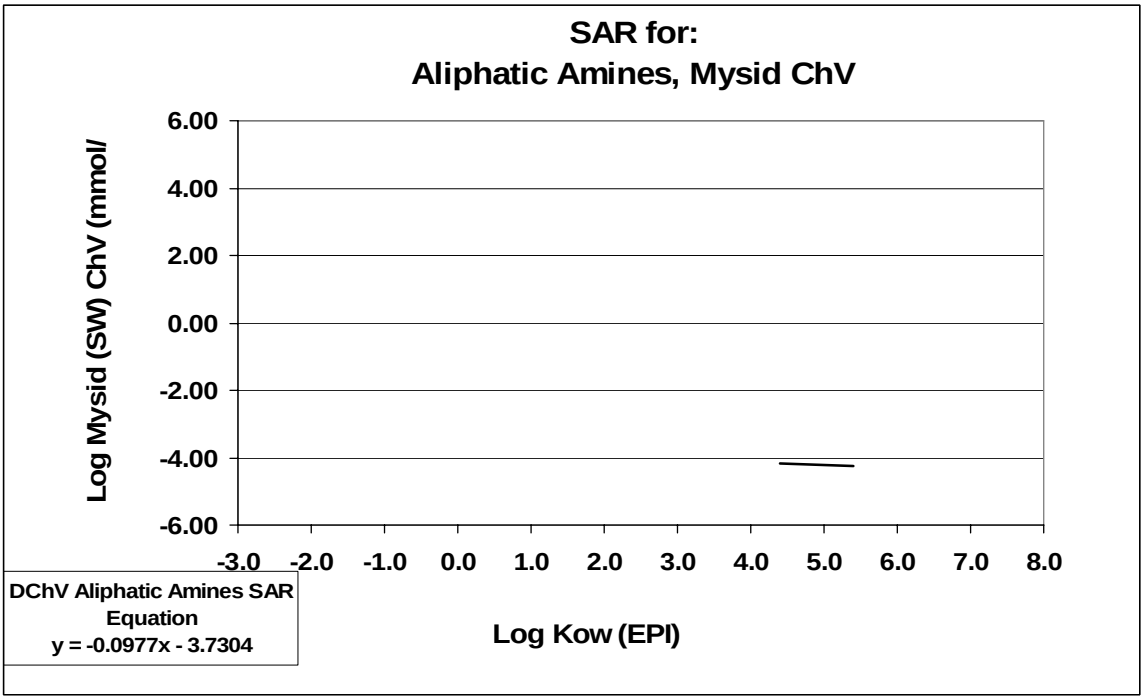
ESTIMATED TOXICITY:
No adequate data were available for the aliphatic amines SAR mysid (SW) chronic value (ChV) endpoint. Predictions for this endpoint are based on the aliphatic amines SAR for the freshwater daphnid ChV endpoint. The SAR equation used to estimate toxicity is:

Log 96-h ChV (mmol/L) = -0.0977 (log Kow) – 3.7304

The ChV is in millimoles per liter (mM/L). To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for aliphatic amines.

LIMITATIONS:
If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

REFERENCES:

GREEN ALGAE (SW) ChV

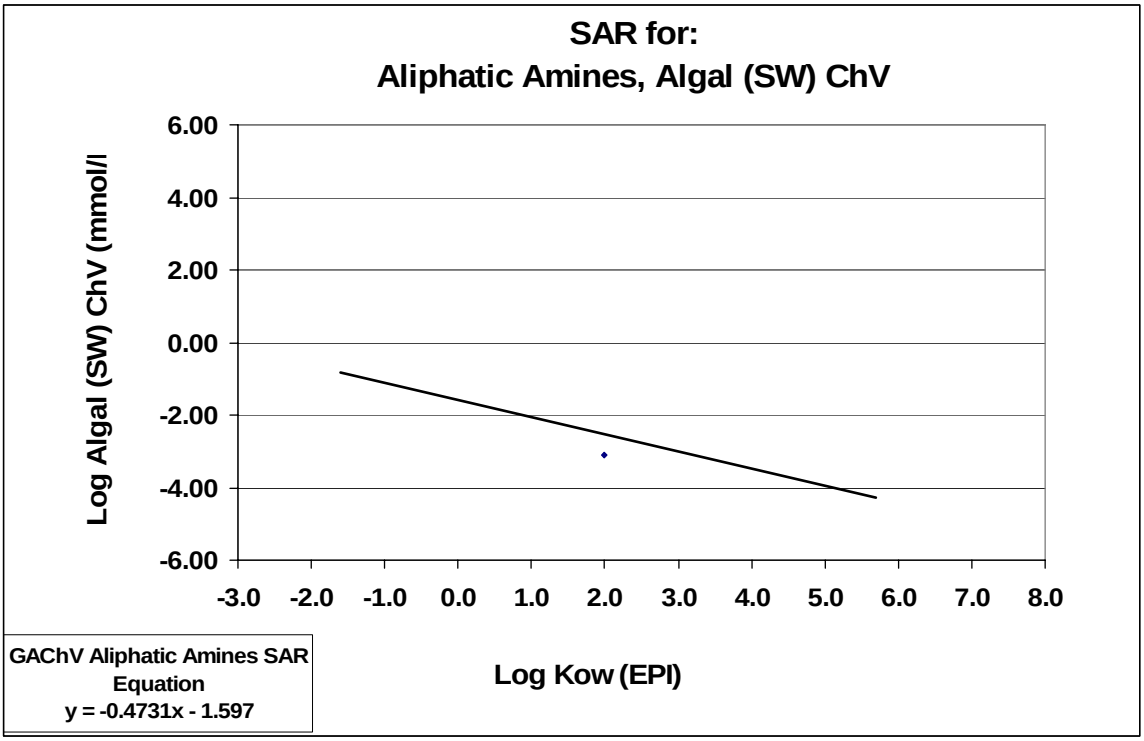
No adequate data were available for the aliphatic amines SAR green algae (SW) chronic value (ChV) endpoint. Predictions for this endpoint are based on the aliphatic amines SAR for the freshwater green algae ChV endpoint. The SAR equation used to estimate toxicity is:

Log 96-h ChV (mmol/L) = -0.4731 (log Kow) – 1.597

The ChV is in millimoles per liter (mM/L). To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 7.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for aliphatic amines.

LIMITATIONS:
If the log Kow value is greater than 7, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	CLogP Kow	SRC log Kow	Meas. log Kow	Algal (SW) ChV (mg/L)	Log Algal (SW) ChV (mmol/L)	Reference (Meas. Kow)	Reference (Algal (SW) ChV)
CBI	CBI	455	3.4	2		0.37	-3.09		P93-___
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
						* indicates no effects at saturation			

REFERENCES:

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data

FISH 96-h LC50 (Mortality)

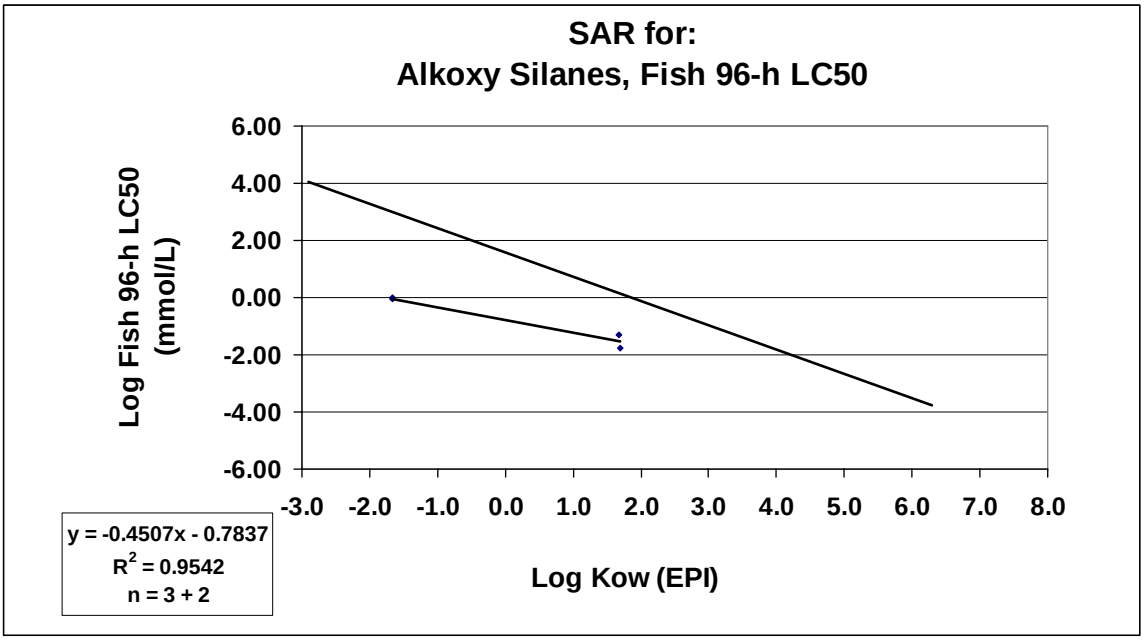
ESTIMATED TOXICITY:
The fish 96-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h LC50 (mmol/L) = -0.4507 (log Kow) - 0.7837

The LC50 is in millimoles per liter (mM/L); N = 3 + 2; and the Coefficient of Determination (R^2) = 0.9542. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 5.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for alkoxy silanes.

LIMITATIONS:
If the log Kow value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish 96-h LC50 (mg/L)	Log Fish 96-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Fish 96-h LC50)
CBI	CBI	222	MF	-1.7		213	-0.02		P90-___
CBI	CBI	222	MF	-1.7		200	-0.05		P90-___
CBI	CBI	263	MF	1.7		13	-1.31		P91-___
CBI	CBI	328	MF	1.7		5.4	-1.78		P00-___
SAR Data Not Included in Regression Equation:									
CBI	CBI	347	MF	6.7		*			P93-___
CBI	CBI	1067	MF	7.3		*			P88-___
Data Not Included in SAR:									
CBI	CBI	307	MF	-0.12		>100	>-0.49		P81-___
CBI	CBI	278	MF	0.56		>74	>-0.57		CBI
CBI	CBI	189	0.52	0.86		>100	>-0.39		P-05-___
CBI	CBI	206	MF	1		>83	>-0.39		P82-___
CBI	CBI	197	MF	2.2		>100	>-0.29		P81-___
						* indicates no effects at saturation			

REFERENCES:

US EPA Memo, 2003

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

DAPHNID 48-h LC50

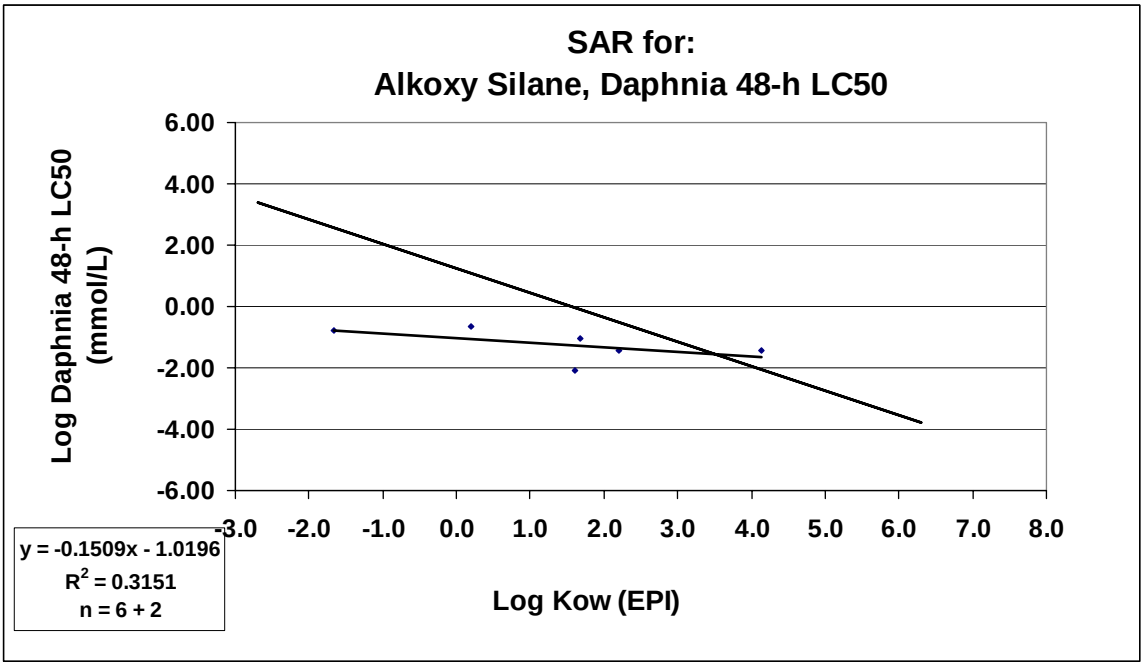
ESTIMATED TOXICITY:
The daphnid 48-h LC50 values used to develop this SAR were measured, and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 48-h LC50 (mmol/L) = -0.1509 (log Kow) – 1.0196

The LC50 is in millimoles per liter (mM/L); N = 6 + 2; and the Coefficient of Determination (R^2) = 0.3151. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 5.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for alkoxy silanes.

LIMITATIONS:
If the log Kow value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Daphnia 48-h LC50 (mg/L)	Log Daphnia 48-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Daphnia 48-h LC50)
CBI	CBI	222	MF	-1.7		37	-0.78		P90-____
CBI	CBI	221	MF	0.2		51	-0.64		P96-____
78-62-6	Dimethyldiethoxysilane	148	MF	1.6	0.61	1.25	-2.07	Hansch C, et al, 1995	May Passino DR, Smith SB, 1987
CBI	CBI	263	MF	1.7		25	-1.02		P91-_____
CBI	CBI	197	MF	2.2		7.6	-1.41		P81-____
CBI	CBI	228	MF	4.1		8.6	-1.42		P91-____/ P91-____
SAR Data Not Included in Regression Equation:									
CBI	CBI	347	MF	6.7		*			P93-____
CBI	CBI	1067	MF	7.3		*			P88-____
Data Not Included in SAR:									
CBI	CBI	278	MF	0.6		>74	>-0.57		CBI
CBI	CBI	189	0.52	0.86		270	0.15		P05-____
CBI	CBI	328	MF	1.7		>2.0	>-2.21		CBI
CBI	CBI	206	MF	1		>83	>-0.39		P82-____
CBI	CBI	307	MF	-0.12		>100	>-0.49		P81-____
						* indicates no effects at saturation			

REFERENCES:

May Passino DR, Smith SB. 1987. Acute bioassays and hazard evaluation of representative contaminants detected in Great Lakes fish. Env. Toxicol. Chem. 6:901-907.

US EPA Memo, 2003

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

GREEN ALGAE 96-h EC50

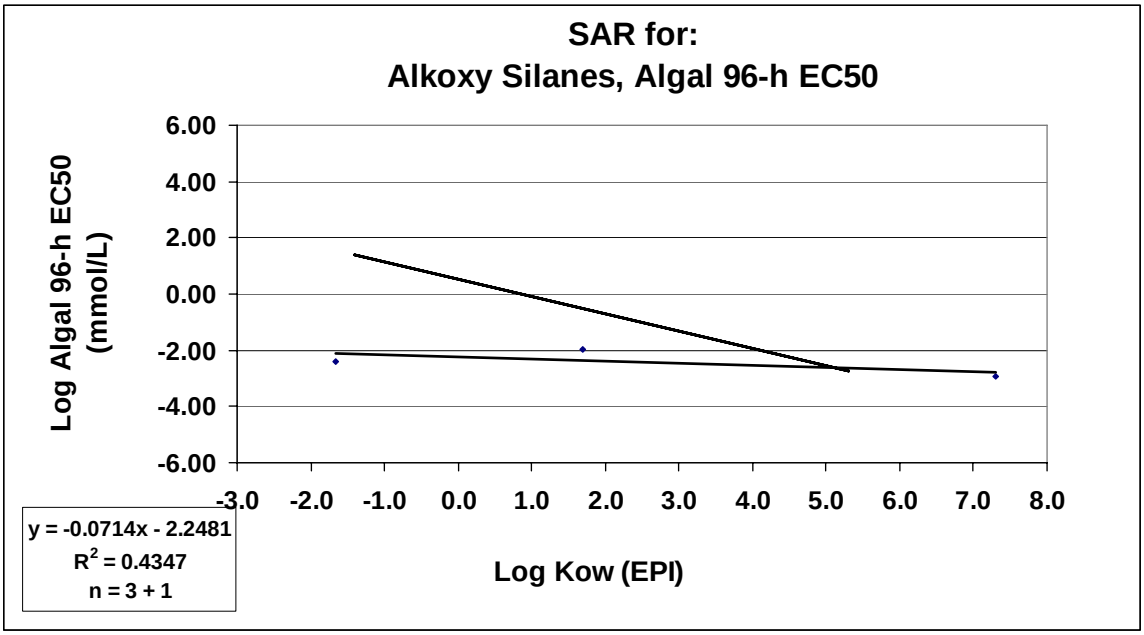
ESTIMATED TOXICITY:
The green algae 96-h EC50 values used to develop this SAR were measured, and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h EC50 (mmol/L) = -0.0714 (log Kow) – 2.2481

The EC50 is in millimoles per liter (mM/L); N = 3 + 1; and the Coefficient of Determination (R^2) = 0.4347. To convert the EC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 6.4
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for alkoxy silanes.

LIMITATIONS:
If the log Kow value is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Algal 96-h EC50 (mg/L)	Log Algal 96-h EC50 (mmol/L)	Reference (Meas. Kow)	Reference (Algal 96-h EC50)
CBI	CBI	222	MF	-1.7		0.9	-2.39		P90-___
CBI	CBI	328	MF	1.7		3.7	-1.95		P00-___
CBI	CBI	1440	MF	7.3		1.7	-2.93		P88-___
SAR Data Not Included in Regression Equation:									
CBI	CBI	347	MF	6.7		*			P93-___
Data Not Included in SAR:									
CBI	CBI	278	MF	0.6		>64	>-0.64		CBI
CBI	CBI	189	0.52	0.86		18	-1.02		P05-___
	* indicates no effects at saturation								

REFERENCES:

US EPA Memo, 2003

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

FISH ChV

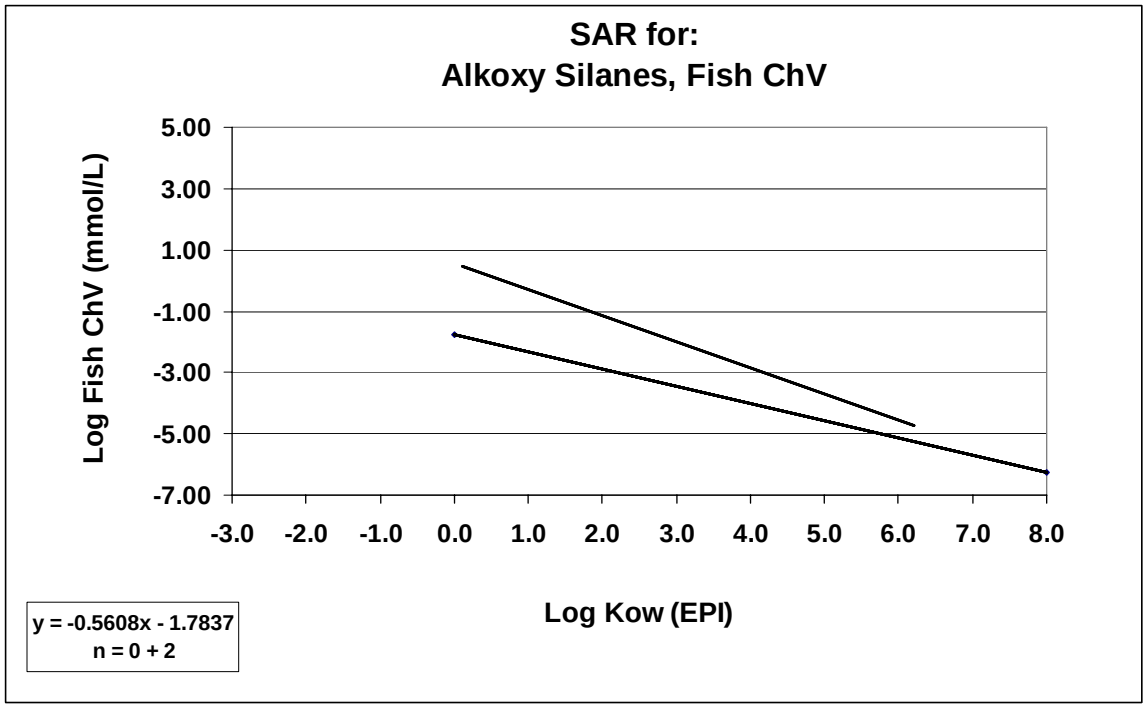
ESTIMATED TOXICITY:
No adequate data were available for the alkoxy silanes fish chronic value (ChV) SAR. Predictions for this endpoint were estimated using the acute-to-chronic ratio, and were based on the acute fish SAR for alkoxysilanes. The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.5608 (log Kow) – 1.7837

The ChV is in millimoles per liter (mM/L). To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for alkoxysilanes.

LIMITATIONS:
If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish ChV (mg/L)	Log Fish ChV (mmol/L)	Reference (Meas. Kow)	Reference (Fish ChV)
	1/10 F96		0	0			-1.78		1/10 F96 Alkoxy Silanes SAR
	Kow Limit		8	8			-6.27	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
						* indicates no effects at saturation			

REFERENCES:

DAPHNID ChV

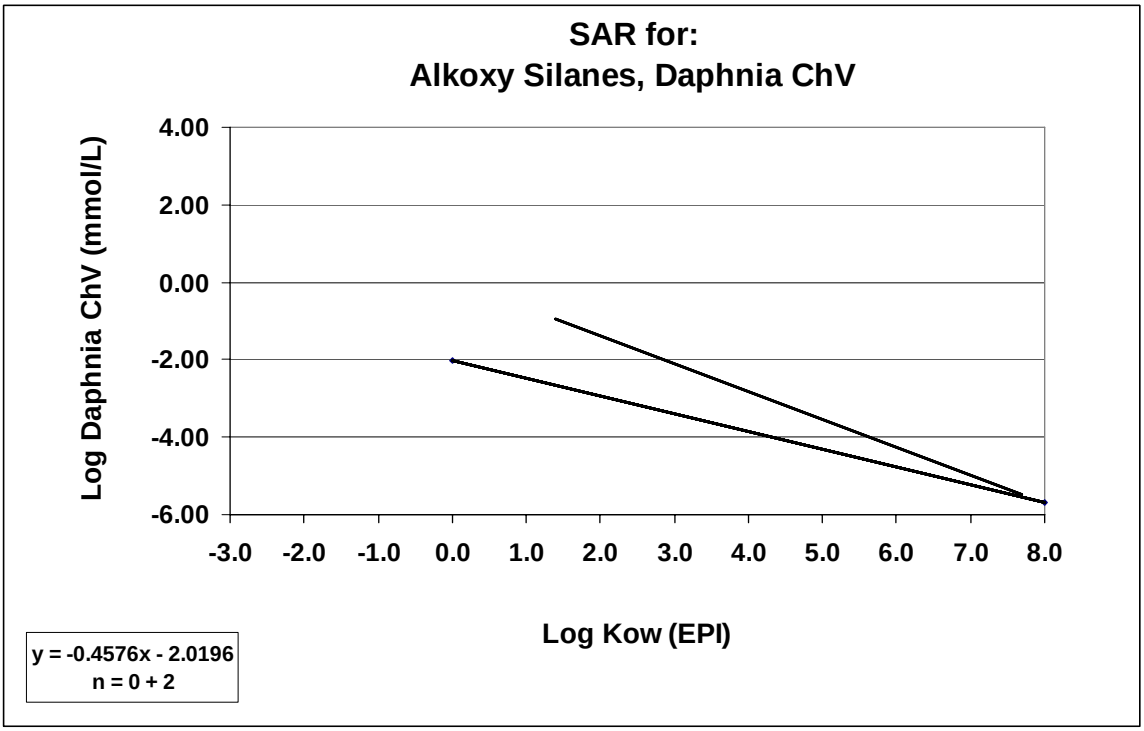
ESTIMATED TOXICITY:
No adequate data were available for the Alkoxysilanes daphnid chronic value SAR endpoint. Predictions for this endpoint were estimated using the acute-to-chronic ratio, and were based on the acute daphnid SAR for alkoxysilanes. The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.4576 (log Kow) – 2.0196

The ChV is in millimoles per liter (mM/L). To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for alkoxysilanes.

LIMITATIONS:
If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Daphnia ChV (mg/L)	Log Daphnia ChV (mmol/L)	Reference (Meas. Kow)	Reference (Daphnia ChV)
	1/10 D48		0	0			-2.02		1/10 D48 Alkoxy Silanes SAR
	Kow Limit		8	8			-5.68	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
CBI	CBI	222	MF	-1.7		>1.0	-2.35		P90-___
						* indicates no effects at saturation			

REFERENCES:

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

GREEN ALGAE ChV

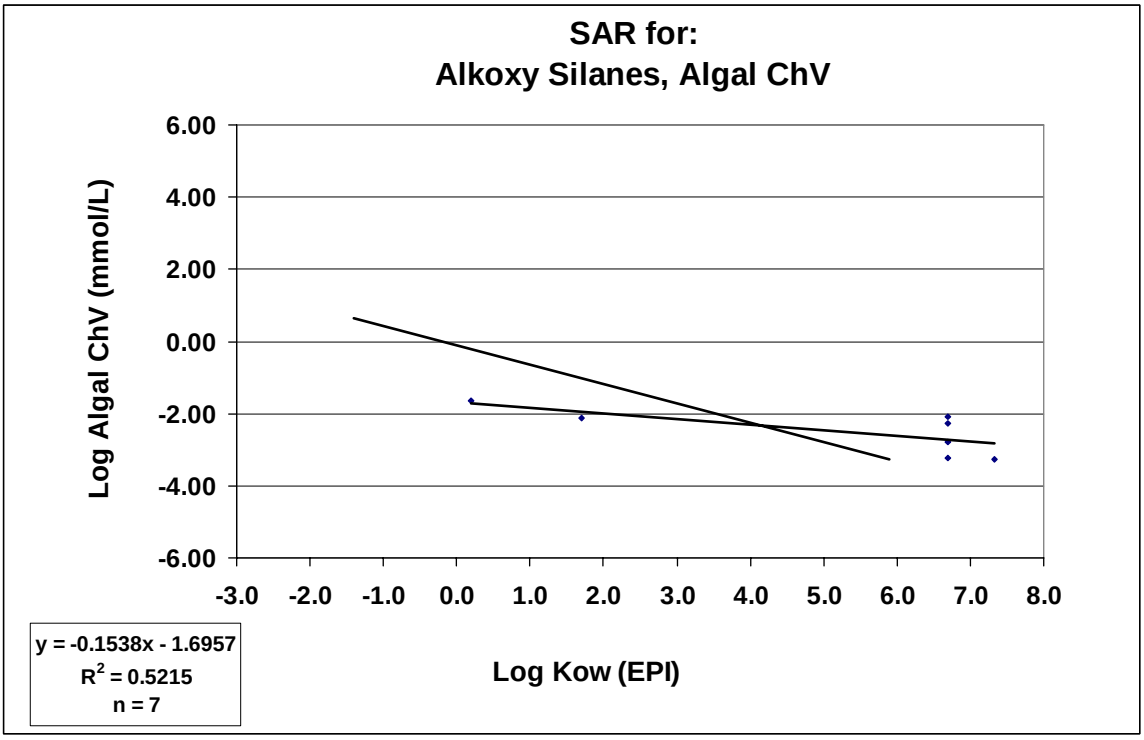
ESTIMATED TOXICITY:
The green algae chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.1538 (log Kow) – 1.6957

The ChV is in millimoles per liter (mM/L); N = 7; and the Coefficient of Determination (R^2) = 0.5215. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

GRAPH:



APPLICATION:
This SAR may be used to estimate toxicity for alkoxy silanes.

LIMITATIONS:
If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Algal ChV (mg/L)	Log Algal ChV (mmol/L)	Reference (Meas. Kow)	Reference (Algal ChV)
CBI	CBI	221	MF	0.2		5	-1.65		P96-___
CBI	CBI	328	MF	1.7		2.5	-2.12		P00-___
CBI	CBI	347	MF	6.7		0.2	-3.24		P93-___
CBI	CBI	347	MF	6.7		0.57	-2.78		P93-___
CBI	CBI	347	MF	6.7		1.8	-2.29		P93-___
CBI	CBI	347	MF	6.7		2.9	-2.08		P93-___
CBI	CBI	1440	MF	7.3		0.8	-3.26		P88-___
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
CBI	CBI	222	MF	-1.7		<1.0	<-2.35		P90-___
CBI	CBI	180	MF	-1.7		0.04	-3.65		P92-___
CBI	CBI	278	MF	0.56		>64	>-0.64		CBI
CBI	CBI	189	0.52	0.86		4.4	-1.63		P05-___
						* indicates no effects at saturation			

REFERENCES:

U.S. EPA Memo, 2003

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

FISH 96-h LC50 (Mortality)

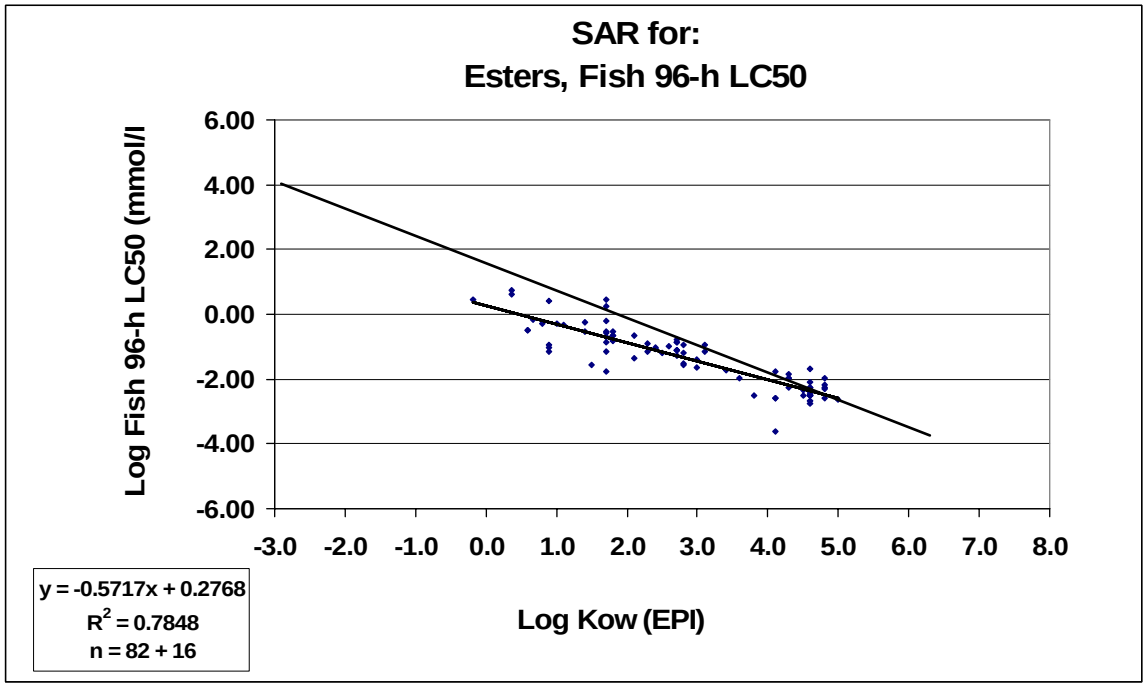
ESTIMATED TOXICITY:
The fish 96-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h LC50 (mmol/L) = -0.5717 (log Kow) + 0.2768

The LC50 is in millimoles per liter (mM/L); N = 81 + 16; and the Coefficient of Determination (R^2) = 0.786. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the ester.

Maximum K_{ow}: 5.0
Maximum MW: 1000

GRAPH:



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 Kow value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish 96-h LC50 (mg/L)	Log Fish 96-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Fish 96-h LC50)
97-64-3	Ethyl lactate	118	0.31	-0.18		320	0.43		Bowmer et al.
79-20-9	Methyl acetate	74	0.14	0.37	0.18	320	0.64	Hansch & Leo, 1985	DUL
79-20-9	Methyl acetate	74	0.14	0.37	0.18	399	0.73	Hansch & Leo, 1985	DUL
111-15-9	2-Ethoxyethyl acetate	132	0.68	0.59		41	-0.51		Bailey et al., 1985
111-15-9	2-Ethoxyethyl acetate	132	0.68	0.59		42.1	-0.50		DUL
CBI	CBI	158	0.27	0.67	0.94	110	-0.16	None given	P00-____
138-22-7	Butyl lactate	146	1.4	0.80		75	-0.29		Bowmer et al.
141-78-6	Ethyl acetate	88	0.70	0.90	0.7	230	0.42	Hansch & Leo, 1985	Veith et al (1984)/ DUL
105-53-3	Diethyl malonate	160	1.1	0.90	0.96	11.8	-1.13	Pomona, 1987	DUL
105-53-3	Diethyl malonate	160	1.1	0.90	0.96	15.4	-1.02	Pomona, 1987	DUL
105-53-3	Diethyl malonate	160	1.1	0.90	0.96	17.4	-0.96	Pomona, 1987	DUL
CBI	CBI	146	1.0	1.0		77	-0.28		P94-_____
CBI	CBI	146	1.2	1.1		70	-0.32		P97-____/Analog
109-60-4	Propyl acetate	102	1.2	1.4	1.24	60	-0.23	Hansch & Leo, 1985	DUL
1129-35-7	Methyl 4-cyanobenzoate	161	1.5	1.4		46.8	-0.54		DUL
5292-45-5	Dimethyl-2-nitroterephthalate	239	1.7	1.5		6.52	-1.56		DUL/Veith et al. (1984)
540-88-5	tert-Butyl acetate	116	1.4	1.7	1.76	327	0.45	Hansch et al., 1995	DUL
CBI/CBI	CBI/CBI	144	0.90	1.7		244	0.23		P93-____/ P93-____
619-50-1	Methyl-p-nitrobenzoate	181	1.9	1.7	1.89	23.8	-0.88	Sotomatsu et al., 1993	DUL
120-61-6	Dimethyl terephthalate	194	2.1	1.7	2.25	14.3	-1.13	Hansch & Leo, 1985	SIDS (2000)
131-11-3	Dimethyl phthalate	194	1.5	1.7	1.6	39	-0.70	Ellington & Floyd, 1997	Staples et. al (1997)
131-11-3	Dimethyl phthalate	194	1.5	1.7	1.6	50	-0.59	Ellington & Floyd, 1997	Staples et. al (1997)
131-11-3	Dimethyl phthalate	194	1.5	1.7	1.6	56	-0.54	Ellington & Floyd, 1997	Staples et. al (1997)
131-11-3	Dimethyl phthalate	194	1.5	1.7	1.6	121	-0.21	Ellington & Floyd, 1997	Staples et. al (1997)/DUL
CBI	CBI	328	2.2	1.7		5.4	-1.78		P00-____
94-09-7	Ethyl-p-aminobenzoate	165	1.9	1.8	1.86	35.4	-0.67	Hansch & Leo, 1985	DUL
94-09-7	Ethyl-p-aminobenzoate	165	1.9	1.8	1.86	36	-0.66	Hansch & Leo, 1985	DUL
886-86-2	Ethyl 3-aminobenzoate, methanesulfonic acid salt	261	1.9	1.8		79	-0.52		DUL
123-86-4	Butyl acetate	116	1.7	1.8	1.78	18	-0.81	Hansch et al., 1995	DUL
2150-47-2	Methyl-2,4-dihydoxybenzoate	168	1.9	2.1		38.5	-0.64		Veith et al (1984)
5372-81-6	Dimethyl-2-amino	209	2.1	2.1		8.94	-1.37		DUL/Veith et al. (1984)
93-89-0	Ethyl benzoate	150	2.6	2.3	2.64	10.8	-1.14	Hansch & Leo, 1986	DUL
42087-80-9	Methyl-4-chloro-2-nitrobenzoate	216	2.4	2.3		27.7	-0.89		DUL
141-28-6	Diethyl adipate	202	1.8	2.4		16.8	-1.08		DUL
141-28-6	Diethyl adipate	202	1.8	2.4		19.3	-1.02		DUL
1126-46-1	Methyl -p-chlorobenzoate	171	2.8	2.5	2.87	11	-1.19	Pagou & Koutselinis, 1994	DUL
706-14-9	gamma-Decanolactone	170	2.4	2.6	2.72	18	-0.98	Hansch & Leo, 1985	DUL
6283-86-9	2-Ethylhexyl lactate	202	3.4	2.7		32	-0.80		Bowmer et al.
84-66-2	Diethyl phthalate	222	2.5	2.7	2.4	12	-1.27	Ellington & Floyd, 1996	Staples et. al (1997)
84-66-2	Diethyl phthalate	222	2.5	2.7	2.4	16.7	-1.12	Ellington & Floyd, 1996	Staples et. al (1997)
84-66-2	Diethyl phthalate	222	2.5	2.7	2.4	16.8	-1.12	Ellington & Floyd, 1996	Staples et. al (1997)
84-66-2	Diethyl phthalate	222	2.5	2.7	2.4	17	-1.12	Ellington & Floyd, 1996	Staples et. al (1997)
84-66-2	Diethyl phthalate	222	2.5	2.7	2.4	30	-0.87	Ellington & Floyd, 1996	Veith et al. (1984)
84-66-2	Diethyl phthalate	222	2.5	2.7	2.4	31.8	-0.84	Ellington & Floyd, 1996	Staples et. al (1997)/DUL
142-92-7	Hexyl acetate	144	2.9	2.8		4	-1.56		DUL
142-92-7	Hexyl acetate	144	2.8	2.8		4.4	-1.51		Veith et al (1984)
123-66-0	Ethyl hexanoate	144	2.8	2.8		8.94	-1.21		Veith et al (1984)/ DUL
5464-71-1	Octyl lactate	202	3.5	2.8		24	-0.93		Bowmer et al.
607-81-8	Diethyl benzylmalonate	250	2.9	3.0	2.76	5.43	-1.66	Hansch & Leo, 1985	DUL
CBI/CBI	CBI/CBI	487	3.4	3.0		20	-1.39		P05-____/P02-____
118-61-6	Ethyl salicylate	166	3.0	3.1	3	19.6	-0.93	Korenman & Danilov, 1990	Veith et al (1984)
2905-69-3	Methyl-2,5-dichlorobenzoate	205	3.2	3.1		14	-1.17		DUL
141-03-7	Dibutyl succinate	230	3.6	3.4		4.46	-1.71		DUL
000000-00-0	N, N-bis(isopropoxycarbonylmet	307	3.8	3.6		3.2	-1.98		8(e)-12513
CBI	CBI	362	3.9	3.8		1.1	-2.52		8(e)-_____/P-90-_____
84-62-8	Diphenyl phthalate	318	4.5	4.1		0.08	-3.60		DUL
84-62-8	Diphenyl-1-phthalate	318	4.5	4.1		0.8	-2.60		Veith et al. (1984)
744-45-6	Diphenyl isophthalate	318	5.1	4.1		0.8	-2.60		Veith et al. (1984)
1929-73-3	2,4-D butoxy ethanol ester	321	4.7	4.1		5.6	-1.76		Mount and Stephan, 1967
110-40-7	Diethyl sebacate	258	3.9	4.3		2.7	-1.98		DUL
110-40-7	Diethyl sebacate	258	3.9	4.3		2.73	-1.98		DUL
105-99-7	Dibutyl adipate	258	3.9	4.3		3.64	-1.85		DUL
CBI	CBI	285	3.7	4.3	4.2	1.6	-2.25	None given	8(e)-____/P91-____
CBI	CBI	270	4.5	4.5		1.26	-2.33		P00-____
84-69-5	Diisobutyl phthalate	278	4.4	4.5	4.1	0.9	-2.49	Hansch & Leo, 1985	Staples et. al (1997)/DUL
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	0.48	-2.76	Ellington & Floyd, 1996	Staples et. al (1997)
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	0.61	-2.66	Ellington & Floyd, 1996	Staples et. al (1997)
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	0.85	-2.51	Ellington & Floyd, 1996	Staples et. al (1997)/DUL
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	0.9	-2.49	Ellington & Floyd, 1996	Staples et. al (1997)
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	0.92	-2.48	Ellington & Floyd, 1996	Staples et. al (1997)
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	1.1	-2.40	Ellington & Floyd, 1996	DUL/Veith et al. (1984)
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	1.1	-2.40	Ellington & Floyd, 1996	Staples et. al (1997)
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	1.54	-2.26	Ellington & Floyd, 1996	Staples et. al (1997)
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	1.6	-2.24	Ellington & Floyd, 1996	Staples et. al (1997)
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	2.2	-2.10	Ellington & Floyd, 1996	Staples et. al (1997)
3126-90-7	Di-n-butyl-m-phthalate	278	5.3	4.6	4.3	0.9	-2.49	Pomona, 1987	Veith et al. (1984)
1962-75-0	Di-n-butyl terephthalate	278	5.3	4.6	5.5	5.53	-1.70	Hansch et al., 1995	DUL
85-68-7	Butylbenzyl phthalate	312	4.8	4.8	4.7	0.82	-2.58	Ellington & Floyd, 1996	Staples et. al (1997)
85-68-7	Butylbenzyl phthalate	312	4.8	4.8	4.7	1.5	-2.32	Ellington & Floyd, 1996	Staples et. al (1997)

85-68-7	Butylbenzyl phthalate	312	4.8	4.8	4.7	1.7	-2.26	Ellington & Floyd, 1996	Staples et. al (1997)
85-68-7	Butylbenzyl phthalate	312	4.8	4.8	4.7	2.1	-2.17	Ellington & Floyd, 1996	Staples et. al (1997)
85-68-7	Butylbenzyl phthalate	312	4.8	4.8	4.7	3.3	-1.98	Ellington & Floyd, 1996	Staples et. al (1997)
	Kow Limit		5	5			-2.65	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
CBI	CBI	509	3	2.3	2.1	*	*	None given	P91-____
CBI	CBI	468	1.6	2.8	3	*	*	None given	P95-____
CBI	CBI	298	3.8	3.9		*	*		P-90-____
CBI	CBI	461	4.2	4.2	2.6	*	*	None given	P00-____
CBI	CBI	290	5.7	5.1	4.4	*	*		P91-____
CBI/CBI	CBI/CBI	252	6.3	5.4		0.043	*-3.77		P01-____/L98-____
117-81-7	Di-(2-ethylhexyl)-phthalate	391	8.6	8.4	7.6	*		DeBruijn et al. 1989	Veith et al. (1984)
137-89-3	Di-n-octyl-m-phthalate	391	9.2	8.4		*	*		Veith et al. (1984)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	*	*	Ellington & Floyd, 1996	Veith et al. (1984)/DUL
4654-26-6	Di-n-octyl-p-phthalate	391	9.5	8.5		*	*		Veith et al. (1984)
CBI	CBI	368	1.3	0.99	0.6	27	-1.13	None given	P93-_____; mixture
CBI	CBI	644	9.3	12		*	*		P90-____
CBI	CBI	595	17	16		*	*		P91-____
84731-63-5	Diisotridecyl dodecanedioate	595	16	16		*	*		Veith et al. (1984)
CBI	CBI	525	11	11		*	*		P-90-____
Data Not Included in SAR:									
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	>1.24	>-2.35	Ellington & Floyd, 1996	Staples et. al (1997)
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	1.2-1.8	-2.36 - -2.19	Ellington & Floyd, 1996	Staples et. al (1997)
85-68-7	Butylbenzyl phthalate	312	4.8	4.8	4.7	>0.78	>-2.6	Ellington & Floyd, 1996	Staples et. al (1997)
84-75-3	Dihexyl phthalate	335	6.8	6.6	6.8	>0.1	>-3.53	Ellington & Floyd, 1996	Staples et. al (1997)
84-75-3	Dihexyl phthalate	335	6.8	6.6	6.8	>0.11	>-3.48	Ellington & Floyd, 1996	Staples et. al (1997)
84-75-3	Dihexyl phthalate	335	6.8	6.6	6.8	>0.2	>-3.22	Ellington & Floyd, 1996	Staples et. al (1997)
84-75-3	Dihexyl phthalate	335	6.8	6.6	6.8	>0.24	>-3.14	Ellington & Floyd, 1996	Staples et. al (1997)
27554-26-3	Diisooctyl phthalate	391	8.6	8.4		>0.13	>-3.48		Staples et. al (1997)
27554-26-3	Diisooctyl phthalate	391	8.6	8.4		>0.14	>-3.45		Staples et. al (1997)
27554-26-3	Diisooctyl phthalate	391	8.6	8.4		>0.23	>-3.23		Staples et. al (1997)
27554-26-3	Diisooctyl phthalate	391	8.6	8.4		>0.29	>-3.13		Staples et. al (1997)
117-81-7	Di-(2-ethylhexyl)-phthalate	391	8.6	8.4	7.6	>19.51	>-1.3	DeBruijn et al. 1989	ETFS
117-81-7	Di-(2-ethylhexyl)-phthalate	391	8.6	8.4	7.6	>100	>-0.59	DeBruijn et al. 1989	ETFS
117-81-7	Di-(2-ethylhexyl)-phthalate	391	8.6	8.4	7.6	>100	>-0.59	DeBruijn et al. 1989	ETFS
117-81-7	Di-(2-ethylhexyl)-phthalate	391	8.6	8.4	7.6	>770	>0.29	DeBruijn et al. 1989	ETFS
117-81-7	Di-(2-ethylhexyl)-phthalate	391	8.6	8.4	7.6	>1106.2	>0.45	DeBruijn et al. 1989	ETFS
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>0.16	>-3.39	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>0.2	>-3.29	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>0.32	>-3.09	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>0.32	>-3.09	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>0.32	>-3.09	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>0.32	>-3.09	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>0.32	>-3.09	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>0.32	>-3.09	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>0.327	>-3.08	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>0.67	>-2.77	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>0.67	>-2.77	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>100	>-0.59	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>100	>-0.59	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>100	>-0.59	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>100	>-0.59	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>100	>-0.59	Ellington & Floyd, 1996	Staples et. al (1997)
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>100	>-0.59	Ellington & Floyd, 1996	EPA, 8e-14321
117-84-0	Dioctyl phthalate	391	8.9	8.5	8.1	>19.5	>-1.30	Ellington & Floyd, 1996	Staples et. al (1997)
111381-90-9 (111381-89-6)	Di(heptyl,nonyl,undecyl) phthalate	419	9.7	9.4		>0.13	>-3.51		Staples et. al (1997)
111381-90-9 (111381-89-6)	Di(heptyl,nonyl,undecyl) phthalate	419	9.7	9.4		>0.17	>-3.39		Staples et. al (1997)
28553-12-0	Diisononyl phthalate	419	9.7	9.4		>0.19	>-3.34		Staples et. al (1997)
111381-90-9 (111381-89-6)	Di(heptyl,nonyl,undecyl) phthalate	419	9.7	9.4		>0.21	>-3.30		Staples et. al (1997)
111381-90-9 (111381-89-6)	Di(heptyl,nonyl,undecyl) phthalate	419	9.7	9.4		>0.23	>-3.26		Staples et. al (1997)
28553-12-0	Diisononyl phthalate	425	9.7	9.4		>0.1	>-3.63		Staples et. al (1997)
28553-12-0	Diisononyl phthalate	425	9.7	9.4		>0.14	>-3.48		Staples et. al (1997)
28553-12-0	Diisononyl phthalate	425	9.7	9.4		>0.16	>-3.42		Staples et. al (1997)
26761-40-0	Diisodecyl phthalate	447	10.7	10.4		>0.37	>-3.08		Staples et. al (1997)
26761-40-0	Diisodecyl phthalate	447	10.7	10.4		>0.47	>-2.98		Staples et. al (1997)
26761-40-0	Diisodecyl phthalate	447	10.7	10.4		>0.62	>-2.86		Staples et. al (1997)
26761-40-0	Diisodecyl phthalate	447	10.7	10.4		>1	>-2.65		Staples et. al (1997)
3648-20-2	Di-undecyl phthalate	475	12	11.5		>0.22	>-3.33		Staples et. al (1997)
3648-20-2	Di-undecyl phthalate	475	12	11.5		>0.73	>-2.81		Staples et. al (1997)
3648-20-2	Di-undecyl phthalate	475	12	11.5		>0.74	>-2.81		Staples et. al (1997)
3648-20-2	Di-undecyl phthalate	475	12	11.5		>1.3	>-2.56		Staples et. al (1997)
3648-20-2	Di-undecyl phthalate	475	12	11.5		>1.4	>-2.53		Staples et. al (1997)
119-06-2	Ditridecyl phthalate	531	14	13.5		>0.12	>-3.65		Staples et. al (1997)
119-06-2	Ditridecyl phthalate	531	14	13.5		>0.14	>-3.58		Staples et. al (1997)
119-06-2	Ditridecyl phthalate	531	14	13.5		>0.15	>-3.55		Staples et. al (1997)
119-06-2	Ditridecyl phthalate	531	14	13.5		>0.26	>-3.31		Staples et. al (1997)
						* indicates no effects at saturation			

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FISH 14-d LC50 (Mortality)

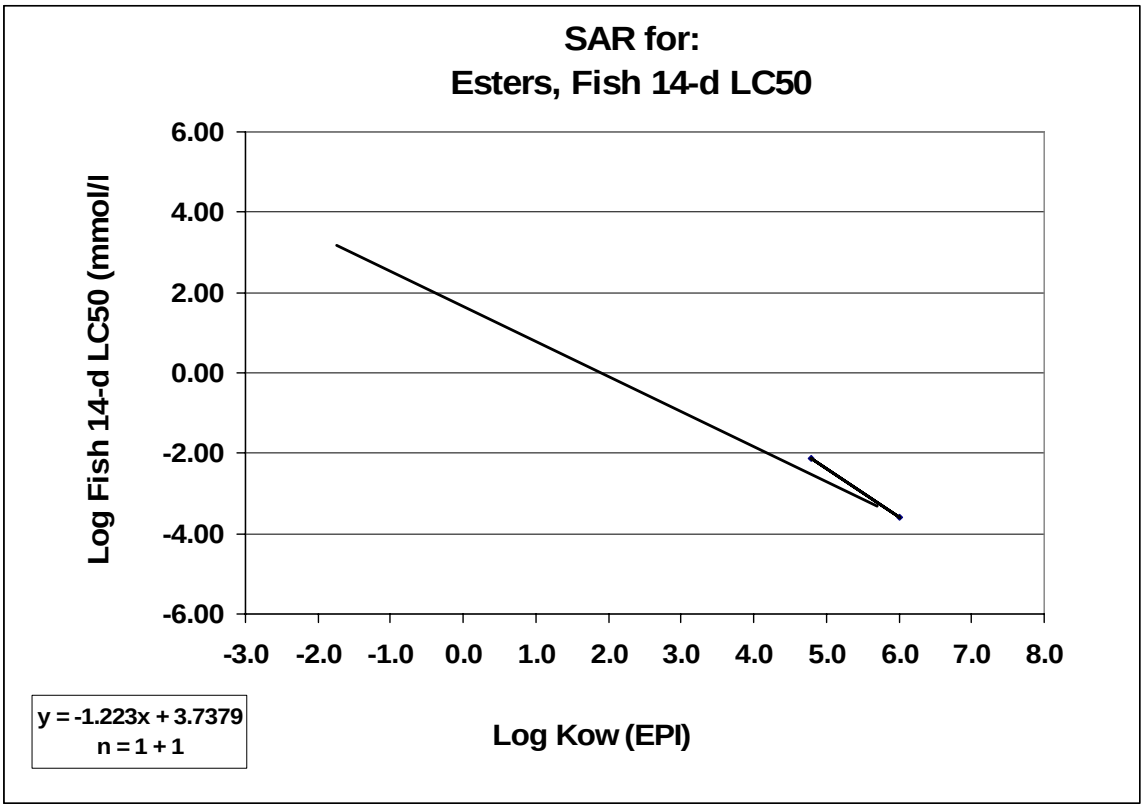
ESTIMATED TOXICITY:
The fish 14-d LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h (mmol/L) = - 1.223 (log Kow) + 3.7379

The LC50 is in millimoles per liter (mM/L); N = 1 + 1; and the Coefficient of Determination (R^2) = N/A. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the ester.

Maximum K_{ow}: 6.0
Maximum MW: 1000

GRAPH:



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 Kow value is greater than 6.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish 14-d LC50 (mg/L)	Log Fish 14-d LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Fish 14-d LC50)
85-68-7	Butylbenzyl phthalate	312	4.8	4.8	4.7	2.3	-2.13	Ellington & Floyd, 1996	Staples et. al (1997)
	Kow Limit		6	6			-3.60	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
						* indicates no effects at saturation			

REFERENCES:
Staples CA, Adams W, Parkerton TF, Gorsuch JW, Biddinger GR, Reinert KH. 1997. Aquatic toxicity of eighteen phthalate esters. Environmental Toxicology and Chemistry, 16 (5): 875-891.

DAPHNID 48-h LC50

ESTIMATED TOXICITY:

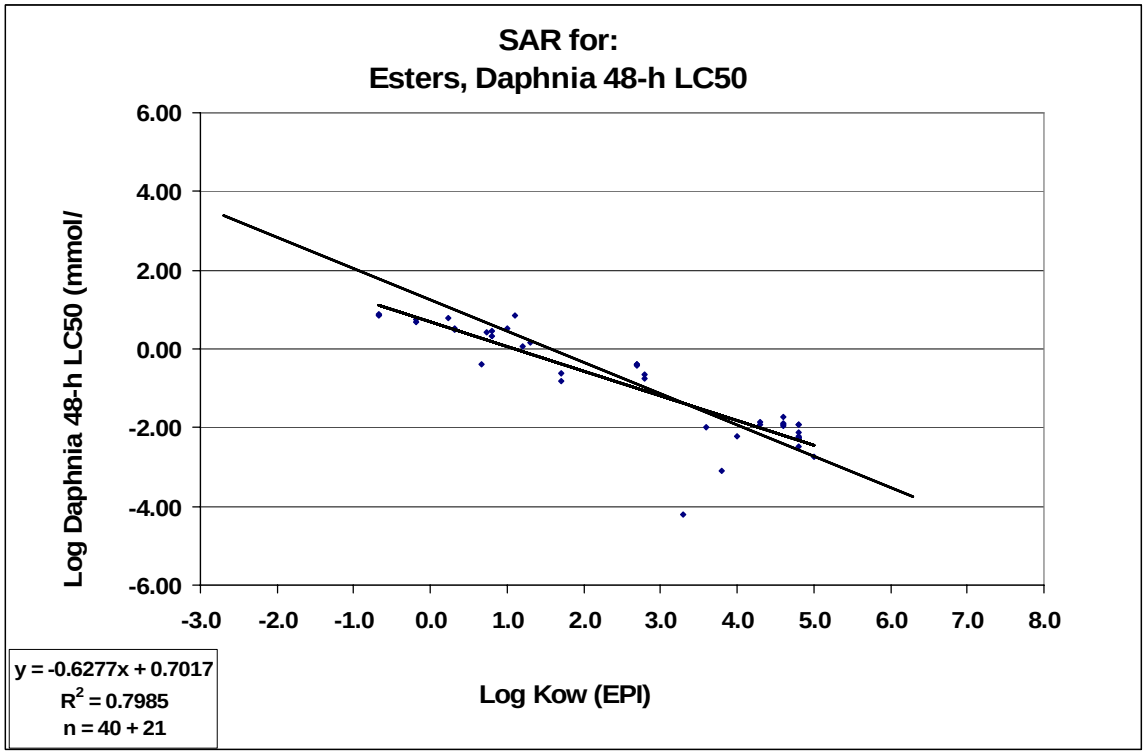
The daphnid 48-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h LC50 (mmol/L) = -0.6277 (log Kow) + 0.7017

The LC50 is in millimoles per liter (mM/L); N = 40 + 21; and the Coefficient of Determination (R^2) = 0.7985. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the ester.

Maximum K_{ow}: 5.0
Maximum MW: 1000

GRAPH:



APPLICATIONS:
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 phenols.

LIMITATIONS:
If the log Kow value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Daphnia 48-h LC50 (mg/L)	Log Daphnia 48-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Daphnia 48-h LC50)
Methyl lactate	104	-0.22	-0.67		749	0.86		Bowmer et al.
Methyl lactate	104	-0.22	-0.67		780	0.88		Bowmer et al.
Ethyl lactate	118	0.33	-0.18		560	0.68		Bowmer et al.
Ethyl lactate	118	0.33	-0.18		683	0.76		Bowmer et al.
Isopropyl lactate	132	0.62	0.23		802	0.78		Bowmer et al.
n-Propyl lactate	132	0.84	0.31		413	0.50		Bowmer et al.
n-Propyl lactate	132	0.84	0.31		423	0.51		Bowmer et al.
CBI	158	0.27	0.67	0.94	63	-0.40	None given	P-00-____
Isobutyl lactate	146	1.2	0.73		395	0.43		Bowmer et al.
Butyl lactate	146	1.4	0.80		320	0.34		Bowmer et al.
Butyl lactate	146	1.4	0.80		423	0.46		Bowmer et al.
CBI	146	1.0	1.0		500	0.53		P94-____
CBI	146	1.2	1.1		1000	0.84		P97-____/Analog
Isoamyl or Isopentyl lactate	160	1.8	1.2		193	0.08		Bowmer et al.
Pentyl lactate	160	1.9	1.3		238	0.17		Bowmer et al.
Dimethyl terephthalate	194	2.1	1.7	2.3	30.4	-0.80	Hansch & Leo, 1985	Datasheet
Dimethyl phthalate	194	1.5	1.7	1.6	45.9	-0.63	Ellington & Floyd, 1997	Staples et. al (1997)
2-Ethylhexyl lactate	202	3.4	2.7		83	-0.39		Bowmer et al.
Diethyl phthalate	222	2.5	2.7	2.4	86	-0.41	Ellington & Floyd, 1996	Staples et. al (1997)
Diethyl phthalate	222	2.5	2.7	2.4	90	-0.39	Ellington & Floyd, 1996	Nabholz (1987)
Octyl lactate	202	3.5	2.8		37	-0.74		Bowmer et al.
Octyl lactate	202	3.5	2.8		45	-0.65		Bowmer et al.
CBI	286	4.0	3.3		0.018	-4.20		X97-____
N, N-	307	3.8	3.6		3.2	-1.98		8(e)-12513
CBI	362	3.9	3.8		0.28	-3.11		8(e)-____/P-90-____
CBI	184	3.6	4.0		1.1	-2.22		P92-____/ 8(e)-____
CBI	244	4.8	4.3		3.3	-1.87		P92-____
CBI	285	3.7	4.3	4.2	3.32	-1.93	None given	8(e)-____/P91-____
Dibutyl phthalate	278	4.7	4.6	4.5	3	-1.97	Ellington & Floyd, 1996	Staples et. al (1997)
Dibutyl phthalate	278	4.7	4.6	4.5	3.4	-1.91	Ellington & Floyd, 1996	Nabholz (1987)
Dibutyl phthalate	278	4.7	4.6	4.5	3.7	-1.88	Ellington & Floyd, 1996	Staples et. al (1997)
Dibutyl phthalate	278	4.7	4.6	4.5	5.2	-1.73	Ellington & Floyd, 1996	Nabholz (1987)
Butyl-benzyl phthalate	312	4.8	4.8	4.7	1	-2.49	Ellington & Floyd, 1996	Nabholz (1987)
Butyl-benzyl phthalate	312	4.8	4.8	4.7	1.6	-2.29	Ellington & Floyd, 1996	Nabholz (1987)
Butyl-benzyl phthalate	312	4.8	4.8	4.7	1.7	-2.26	Ellington & Floyd, 1996	Nabholz (1987)
Butyl-benzyl phthalate	312	4.8	4.8	4.7	1.8	-2.24	Ellington & Floyd, 1996	Staples et. al (1997)
Butyl-benzyl phthalate	312	4.8	4.8	4.7	1.83	-2.23	Ellington & Floyd, 1996	Nabholz (1987)
Butyl-benzyl phthalate	312	4.8	4.8	4.7	2.4	-2.11	Ellington & Floyd, 1996	Nabholz (1987)
Butyl-benzyl phthalate	312	4.8	4.8	4.7	3.7	-1.93	Ellington & Floyd, 1996	Nabholz (1987)
Butyl-benzyl phthalate	312	4.8	4.8	4.7	3.7	-1.93	Ellington & Floyd, 1996	Staples et. al (1997)
Kow Limit		5	5			-2.73	NO Cutoff	NO SAR
Included in Regression Equation:								
CBI	468	1.6	2.8	3	*	*	None given	P-95-____
CBI	298	3.8	3.9		*	*		P-90-____
CBI	252	6.3	5.4		*	*		P01-____
CBI	284	5.4	5.5	4.7	2.7	-2.02	None given	P95-____
Butyl 2-ethylhexyl phthalate	334	6.6	6.5		*			Nabholz (1987)
Dihexyl phthalate	335	6.8	6.6		*			Nabholz (1987)

Diisooctyl phthalate	390	8.6	8.4		*			Nabholz (1987)
Di-(2-ethylhexyl)-phthalate	391	8.6	8.4	7.6	*		DeBruijn et al. 1989	Nabholz (1987)/ Staples et. al (1
Di-(2-ethylhexyl)-phthalate	391	8.6	8.4	7.6	*4.69	*3.26	DeBruijn et al. 1989	ETFS
Di-(n-hexyl, n-octyl, n-decyl)- phthalate	390	8.9	8.5		*			Nabholz (1987)
Di-(n-octyl)-phthalate	391	8.9	8.5		*			Nabholz (1987)
Di-(heptyl, nonyl, undecyl)-phthalate	419	9.7	9.4		*			Nabholz (1987)
Diisononyl phthalate	419	9.7	9.4		*			Nabholz (1987)
Diisodecyl phthalate	447	11	10		*			Nabholz (1987)
CBI	525	11	11		*	*		P-90-____
Diundecyl phthalate	475	12	12		*			Nabholz (1987)
Ditridecyl phthalate	531	14	13		*			Nabholz (1987)
CBI	290	5.7	-	4.4	*	*	None given	P-91-____
CBI	455	-	-		*	*		P-90-____/T-89-____
CBI	509 (n=1)	>= 3.0	-	2.1	*	*	None given	P-91-____
ıded in SAR:								
Dimethyl phthalate	194	1.5	1.7		>52	>-0.57		Nabholz (1987)
Warfarin	308	2.9	2.2	2.6	0.288	-3.03	Sangster, 1994	Lilius et al., 1995; 24-hour study duration.
CBI	487	3.4	3		>90	>-0.73		P05-____/P02-____
Butyl-benzyl phthalate	312	4.8	4.8		>0.96	>-2.51		Staples et. al (1997)
Butyl (2-ethylhexyl) phthalate	334	6.6	6.5		>0.07	>-3.68		Staples et. al (1997)
Dihexyl phthalate	335	6.8	6.6		>0.18	>-3.27		Staples et. al (1997)
Diisoctyl phthalate	390	8.6	8.4		>0.16	>-3.39		Staples et. al (1997)
Di-(2-ethylhexyl) phthalate	391	8.6	8.4		>0.16	>-3.39		Staples et. al (1997)
Di-(2-ethylhexyl) phthalate	391	8.6	8.4		>1	>-2.59		Staples et. al (1997)
Di-(n-hexyl, n-octyl, n-decyl) phthalate	390	8.9	8.5		>0.33	>-3.07		Staples et. al (1997)
Dioctyl phthalate	391	8.9	8.5		>10	>-1.59		Staples et. al (1997)
Di-(heptyl, nonyl, undecyl)-phthalate	419	9.7	9.4		>0.04	>-4.02		Staples et. al (1997)
Diisononyl phthalate	419	9.7	9.4		>0.06	>-3.84		Staples et. al (1997)
Diisononyl phthalate	419	9.7	9.4		>1	>-2.62		Staples et. al (1997)
Diisodecyl phthalate	447	11	10		>0.02	>-4.35		Staples et. al (1997)
Diisodecyl phthalate	447	11	10		>1	>-2.65		Staples et. al (1997)
Diundecyl phthalate	475	12	12		>0.02	>-4.38		Staples et. al (1997)
Ditridecyl phthalate	531	14	13		>0.05	>-4.03		Staples et. al (1997)
Ditridecyl phthalate	531	14	13		>1	>-2.73		Staples et. al (1997)
					* indicates no effects at saturation			

REFERENCES:

Bowmer CT, Hooftman RN, Hanstveit AO, Venderbosch PWM, Van der Hoeven N. 1998. The ecotoxicity and the biodegradability of lactic acid, alkyl lactate esters and lactate salts. Chemosphere 37(7):1317-1333.

Nabholz JV. 1987. The acute and chronic toxicity of dialkyl phthalate esters to daphnids. Interagency memorandum to “Whom it may concern”. Washington DC: Office of Toxic Substances, Environmental Effects Branch, Health and Environmental Review Division (TS-796), United States Environmental Protection Agency, 20460-0001.

Staples CA, Adams W, Parkerton TF, Gorsuch JW, Biddinger GR, Reinert KH. 1997. Aquatic toxicity of eighteen phthalate esters. Environmental Toxicology and Chemistry, 16 (5): 875-891.

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

GREEN ALGAE 96-h EC50 (Growth)

ESTIMATED TOXICITY:

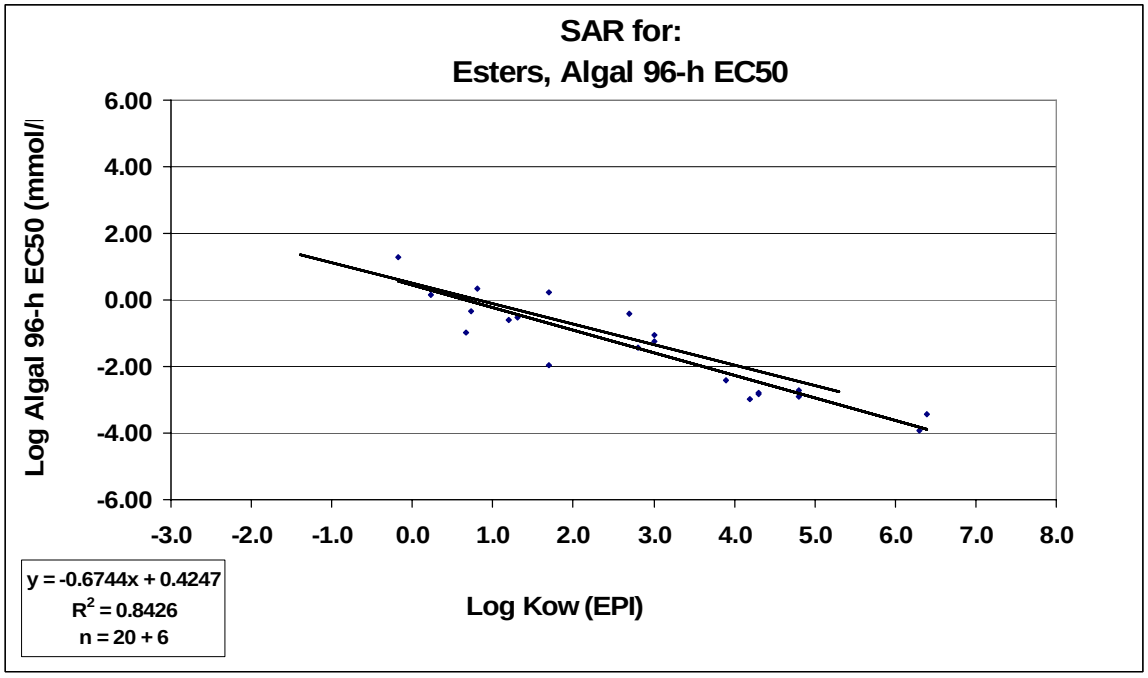
The green algae 96-h EC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h EC50 (mmol/L) = -0.6744 log (Kow) + 0.4247

The EC50 is in millimoles per liter (mM/L); N = 20 + 6; and the Coefficient of Determination (R^2) = 0.8426. To convert the EC50 from mM/L to mg/L, multiply by the molecular weight of the ester.

Maximum K_{ow}: 6.4
Maximum MW: 1000

GRAPH:



APPLICATIONS:
This SAR may be used to estimate toxicity for the following esters.

5. Acetates
6. Benzoates
7. Dicarboxylic aliphatics
8. Phthalates, derived from aliphatic alcohols and phenols.

LIMITATIONS:
If the log Kow value is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Algal 96-h EC50 (mg/L)	Log Algal 96-h EC50 (mmol/L)	Reference (Meas. Kow)	Reference (Algal 96-h EC50)
97-64-3	Ethyl lactate	118	0.33	-0.18		2300	1.29		Bowmer et al.
617-51-6	Isopropyl lactate	132	0.62	0.23		180	0.13		Bowmer et al.
CBI	CBI	158	0.27	0.67	0.94	16	-0.99	None given	P00-____
585-24-0/ 68166-83-6/ 77027-84-0	Isobutyl lactate	146	1.2	0.73		64	-0.36		Bowmer et al.
138-22-7	Butyl lactate	146	1.4	0.80		329	0.35		Bowmer et al.
19329-89-6	Isoamyl or Isopentyl lactate	160	1.8	1.2		41	-0.59		Bowmer et al.
6382-06-5	Pentyl lactate	160	1.9	1.3		46	-0.54		Bowmer et al.
131-11-3	Dimethyl phthalate	194	1.5	1.7	1.6	313	0.21	Ellington & Floyd, 1997	Staples et. al (1997)
CBI	CBI	328		1.7		3.7	-1.95		P00-____
84-66-2	Diethyl phthalate	222	2.5	2.7	2.4	85.6	-0.41	Ellington & Floyd, 1996	Staples et. al (1997)
5464-71-1	Octyl lactate	202	3.5	2.8		7.6	-1.42		Bowmer et al.
CBI	CBI	487	3.4	3.0		28	-1.24		P02-____
CBI	CBI	487	3.4	3.0		42	-1.06		P05-____/P02-____
CBI	CBI	362	3.8	3.9		1.4	-2.41		8(e)-____/P-90-____
CBI	CBI	461	MF	4.2	2.6	0.48	-2.98	None given	P-00-____
CBI	CBI	244	4.8	4.3		0.4	-2.79		P92-____
CBI	CBI	285	3.7	4.3	4.2	0.41	-2.84	None given	8(e)-____/P91-____
85-68-7	Butyl-benzyl phthalate	312	4.8	4.8	4.7	0.4	-2.89	Ellington & Floyd, 1996	Staples et. al (1997)
85-68-7	Butyl-benzyl phthalate	312	4.8	4.8	4.7	0.6	-2.72	Ellington & Floyd, 1996	Staples et. al (1997)
110-33-8	Dihexyl adipate	315	6.0	6.3		0.038	-3.92		8(e)-9618
	Kow Limit		6.4	6.4			-3.43	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
CBI	CBI	468	1.6	2.8	2.96 @25C, pH5.7	*	*	None given	P-95-____
103-09-3	2-Ethylhexyl acetate	172	3.7	3.7		*	*		Datasheet
CBI	CBI	252	6.3	5.4		*	*		P01-____
CBI	CBI	284	5.4	5.5	4.7	*	*	None given	P-95-____
CBI	CBI	262	6.7	5.6	6.64	*	*	HPLC	P90-____
Data Not Included in SAR:									
84-66-2	Diethyl phthalate	222	2.5	2.9		>100	>-0.346		Staples et. al (1997)
84-74-2	Dibutyl phthalate	278	4.7	4.6		>13	>1.33		Staples et. al (1997)
						* indicates no effects at saturation			

REFERENCES:

Bowmer CT, Hooftman RN, Hanstveit AO, Venderbosch PWM, Van der Hoeven N. 1998. The ecotoxicity and the biodegradability of lactic acid, alkyl lactate esters and lactate salts. Chemosphere 37(7):1317-1333.Confidential Business Information

Staples CA, Adams W, Parkerton TF, Gorsuch JW, Biddinger GR, Reinert KH. 1997. Aquatic toxicity of eighteen phthalate esters. Environmental Toxicology and Chemistry, 16 (5): 875-891.

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U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

FISH 32/33-d ChV

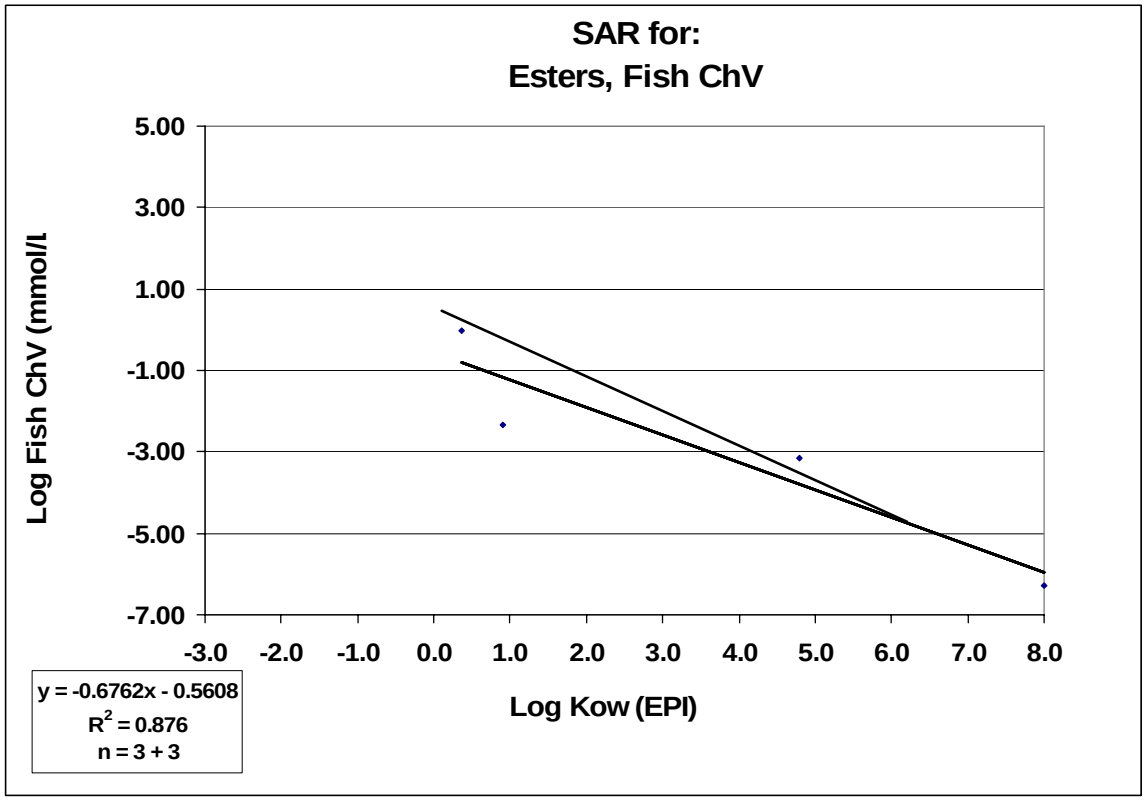
ESTIMATED TOXICITY:
The fish chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.6762 log Kow - 0.5608

The ChV is in millimoles per liter (mM/L); N = 3 + 3; and the Coefficient of Determination (R^2) = 0.876. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

GRAPH:



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 Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish ChV (mg/L)	Log Fish ChV (mmol/L)	Reference (Meas. Kow)	Reference (Fish ChV)
79-20-9	Methyl acetate	74	0.18	0.37	0.18	72.1	-0.01	Hansch & Leo, 1985	DUL
105-53-3	Diethyl malonate	160	1.1	0.9	0.96	0.76	-2.32	Pomona, 1987	USEPA, 1991/ DUL
85-68-7	Butyl-benzyl phthalate	312	4.8	4.8	4.7	0.22	-3.15	Ellington & Floyd, 1996	Staples et. al (1997)
	Kow Limit		8	8			-6.27	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
CBI	CBI	262	6.7	5.6	6.64	*	*	HPLC	P90-___
117-81-7	Di-(2-ethylhexyl)-phthalate	391	8.6	8.4	7.6	*31.8	*1.1	DeBruijn et al. 1989	ETFS
Data Not Included in SAR:									
141-78-6	Ethyl acetate	88	0.71	0.86	0.73	< 9.65	<-0.96	Hansch & Leo, 1985	DUL
1929-73-3	2,4-D butoxy ethanol ester	321	4.7	4.1		0.67	-2.68		Mount and Stephan, 1967; incorrect duration.
117-81-7	Di-(2-ethylhexyl)-phthalate	391	8.6	8.4	7.6	>0.5	>-2.89	DeBruijn et al. 1989	ETFS
						* indicates no effects at saturation			

REFERENCES:
Mount and Stephan.1967. A method establishing acceptable toxicant limits for fish-malathion and the butoxyethanol ester of 2,4-D. Trans. Amer. Fish. Soc. 96 (2) 185 - 193 Mount and Stephan, 1967

Staples CA, Adams W, Parkerton TF, Gorsuch JW, Biddinger GR, Reinert KH. 1997. Aquatic toxicity of eighteen phthalate esters. Environmental Toxicology and Chemistry, 16 (5): 875-891.

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

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

DAPHNID 21-d ChV

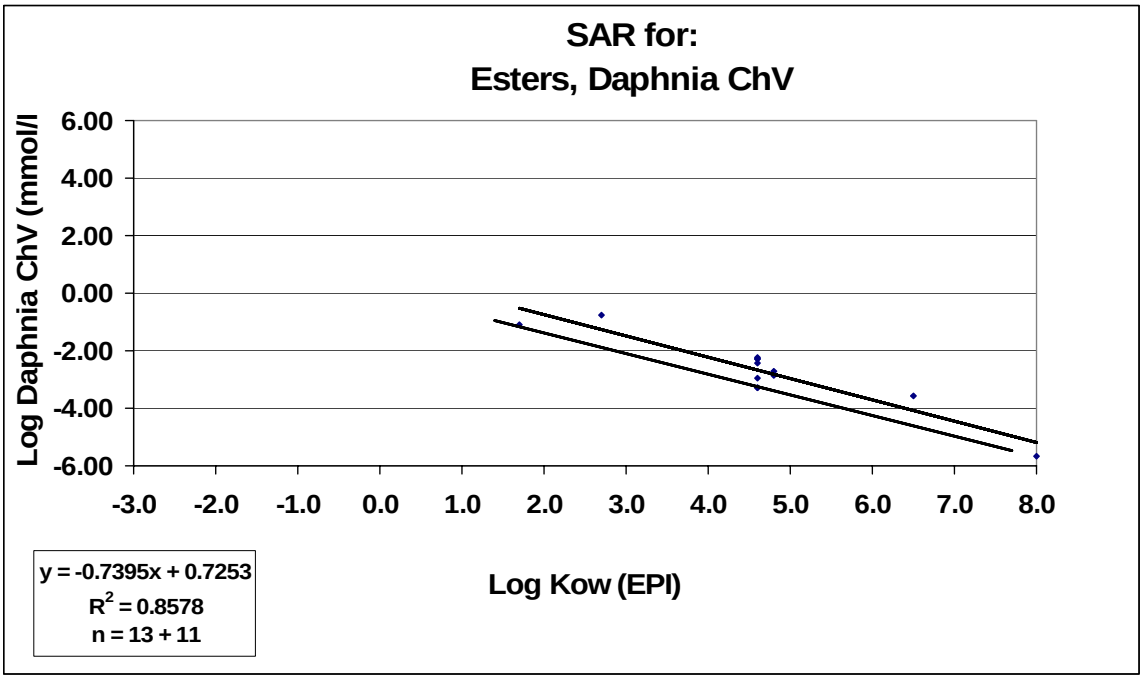
ESTIMATED TOXICITY:
The daphnid ChV values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.7395 log Kow + 0.7253

The ChV is in millimoles per liter (mM/L); N = 13 + 11; and the Coefficient of Determination (R^2) = 0.8578. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1,000

GRAPH:



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 Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Daphnia ChV (mg/L)	Log Daphnia ChV (mmol/L)	Reference (Meas. Kow)	Reference (Daphnia ChV)
131-11-3	Dimethyl phthalate	194	1.5	1.7	1.6	14.9	-1.11	Ellington & Floyd, 1996	Nabholz (1987)/ Staples et. al (1
84-66-2	Diethyl phthalate	222	2.5	2.7	2.4	38.4	-0.76	Ellington & Floyd, 1996	Nabholz (1987)/ Staples et. al (1
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	0.14	-3.30	Ellington & Floyd, 1996	Nabholz (1987)/ Staples et. al (1
3126-90-7	Di-n-butyl-iso phthalate	278	5.3	4.6		0.15	-3.27		Nabholz (1987)
84-72-2	Dibutyl phthalate	278	4.7	4.6	4.5	0.32	-2.94	Ellington & Floyd, 1996	Nabholz (1987)/ Staples et. al (1
84-72-2	Dibutyl phthalate	278	4.7	4.6	4.5	1	-2.44	Ellington & Floyd, 1996	Nabholz (1987)
84-72-2	Dibutyl phthalate	278	4.7	4.6	4.5	1.4	-2.30	Ellington & Floyd, 1996	Nabholz (1987)/ Staples et. al (1
84-72-2	Dibutyl phthalate	278	4.7	4.6	4.5	1.55	-2.25	Ellington & Floyd, 1996	Staples et. al (1997)
84-72-2	Dibutyl phthalate	278	4.7	4.6	4.5	1.5	-2.27	Ellington & Floyd, 1996	Nabholz (1987)
85-68-7	Butyl-benzyl phthalate	312	4.8	4.8	4.7	0.44	-2.85	Ellington & Floyd, 1996	Nabholz (1987)/ Staples et. al (1
85-68-7	Butyl-benzyl phthalate	312	4.8	4.8	4.7	0.63	-2.69	Ellington & Floyd, 1996	Nabholz (1987)/ Staples et. al (1
85-69-8	Butyl (2-ethylhexyl) phthalate	334	6.6	6.5		0.088	-3.58		Staples et. al (1997)
	Kow Limit		8	8			-5.69	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
111381-90-9 (111381-89-6)	Di(heptyl,nonyl,undecyl) phthalate	419	9.7	9.4		*	*		Nabholz (1987)
117-81-7	Di-(2-ethylhexyl) phthalate	391	8.6	8.4		*	*		Nabholz (1987)
117-84-0	Dioctyl phthalate	391	8.9	8.5		*	*		Nabholz (1987)
119-06-2	Ditridecyl phthalate	531	14	13		*	*		Nabholz (1987)
123-79-5	Dioctyl adipate	371	8.1	8.3		35	-1.03		8(e)-9781
CBI	CBI	262	6.7	5.6	6.64	*	*	HPLC	P90-___
25724-58-7 (68515-51-5)	Di-(n-hexyl, n-octyl, n-decyl)- phthalate	390	8.9	8.5		*	*		Nabholz (1987)
26761-40-0	Diisodecyl phthalate	447	11	10		*	*		Nabholz (1987)
27554-26-3	Diisooctyl phthalate	390	8.6	8.4		*	*		Nabholz (1987)
28553-12-0	Diisononyl phthalate	419	9.7	9.4		*	*		Nabholz (1987)
CBI	CBI	547	12	12		*	*		P-94-___
3648-20-2	Diundecyl phthalate	475	12	12		*	*		Nabholz (1987)
84-75-3	Dihexyl phthalate	335	6.8	6.6	6.8	*	*	Ellington & Floyd, 1996	Nabholz (1987)
85-69-8	Butyl 2-ethylhexyl phthalate	334	6.6	6.5		*	*		Nabholz (1987)
Data Not Included in SAR:									
117-81-7	Di-(2-ethylhexyl)-phthalate	391	8.6	8.4	7.6	>0.0856	>-3.66	DeBruijn et al. 1989	ETFS
						* indicates no effects 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: Office of Toxic Substances, Environmental Effects Branch, Health and Environmental Review Division (TS-796), United States Environmental Protection Agency, 20460-0001.

Staples CA, Adams W, Parkerton TF, Gorsuch JW, Biddinger GR, Reinert KH. 1997. Aquatic toxicity of eighteen phthalate esters. Environmental Toxicology and Chemistry, 16 (5): 875-891.

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

GREEN ALGAE ChV

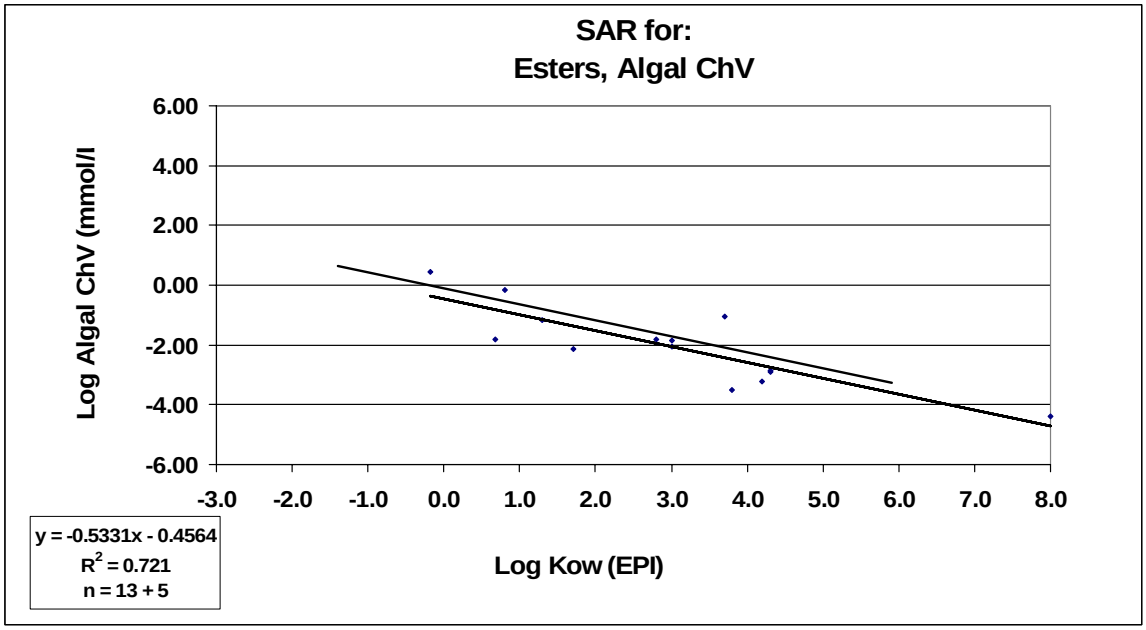
ESTIMATED TOXICITY:
The green algae chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.5331 (log Kow) - 0.4564

The ChV is in millimoles per liter (mM/L); N = 13 + 5; and the Coefficient of Determination (R^2) = 0.721. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1,000

GRAPH:



APPLICATIONS:
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 Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Algal ChV (mg/L)	Log Algal ChV (mmol/L)	Reference (Meas. Kow)	Reference (Algal ChV)
97-64-3	Ethyl lactate	118	0.33	-0.18		320	0.43		Bowmer et al.
CBI	CBI	158	0.27	0.67	0.94	2.5	-1.80	None given	P-00-____
138-22-7	Butyl lactate	146	1.4	0.8		100	-0.16		Bowmer et al.
6382-06-5	Pentyl lactate	160	1.9	1.3		11	-1.16		Bowmer et al.
CBI	CBI	328		1.7		2.5	-2.12		P00-____
5464-71-1	Octyl lactate	202	3.5	2.8		3.2	-1.80		Bowmer et al.
CBI	CBI	487	3.4	3		4.5	-2.03		P02-____
CBI	CBI	487	3.4	3.0		7	-1.84		P05-____/P02-____
103-09-3	2-Ethylhexyl acetate	172	3.7	3.7		15	-1.06		Datasheet
CBI	CBI	362	3.9	3.8		0.11	-3.52		8(e)-____/P-90-____
CBI	CBI	461	MF	4.2	2.6	0.27	-3.23	None given	P-00-
CBI	CBI	244	4.8	4.3		0.3	-2.91		P92-____
CBI	CBI	285	3.7	4.3	4.2	0.39	-2.86	None given	P91-____
	Kow Limit		8	8			-4.38	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
CBI	CBI	468	1.6	2.8	3	*	*	None given	P95-____
CBI	CBI	252	6.3	5.4		*	*		P01-____
CBI	CBI	284	5.4	5.5	4.7	*	*	None given	P95-____
CBI	CBI	262	6.7	5.6	6.64	*	*	HPLC	P90-____
Data Not Included in SAR:									
617-51-6	Isopropyl lactate	132	0.62	0.23		<100	<-0.12		Bowmer et al.
585-24-0/ 68166-83-6/ 77027-84-0	Isobutyl lactate	146	1.3	0.69		<32	<-0.66		Bowmer et al.
585-24-0/ 68166-83-6/ 77027-84-0	Isobutyl lactate	146	1.3	0.73		<32			Bowmer et al.
19329-89-6	Isoamyl or Isopentyl lactate	160	1.8	1.2		<10	<-1.2		Bowmer et al.
	* indicates no effects at saturation								

REFERENCES:

Bowmer CT, Hooftman RN, Hanstveit AO, Venderbosch PWM, Van der Hoeven N. 1998. The ecotoxicity and the biodegradability of lactic acid, alkyl lactate esters and lactate salts. Chemosphere 37(7):1317-1333.Confidential Business InformationConfidential Business Information

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

FISH (SW) 96-h LC50 (Mortality)

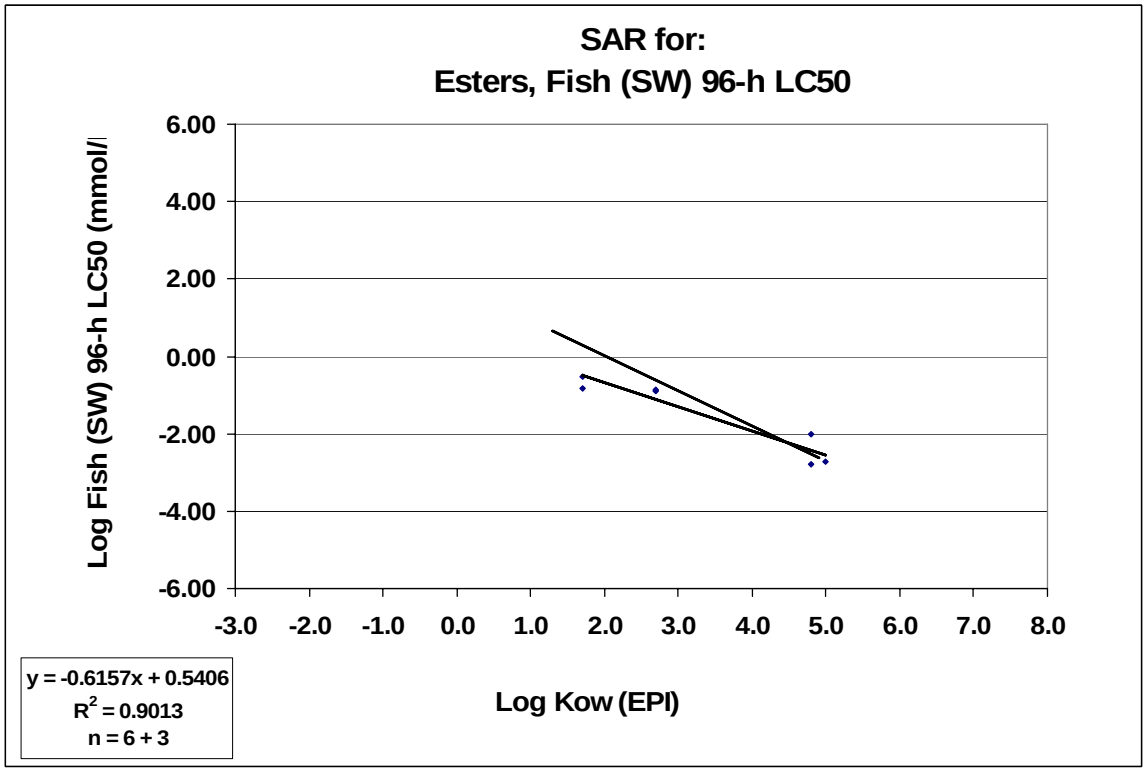
ESTIMATED TOXICITY:
The saltwater fish 96-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h LC50 (mmol/L) = - 0.6157 (log Kow) + 0.5406

The LC50 is in millimoles per liter (mM/L); N = 6 + 3; and the Coefficient of Determination (R^2) = 0.9013. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 5
Maximum MW: 1,000

GRAPH:



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 Kow value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish (SW) 96-h LC50 (mg/L)	Log Fish (SW) 96-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Fish SW 96-h LC50)
131-11-3	Dimethyl phthalate	194	1.5	1.7	1.6	29	-0.83	Ellington & Floyd, 1996	Staples et al. (1997)
131-11-3	Dimethyl phthalate	194	1.5	1.7	1.6	57.31	-0.53	Ellington & Floyd, 1996	Zaroogian et al. (1985)
84-66-2	Diethyl phthalate	222	2.5	2.7	2.4	29.979	-0.87	Ellington & Floyd, 1996	Zaroogian et al. (1985)
84-66-2	Diethyl phthalate	222	2.5	2.7	2.4	29	-0.88	Ellington & Floyd, 1996	Staples et. al (1997)
85-68-7	Butylbenzyl phthalate	312	4.8	4.8	4.7	0.51	-2.79	Ellington & Floyd, 1996	Staples et. al (1997)
85-68-7	Butylbenzyl phthalate	312	4.8	4.8	4.7	3	-2.02	Ellington & Floyd, 1996	Staples et al. (1997)
	Kow Limit		5	5			-2.71	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
51630-58-1	Fenvalerate	420	6.8	6.8	6.2	0.004	-5.02	Hansch & Leo, 1985	Zaroogian et al., 1985
52645-53-1	Permethrin	391	7.1	7.4	6.5	0.068	-3.76	Hansch & Leo, 1985	Zaroogian et al., 1985
Data Not Included in SAR:									
131-11-3	Dimethyl phthalate	194	1.5	1.7		100-115	-0.29 - -0.23		Staples et. al (1997)
84-74-2	Dibutyl phthalate	278	4.7	4.6		>0.6	>-2.67		Staples et. al (1997)
85-68-7	Butylbenzyl phthalate	312	4.8	4.8		>0.68	>-2.66		Staples et. al (1997)
85-69-8	Butyl 2-ethylhexyl phthalate	334	6.6	6.5		>1.36	>-2.39		Staples et. al (1997)
84-75-3	Dihexyl phthalate	335	6.8	6.6	6.8	>0.78	>-2.63	Ellington & Floyd, 1996	Staples et. al (1997)
27554-26-3	Diisooctyl phthalate	390	8.6	8.4		>0.48	>-2.91		Staples et. al (1997)
117-81-7	Di-(2-ethylhexyl) phthalate	391	8.6	8.4	8.1	>0.17	>-3.36	DeBruijn et al. 1989	Staples et. al (1997)
25724-58-7 (68515-51-5)	Di-(n-hexyl, n-octyl, n-decyl)- phthalate	390	8.9	8.5		>0.37	>-3.02		Staples et. al (1997)
28553-12-0	Diisononyl phthalate	419	9.7	9.4		>0.52	>-2.91		Staples et. al (1997)
26761-40-0	Diisodecyl phthalate	447	11	10		>0.47	>-2.98		Staples et. al (1997)
3648-20-2	Diundecyl phthalate	475	12	12		>0.22	>-3.33		Staples et. al (1997)
119-06-2	Ditridecyl phthalate	531	14	14		>0.65	>-2.91		Staples et. al (1997)
						* indicates no effects at saturation			

REFERENCES:

Staples CA, Adams W, Parkerton TF, Gorsuch JW, Biddinger GR, Reinert KH. 1997. Aquatic toxicity of eighteen phthalate esters. Environmental Toxicology and Chemistry, 16 (5): 875-891.

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

MYSID SHRIMP (SW) 96-h LC50 (Mortality)

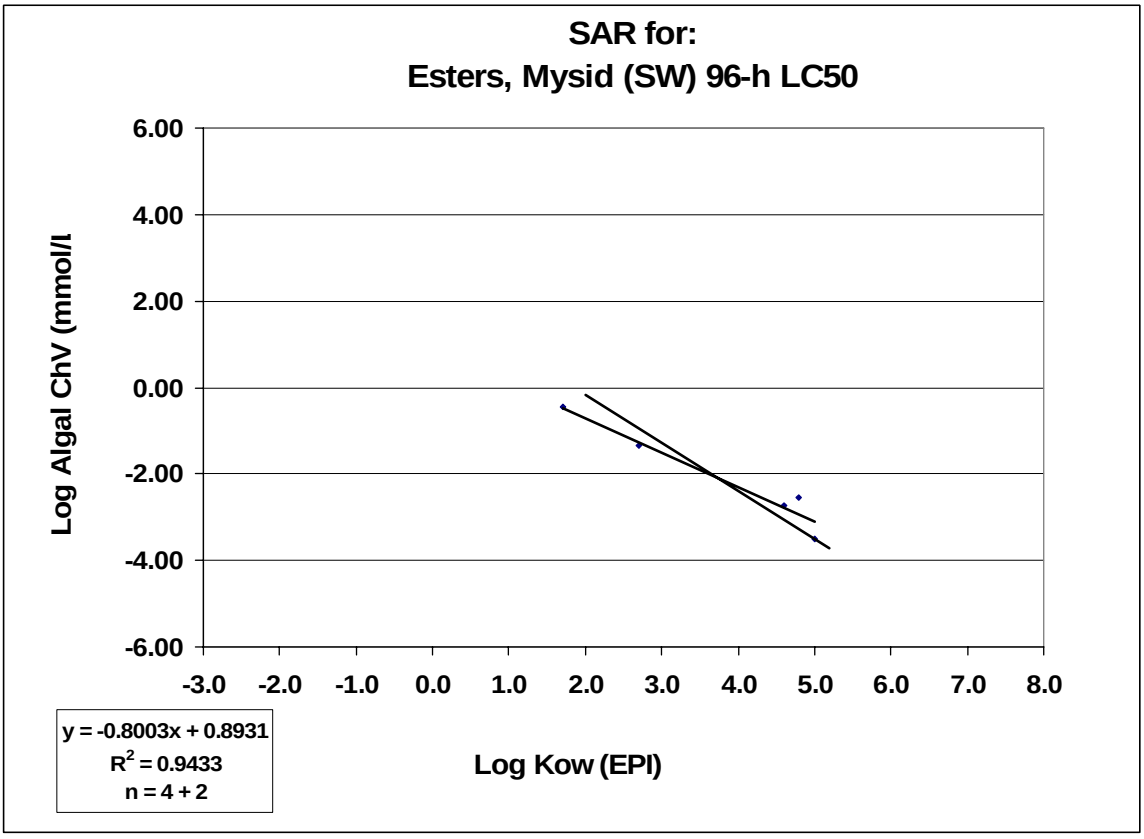
ESTIMATED TOXICITY:
The saltwater mysid shrimp 96-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h LC50 (mmol/L) = - 0.8003 (log Kow) + 0.8931

The LC50 is in millimoles per liter (mM/L); N = 4 + 2; and the Coefficient of Determination (R^2) = 0.9433. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 5
Maximum MW: 1,000

GRAPH:



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 Kow value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Mysid (SW) Inv 96-h LC50 (mg/L)	Log Mysid (SW) Inv 96-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Mysid SW Inv 96-h LC50)
131-11-3	Dimethyl phthalate	194	1.5	1.7	1.6	68.6	-0.45	Ellington & Floyd, 1996	Staples et. al (1997)
84-66-2	Diethyl phthalate	222	2.5	2.7	4.5	10.3	-1.33	Ellington & Floyd, 1996	Staples et. al (1997)
84-74-2	Dibutyl phthalate	278	4.7	4.6	4.5	0.5	-2.75	Ellington & Floyd, 1996	Staples et. al (1997)
85-68-7	Butyl-benzyl phthalate	312	4.8	4.8	4.7	0.9	-2.54	Ellington & Floyd, 1996	Staples et. al (1997)
	Kow Limit		5	5			-3.51	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
51630-58-1	Fenvalerate	420	6.8	6.8	6.2	0.0001	-6.62	Hansch et al., 1995	Zaroogian et al., 1985
Data Not Included in SAR:									
85-69-8	Butyl 2-ethylhexyl phthalate	334	6.6	6.5		>0.5	>-2.82		Staples et. al (1997)
84-75-3	Dihexyl phthalate	335	6.8	6.6	6.8	>0.32	>-3.02	Ellington & Floyd, 1996	Staples et. al (1997)
103-23-1	Di(2-ethylhexyl) adipate	371	7.9	8.1		> 0.23	>-3.2		8(e)-10258
27554-26-3	Diisooctyl phthalate	390	8.6	8.4		>0.55	>-2.85		Staples et. al (1997)
117-81-7	Di-(2-ethylhexyl) phthalate	391	8.6	8.4	7.6	>0.37	>-3.02	DeBruijn et al. 1989	Staples et. al (1997)
25724-58-7	Di-(n-hexyl, n-octyl, n-	390	8.9	8.5		>0.26	>-3.18		Staples et. al (1997)
28553-12-0	Diisononyl phthalate	419	9.7	9.4		>0.39	>-3.03		Staples et. al (1997)
26761-40-0	Diisodecyl phthalate	447	11	10		>0.08	>-3.75		Staples et. al (1997)
3648-20-2	Diundecyl phthalate	475	12	12		>0.29	>-3.21		Staples et. al (1997)
119-06-2	Ditridecyl phthalate	531	14	14		>0.8	>-2.81		Staples et. al (1997)
						* indicates no effects at saturation			

REFERENCES:

Staple CA, Adams W, Parkerton TF, Gorsuch JW, Biddinger GR, Reinert KH. 1997. Aquatic toxicity of eighteen phthalate esters. Environmental Toxicology and Chemistry, 16 (5): 875-891.

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

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

FISH (SW) ChV

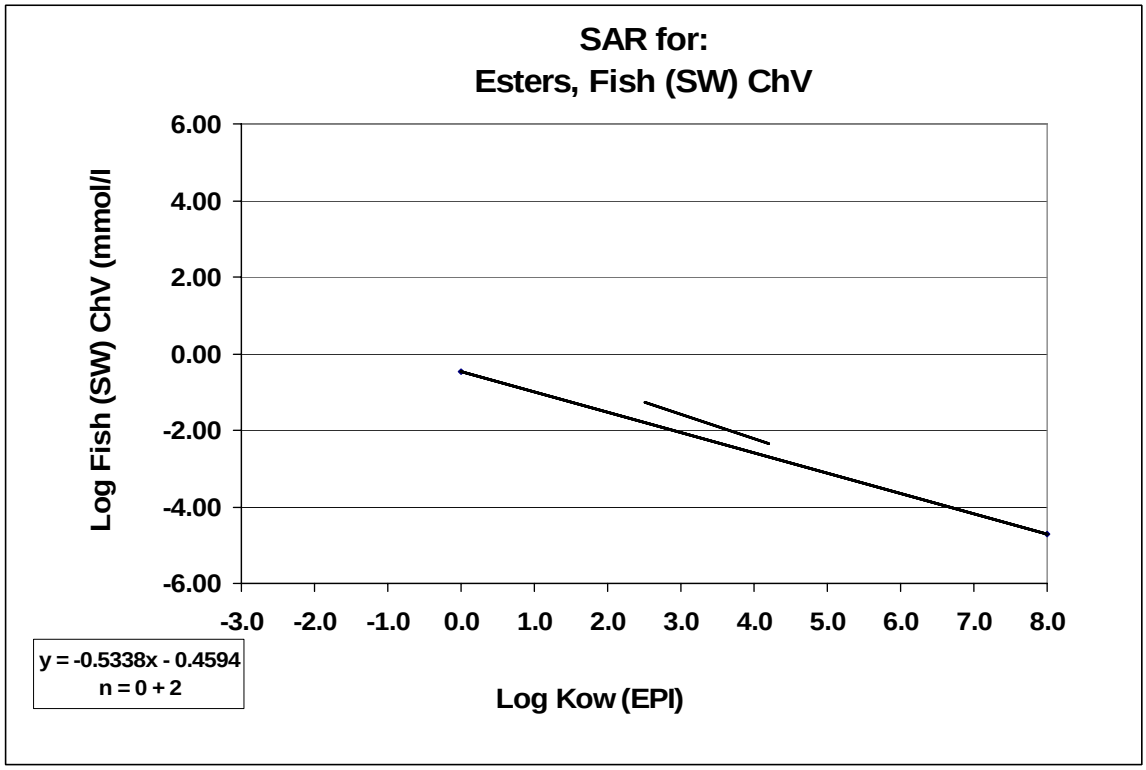
ESTIMATED TOXICITY:
The fish (SW) chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = - 0.5338 (log Kow) - 0.4594

The ChV is in millimoles per liter (mM/L); N = 0 + 2; and the Coefficient of Determination (R^2) = N/A. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8
Maximum MW: 1,000

GRAPH:



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 Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish (SW) ChV (mg/L)	Log Fish (SW) ChV (mmol/L)	Reference (Meas. Kow)	Reference (Fish SW ChV)
			0	0			-0.46		1/10 F96 (SW) Esters SAR
	Kow Limit		8	8			-4.73	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
						* indicates no effects at saturation			

REFERENCES:

MYSID SHRIMP (SW) ChV

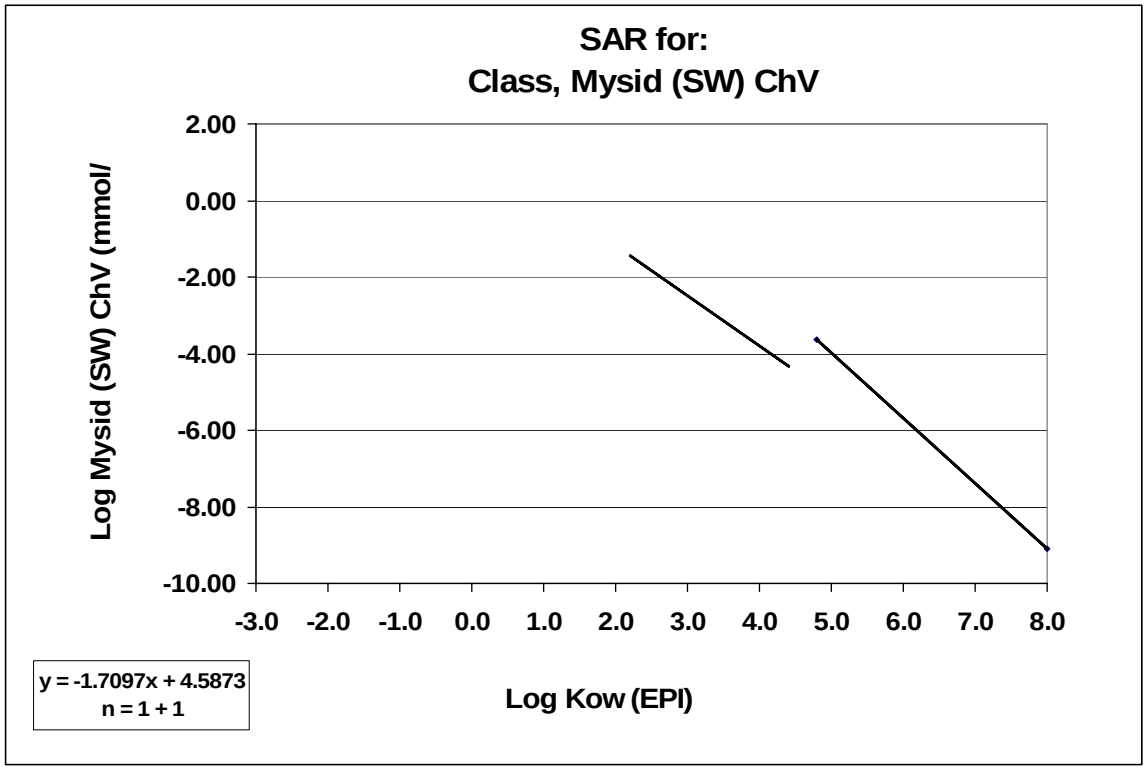
ESTIMATED TOXICITY:
The saltwater mysid shrimp ChV values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -1.7097 (log Kow) + 4.5873

The ChV is in millimoles per liter (mM/L); N = 1 + 1; and the Coefficient of Determination (R^2) = N/A. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8
Maximum MW: 1000

GRAPH:



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 Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Mysid (SW) ChV (mg/L)	Log Mysid (SW) ChV (mmol/L)	Reference (Meas. Kow)	Reference (Mysid SW ChV)
85-68-7	Butyl-benzyl phthalate	312	4.8	4.8	4.7	0.075	-3.62	Ellington & Floyd, 1999	Staples et. al (1997)
	Kow Limit		8	8			-9.09	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
						* indicates no effects at saturation			

REFERENCES:

Staples CA, Adams W, Parkerton TF, Gorsuch JW, Biddinger GR, Reinert KH. 1997. Aquatic toxicity of eighteen phthalate esters. Environmental Toxicology and Chemistry, 16 (5): 875-891.

EARTHWORM 14-d LC50 (Mortality)

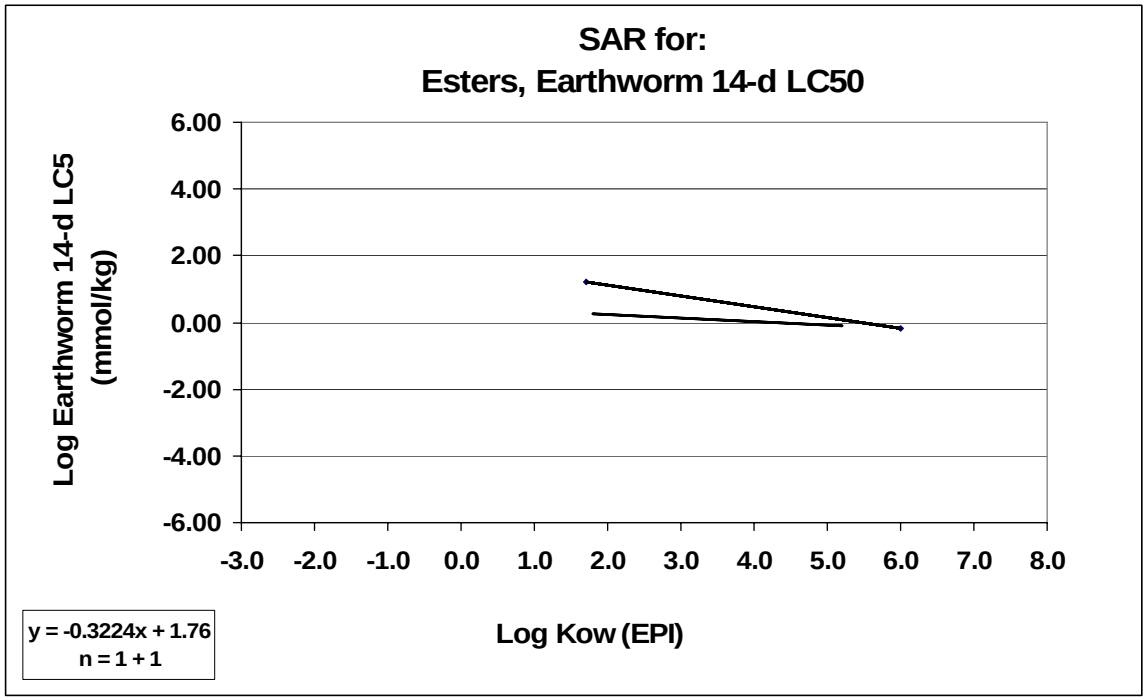
ESTIMATED TOXICITY:
The earthworm 14-d LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.3224 (log Kow) + 1.76

The LC50 is in millimoles per kilogram dry weight soil (mM/kg dry weight); N = 1+ 1; and the Coefficient of Determination (R^2) = N/A. To convert the LC50 from mM/kg to mg/kg, multiply by the molecular weight of the compound.

Maximum K_{ow}: 6
Maximum MW: 1000

GRAPH:



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 Kow value is greater than 6.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

DATA:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Earthworm LC50 (mg/kg)	Log Earthworm LC50 (mmol/kg)	Reference (Meas. Kow)	Reference Earthworm (LC50)
113-11-3	Dimethyl phthalate	194	1.5	1.7	1.6	3160	1.21	Ellington & Floyd, 1996	Neuhauser et al., 1985
	Kow Limit		6	6			-0.17	NO Cutoff	NO SAR
SAR Data Not Included in Regression Equation:									
CBI	CBI	468	1.6	2.8	3	*	*	None given	P-95-___
Data Not Included in SAR:									
* indicates no effects at saturation									

REFERENCES:

Neuhauser, E.F., Loehr, R.C., Malecki, M.R., Milligan, D.L. and Durkin, P.R. 1985. The toxicity of selected organic chemicals to the earthworm *Eisenia fetida*. Journal of Environmental Quality 14: 383-388.

FISH 96-h LC50

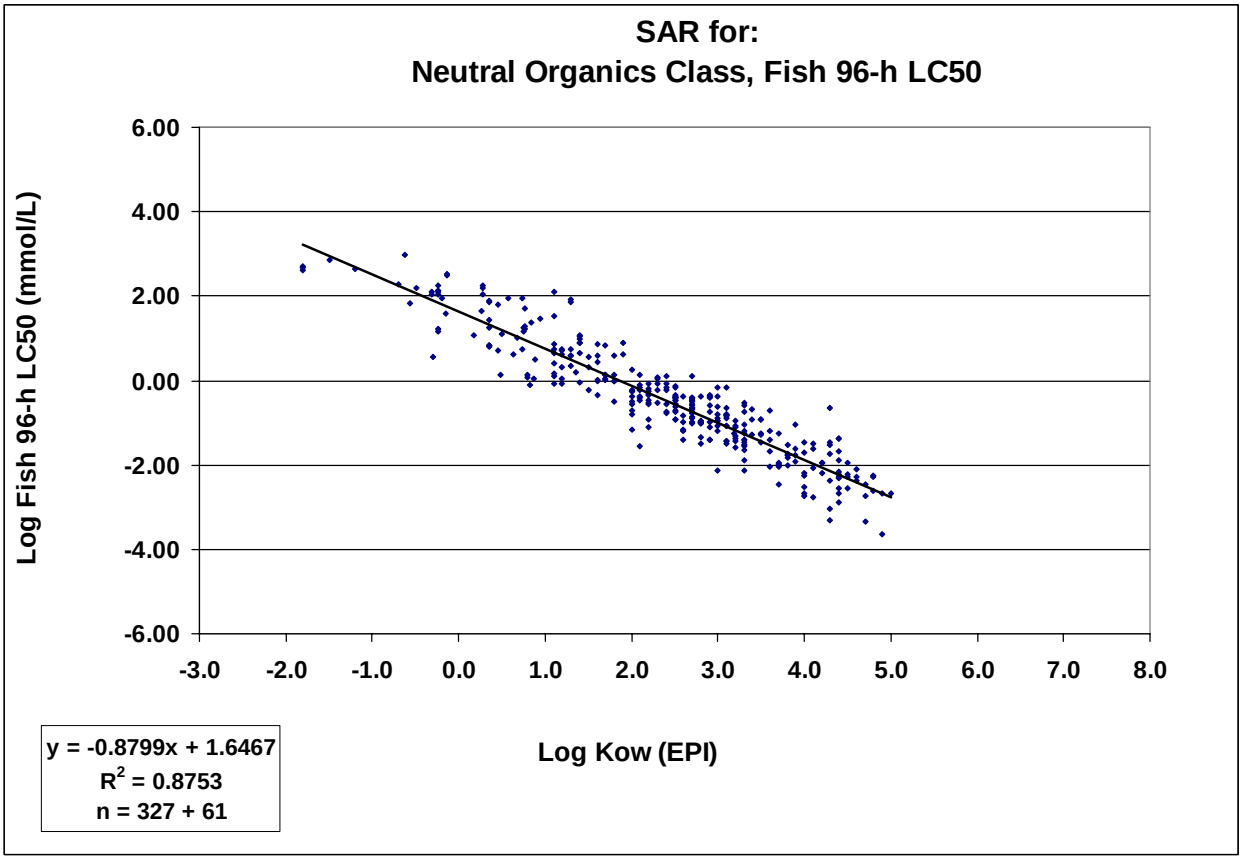
ESTIMATED TOXICITY:
The fish 96-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log LC50 (mmol/L) = -0.8799 log K_{ow} + 1.6467

The LC50 is in millimoles per liter (mM/L); N = 327 + 61; and the Coefficient of Determination (R^2) = 0.8753. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 5.0
Maximum MW: 1000

Graph:



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 Kow value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	F 96-h LC50 (mg/L)	Log F 96-h LC50 (mmol/L)	Reference (meas. Kow)	Reference (LC50)
112-27-6	Triethylene Glycol	150	-1.2	-1.8		59,900	2.60		DUL
112-27-6	Triethylene Glycol	150	-1.2	-1.8		70,200	2.67		DUL
112-27-6	Triethylene Glycol	150	-1.2	-1.8		77,400	2.71		DUL
111-46-6	2-Hydroxyethyl Ether	106	-1.3	-1.5		75200	2.85		DUL
67-68-5	Dimethyl Sulfoxide	78	-1.4	-1.2	-1.35	34000	2.64	Hansch & Leo, 1985	DUL
111-90-0	2-(2-Ethoxyethoxy)ethanol	134	-0.15	-0.69	-0.54	26,500	2.30	Funasaki et al., 1984	DUL
67-56-1	Methanol	32	-0.76	-0.63	-0.77	29400	2.96	Hansch & Leo, 1985	DUL
110-88-3	s-Trioxane	90	-0.56	-0.56	-0.43	5950	1.82	Hansch et al., 1995	DUL
127-19-5	N,N-Dimethyl acetamide	87	-0.96	-0.49	-0.77	13300	2.18	Hansch & Leo, 1985	CAS - Kennedy, 1986
123-91-1	1,4-Dioxane	88	-0.49	-0.32	-0.27	9850	2.05	Hansch & Leo, 1985	DUL
123-91-1	1,4-Dioxane	88	-0.49	-0.32	-0.27	10800	2.09	Hansch & Leo, 1985	DUL
CBI	CBI	116	0	-0.3		431	0.57		P90-____
67-64-1	Acetone	58	-0.21	-0.24	-0.24	10700	2.27	Hansch & Leo, 1985	CAS -Mount & Stephan, 1967
67-64-1	Acetone	58	-0.21	-0.24	-0.24	8120	2.15	Hansch & Leo, 1985	DUL
67-64-1	Acetone	58	-0.21	-0.24	-0.24	7280	2.10	Hansch & Leo, 1985	DUL
67-64-1	Acetone	58	-0.21	-0.24	-0.24	6210	2.03	Hansch & Leo, 1985	DUL
126-33-0	Sulfolane	120	-0.9	-0.24	-0.77	1760	1.17	Hansch & Leo, 1985	Shell, 1984
126-33-0	Sulfolane	120	-0.9	-0.24	-0.77	1930	1.21	Hansch & Leo, 1985	Shell, 1984
109-87-5	Dimethoxymethane	76	-0.43	-0.19	0	6990	1.96	Hansch & Leo, 1985	DUL
75-05-8	Acetonitrile	41	-0.39	-0.15	-0.34	1640	1.60	Hansch & Leo, 1985	DUL
64-17-5	Ethanol	46	-0.24	-0.14	-0.31	15300	2.52	Hansch & Leo, 1985	DUL
64-17-5	Ethanol	46	-0.24	-0.14	-0.31	14200	2.49	Hansch & Leo, 1985	DUL
CBI	CBI	128	0.2	0.18	0.05	1470	1.06	P92-____	P92-____
78-93-3	2-Butanone	72	0.26	0.26	0.29	3220	1.65	Hansch & Leo, 1985	DUL
67-63-0	2-Propanol	60	0.07	0.28	0.05	9640	2.21	Hansch & Leo, 1985	DUL
67-63-0	2-Propanol	60	0.07	0.28	0.05	10400	2.24	Hansch & Leo, 1985	DUL
67-63-0	2-Propanol	60	0.07	0.28	0.05	6550	2.04	Hansch & Leo, 1985	DUL
107-12-0	Propionitrile	55	0.14	0.35	0.16	1520	1.44	Hansch & Leo, 1985	DUL
71-23-8	1-Propanol	60	0.29	0.35	0.25	4630	1.89	Hansch & Leo, 1985	DUL
71-23-8	1-Propanol	60	0.29	0.35	0.25	4480	1.87	Hansch & Leo, 1985	DUL
100-70-9	2-Cyanopyridine	104	0.27	0.35	0.45	726	0.84	Sangster, 1994	DUL
111-69-3	1,4-Dicyanobutane	108	-0.42	0.35	-0.32	1930	1.25	Tanii & Hashimoto, 1986	DUL, CAS
111-69-3	1,4-Dicyanobutane	108	-0.42	0.35	-0.32	670	0.79	Tanii & Hashimoto, 1985	CAS
111-69-3	1,4-Dicyanobutane	108	-0.42	0.35	-0.32	720	0.82	Tanii & Hashimoto, 1985	CAS
4412-91-3	3-Furanmethanol	98	0.28	0.45	0.3	508	0.71	Hansch, C. et al. 1995	Veith et al., 1983
CBI	CBI	118	-0.4	0.46		7400	1.80		P92-____
1122-54-9	4-Acetylpyridine	121	0.48	0.49	0.48	168	0.14	Hansch & Leo, 1985	DUL
685-91-6	N,N-Diethylacetamide	115	0.26	0.5	0.34	1500	1.12	Hansch & Leo, 1985	DUL
107-41-5	2-Methyl-2,4-pentanediol	118	-0.68	0.58		10700	1.96		DUL
120-07-0	N-Phenyldiethanolamine	181	0.6	0.63		735	0.61		DUL
563-80-4	3-Methyl-2-butanone	86	0.57	0.67	0.84	864	1.00	Hansch et al., 1995	DUL
75-65-0	2-Methyl-2-Propanol	74	0.47	0.73	0.35	6410	1.94	Hansch & Leo, 1985	DUL
55-21-0	Benzamide	121	0.66	0.74	0.64	661	0.74	Hansch & Leo, 1985	DUL
96-22-0	3-Pentanone	86	0.79	0.75	0.99	1540	1.25	Hansch & Leo, 1985	DUL
107-87-9	2-Pentanone	86	0.91	0.75	0.91	1240	1.16	Hansch & Leo, 1985	DUL
693-93-6	4-Methyloxazole	83	0.09	0.76		1390	1.22		DUL
78-83-1	2-Methy-1-propanol	74	0.69	0.77	0.76	1430	1.29	Hansch & Leo, 1985	DUL
78-92-2	(+-)-2-Butanol	74	0.60	0.77	0.61	3670	1.69	Hansch & Leo, 1985	DUL
110-86-1	Pyridine	79	0.65	0.8	0.65	106	0.13	Hansch & Leo, 1985	DUL

110-86-1	Pyridine	79	0.65	0.8	0.65	93.8	0.07	Hansch & Leo, 1985	DUL
3424-93-9	o-Methoxybenzamide	151	0.86	0.82	0.86	120	-0.10	Hansch & Leo, 1985	DUL
71-36-3	1-Butanol	74	0.82	0.84	0.88	1730	1.37	Hansch & Leo, 1985	DUL
2859-67-8	3-(3-Pyridyl)-1-propanol	137	0.22	0.87	0.6	150	0.04	Hansch & Leo, 1985	DUL
109-97-7	Pyrrole	67	0.76	0.88	0.75	210	0.50	Hansch & Leo, 1985	DUL
109-99-9	Tetrahydrofuran	72	0.33	0.94	0.46	2160	1.48	Hansch & Leo, 1985	DUL
60-29-7	Diethyl Ether	74	0.87	1.1	0.89	2560	1.54	Hansch & Leo, 1985	DUL
108-94-1	Cyclohexanone	98	0.81	1.1	0.81	527	0.73	Hansch & Leo, 1985	DUL
108-94-1	Cyclohexanone	98	0.81	1.1	0.81	732	0.87	Hansch & Leo, 1985	DUL
75-97-8	3,3-Dimethyl-2-butanone	100	0.97	1.1	1.20	87	-0.06	Hansch et al., 1995	DUL
932-16-1	2-Acetyl-1-methylpyrrole	123	0.84	1.1		157	0.11		DUL
100-79-8	Solketal	132	0.19	1.1		16700	2.10		DUL
122-99-6	2-Phenoxyethanol	138	1.2	1.1	1.16	344	0.40	Hansch & Leo, 1985	DUL
920-66-1	1,1,1,3,3,3-Hexafluoro-2-propanol	168	1.6	1.1	1.66	244	0.16	Pomona, 1987	DUL
29911-28-2	Dipropylene glycol n-butyl ether	190	0.12	1.1	1.7	840	0.65	Datasheet	SIDS
108-10-1	4-Methyl-2-pentanone	100	1.2	1.2	1.31	505	0.70	Tanii & Hashimoto, 1986	DUL
108-10-1	4-Methyl-2-pentanone	100	1.2	1.2	1.31	540	0.73	Tanii & Hashimoto, 1986	DUL
591-78-6	2-Hexanone	100	1.4	1.2	1.38	428	0.63	Hansch & Leo, 1985	DUL
115-20-8	2,2,2-trichloroethanol	149	1.5	1.2	1.4	299	0.30	Hansch, C. et al. 1995	Veith et al., 1983
13909-73-4	2', 3', 4'-Trimethoxyacetophenone	210	1.6	1.2	1.63	172	-0.09	Hansch et al., 1995	DUL
13909-73-4	2', 3', 4'-Trimethoxyacetophenone	210	1.6	1.2	1.63	229	0.04	Hansch et al., 1995	DUL
75-09-2	Dichloromethane	85	1.2	1.3	1.25	330	0.59	Hansch & Leo, 1985	DUL
71-41-0	1-Pentanol	88	1.4	1.3	1.51	472	0.73	Sangster, 1994	DUL
629-40-3	1,6-Dicyanohexane	136	0.63	1.3	0.59	528	0.59	Tanii & Hashimoto, 1985	DUL
126-81-8	5, 5-Dimethyl-1,3-cyclohexanedione	140	0.59	1.3		11500	1.91		DUL
383-63-1	Ethyl trifluoroacetate	142	1.3	1.3	1.18	10000	1.85	Hansch & Leo, 1985	DUL
CBI	CBI	248	1.9	1.3		564	0.36		P88-___
108-99-6	3-Picoline	93	1.1	1.35	1.2	144	0.19	Hansch & Leo, 1985	DUL
110-00-9	Furan	68	1.3	1.4	1.34	61	-0.05	Hansch & Leo, 1985	DUL
1634-04-4	tert-Butyl Methyl Ether	88	1.1	1.4	0.94	672	0.88	Hansch et al., 1995	DUL
1634-04-4	tert-Butyl Methyl Ether	88	1.1	1.4	0.94	706	0.90	Hansch et al., 1995	Veith et al., 1983
1634-04-4	tert-Butyl Methyl Ether	88	1.1	1.4	0.94	980	1.05	Hansch et al., 1995	CAS-Wetal, 2001
1634-04-4	tert-Butyl Methyl Ether	88	1.1	1.4	0.94	1057	1.08	Hansch et al., 1995	CAS-Wetal, 2001
108-89-4	4-Picoline	93	1.1	1.4	1.22	403	0.64	Hansch & Leo, 1985	DUL
109-06-8	2-Picoline	93	1.1	1.4	1.11	897	0.98	Hansch & Leo, 1985	DUL
497-37-0	exo-Norborneol	112	1	1.5		228	0.31		DUL
67-66-3	Chloroform	119	2.0	1.5	1.97	70.7	-0.23	Hansch & Leo, 1985	DUL
29553-26-2	2-Methyl-3,3,4,4-tetrafluoro-2-butanol	160	1	1.5		582	0.56		DUL
108-93-0	Cyclohexanol	100	1.3	1.6	1.23	704	0.85	Hansch & Leo, 1985	DUL
928-96-1	cis-3-Hexen-1-ol	100	1.4	1.6		381	0.58		DUL
928-97-2	trans-3-Hexen-1-ol	100	1.4	1.6		271	0.43		DUL
100-61-8	N-Methylaniline	107	1.6	1.6	1.66	100	-0.03	Hansch & Leo, 1985	DUL
5683-33-0	2-Dimethylaminopyridine	122	1.7	1.6	1.65	127	0.02	Yamagami et al., 1990	DUL
22726-00-7	m-Bromobenzamide	200	1.7	1.6	1.65	92.7	-0.33	Hansch et al., 1995	DUL
77-74-7	3-Methyl-3-pentanol	102	1.5	1.7		672	0.82		DUL
110-12-3	5-Methyl-2-hexanone	114	1.8	1.7	1.88	159	0.14	Tanii & Hashimoto, 1986	DUL
110-43-0	2-Heptanone	114	1.9	1.7	1.98	131	0.06	Hansch & Leo, 1985	DUL
98-86-2	Acetophenone	120	1.6	1.7	1.58	162	0.13	Hansch & Leo, 1985	DUL
CBI	CBI	172	1.7	1.7		180	0.02		P94-___
107-06-2	1,2-Dichloroethane	99	1.5	1.8	1.48	136	0.14	Hansch & Leo, 1985	DUL
111-27-3	1-Hexanol	102	1.9	1.8	2.03	97.7	-0.02	Hansch & Leo, 1985	DUL
100-71-0	2-Ethylpyridine	107	1.7	1.8	1.69	414	0.59	Hansch & Leo, 1985	DUL
98-95-3	Nitrobenzene	123	1.9	1.8	1.85	119	-0.01	Hansch & Leo, 1985	DUL
459-59-6	4-Fluoro-N-methylaniline	125	2.1	1.8		38.4	-0.51		DUL
108-20-3	Isopropyl Ether	102	1.5	1.9	1.52	786	0.89	Funasaki et al., 1985	DUL
20662-84-4	2,4,5-Trimethyloxazole	111	2.2	1.9		448	0.61		DUL
71-43-2	Benzene	78	2.1	2.0	2.13	12.6	-0.79	Hansch & Leo, 1985	DUL
71-43-2	Benzene	78	2.1	2.0	2.13	24.6	-0.50	Hansch & Leo, 1985	DUL
71-43-2	Benzene	78	2.1	2.0	2.13	5.3	-1.17	Hansch & Leo, 1985	CAS - ETFS
71-43-2	Benzene	78	2.1	2.0	2.13	22	-0.55	Hansch & Leo, 1985	CAS - ETFS
71-43-2	Benzene	78	2.1	2.0	2.13	33	-0.37	Hansch & Leo, 1985	CAS - ETFS
18368-63-3	6-Chloro-2-picoline	128	1.9	2		232	0.26		DUL
350-46-9	1-Fluoro-4-nitrobenzene	141	2	2	1.8	28.4	-0.70	Hansch & Leo, 1985	DUL
761-65-9	N,N-Dibutylformamide	157	2.1	2		89.3	-0.25		DUL
14548-46-0	4-Benzoylpyridine	183	2	2	1.98	103	-0.25	Hansch & Leo, 1985	DUL
79-00-5	1,1,2-Trichloroethane	133	2.1	2.0	1.89	81.6	-0.21	Pomona, 1987	DUL
600-36-2	2,4-Dimethyl-3-pentanol	116	1.9	2.1		163	0.15		DUL
529-19-1	o-Tolunitrile	117	2.2	2.1	2.2	44.7	-0.42	Pomona, 1987	DUL
110-93-0	6-Methyl-5-hepten-2-one	126	1.8	2.1		85.7	-0.17		DUL
91-22-5	Quinoline	129	2.0	2.1	2.03	77.8	-0.22	Hansch & Leo, 1985	DUL
552-41-0	2'-hydroxy-4'-methoxyacetophenone	166	2	2.1	2	54.9	-0.48	BioByte, 1995	Veith et al., 1983
6001-64-5	1,1,1-Trichloro-2-methyl-2-propanol Hydrate	177	2	2.1	2.03	135	-0.12	Hansch & Leo, 1985	DUL
5465-65-6	4'-Chloro-3'-nitroacetophenone	200	2	2.1		5.5	-1.56		DUL
945-51-7	Phenyl Sulfoxide	202	2.1	2.1	2.06	87.3	-0.36	Hansch & Leo, 1985	DUL

121-69-7	N,N-Dimethylaniline	121	2.3	2.2	2.31	78.2	-0.19	Hansch & Leo, 1985	DUL
121-69-7	N,N-Dimethylaniline	121	2.3	2.2	2.31	52.6	-0.36	Hansch & Leo, 1985	DUL
106-94-5	1-Bromopropane	123	2.1	2.2	2.1	67.3	-0.26	Hansch & Leo, 1985	DUL
111-13-7	2-Octanone	128	2.4	2.2	2.37	36	-0.55	Tanii & Hashimoto, 1986	DUL
95-16-9	Benzothiazole	135	2.2	2.2	1.99	64	-0.32	Brown & Lee, 1992	CAS
150-78-7	p-Dimethoxybenzene	138	2.2	2.2	2.04	117	-0.07	Dunn et al., 1983	DUL
79-34-5	1,1,2,2-Tetrachloroethane	168	2.6	2.2	2.39	20.3	-0.92	Hansch & Leo, 1985	DUL
25322-20-7	Tetrachloroethane	168	2.6	2.2	2.4	13.5	-1.09	Hansch, C. et al. 1995	Veith et al., 1983
91-88-3	2-(N-Ethyl-m-toluidino)ethanol	179	2.4	2.2		52.9	-0.53		DUL
621-08-9	Benzyl Sulfoxide	230	2	2.2	1.99	80.1	-0.46	Hansch et al., 1995	DUL
78-87-5	1,2-Dichloropropane	113	2.0	2.3	1.98	127	0.05	Sangster, 1994	DUL
142-28-9	1,3-Dichloropropane	113	1.7	2.3	2	94.2	-0.08	Hansch & Leo, 1985	DUL
142-28-9	1,3-Dichloropropane	113	1.7	2.3	2	131	0.06	Hansch & Leo, 1985	DUL
111-70-6	1-Heptanol	116	2.4	2.3	2.62	34.5	-0.53	Sangster, 1994	DUL
134-62-3	N,N-Diethyl-m-toluamide	191	2.2	2.3	2.18	110	-0.24	Sangster, 1993	DUL
1717-00-6	1,1-Dichloro-1-fluoro ethane	117	2	2.4		150	0.11		FYI-695
CBI	CBI	117	2	2.4		20	-0.77		P88-____
104-90-5	5-Ethyl-2-methylpyridine (2-picoline, 5-ethyl)	121	2.5	2.4		81.1	-0.17		DUL, CAS
104-90-5	5-Ethyl-2-methylpyridine	121	2.5	2.4		70	-0.24		CAS
99-08-1	m-Nitrotoluene	137	2.4	2.4	2.45	25.6	-0.73	Hansch & Leo, 1985	DUL
56-23-5	Carbon Tetrachloride	154	2.9	2.4	2.83	41.4	-0.57	Hansch & Leo, 1985	DUL
4916-57-8	1,2-Bis(4-pyridyl)ethane	184	1.6	2.4		151	-0.09		DUL
108-88-3	Toluene	92	2.6	2.5	2.73	36.2	-0.41	Hansch & Leo, 1985	DUL
108-88-3	Toluene	92	2.6	2.5	2.73	31.7	-0.46	Hansch & Leo, 1985	DUL
108-88-3	Toluene	92	2.6	2.5	2.73	17.5	-0.72	Hansch & Leo, 1985	CAS - ETFS
108-88-3	Toluene	92	2.6	2.5	2.73	38.1	-0.38	Hansch & Leo, 1985	CAS - ETFS
625-86-5	2,5-Dimethylfuran	96	2.3	2.5	2.24	71.1	-0.13	Hansch et al., 1995	DUL
271-89-6	2,3-Benzofuran	118	2.7	2.5	2.67	14	-0.93	Hansch & Leo, 1985	DUL
496-16-2	2,3-Dihydrobenzofuran	120	2	2.5	2.14	81.7	-0.17	Hansch & Leo, 1985	DUL
79-01-6	1,1,2-trichloroethylene	131	2.6	2.5	2.4	44.1	-0.47	Hansch, C. et al., 1995	Veith et al., 1983
589-09-3	N-Allylaniline	133	2.2	2.5		35.9	-0.57		DUL
96-18-4	1,2,3-Trichloropropane	147	2	2.5	2.27	66.5	-0.34	Chem Inspect Test Inst. 199	DUL
5395-75-5	3,6-Dithiaoctane	150	2.5	2.5		60.2	-0.40		DUL
88-73-3	1-Chloro-2-nitrobenzene	158	2.4	2.5	2.2	29.6	-0.73	Hansch & Leo, 1985	DUL
121-73-3	1-Chloro-2-nitrobenzene	158	2.6	2.5	2.46	18.8	-0.92	Hansch et al., 1995	DUL
368-77-4	a,a,a-Trifluoro-m-tolunitrile	171	2.5	2.5		47.7	-0.55		DUL
447-60-9	a,a,a-Trifluoro-o-tolunitile	171	2.5	2.5		42.2	-0.61		DUL
CBI	CBI	530	2.7	2.5		206	-0.41		P98-____
108-90-7	Chlorobenzene	113	2.9	2.6	2.84	16.9	-0.83	Sangster, 1994	DUL
108-90-7	Chlorobenzene	113	2.9	2.6	2.84	4.5	-1.40	Sangster, 1994	CAS-Bailey et al., 1985
108-90-7	Chlorobenzene	113	2.9	2.6	2.84	7.4	-1.18	Sangster, 1994	CAS-Bailey et al., 1985
83-34-1	3-Methyindole	131	2.2	2.6	2.60	8.84	-1.17	Hansch & Leo, 1985	DUL
700-58-3	2-Adamantanone	150	1.5	2.6		60.8	-0.39		DUL
939-23-1	4-Phenylpyridine	155	2.5	2.6	2.59	16.1	-0.98	Hansch & Leo, 1985	DUL
95-52-3	2-Fluorotoluene	110	2.8	2.7		19.3	-0.76		DUL
95-52-3	2-Fluorotoluene	110	2.8	2.7		19.6	-0.75		DUL
15045-43-9	2, 2, 5, 5-Tetramethyltetrahydrofuran	128	2.1	2.7	2.06	168	0.12	Hansch et al., 1995	DUL
104-76-7	2-Ethylhexanol	130	2.8	2.7		28.2	-0.66		DUL
104-76-7	2-Ethylhexanol	130	2.8	2.7		17.1	-0.88		CAS-SIDS
104-76-7	2-Ethylhexanol	130	2.8	2.7		28	-0.67		CAS-SIDS
104-76-7	2-Ethylhexanol	130	2.8	2.7		29.6	-0.64		CAS-SIDS
104-76-7	2-Ethylhexanol	130	2.8	2.7		34	-0.58		CAS-SIDS
71-55-6	1,1,1-Trichloroethane	133	2.5	2.7	2.49	52.9	-0.40	Hansch & Leo, 1985	DUL
71-55-6	1,1,1-Trichloroethane	133	2.5	2.7	2.49	42.3	-0.50	Hansch & Leo, 1985	DUL
99-97-8	N,N-Dimethyl-p-toluidine	135	2.8	2.7	2.81	52	-0.41	Sangster, 1993	DUL
99-97-8	N,N-Dimethyl-p-toluidine	135	2.8	2.7	2.81	46	-0.47	Sangster, 1993	DUL
102-27-2	N-Ethyl-m-toluidine	135	2.7	2.7		49.5	-0.44		DUL
109-65-9	1-Bromobutane	137	2.7	2.7	2.75	36.7	-0.57	Hansch & Leo, 1985	DUL
502-56-7	5-Nonanone	142	3	2.7		31	-0.66		DUL
821-55-6	2-Nonanone	142	3	2.7	3.14	15.2	-0.97	Hansch et al., 1995	DUL
5673-07-4	2,6-Dimethoxytoluene	152	2.9	2.7	2.87	20.2	-0.88	Nakagawa et al., 1992	DUL
6575-09-3	2-Chloro-6-methylbenzonitrile	152	2.8	2.7		15.1	-1.00		DUL
110-56-5	1,4-Dichlorobutane	127	2.2	2.8		51.6	-0.39		DUL
111-87-5	n-Octanol	130	2.9	2.8	3	13.5	-0.98	Hansch et al., 1995	Broderius et al., 2005
111-87-5	n-Octanol	130	2.9	2.8	3	13.5	-0.98	Hansch et al., 1995	DUL
111-87-5	n-Octanol	130	2.9	2.8	3	14.6	-0.95	Hansch et al., 1995	DUL
111-87-5	n-Octanol	130	2.9	2.8	3	13.1	-1.00	Hansch et al., 1995	DUL
111-87-5	n-Octanol	130	2.9	2.8	3	14	-0.97	Hansch et al., 1995	DUL
111-87-5	n-Octanol	130	2.9	2.8	3	13.1	-1.00	Hansch et al., 1995	DUL
111-87-5	n-Octanol	130	2.9	2.8	3	13	-1.00	Hansch et al., 1995	DUL
CBI	CBI	172	3	2.8	2.74	5.4	-1.50	Hansch et al., 1995	P93-____
CBI	CBI	172	3	2.8	2.74	17	-1.01	Hansch et al., 1995	P93-____
80965-30-6	4-(4-Methyl-1-piperidinyl) pyridine	176	3.3	2.8		7.8	-1.35		P83-____; 8(e)-____
592-46-1	2,4-Hexadiene	82	3	2.9	2.8	20.6	-0.60	Hansch et al., 1995	DUL

498-66-8	Norbornylene	94	2.6	2.9		10	-0.97		DUL
100-42-5	Styrene	104	2.9	2.9	2.95	4.02	-1.41	Hansch & Leo, 1985	DUL
111-47-7	n-Propyl Sulfide	118	3	2.9		21.7	-0.74		DUL
464-45-9	[(1S)-endo]-(-)-Borneol	154	2.6	2.9	2.32	67.8	-0.36	Hansch et al., 1995	DUL
464-45-9	[(1S)-endo]-(-)-Borneol	154	2.6	2.9	2.32	59	-0.42	Hansch et al., 1995	DUL
103-05-9	Benzyl-tert-butanol	164	2.4	2.9		66.4	-0.39		DUL
709-98-8	Propanil	218	3.3	2.9	3.07	8.6	-1.40	Hansch & Leo, 1985	DUL
14548-45-9	4-Bromophenyl 3-Pyridyl Ketone	262	3	2.9		20.4	-1.11		DUL
100-41-4	Ethylbenzene	106	3.2	3	3.15	12.1	-0.94	Hansch & Leo, 1985	DUL
100-41-4	Ethylbenzene	106	3.2	3	3.15	9.09	-1.07	Hansch & Leo, 1985	DUL
100-41-4	Ethylbenzene	106	3.2	3	3.15	14	-0.88	Hansch & Leo, 1985	CAS - ETFS
100-41-4	Ethylbenzene	106	3.2	3	3.15	45.3	-0.37	Hansch & Leo, 1985	CAS - ETFS
100-41-4	Ethylbenzene	106	3.2	3	3.15	70.4	-0.18	Hansch & Leo, 1985	CAS - ETFS
142-96-1	Butyl Ether	130	3	3	3.21	32.3	-0.60	Hansch et al., 1995	DUL
464-48-2	(1S)-(-)-Camphor	152	2.2	3		17	-0.95		DUL
363-72-4	Pentafluorobenzene	168	2.9	3	2.53	27	-0.79	Hetel, 1995	DUL
2234-16-4	2', 4'-Dichloroacetophenone	189	2.7	3		11.7	-1.21		DUL
75-47-8	Iodoform	394	3.5	3.0		2.92	-2.13		DUL
513-81-5	2,3-Dimethyl-1,3-butadiene	82	2.7	3.1		6.91	-1.07		DUL
95-47-6	o-Xylene	106	3.1	3.1	3.12	16.4	-0.81	Hansch & Leo, 1985	DUL
95-47-6	o-Xylene	106	3.1	3.1	3.12	16.4	-0.81	Hansch & Leo, 1985	DUL
106-42-3	p-Xylene	106	3.1	3.1	3.15	8.87	-1.08	Hansch & Leo, 1985	DUL
108-38-3	m-Xylene	106	3.1	3.1	3.2	16	-0.82	Hansch & Leo, 1985	DUL
1330-20-7	Xylene, Mixed	106	3.1	3.1	3.12	13.4	-0.90	Hansch & Leo, 1985	DUL
1330-20-7	Xylene, Mixed	106	3.1	3.1	3.12	24.5	-0.64	Hansch & Leo, 1985	CAS-Bailey et al., 1985
1330-20-7	Xylene, Mixed	106	3.1	3.1	3.12	15.7	-0.83	Hansch & Leo, 1985	CAS-Bailey et al., 1985
470-82-6	Cineole	154	2.8	3.1	2.5	102	-0.18	Hansch et al., 1995	DUL
76-01-7	Pentachloroethane	202	3.6	3.1	3.22	6.65	-1.48	Hansch et al., 1995	Broderius et al., 2005
76-01-7	Pentachloroethane	202	3.6	3.1	3.22	7.35	-1.44	Hansch et al., 1995	Broderius et al., 2005
76-01-7	Pentachloroethane	202	3.6	3.1	3.22	7.53	-1.43	Hansch et al., 1995	DUL
110-82-7	Cyclohexane	84	3.4	3.2	3.44	4.53	-1.27	Hansch & Leo, 1985	DUL
91-20-3	Napthalene	128	3.3	3.2	3.3	6.14	-1.32	Hansch & Leo, 1985	DUL
91-66-7	N, N-Diethylaniline	149	3.2	3.2	3.31	16.4	-0.96	Hansch & Leo, 1985	DUL
693-54-9	2-Decanone	156	3.5	3.2	3.73	5.7	-1.44	Tanii et al., 1986	DUL
693-54-9	2-Decanone	156	3.5	3.2	3.73	4.1	-1.58	Tanii et al., 1986	DUL
119-61-9	Benzophenone	182	3.2	3.2	3.18	15.3	-1.08	Hansch & Leo, 1985	DUL
119-61-9	Benzophenone	182	3.2	3.2	3.18	14.2	-1.11	Hansch & Leo, 1985	DUL
CBI	CBI	221	3.4	3.2		9.3	-1.38		P92-___
110-54-3	Hexane	86	3.9	3.3	3.9	2.5	-1.54	Hansch & Leo, 1985	DUL
2243-27-8	n-Octyl Cyanide	139	3.3	3.3	3.12	4.91	-1.45	Tanii & Hashimoto, 1984	DUL
2243-27-8	n-Octyl Cyanide	139	3.3	3.3	3.12	5.61	-1.39	Tanii & Hashimoto, 1984	DUL
628-76-2	1,5-Dichloropentane	141	2.8	3.3		25.3	-0.75		DUL
143-08-8	1-Nonanol	144	3.5	3.3	3.77	5.7	-1.40	Tewari et al., 1982	DUL
95-50-1	1,2-Dichlorobenzene	147	3.5	3.3	3.43	9.47	-1.19	Hansch et al., 1995	DUL
106-46-7	p-Dichlorobenzene	147	3.6	3.3	3.44	1.12	-2.12	Hansch et al., 1995	CAS - ETFS
106-46-7	p-Dichlorobenzene	147	3.6	3.3	3.44	4	-1.57	Hansch et al., 1995	CAS - ETFS
106-46-7	p-Dichlorobenzene	147	3.6	3.3	3.44	4.28	-1.54	Hansch et al., 1995	CAS - ETFS
541-73-1	1,3-Dichlorobenzene	147	3.6	3.3	3.53	8.03	-1.26	Hansch et al., 1995	DUL
122-39-4	Diphenylamine	169	3.6	3.3	3.5	2.2	-1.89	Hansch & Leo, 1985	U.S. EPA RED
122-39-4	Diphenylamine	169	3.6	3.3	3.5	3.79	-1.65	Hansch & Leo, 1985	DUL
2362-61-0	trans-2-Phenyl-1-cyclohexanol	176	2.7	3.3		44.4	-0.60		DUL
CBI	CBI	197	2.4	3.3		17.8	-1.04		Z02-___
76-29-9	[(1R)-endo]-(+)-3-Bromocamphor	231	2.6	3.3		68.5	-0.53		DUL
4180-23-8	trans-Anethole	148	3.3	3.4		7.5	-1.30		DUL Terpene Study
CBI	CBI	154	2.4	3.4	2.87	33	-0.67	Li & Perdue, 1995	P89-___
2216-51-5	(1R, 2S, 5R)-(-)-Menthol	156	3.2	3.4	3.3	18.9	-0.92	Chem Inspect Test Inst., 199	DUL
98-82-8	Isopropylbenzene	120	3.7	3.5	3.66	6.32	-1.28	Hansch & Leo, 1985	DUL
822-86-6	trans-1,2-Dichlorocyclohexane	153	3.3	3.5	3.21	18.4	-0.92	Hansch & Leo, 1985	DUL
822-86-6	trans-1,2-Dichlorocyclohexane	153	3.3	3.5	3.18	18.4	-0.92	Hansch & Leo, 1985	DUL
54576-32-8	3,8-Dithadecane	178	3.1	3.5		6.06	-1.47		DUL
56348-40-4	2,9-Dithiadecane	178	3.1	3.5		10.1	-1.25		DUL
95-63-6	1,2,4-Trimethylbenzene	120	3.6	3.6	3.63	7.72	-1.19	Hansch et al., 1995	DUL
107-47-1	tert-Butyl-sulfide	146	3.3	3.6		29.1	-0.70		DUL
1126-79-0	Butyl Phenyl Ether	150	3.6	3.6		5.77	-1.41		DUL
111-25-1	1-Bromohexane	165	3.7	3.6	3.8	3.45	-1.68	Hansch & Leo, 1985	DUL
13608-87-2	2', 3', 4'-Trichloroacetophenone	223	3.2	3.6		2	-2.05		DUL
CBI	CBI	100	4.3	3.7		0.97	-2.01		P02-___
4253-89-8	Isopropyl Disulfide	150	3.4	3.7		8.31	-1.26		DUL
132-64-9	Dibenzofuran	168	4.1	3.7	4.12	1.78	-1.97	Hansch & Leo, 1985	DUL
132-64-9	Dibenzofuran	168	4.1	3.7	4.12	1.85	-1.96	Hansch & Leo, 1985	DUL
112-12-9	2-Undecanone	170	4	3.7	4.09	1.5	-2.05	Tanii & Hashimoto, 1986	DUL
89-69-0	1,2,4-Trichloro-5-nitrobenzene	226	3.7	3.7	3.48	0.78	-2.46	8(e)-14895	8(e)-14895
629-19-6	Propyl Disulfide	150	3.9	3.8		2.62	-1.76		DUL
92-52-4	Biphenyl	154	4	3.8	3.98	1.5	-2.01	Sangster, 1993	8(e)-3066
92-52-4	Biphenyl	154	4	3.8	3.98	4.7	-1.52	Sangster, 1993	8(e)-3066

112-30-1	1-Decanol	158	4	3.8	4.57	2.4	-1.82	Pomona, 1987	DUL
95-75-0	3,4-Dichlorotoluene	161	3.9	3.8	3.95	2.91	-1.74	Biobyte, 1995	DUL
583-53-9	1,2-Dibromobenzene	236	3.7	3.8	3.64	4.05	-1.77	Hansch & Leo, 1985	DUL
544-40-1	n-Butyl Sulfide	146	4	3.9		3.58	-1.61		DUL
120-82-1	1,2,4-Trichlorobenzene	181	4.2	3.9	4.02	2.99	-1.78	Hansch et al., 1995	DUL
620-88-2	4-Nitrophenyl Phenyl Ether	215	4.3	3.9	3.92	2.65	-1.91	Nandihalli et al., 1993	DUL
CBI	CBI	242	2.9	3.9		22	-1.04		P93-____
CBI	CBI	107	4.9	4	2.76, 5.18	0.31	-2.54	Datasheet	P04-____/P04-____
764-13-6	2,5-Dimethyl-2,4-hexadiene	110	3.8	4.0	3.5	3.78	-1.46	Chem Inspect Test Inst., 199	DUL
281-23-2	Adamantane	136	4	4.0	4.24	0.285	-2.68	Sangster, 1994	DUL
693-65-2	Dipentyl ether	158	4	4.0		3.14	-1.70		DUL
67-72-1	Hexachloroethane	237	4.6	4.0	4.14	1.53	-2.19	Hansch et al., 1995	DUL
67-72-1	Hexachloroethane	237	4.6	4.0	4.14	1.32	-2.25	Hansch et al., 1995	DUL
2176-62-7	Pentachloropyridine	251	3.8	4.0	3.53	0.47	-2.73	Hansch & Leo, 1985	Veith & Broderius
141-93-5	1,3-Diethylbenzene	134	4.2	4.1	4.57	4.15	-1.51	Sherblom & Eganhouse, 198	DUL
101-84-8	Phenyl Ether	170	4.2	4.1	4.21	4	-1.63	Hansch & Leo, 1985	DUL
629-04-9	1-Bromoheptane	179	4.3	4.1	4.36	1.47	-2.09	Hansch & Leo, 1985	DUL
55792-61-5	2'-(Octyloxy)-acetanilide	263	4.3	4.1		0.45	-2.77		DUL
83-32-9	Acenapthene	154	3.8	4.2	3.9	1.73	-1.95	Hansch & Leo, 1985	DUL
6175-49-1	2-Dodecanone	184	4.6	4.2		1.18	-2.19		DUL
CBI	CBI	198	5	4.2		2.3	-1.94		P95-____
85-01-8	Phenanthrene	178	4.5	4.3	4.46	3.2	-1.75	Hansch & Leo, 1985	CAS-Edsall, 1991
882-33-7	Phenyl Disulfide	218	4.4	4.3	4.41	0.11	-3.30	Hansch & Leo, 1985	DUL
CBI	CBI	225	3.5	4.3		6.8	-1.52		P92-____
81-19-6	a,a-2,6-Tetrachlorotoluene	230	4.6	4.3		0.97	-2.37		Veith et al., 1983
CBI	CBI	230	3.2	4.3		53	-0.64		P00-____
3558-69-8	2,6-Diphenylpyridine	231	4.8	4.3	4.82	0.212	-3.04	Hansch & Leo, 1985	DUL
CBI	CBI	344	2.9	4.3		11.5	-1.48		P97-____
4795-86-2	(1S)-(-)-trans-pinane	138	4.7	4.4		5.7	-1.38		CAS-Edsall, 1991
85-01-8	Phenanthrene	178	4.5	4.4	4.46	0.234	-2.88	Hansch & Leo, 1985	CAS - ETFS
85-01-8	Phenanthrene	178	4.5	4.4	4.46	0.375	-2.68	Hansch & Leo, 1985	CAS - ETFS
2051-60-7	2-Chlorobiphenyl	189	4.5	4.4	4.53	0.54	-2.54	Hansch et al., 1995	8(e)-3066
2051-60-7	2-Chlorobiphenyl	189	4.5	4.4	4.53	4	-1.67	Hansch et al., 1995	8(e)-3066
2051-60-7	2-Chlorobiphenyl	189	4.5	4.4	4.53	1.1	-2.24	Hansch et al., 1995	8(e)-3066
2051-61-8	3-Chlorobiphenyl	189	4.7	4.4	4.58	1	-2.28	Hansch et al., 1995	8(e)-3066
2051-62-9	4-Chlorobiphenyl	189	4.7	4.4	4.61	0.9	-2.32	Hansch et al., 1995	8(e)-3066
2051-61-8	3-Chlorobiphenyl	189	4.7	4.4	4.58	7.8	-1.38	Hansch et al., 1995	8(e)-3066
2051-61-8	3-Chlorobiphenyl	189	4.7	4.4	4.58	2.4	-1.90	Hansch et al., 1995	8(e)-3066
2051-62-9	4-Chlorobiphenyl	189	4.7	4.4	4.61	1.3	-2.16	Hansch et al., 1995	8(e)-3066
538-68-1	Amylbenzene	148	4.8	4.5	4.9	1.71	-1.94	Hansch & Leo, 1985	DUL
330-93-8	p-Fluorophenyl Ether	206	4.7	4.5		1.2	-2.23		DUL
330-93-8	p-Fluorophenyl Ether	206	4.7	4.5		1.06	-2.29		DUL
28675-08-3	2,4-Dichlorodiphenyl ether	239	5.6	4.5	5	0.66	-2.56	Kurz & Ballschmiter, 1999	Chui, 1990
110-06-5	t-Butyl Disulfide	178	4.2	4.6		1.37	-2.11		DUL
111-83-1	1-Bromooctane	193	4.8	4.6	4.89	0.838	-2.36	Hansch & Leo, 1985	DUL
634-66-2	1,2,3,4-Tetrachlorobenzene	216	4.6	4.6	4.6	1.1	-2.29	Hansch, C. et al. 1995	Veith et al., 1983
22094-81-1	Bicyclo(2.2.1)hept-2-ene, 5-butyl-	150	4.7	4.7		0.07	-3.33		8(e)-14623
593-08-8	2-Tridecanone	198	5.1	4.7		0.36	-2.74		DUL
7005-72-3	4-Chlorodiphenyl ether	205	5.1	4.7	4.7	0.73	-2.45	Kurz & Ballschmiter, 1999	Chui, 1990
5989-27-5	(R)-(+)-Limonene	136	4.3	4.8	4.6	0.702	-2.29	Li & Perdue, 1995	DUL
2437-25-4	n-Undecyl Cyanide	181	4.9	4.8		0.43	-2.62		DUL
112-53-8	1-Dodecanol	186	5.1	4.8	5.1	1.01	-2.27	Hansch, C. et al. 1995	Veith et al., 1983
955-83-9	2,5-Diphenylfuran	220	5.5	4.9		0.05	-3.64		DUL
CBI	CBI	382	4.7	4.9		0.825	-2.67		8(e)-____
1647-16-1	1,9-Decadiene	138	5	5		0.29	-2.68		DUL
SAR data not included in regression equation:									
CBI	CBI	303	MF	2.5	2.73	*	*	NS	P02-____
CBI	CBI	387	1.7	2.5		*	*		P85-____
CBI	CBI	663	1.9	2.5		*	*		L96-____
CBI	CBI	303		3.1		*	*		P04-____
CBI	CBI	250	2.7	3.2		*	*		P95-____
3085-42-5	4-Chlorophenyl Sulfoxide	271	3.7	3.4		*	*		DUL
90-47-1	Xanthone	196	2.5	3.8	3.39	*	*	Hansch et al., 1995	DUL
1120-16-7	Dodecanamide	199	4.1	3.8		*	*		DUL
624-38-4	1,4-Diiodobenzene	330	4.4	4.3	4.11	*	*	Hansch et al., 1995	DUL
462-18-0	7-Tridecanone	198	5	4.7		*	*		DUL
955-83-9	2,5-Diphenylfuran	220	5.5	4.9		*	*		DUL
CBI	CBI	246	MF	4.9		*	*		P03-____
CBI	CBI	465	9.3	4.9		*	*		L03-____
CBI	CBI	200	5.1	5.1		0.055	-3.56		P06-____; 8(e)-____
603-34-9	Triphenylamine	245	5.7	5.1	5.74	*	*	Hansch & Leo, 1985	DUL
27548-92-0	Isotridecan-1-ol	200	5.2	5.2		0.55	-2.56		8(e)-15285
68526-86-3	C11-14 isoalcohols, C13-rich	200	5.2	5.2		0.8	-2.40		8(e)-15284
3081-01-4	N-(1,4-dimethylpentyl)-N'-phenyl-p-phenylenediamine	282	5.9	5.2		0.3	-2.97		8(e)-8901

3081-01-4	N-(1,4-dimethylpentyl)-N'-phenyl-p-phenylenediamine	282	5.9	5.2		0.42	-2.83		8(e)-9279
3081-01-4	N-(1,4-dimethylpentyl)-N'-phenyl-p-phenylenediamine	282	5.9	5.2		0.14	-3.30		8(e)-9412
3081-01-4	N-(1,4-dimethylpentyl)-N'-phenyl-p-phenylenediamine	282	5.9	5.2		0.49	-2.76		8(e)-9279
3081-01-4	N-(1,4-dimethylpentyl)-N'-phenyl-p-phenylenediamine	282	5.9	5.2		0.4	-2.85		8(e)-9018
3081-01-4	N-(1,4-dimethylpentyl)-N'-phenyl-p-phenylenediamine	282	5.9	5.2		0.42	-2.83		8(e)-10299
3081-01-4	N-(1,4-dimethylpentyl)-N'-phenyl-p-phenylenediamine	282	5.9	5.2		0.8	-2.55		8(e)-9898
112-70-9	1-Tridecanol	200	5.6	5.3		*	*		DUL
886-65-7	1,4-Diphenyl-1,3-butadiene	206	5	5.3		*	*		DUL
CBI	CBI	253	4.5	5.3		0.59	-2.63		Z02-____
CBI	CBI	258	4.2	5.3		12	-1.33		P00-____
103-19-5	p-Tolyl Disulfide	246	5.4	5.4		*	*		DUL
218-01-9	Chrysene	228	5.7	5.5	5.81	0.0609	-3.57	De Maagd et al., 1998	CAS - ETFS
CBI	CBI	290	5.5	5.6		*	*		P97-____
31242-94-1	2,4,5,4'-Tetrachloro diphenyl ether	308	6.9	5.8	5.88	*	*	Kurz & Ballschmiter, 1999	Chui, 1990
92-51-3	Dicyclohexyl	166	5.9	5.9		*	*		DUL
CBI	CBI	269	5.8	5.9		*	*		L06-____
CBI	CBI	226	6.7	6.1		*	*		P91-____
CBI	CBI	232	6.7	6.2		*	*		P90-____, -____, -____, S03-
2437-79-8	2,2',4,4'-Tetrachlorobiphenyl	292	6.4	6.3	6.29	0.12	-3.39	Hansch & Leo, 1985	8(e)-3066
2437-79-8	2,2',4,4'-Tetrachlorobiphenyl	292	6.4	6.3	6.29	0.12	-3.39	Hansch & Leo, 1985	8(e)-3066
CBI	CBI	338	6.1	6.3		*	*		P89-____
CBI	CBI	260	6.8	6.4		*	*		P92-____
CBI	CBI	182	7	6.5		*	*		P00-____
CBI	CBI	352	5.4	6.5		*	*		L91-____
629-82-3	Dioctyl ether	42	7.2	6.9		*	*		Veith et al., 1983
CBI	CBI	525		6.9	5.1	*	*	Rekker	P00-____
31242-93-0	2,4,4'-Trichlorodiphenyl ether	274	7.9	7.1	6.82	*	*	Kurz & Ballschmiter, 1999	Chui, 1990
CBI	CBI	525	7.2	7.1		*	*		P98-____
143-28-2	cis-Octadecen-1-ol	268	7.7	7.5		*	*		DUL
85-22-3	2,3,4,5,6-Pentabromoethylbenzene	501	6.7	7.5		*	*		DUL
CBI	CBI	463	8.3	7.8		*	*		P87-____
CBI	CBI	332	8.6	8.2		*	*		P92-____
3808-87-5	2,4,5-Trichlorophenyl Disulfide	425	8.5	8.2		*	*		DUL
CBI	CBI	425	7.5	8.2		*	*		P91-____
CBI	CBI	242	9.3	8.6		*	*		P98-____
CBI	CBI	335	6.4	8.8		*	*		P95-____
CBI	CBI	431	11	10		*	*		L05-____
CBI	CBI	311	12	11		*	*		P88-____
CBI	CBI	345	12	11		*	*		P99-____
CBI	CBI	517	12.2	11		*	*		P98-____
CBI	CBI	736	16	11		*	*		P91-____
CBI	CBI	694	15	12		*	*		P88-____
CBI	CBI	868	12	13		*	*		P94-____
Data not used in SAR:									
CBI	CBI	488	-1.6	-4.3		10000	1.31		P95-____; NOEC
CBI	CBI	320	-3.2	-3.8		830	0.41		P93-____; NOEC
87-72-9	L-Arabinose	150	-2.9	-2.9	-3.02	37700	2.40	Hansch & Leo, 1985	DUL; L-confirmation results in excess toxicity
CBI	CBI	118	0.49	0.46	0.39	>1000		Binstein et al., 1993	P89-____; inequality
994-05-8	tert-Amyl Methyl Ether	102	1.6	1.9		580	0.75		8FYI-1052; not verified
CBI	CBI		MF	2.4		*	*		P92-____; SRC log kow too low
CBI	CBI	216	2.5	3.4		140	-0.19		P93-____; 48-h test
CBI	CBI	334	0.76	3.5		22	-1.18		L02-____; 48-h test
CBI	CBI	196	1.6	3.5		150	-0.12		PC1822; 48-h test
101-84-8	Diphenyl ether	170	4.2	4.1	4.21	1.7	-2.00	Hansch & Leo, 1985	LeBlanc, 1984; no duration
58-89-9	Lindane	291	3.8	4.3	3.72	0.1	-3.46	Hansch & Leo, 1985	ETFS; excess toxicity
CBI	CBI	182	5	4.6	4.56	3.5	-1.72	P92-1356-1	P92-____; EC>SH2O and 48-h
CBI	CBI	425	MF	5		91	-0.67		P92-____; 48-h test
63393-82-8	Doanol-25/alcohols, C12-15 alkyl	186	5.6	5.3		43	-0.64		8(e)-4803; unspecified purity
CBI	CBI	341	5.2	5.6		*	*		P90-____; 48-h test
CBI	CBI	260	6.8	6.4	5.3	*	*		P92-____
CBI	CBI	272	7.2	6.6		*	*		P92-____; EC>SH2O and 72-h
8001-35-2	Toxaphene	414	4.3	6.8		0.004	-5.01		ETFS; excess toxicity
3007-74-7	Dodecylaniline	261	7.5	7		high			8(e)-9166; unspecified value
CBI	CBI	515	6.8	7	3.26	<0.100		P02-306	P02-____; NOEC
CBI	CBI	378	MF	9		*	*		L99-____; 48-h test
CBI	CBI	475	10	9.6	>5.11	*	*	P92-465	P92-____; 48-h test
CBI	CBI	789	11	12		*	*		P94-____; 48-h test
CBI	CBI	971	11	14		*	*		P89-____; 48-h test
1336-36-3	PCBs					0.002			ETFS; unspecified structure
CBI	CBI	172	3	2.8	2.74	18	≤-0.98	Hansch et al., 1995	P93-____
								* indicates no effects at saturation	

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FISH 14-d LC50

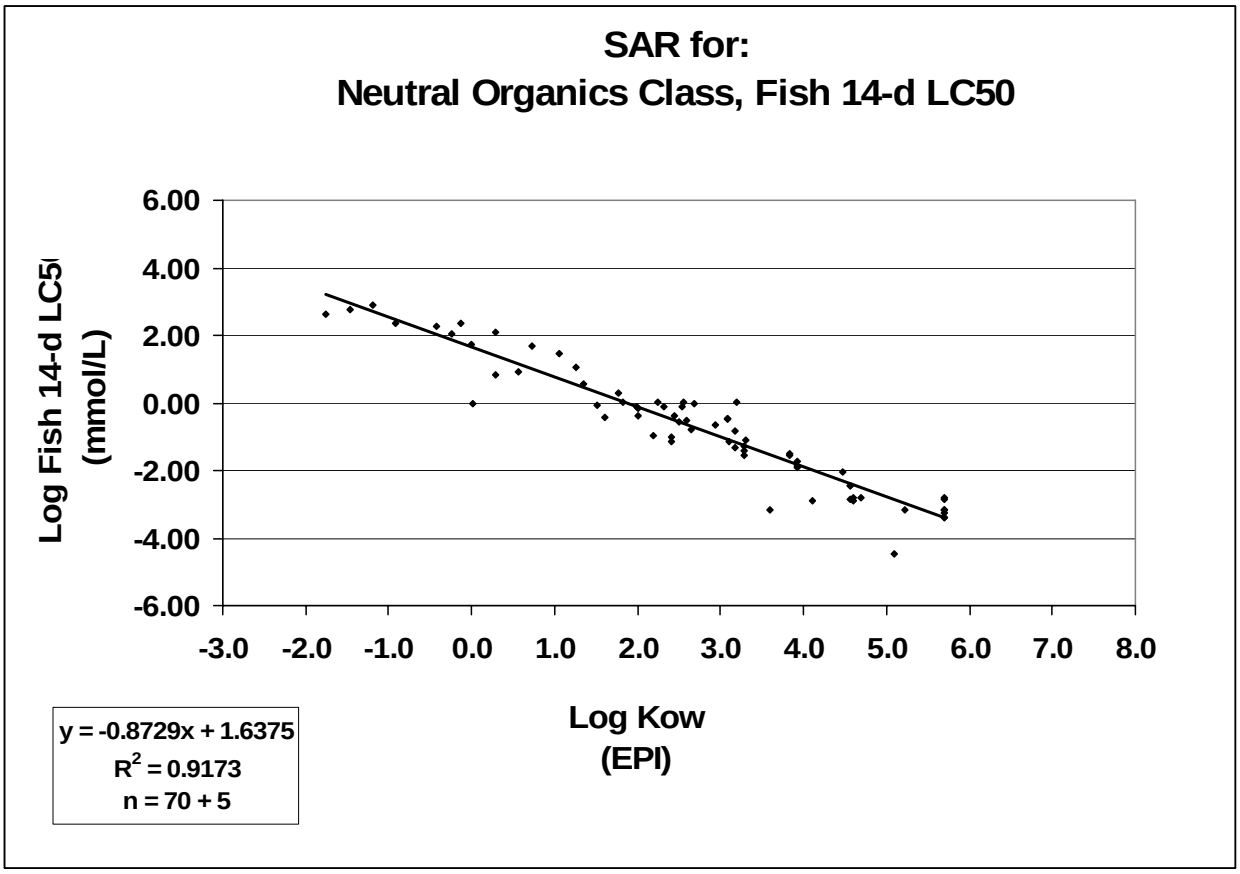
ESTIMATED TOXICITY:
The fish 14-d LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 14-d LC50 (mmol/L) = -0.8729 log K_{ow} + 1.6375

The LC50 is in millimoles per liter (mM/L); N = 70 + 5; and the Coefficient of Determination (R^2) = 0.9173. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 6.0
Maximum MW: 1000

Graph:



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 Kow value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	F 14-d LC50 (mg/L)	Log F 14-d LC50 (mmol/L)	Reference (Meas. Kow)	Reference (LC50)
112-27-6	Trigol (triethyleneglycol)	150	-1.2	-1.8		62601	2.62		Konemann, 1981
111-46-6	Digol (diethyleneglycol)	106	-0.31	-1.5		61066	2.76		Konemann, 1981
107-21-1	Ethanediol (ethyleneglycol)	62	-1.4	-1.2	-1.36	49304	2.90	Hansch & Leo, 1985	Konemann, 1981
109-86-4	2-Methoxyethanol	76	-0.75	-0.91	-0.77	17434	2.36	Hansch & Leo, 1985	Konemann, 1981
110-80-5	2-Ethoxyethanol	90	-0.22	-0.42	-0.32	16399	2.26	Hansch et al., 1995	Konemann, 1981
67-64-1	Acetone	58	-0.21	-0.24	-0.24	6368	2.04	Hansch & Leo, 1985	Konemann, 1981
64-17-5	Ethanol	46	-0.24	-0.14	-0.31	11051	2.38	Hansch & Leo, 1985	Konemann, 1981
109-59-1	2-Isopropoxyethanol	104	0.09	0	0.05	5466	1.72	Hansch & Leo, 1985	Konemann, 1981
143-22-6	Butyltrigol	206	1	0.0		197	-0.02		Konemann, 1981
67-63-0	Propanol-2	60	0.08	0.28	0.05	7061	2.07	Hansch & Leo, 1985	Konemann, 1981
112-34-5	Butyldigol	162	0.91	0.29	0.56	1149	0.85	Funasaki et al., 1984	Konemann, 1981
111-76-2	2-Butoxyethanol	118	0.84	0.57	0.83	983	0.92	Hansch & Leo, 1985	Konemann, 1981
75-65-0	2-Methylpropanol-2	74	0.47	0.73	0.35	3548	1.68	Hansch & Leo, 1985	Konemann, 1981
60-29-7	Diethylether	74	0.87	1.1	0.89	2138	1.46	Hansch & Leo, 1985	Konemann, 1981
584-02-1	Pentanol-3	88	1.1	1.3	1.21	989	1.05	Hansch & Leo, 1985	Konemann, 1981
75-09-2	Dichloromethane	85	1.2	1.3	1.25	294	0.54	Hansch & Leo, 1985	Konemann, 1981
67-66-3	Chloroform	119	2.0	1.5	1.97	102	-0.07	Hansch & Leo, 1985	Konemann, 1981
111-44-4	2,2'-Dichlorodiethylether	143	1	1.6	1.29	54	-0.42	Hansch & Leo, 1985	Konemann, 1981
75-34-3	1,1-Dichloroethane	99	1.8	1.8	1.79	202	0.31	Hansch & Leo, 1985	Konemann, 1981
107-06-2	1,2-Dichloroethane	99	1.5	1.8	1.48	106	0.03	Hansch & Leo, 1985	Konemann, 1981
71-43-2	Benzene	78	2.1	2.0	2.13	63	-0.09	Hansch & Leo, 1985	Konemann, 1981
79-00-5	1,1,2-Trichloroethane	133	2.1	2.0	1.89	94	-0.15	Pomona, 1987	Konemann, 1981
25323-89-1	Trichloroethane	133	2.1	2.0	1.89	56	-0.38	Pomona, 1987	Konemann, 1981
25322-20-7	Tetrachloroethane	168	2.6	2.2	2.39	18	-0.97	Hansch & Leo, 1985	Konemann, 1981
78-87-5	1,2-Dichloropropane	113	2.0	2.3	1.89	116	0.01	Sangster, 1994	Konemann, 1981
142-28-9	1,3-Dichloropropane	113	1.7	2.3	2	84	-0.13	Hansch & Leo, 1985	Konemann, 1981
78-88-6	2, 3-Dichloro-1-propene	111	2	2.4		11	-1.00		Konemann, 1981
544-00-7	2,4-Dichloroaniline	162	2.7	2.4	2.78	11.7	-1.14	Sangster, 1994	Konemann, 1981
56-23-5	Tetrachloromethane	154	2.9	2.4	2.83	67	-0.36	Hansch & Leo, 1985	Konemann, 1981
96-18-4	1,2,3-Trichloropropane	147	2.0	2.5	2.27	42	-0.55	Chem Inspect Test Inst., 1992	Konemann, 1981
108-88-3	Toluene	92	2.6	2.5	2.73	68	-0.13	Hansch & Leo, 1985	Konemann, 1981
109-69-3	1-Chlorobutane	93	2.5	2.6	2.64	97	0.02	Hansch & Leo, 1985	Konemann, 1981
110-57-6	trans-1,4-Dichloro-2-butene	125	1.8	2.6		40	-0.50		Konemann, 1981
108-90-7	Monochlorobenzene	113	2.9	2.6	2.84	19	-0.77	Sangster, 1994	Konemann, 1981
71-55-6	1,1,1-Trichloroethane	133	2.5	2.7	2.49	133	0.00	Hansch & Leo, 1985	Konemann, 1981
630-20-6	1,1,2,2-Tetrachloroethane	168	3.0	2.9		37	-0.66		Konemann, 1981
95-47-6	o-Xylene	106	3.1	3.1	3.12	35	-0.48	Hansch & Leo, 1985	Konemann, 1981
106-42-3	p-Xylene	106	3.1	3.1	3.15	35	-0.48	Hansch & Leo, 1985	Konemann, 1981
108-38-3	m-Xylene	106	3.1	3.1	3.2	38	-0.45	Hansch & Leo, 1985	Konemann, 1981
76-01-7	Pentachloroethane	202	3.6	3.1	3.22	15	-1.13	Hansch et al., 1995	Konemann, 1981
106-43-4	4-Chlorotoluene	127	3.4	3.2	3.33	5.9	-1.33	Hansch & Leo, 1985	Konemann, 1981
108-41-8	3-Chlorotoluene	127	3.4	3.2	3.28	18	-0.84	Hansch & Leo, 1985	Konemann, 1981
110-82-7	Cyclohexane	84	3.4	3.2	3.44	84	0.00	Hansch & Leo, 1985	Konemann, 1981
95-50-1	1,2-Dichlorobenzene	147	3.4	3.3	3.43	5.9	-1.40	Hansch et al., 1995	Konemann, 1981
106-46-7	1,4-Dichlorobenzene	147	3.6	3.3	3.44	4.0	-1.57	Hansch et al., 1995	Konemann, 1981
541-73-1	1,3-Dichlorobenzene	147	3.6	3.3	3.53	7.4	-1.30	Hansch et al., 1995	Konemann, 1981
628-76-2	1,5-Dichloropentane	141	2.8	3.3		11.20	-1.10		Konemann, 1981
626-16-4	alpha, alpha'-Dichloro-m-xylene	175	3.3	3.6	2.72	0.12	-3.16	Hansch & Leo, 1985	Konemann, 1981
95-73-8	2,4-Dichlorotoluene	161	4.1	3.8	4.24	4.6	-1.54	Hansch & Leo, 1985	Konemann, 1981

95-75-0	3,4-Dichlorotoluene	161	3.9	3.8	3.95	5.1	-1.50	BioByte, 1995	Konemann, 1981
87-61-6	1,2,3-Trichlorobenzene	181	4.1	3.9	4.05	2.3	-1.89	Sangster, 1994	Konemann, 1981
108-70-3	1,3,5-Trichlorobenzene	181	4.3	3.9	4.19	3.3	-1.74	Hansch & Leo, 1985	Konemann, 1981
120-82-1	1,2,4-Trichlorobenzene	181	4.2	3.9	4.02	2.4	-1.88	Hansch et al., 1995	Konemann, 1981
94-99-5	2,4,a-Trichlorotoluene	195	4.1	4.1	3.82	0.2	-2.91	Hansch & Leo, 1985	Konemann, 1981
6639-30-1	2,4,5-Trichlorotoluene	195	4.6	4.5	4.56	1.7	-2.06	BioByte, 1995	Konemann, 1981
68953-84-4	1,4-Benzenediamine, N,N'-mixed	274	5.7	4.6		0.4	-2.89		8(e)-13284
68953-84-4	1,4-Benzenediamine, N,N'-mixed	274	5.7	4.6		0.4	-2.80		8(e)-13284
95-94-3	1,2,4,5-Tetrachlorobenzene	216	4.8	4.6	4.64	0.30	-2.85	Hansch & Leo, 1985	Konemann, 1981
634-66-2	1,2,3,4-Tetrachlorobenzene	216	4.6	4.6	4.6	0.80	-2.43	Hansch & Leo, 1985	Konemann, 1981
634-90-2	1,2,3,5-Tetrachlorobenzene	216	4.8	4.6	4.56	0.80	-2.43	Hansch & Leo, 1985	Konemann, 1981
87-68-3	Hexachlorobutadiene	261	4.9	4.7	4.78	0.39	-2.83	Hansch et al., 1995	Konemann, 1981
556-67-2	Octamethylcyclotetrasiloxane	297	7	5.1	5.1	0.01	-4.47	TSCATS	8(e)-11384
608-93-5	Pentachlorobenzene	250	5.2	5.2	5.17	0.18	-3.15	Hansch & Leo, 1985	Konemann, 1981
15862-07-4	2,4,5-Trichlorobiphenyl	258	5.8	5.7	5.81	0.18	-3.16	Hansch & Leo, 1985	Konemann, 1981
16606-02-3	2,4',5-Trichlorobiphenyl	258	5.9	5.7	5.69	0.18	-3.16	Hansch & Leo, 1985	Konemann, 1981
35693-92-6	2,4,6-Trichlorobiphenyl	258	5.7	5.7	5.47	0.40	-2.81	Hansch & Leo, 1985	Konemann, 1981
37680-65-2	2,2',5-Trichlorobiphenyl	258	5.7	5.7	5.55	0.10	-3.41	Hansch & Leo, 1985	Konemann, 1981
55702-45-9	2,3,6-Trichlorobiphenyl	258	5.5	5.7	5.67	0.15	-3.24	Hansch & Leo, 1985	Konemann, 1981
55702-46-0	2,3,4-Trichlorobiphenyl	258	5.7	5.7	5.86	0.35	-2.87	BioByte, 1995	Konemann, 1981
55712-37-3	2,3',4-Trichlorobiphenyl	258	5.9	5.7		0.10	-3.41		Konemann, 1981
SAR data not used in regression equation:									
38444-81-4	2,3',5-Trichlorobiphenyl	258	5.9	5.7	5.76	*	*	Hansch & Leo, 1985	Konemann, 1981
118-74-1	Hexachlorobenzene	285	5.7	5.9	5.73	*	*	DeBruijn et al., 1989	Konemann, 1981
15968-05-5	2,6,2',6'-Tetrachlorobiphenyl	292	5.9	6.3	5.94	*	*	DeBruijn et al., 1989	Konemann, 1981
33284-53-6	2,3,4,5-Tetrachlorobiphenyl	292	6.3	6.3	6.41	*	*	Hansch & Leo, 1985	Konemann, 1981
CBI	CBI	260	6.8	6.4		*	*		P92-____
Data not used in SAR:									
CBI	CBI	216	2.5	3.4		98.0	-0.34		P93-____; ??????
CBI	CBI	182	5	4.6	4.56	2.5	-1.86	P92-1356	P92-____; EC>SH2O
						* indicates no effects at saturation			

References:
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U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

DAPHNID 48-h LC50

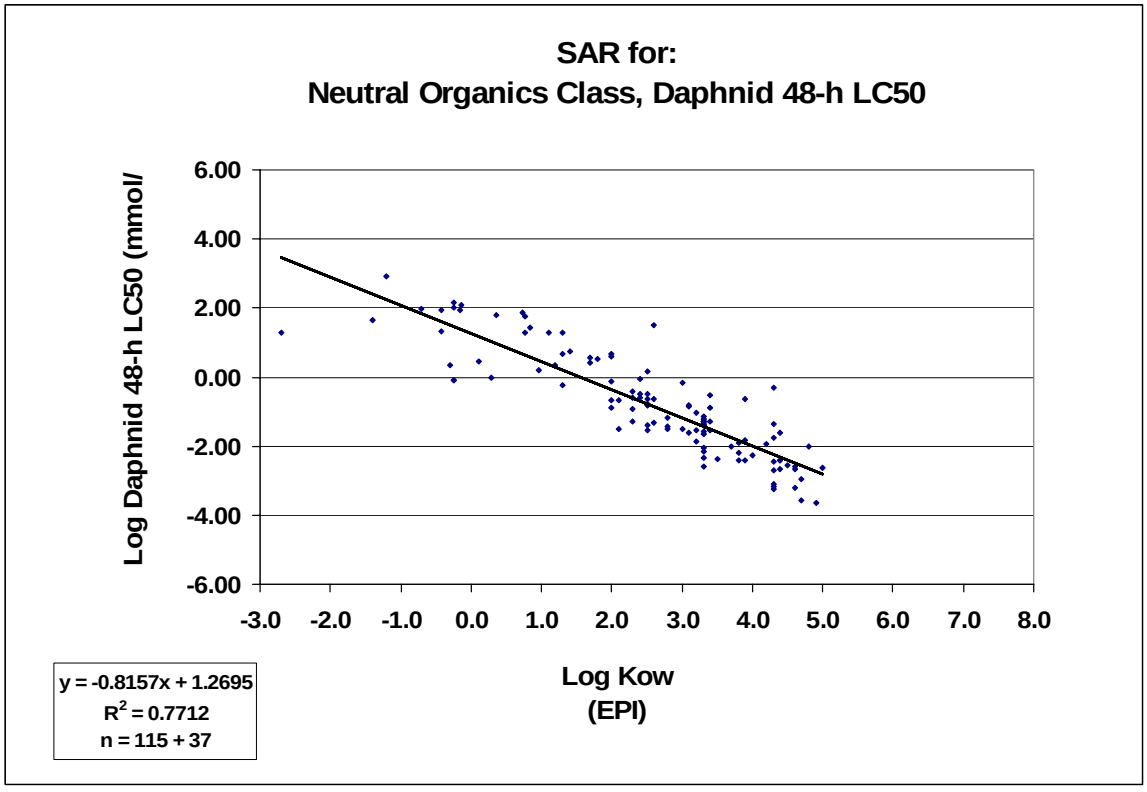
ESTIMATED TOXICITY:
The daphnid 48-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 48-h LC50 = -0.8157 (log K_{ow}) + 1.2695

The LC50 is in millimoles per liter (mM/L); N = 115 + 37; and the Coefficient of Determination (R^2) = 0.7712. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 5.0
Maximum MW: 1000

Graph:



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 Kow value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	CLogP Kow	SRC Kow	Meas. Kow	Daphnid 48-h LC50 (mg/L)	Log Daphnid 48-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (LC50)
CBI	CBI	224	-2	-2.7		4400	1.29		P95-___
CBI	CBI	355	-2.8	-1.4		15600	1.64		P97-___
107-21-1	Ethanediol	62	-1.4	-1.2	-1.36	50452	2.91	Hansch & Leo, 1985	Hermens et al., 1984
504-63-2	1,3-Propandiol	76	-1.7	-0.71	-1.04	7417	1.99	Hansch, et al., 1995	Kuhn, 1989
110-80-5	2-Ethoxyethanol	90	-0.22	-0.42	-0.32	7670	1.93	Hansch et al., 1995	Hermens et al., 1984
110-80-5	2-Ethoxyethanol	90	-0.22	-0.42	-0.32	1903	1.33	Hansch et al., 1995	Hermens et al., 1984 (Rose et al.)
CBI	CBI	116	0	-0.3		252	0.34		P90-___
67-64-1	Acetone	58	-0.21	-0.24	-0.24	6081	2.02	Hansch & Leo, 1985	Hermens et al., 1984
CBI	CBI	58	-2.08	-0.24	-0.24	8600	2.17	Hansch & Leo, 1985	P98-___
126-33-0	Sulfolane (sulfone)	120	-0.9	-0.24	-0.77	95	-0.10	Hansch, et al., 1995	Shell, 1984
126-33-0	Sulfolane (sulfone)	120	-0.9	-0.24	-0.77	94	-0.11	Hansch, et al., 1995	Shell, 1984
75-05-8	Acetonitrile	41	-0.34	-0.15	-0.34	3600	1.94	Hansch & Leo, 1985	Tong et al., 1996
64-17-5	Ethanol	46	-0.24	-0.14	-0.31	5413	2.07	Hansch & Leo, 1985	Hermens et al., 1984
107-07-3	2-Chloroethanol	81	-0.17	0.11	0.03	227	0.45	Hansch, et al., 1995	Kuhn, 1989
CBI	CBI	162	0.47	0.29		160	-0.01		L92-___
71-23-8	n-Propanol	60	0.29	0.35	0.25	3644	1.78	Hansch, et al., 1995	Kuhn, 1989
75-65-0	tert-Butanol	74	0.47	0.73	0.35	5504	1.87	Hansch, et al., 1995	Kuhn, 1989
78-83-1	Isobutanol	74	0.69	0.77	0.76	1439	1.29	Hansch, et al., 1995	Kuhn, 1989
78-92-2	sec-Butanol	74	0.6	0.77	0.61	4227	1.76	Hansch, et al., 1995	Kuhn, 1989
71-36-3	n-Butanol	74	0.82	0.84	0.88	1983	1.43	Hansch, et al., 1995	Kuhn, 1989
96-13-9	2,3-Dibromopropanol	218	0.63	0.96		338	0.19		Kuhn, 1989
60-29-7	Diethylether	74	0.87	1.1	0.89	1380	1.27	Hansch & Leo, 1985	Hermens et al., 1984
115-20-8	2,2,2-Trichloroethanol	88	1.5	1.2	1.42	198	0.35	Hansch, et al., 1995	Kuhn, 1989
75-09-2	Methylene chloride/dichlorom	85	1.2	1.3	1.25	1682	1.30	Hansch et al., 1995	Kuhn, 1989
71-41-0	Pentanol	88	1.4	1.3	1.5	52.8	-0.22	Sangster, 1994	Hermens et al., 1984 (Rose et al.)
71-41-0	Pentanol	149	1.3	1.3	1.51	714	0.68	Sangster, 1994	Kuhn, 1989
1634-04-4	Methyl tert-butyl ether	88	1	1.4	0.94	472	0.73	Hansch & Leo, 1985	CAS-Wetal, 2001
CBI	CBI	84	1.6	1.7		300	0.55		P92-___
CBI	CBI	172	1.7	1.7		440	0.41		P94-___
107-06-2	1,2-Dichloroethane	99	1.5	1.8	1.48	324	0.51	Hansch et al., 1995	Kuhn, 1989
71-43-2	Benzene	78	2.1	2	2.13	56.6	-0.14	Hansch & Leo, 1985	Hermens et al., 1984
71-43-2	Benzene	78	2.1	2	2.13	10.3	-0.88	Hansch & Leo, 1985	Hermens et al., 1984 (Rose et al.)
71-43-2	Benzene	78	2.1	2	2.13	17	-0.66	Hansch & Leo, 1985	CAS-Niederlehner et al., 1998
71-43-2	Benzene	78	2.1	2	2.13	380	0.69	Hansch & Leo, 1985	CAS-ETFS
71-43-2	Benzene	78	2.1	2	2.13	300	0.59	Hansch & Leo, 1985	CAS-ETFS
91-22-5	Quinoline	129	2	2.1	2.03	28.5	-0.66	Hansch & Leo, 1985	CAS-Parkhurst, 1981; Eastmond, 1984
119-65-3	Isoquinoline	129	1.8	2.1	2.08	4.1	-1.50	Hansch & Leo, 1985	CAS-Parkhurst, 1981
78-87-5	1,2-Dichloropropane	113	2	2.3	1.98	45	-0.40	Sangster, 1994	Hermens et al., 1984
78-87-5	1,2-Dichloropropane	113	2	2.3	1.98	13.8	-0.91	Sangster, 1994	Hermens et al., 1984 (Rose et al.)
111-70-6	Heptanol	116	2.4	2.3	2.62	6.15	-1.28	Sangster, 1994	Hermens et al., 1984 (Rose et al.)
3622-84-2	Benzenesulfonamide, N-buty	213	2.5	2.3	2.1	56	-0.58	PSIDS	SIDS
1717-00-6	1,1-Dichloro-1-fluoroethane	117	2	2.4		29.6	-0.60		FYI-695
CBI	CBI	117	2	2.4		100	-0.07		P88-___
104-90-5	2-Picoline, 5-ethyl	121	2.5	2.4		39.6	-0.49		CAS
108-88-3	Toluene	92	2.6	2.5	2.73	14.9	-0.79	Hansch & Leo, 1985	Hermens et al., 1984
108-88-3	Toluene	92	2.6	2.5	2.73	3.8	-1.38	Hansch & Leo, 1985	CAS-Niederlehner et al., 1998
108-88-3	Toluene	92	2.6	2.5	2.73	137	0.17	Hansch & Leo, 1985	CAS-ETFS
79-01-6	1,1,2-Trichloroethene	131	2.6	2.5	2.42	20.8	-0.80	Hansch & Leo, 1985	Hermens et al., 1984
96-18-4	1,2,3-Trichloropropane	147	2	2.5	2.27	35.4	-0.62	Chem Inspect Test Inst., 199	Hermens et al., 1984

96-18-4	1,2,3-Trichloropropane	147	2	2.5	2.27	35.4	-0.62	Chem Inspect Test Inst., 199	Hermens et al., 1984
96-18-4	1,2,3-Trichloropropane	147	2	2.5	2.27	4.13	-1.55	Chem Inspect Test Inst., 199	Hermens et al., 1984 (Rose et al.)
CBI	CBI	303	MF	2.5	2.73	46.2	-0.82	NS	P02-___
CBI	CBI	530	2.7	2.5		167	-0.50		P98-___
109-69-3	1-Chlorobutane	93	2.5	2.6	2.64	3020	1.51	Hansch, et al., 1995	Kuhn, 1989
108-90-7	Monochlorobezene	113	2.9	2.6	2.84	25.8	-0.64	Sangster, 1994	Hermens et al., 1984
108-90-7	Monochlorobezene	113	2.9	2.6	2.84	5.33	-1.33	Sangster, 1994	Hermens et al., 1984 (Rose et al.)
111-87-5	Octanol	130	2.9	2.8	3	4.12	-1.50	Hansch et al., 1995	Hermens et al., 1984 (Rose et al.)
CBI	CBI	172	3	2.8	2.74	6.3	-1.44	Hansch et al., 1995	P93-___
CBI	CBI	172	3	2.8	2.74	11.3	-1.18	Hansch et al., 1995	P93-___
100-41-4	Ethylbenzene	106	3.2	3	3.15	75	-0.15	Hansch & Leo, 1985	CAS-ETFS
100-41-4	Ethylbenzene	106	3.2	3	3.15	3.2	-1.52	Hansch & Leo, 1985	CAS-Niederlehner et al., 1998
108-38-3	m-Xylene	106	3.1	3.1	3.2	14.3	-0.87	Hansch & Leo, 1985	Hermens et al., 1984
108-38-3	m-Xylene	106	3.1	3.1	3.2	2.49	-1.63	Hansch & Leo, 1985	Hermens et al., 1984 (Rose et al.)
CBI	CBI	303		3.1		47	-0.81		P04-___
106-43-4	4-Chlorotoluene	127	3.4	3.2	3.33	3.6	-1.55	Hansch & Leo, 1985	Hermens et al., 1984
106-43-4	4-Chlorotoluene	127	3.4	3.2	3.33	1.7	-1.87	Hansch & Leo, 1985	Hermens et al., 1984 (Rose et al.)
CBI	CBI	221	3.4	3.2		20	-1.04		P92-___
143-08-8	Nonanol	144	3.5	3.3	3.77	0.359	-2.60	Tewari et al., 1982	Hermens et al., 1984 (Rose et al.)
95-50-1	1,2-Dichlorobenzene	147	3.5	3.3	3.43	3.8	-1.59	Hansch et al., 1995	Hermens et al., 1984
95-50-1	1,2-Dichlorobenzene	147	3.5	3.3	3.43	3.29	-1.65	Hansch et al., 1995	Deneer et al., 1988
95-50-1	1,2-Dichlorobenzene	147	3.5	3.3	3.43	6.56	-1.35	Hansch et al., 1995	Deneer et al., 1988
95-50-1	1,2-Dichlorobenzene	147	3.5	3.3	3.43	7.34	-1.30	Hansch et al., 1995	Deneer et al., 1988
95-50-1	1,2-Dichlorobenzene	147	3.5	3.3	3.43	7.75	-1.28	Hansch et al., 1995	Deneer et al., 1988
95-50-1	1,2-Dichlorobenzene	147	3.5	3.3	3.43	5.7	-1.41	Hansch et al., 1995	Deneer et al., 1988
95-50-1	1,2-Dichlorobenzene	147	3.5	3.3	3.43	7.79	-1.28	Hansch et al., 1995	Deneer et al., 1988
95-50-1	1,2-Dichlorobenzene	147	3.5	3.3	3.43	8.67	-1.23	Hansch et al., 1995	Deneer et al., 1988
95-50-1	1,2-Dichlorobenzene	147	3.5	3.3	3.43	0.66	-2.35	Hansch et al., 1995	Hermens et al., 1984 (Rose et al.)
106-46-7	1,4-Dichlorobenzene	147	3.6	3.3	3.44	11	-1.13	Hansch et al., 1995	CAS-ETFS
106-46-7	1,4-Dichlorobenzene	147	3.6	3.3	3.44	1.29	-2.06	Hansch et al., 1995	Hermens et al., 1984 (Rose et al.)
122-39-4	Diphenylamine	169	3.6	3.3	3.5	1.2	-2.15	Hansch & Leo, 1985	U.S. EPA RED
CBI	CBI	197	2.4	3.3		7.6	-1.41		Z02-___
4180-23-8	trans-Anethole	148	3.3	3.4		7.8	-1.28		DUL Terpene Study
CBI	CBI	154	2.4	3.4	2.87	47	-0.52	Li & Perdue, 1995	P89-___
CBI	CBI	174	3.3	3.4	2.9	23	-0.88	HPLC	P05-___
15972-60-8	Alachlor	270	2.4	3.4	3.52	7.9	-1.53	Hansch, et al., 1995	Oris et al.
101-96-2	N,N'-Di-sec-butyl-p-phenylen	220	3.9	3.5		0.95	-2.36		8(e)-16281
CBI	CBI	100	4.3	3.7		0.97	-2.01		P02-___
92-52-4	Biphenyl	154	4	3.8	3.98	1.9	-1.91	Sangster, 1993	8(e)-3066
95-73-8	2,4-Dichlorotoluene	161	4.1	3.8	4.24	0.62	-2.41	Hansch & Leo, 1985	Hermens et al., 1984
95-73-8	2,4-Dichlorotoluene	161	4.1	3.8	4.24	1.02	-2.20	Hansch & Leo, 1985	Hermens et al., 1984 (Rose et al.)
120-82-1	1,2,4-Trichlorobenzene	182	4.2	3.9	4.02	2.7	-1.83	Hansch et al., 1995	Hermens et al., 1984
120-82-1	1,2,4-Trichlorobenzene	182	4.2	3.9	4.02	0.7	-2.41	Hansch et al., 1995	Hermens et al., 1984 (Rose et al.)
CBI	CBI	242	2.9	3.9		57	-0.63		P93-___
CBI	CBI	107	4.9	4	2.76, 5.18	0.56	-2.28	Datasheet	P04-____/P04-___
CBI	CBI	198	5	4.2		0.34	-1.94		P95-___
571-58-4	1,4-Dimethylnaphthalene	156	4.3	4.3	4.37	0.54	-2.46	Hansch & Leo, 1985	8(e)-12746
85-01-8	Phenanthrene	178	4.5	4.3	4.46	0.35	-2.71	Hansch & Leo, 1985	CAS- Smith et al., 1988
85-01-8	Phenanthrene	178	4.5	4.3	4.46	0.1	-3.25	Hansch & Leo, 1985	CAS-ETFS
85-01-8	Phenanthrene	178	4.5	4.3	4.46	0.117	-3.18	Hansch & Leo, 1985	CAS-ETFS
CBI	CBI	225	3.5	4.3		3.8	-1.77		P92-___
CBI	CBI	230	3.2	4.3		113	-0.31		P00-___
1836-75-5	Nitrofen	284	5.6	4.3	4.64	0.217	-3.12	Sangster, 1994	Oris et al.
CBI	CBI	344	2.9	4.3		15	-1.36		P97-___
4795-86-2	(is)-(-)-trans-Pinane	138	4.7	4.4		3.3	-1.62		CAS-Smith et al., 1988
2051-60-7	2-Chlorobiphenyl	189	4.5	4.4	4.53	0.76	-2.40	Hansch et al., 1995	8(e)-3066
2051-61-8	3-Chlorobiphenyl	189	4.7	4.4	4.58	0.42	-2.65	Hansch et al., 1995	8(e)-3066
2051-62-9	4-Chlorobiphenyl	189	4.7	4.4	4.61	0.75	-2.40	Hansch et al., 1995	8(e)-3066
6639-30-1	2,4,5-Trichlorotoluene	195	4.6	4.5	4.56	0.55	-2.55	BioByte, 1995	Hermens et al., 1984
634-66-2	1,2,3,4-Tetrachlorobenzene	216	4.6	4.6	4.6	0.54	-2.60	Hansch & Leo, 1985	Hermens et al., 1984
634-66-2	1,2,3,4-Tetrachlorobenzene	216	4.6	4.6	4.6	0.13	-3.22	Hansch & Leo, 1985	Hermens et al., 1984 (Rose et al.)
68953-84-4	1,4-Benzenediamine, N,N'-m	274	5.7	4.6		0.59	-2.67		8(e)-13284
22094-81-1	Bicyclo(2.2.1)hept-2-ene, 5-b	150	4.7	4.7		0.04	-3.57		8(e)-14623
CBI	CBI	186	5.1	4.7		0.2	-2.97		P00-___
23184-66-9	Butachlor	312	4	4.8	4.5	3	-2.02	Hansch et al., 1995	Oris et al.
206-44-0	Fluoranthene	202	5	4.9	5.16	0.045	-3.65	Hansch et al., 1995	Oris et al.
603-35-0	Triphenylphosphine	262	MF	5	5.69	0.6	-2.64	Hansch et al., 1995	8(e)-0014
SAR data not included in regression equation:									
CBI	CBI	387	1.7	2.5		*	*		P85-___
CBI	CBI	663	1.9	2.5		*	*		L96-___
1912-24-9	Atrazine	216	2.4	2.8	2.61	*	*	Hansch, et al., 1995	Oris et al.
CBI	CBI	250	2.7	3.2		*	*		P95-___
CBI	CBI	296	5	4.5		*	*		P03-___
68953-84-4	1,4-Benzenediamine, N,N'-m	274	5.7	4.6		*	*		8(e)-13284

CBI	CBI	246	MF	4.9		*	*		P03-___
CBI	CBI	465	9.3	4.9		*	*		L03-___
CBI	CBI	200	5.1	5.1		0.39	-2.71		P06-___; 8(e)-___
68526-86-3	C11-14 isoalcohols, C13-rich	200	5.2	5.2		0.275	-2.86		8(e)-15318
608-93-5	Pentachlorobenzene	250	5.2	5.2	5.17	0.12	-3.32	Hansch & Leo, 1985	Hermens et al., 1984
608-93-5	Pentachlorobenzene	250	5.2	5.2	5.17	0.01	-4.40	Hansch & Leo, 1985	Hermens et al., 1984 (Rose et al.)
608-93-5	Pentachlorobenzene	250	5.2	5.2	5.17	*	*	Hansch, et al., 1985	Oris et al.
3081-01-4	N-(1,4-dimethylpentyl)-N'-phenyl-p-phenylenediamine	282	5.9	5.2		0.21	-3.13		8(e)-9897,8(e)-10181
CBI	CBI	258	4.2	5.3		38	-0.83		P00-___
CBI	CBI	290	5.5	5.6		*	*		P97-___
CBI	CBI	226	6.7	6.1		*	*		P91-___
CBI	CBI	228	6.5	6.1		*	*		P98-___
CBI	CBI	232	6.7	6.2		0.087	-3.43		P90-___, P90-___, P90-___
2437-79-8	2,2',4,4'-Tetrachlorobiphenyl	292	6.4	6.3	6.29	0.04	-3.86	Hansch & Leo, 1985	8(e)-3066
CBI	CBI	338	6.1	6.3		*	*		P89-___
CBI	CBI	260	6.8	6.4		*	*		P92-___
CBI	CBI	260	6.8	6.4		*	*		P92-___
CBI	CBI	352	5.4	6.5		*	*		L91-___
CBI	CBI	525		6.9	5.1	*	*	Rekker	P00-___
CBI	CBI	525	7.2	7.1		*	*		P98-___
CBI	CBI	271	8	7.6		*	*		P98-___
CBI	CBI	463	8.3	7.8		*	*		P87-___
CBI	CBI	425	7.5	8.2		*	*		P91-___
CBI	CBI	242	9.3	8.6		*	*		P98-___
CBI	CBI	431	11	10		*	*		L05-___
CBI	CBI	519	11	10		*	*		P05-___
CBI	CBI	311	12	11		*	*		P88-___
CBI	CBI	345	12	11		*	*		P99-___
CBI	CBI	736	16	11		*	*		P91-___
CBI	CBI	694	15	12		*	*		P88-___
CBI	CBI	868	12	13		*	*		P94-___
Data not used in SAR:									
CBI	CBI	488	-1.6	-4.3		>6000			P95-___; inequality
CBI	CBI	320	-3.2	-3.8		820	0.41		P93-___; LC20
994-05-8	tert-Amyl methyl ether	102	1.6	1.9		100	-0.01		8FYI-1047; not verified
CBI	CBI	250	mf	2.4		*	*		P92-___; SRC log Kow too low
101-84-8	Diphenyl ether	170	4.2	4.1	4.21	0.67	-2.40	Hansch & Leo, 1985	LeBlanc, 1984; no duration
CBI	CBI	182	5	4.6	4.56	2.5	-1.86	P92-1356	P92-___; EC>SH2O
CBI	CBI	182	5	4.6	4.56	1.5	-2.08	P92-1356-1	P92-___; EC>SH2O
CBI	CBI	182	5	4.6	4.56	1.0	-2.27	P92-1356	P92-___; EC>SH2O and 24h test
68908-88-3	Benzylated ethylbenzene	196	5.5	5.1		0.45	-2.64		8(e)-9548; EC>SH2O
72-43-5	Methoxychlor	346	5.2	5.7	5.08	0.014	-4.39	Hansch et al., 1995	Oris et al.; excess toxicity
50-32-8	Benzo[a]pyrene	252	6	6.1	6.13	0.005	-4.70	DeMaagd et al., 1998	ETFS; excess toxicity
CBI	CBI	272	7.2	6.6		1.5	-2.26		P92-___; EC>SH2O
8001-35-2	Toxaphene	414	4.3	6.8		0.01	-4.62		ETFS; excess toxicity
CBI	CBI	515	6.8	7	3.26	<0.120		P02-306	P02-___; NOEC
68425-15-0	Di-tert-dodecylpolysulfides								8(e)-14121; no specific value
CBI	CBI	1320				1000	-0.12		P94-___; NOEC
CBI	CBI					0.1			P92-___; no structure
							* indicates no effects at saturation		

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GREEN ALGAE 96-h EC50

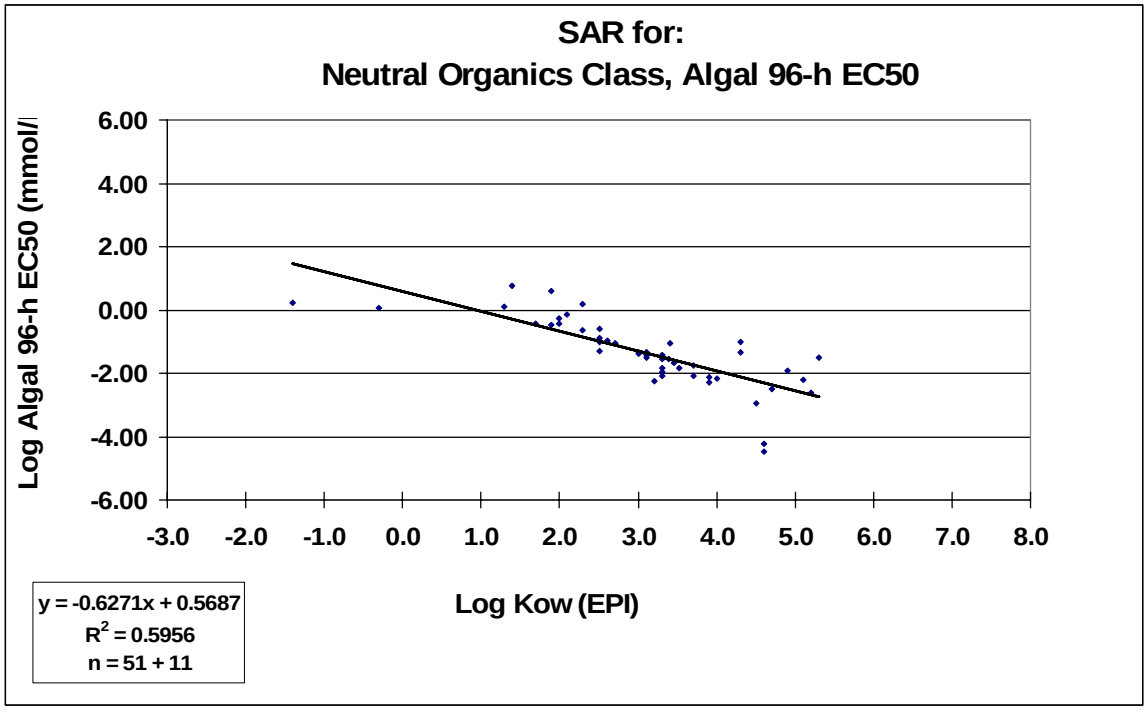
ESTIMATED TOXICITY:
The green algae 96-h EC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h EC50 (mmol/L) = -0.6271 log K_{ow} + 0.5687

The EC50 is in millimoles per liter (mM/L); N = 51 + 11; and the Coefficient of Determination (R^2) = 0.5956. To convert the EC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 6.4
Maximum MW: 1000

Graph:



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 Kow value is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Algal 96-h EC50 (mg/L)	Log Algal 96-h EC50 (mmol/L)	Reference (Meas. Kow)	Reference (EC50)
CBI	CBI	355	-2.8	-1.4		580	0.21		P97-___
CBI	CBI	116	0	-0.3		130	0.05		P90-___
CBI	CBI	248	1.9	1.3		315	0.10		P88-___
1634-04-4	Methyl tert-butyl ether	88	1	1.4	0.94	491	0.75	Hansch & Leo, 1985	CAS-Wetal, 2001
CBI	CBI	172	1.7	1.7		65	-0.42		P94-___
CBI	CBI	102	1.6	1.9	1.55	392	0.58	Datasheet	P98-___
CBI	CBI	271	2.1	1.9		93	-0.46		L96-___
71-43-2	Benzene	78	2.1	2	2.13	29	-0.43	Hansch & Leo, 1985	Galassi, 1988
71-43-2	Benzene	78	2.1	2	2.13	41	-0.28	Hansch & Leo, 1985	Herman, 1990
91-22-5	Quinoline	129	2	2.1	2.03	90	-0.16	Hansch & Leo, 1985	CAS-Kuhn & Pattard, 1990
78-87-5	1,2-Dichloropropane	113	2	2.3	1.98	172	0.18	Sangster, 1994	U.S.EPA, OPP
3622-84-2	Benzenesulfonamide, N-I	213	2.5	2.3	2.1	49	-0.64	PSIDS	SIDS
108-88-3	Toluene	92	2.6	2.5	2.73	12.5	-0.87	Hansch & Leo, 1985	Galassi, 1988
108-88-3	Toluene	92	2.6	2.5	2.73	9.4	-0.99	Hansch & Leo, 1985	Herman, 1990
CBI	CBI	303	MF	2.5	2.73	15	-1.31	NS	P02-___
CBI	CBI	530	2.7	2.5		128	-0.62		P98-___
108-90-7	Chlorobenzene	113	2.9	2.6	2.84	12.5	-0.96	Sangster, 1994	Calamari, 1983
104-76-7	2-Ethylhexanol	130	2.8	2.7		12	-1.03		CAS-SIDS
100-41-4	Ethylbenzene	106	3.2	3	3.15	4.6	-1.36	Hansch & Leo, 1985	Galassi, 1988
100-41-4	Ethylbenzene	106	3.2	3	3.15	4.8	-1.34	Hansch & Leo, 1985	Herman, 1990
95-47-6	o-Xylene	106	3.1	3.1	3.12	4.7	-1.35	Hansch & Leo, 1985	Galassi, 1988
95-47-6	o-Xylene	106	3.1	3.1	3.12	4.2	-1.40	Hansch & Leo, 1985	Herman, 1990
106-42-3	p-Xylene	106	3.1	3.1	3.15	3.2	-1.52	Hansch & Leo, 1985	Galassi, 1988
106-42-3	p-Xylene	106	3.1	3.1	3.15	4.4	-1.38	Hansch & Leo, 1985	Herman, 1990
108-38-3	m-Xylene	106	3.1	3.1	3.2	4.9	-1.34	Hansch & Leo, 1985	Galassi, 1988
108-38-3	m-Xylene	106	3.1	3.1	3.2	3.9	-1.43	Hansch & Leo, 1985	Herman, 1990
CBI	CBI	221	3.4	3.2		1.27	-2.24		P92-___
95-50-1	1,2-Dichlorobenzene	147	3.5	3.3	3.43	2.2	-1.82	Hansch et al., 1995	Calamari, 1983
106-46-7	1,4-Dichlorobenzene	147	3.6	3.3	3.44	1.6	-1.96	Hansch et al., 1995	Calamari, 1983
85-02-9	5,6-Benzoquinoline	179	3.2	3.3	3.43	1.55	-2.06	Hansch & Leo, 1985	CAS- van Vlaardingen, 1996
229-87-8	Phenanthridine	179	3.2	3.3	3.48	5.24	-1.53	Hansch et al., 1995	CAS- van Vlaardingen, 1996
230-27-3	Benzo[h]quinoline	179	3.2	3.3	3.43	6.65	-1.43	Sangster, 1993	CAS- van Vlaardingen, 1996
4180-23-8	trans-Anethole	148	3.3	3.4		4.24	-1.54		DUL Terpene Study
CBI	CBI	154	2.4	3.4	2.87	14	-1.04	Li & Perdue, 1995	P89-___
98-82-8	Isopropyl benzene	120	3.6	3.45	3.66	2.6	-1.66	Hansch et al., 1995	Galassi, 1988
103-65-1	n-Propylbenzene	120	3.7	3.52	3.69	1.8	-1.82	Sangster, 1994	Galassi, 1988
CBI	CBI	100	4.3	3.7		0.8	-2.10		P02-___
89-69-0	1,2,4-Trichloro-5-nitroben	226	3.7	3.7	3.48	4	-1.75	8(e)	8(e)-14895
87-61-6	1,2,3-Trichlorobenzene	181	4	3.9	4.05	0.9	-2.30	Sangster, 1994	Calamari, 1983
120-82-1	1,2,4-Trichlorobenzene	181	4.2	3.9	4.02	1.4	-2.11	Hansch et al., 1995	Calamari, 1983
CBI	CBI	107	4.9	4	2.76, 5.18	0.74	-2.16	Datasheet	P04-___/P04-___
CBI	CBI	230	3.2	4.3		11	-1.32		P00-___
CBI	CBI	344	2.9	4.3		34	-1.01		P97-___
35148-18-6	Z-9-Dodecanol	184	4.5	4.5		0.2	-2.96		8(e)-16211
68953-84-4	1,4-Benzenediamine, N,N	274	5.7	4.6		0.017	-4.21		8(e)-13284
68953-84-4	1,4-Benzenediamine, N,N	274	5.7	4.6		0.009	-4.48		8(e)-13284
125904-11-2	Dibromostyrene	262	4.6	4.7		0.84	-2.49		8(e)-16032
CBI	CBI	246	MF	4.9		3.1	-1.90		P03-___
CBI	CBI	200	5.1	5.1		1.3	-2.19		P06-___; 8(e)-___

3081-01-4	N-(1,4-dimethylpentyl)-N'phenyl-p-phenylenediamine	282	5.9	5.2		0.7	-2.61		8(e)-9170
CBI	CBI	258	4.2	5.3		8.4	-1.49		P00-____
SAR data not included in regression equation:									
CBI	CBI	250	2.7	3.2		*	*		P95-____
CBI	CBI	465	9.3	4.9		*	*		L03-____
118-74-1	Hexachlorobenzene	285	5.7	5.9	5.73	*	*	DeBruijn et al., 1989	Calamari, 1983
CBI	CBI	228	6.5	6.1		*	*		P98-____
CBI	CBI	232	6.7	6.2		*	*		P90-____, P90-____, P90-____, S03-____
CBI	CBI	260	6.8	6.4		*	*		P92-____
CBI	CBI	525	7.2	7.1		*	*		P98-____
CBI	CBI	425	7.5	8.2		*	*		P91-____
CBI	CBI	431	11	10		*	*		L05-____
CBI	CBI	311	12	11		*	*		P88-____
CBI	CBI	868	12	13		*	*		P94-____
Data not included in SAR:									
74-85-1	Ethylene	28	1.2	1.3	1.13	40	0.15	Hansch & Leo, 1985	VN sheet/SIDS; 72-h test
994-05-8	tert-Amyl methyl ether	102	1.6	1.9		0.11	-2.97		8FYI-1050; not verified
CBI	CBI	250	mf	2.4		*	*		P92-____; SRC log Kow too
101-84-8	Diphenyl ether	170	4.2	4.1	4.21	0.8	-2.33	Hansch & Leo, 1985	LeBlanc, 1984; no duration
CBI	CBI	182	5	4.6	4.56	0.5	-2.60	P92-1356-1	P92-____; EC>SH2O and 14-
CBI	CBI	196	5.6	5.2		0.46	-2.63		P92-____; EC>SH2O and 14-
CBI	CBI	290	5.5	5.6		0.022	-4.12		P97-____; VN Flag
CBI	CBI	272	7.2	6.6		1.2	-2.36		P92-____; EC>SH2O and 14-
CBI	CBI	694	15	12		0.056	-4.09		P88-____; EC>SH2O
CBI	CBI	210	6.2			1.2	-2.24		P92-____; EC>SH2O and 14-day test
* indicates no effects at saturation									

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FISH 30-d ChV

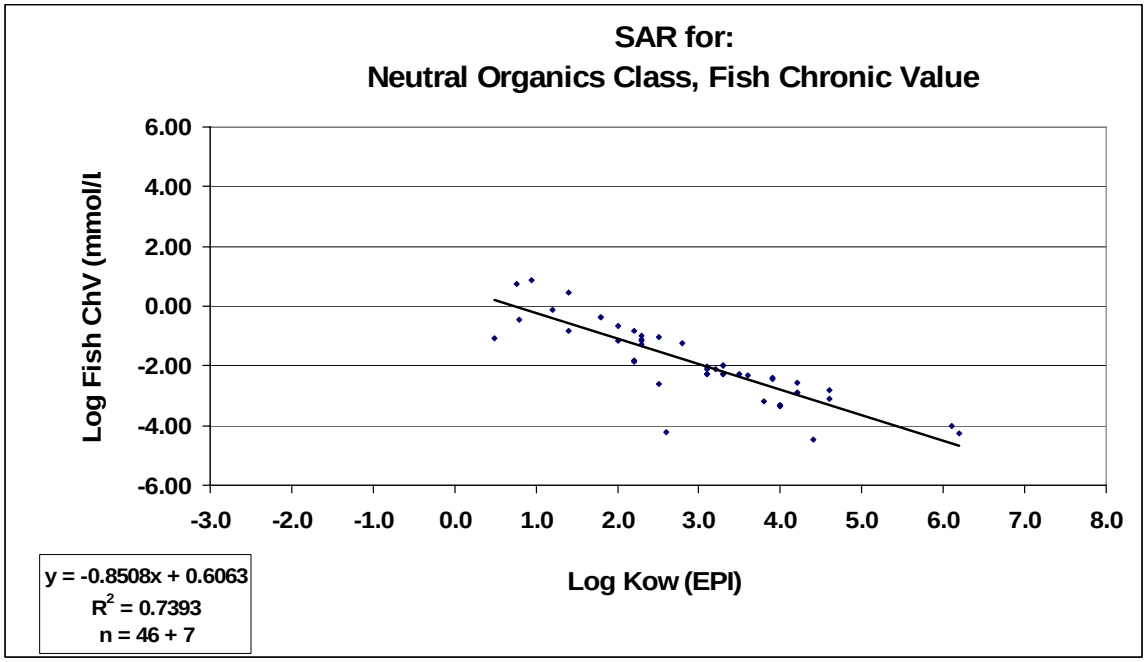
ESTIMATED TOXICITY:
The fish 30-d chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = - 0.8508 log K_{ow} + 0.6063

The ChV is in millimoles per liter (mM/L); N = 46 + 7; and the Coefficient of Determination (R^2) = 0.7393. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

Graph:



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 Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	30-d Fish ChV(mg/L)	Log 30-d Fish ChV (mmol/L)	Reference (Meas. Kow)	Reference (ChV)
1122-54-9	4-Acetylpyridine	121	0.48	0.49	0.48	10.3	-1.07	Hansch & Leo, 1985	DUL
78-83-1	2-Methy-1-propanol	74	0.69	0.77	0.76	416	0.75	Hansch & Leo, 1985	DUL
110-86-1	Pyridine	79	0.65	0.8	0.65	28	-0.45	Hansch & Leo, 1985	DUL
109-99-9	Tetrahydrofuran	72	0.46	0.94	0.46	513	0.85	Hansch & Leo, 1985	DUL
108-10-1	4-Methyl-2-pentanone	100	1.3	1.2	1.31	77.4	-0.11	Tanii & Hashimoto, 1986	DUL
110-00-9	Furan	68	1.3	1.4	1.34	10	-0.83	Hansch & Leo, 1985	DUL
1634-04-4	Methyl tert-butyl ether	88	1	1.4	0.94	245	0.44	Hansch & Leo, 1985	CAS-Wong et al, 2001
107-06-2	1,2-Dichloroethane	99	1.5	1.8	1.48	40.6	-0.39	Hansch & Leo, 1985	DUL
107-06-2	1,2-Dichloroethane	99	1.5	1.8	1.48	41	-0.38	Hansch & Leo, 1985	Benoit et al.. 1982
79-00-5	1,1,2-Trichloroethane	133	2.1	2.01	1.89	27.8	-0.68	Pomona, 1987	DUL
79-00-5	1,1,2-Trichloroethane	133	2.1	2.01	1.89	9.4	-1.15	Pomona, 1987	Ahmad et al., 1984
150-78-7	p-Dimethoxybenzene	138	2.2	2.2	2.04	21.2	-0.81	Dunn et al., 1983	DUL
79-34-5	1,1,2,2-Tetrachloroethane	168	2.6	2.2	2.39	2.5	-1.83	Hansch & Leo, 1985	DUL
79-34-5	1,1,2,2-Tetrachloroethane	168	2.6	2.2	2.39	2.4	-1.84	Hansch & Leo, 1985	Ahmad et al., 1984
78-87-5	1,2-Dichloropropane	113	2.0	2.3	1.98	8.28	-1.14	Sangster, 1994	DUL
78-87-5	1,2-Dichloropropane	113	2.0	2.3	1.98	8.1	-1.14	Sangster, 1994	Benoit et al.. 1982
142-28-9	1,3-Dichloropropane	113	1.7	2.3	2	5.83	-1.29	Hansch & Leo, 1985	DUL
142-28-9	1,3-Dichloropropane	113	1.7	2.3	2	11	-1.01	Hansch & Leo, 1985	Benoit et al., 1982
108-88-3	Toluene	92	2.6	2.5	2.73	8.69	-1.02	Hansch & Leo, 1985	DUL
88-73-3	1-Chloro-2-nitrobenzene	158	2.4	2.5	2.2	0.375	-2.62	Hansch & Leo, 1985	DUL
108-90-7	2-Chlorobenzene	113	2.9	2.6	2.84	0.0067	-4.23	Sangster, 1994	CAS-SRC
111-87-5	n-Octanol	130	2.9	2.8	3	7.15	-1.26	Hansch et al., 1995	Broderius et al., 2005
76-01-7	Pentachloroethane	202	3.6	3.1	3.22	1.63	-2.09	Hansch et al., 1995	Broderius et al., 2005
76-01-7	Pentachloroethane	202	3.6	3.1	3.22	1.99	-2.01	Hansch et al., 1995	Broderius et al., 2005
76-01-7	Pentachloroethane	202	3.6	3.1	3.22	1.1	-2.26	Hansch et al., 1995	Ahmad et al., 1984
76-01-7	Pentachloroethane	202	3.6	3.1	3.22	1.09	-2.27	Hansch et al., 1995	DUL
119-61-9	Benzophenone	182	3.2	3.2	3.18	1.35	-2.13	Hansch & Leo, 1985	DUL
541-73-1	1,3-Dichlorobenzene	147	3.6	3.3	3.53	1.51	-1.99	Hansch et al., 1995	DUL
541-73-1	1,3-Dichlorobenzene	147	3.6	3.3	3.53	1.5	-1.99	Hansch et al., 1995	Carlson and Kosian, 1987
106-46-7	p-Dichlorobenzene	147	3.6	3.3	3.44	0.763	-2.28	Hansch et al., 1995	CAS - ETFS
106-46-7	p-Dichlorobenzene	147	3.6	3.3	3.44	0.751	-2.29	Hansch et al., 1995	DUL
822-86-6	trans-1,2-Dichlorocyclohexane	153	3.3	3.5	3.21	0.774	-2.30	Hansch & Leo, 1985	DUL
98-56-6	Parachloro benzo trifluoride	181	3.7	3.6		0.87	-2.32		8(e)-2491
95-75-0	3,4-Dichlorotoluene	161	4	3.8	3.95	0.108	-3.17	BioByte, 1995	DUL
120-82-1	1,2,4-Trichlorobenzene	181	4.2	3.9	4.02	0.689	-2.42	Hansch et al., 1995	DUL
120-82-1	1,2,4-Trichlorobenzene	181	4.2	3.9	4.02	0.68	-2.43	Hansch et al., 1995	Carlson, 1987
67-72-1	Hexachloroethane	237	4.6	4.0	4.14	0.109	-3.34	Hansch et al., 1995	DUL
67-72-1	Hexachloroethane	237	4.6	4.0	4.14	0.12	-3.30	Hansch et al., 1995	Ahmad et al., 1984
83-32-9	Acenaphthene	154	3.8	4.2	3.92	0.412	-2.57	Hansch & Leo, 1985	CAS-ETFS
83-32-9	Acenaphthene	154	3.8	4.2	3.92	0.199	-2.89	Hansch & Leo, 1985	DUL
83-32-9	Acenaphthene	154	3.8	4.2	3.92	0.2	-2.89	Hansch & Leo, 1985	Lemke et al., 1983
85-01-8	Phenanthrene	178	4.5	4.4	4.46	0.0063	-4.45	Hansch & Leo, 1985	CAS - ETFS
634-66-2	1,2,3,4-Tetrachlorobenzene	216	4.6	4.6	4.6	0.164	-3.12	Hansch, C. et al. 1995	DUL
634-66-2	1,2,3,4-Tetrachlorobenzene	216	4.6	4.6	4.6	0.32	-2.83	Hansch, C. et al. 1995	Carson and Kosian, 1987
CBI	CBI	226	6.7	6.1		0.022	-4.01		P91-____
CBI	CBI	232	6.7	6.2		0.013	-4.25		P90-____, P90-____, P90-____, S03-____
SAR data not included in regression equation:									
608-93-5	Pentachlorobenzene	285		5.2	5.17	*	*	Hansch et al., 1995	DUL
608-93-5	Pentachlorobenzene	285		5.2	5.17	*	*	Hansch et al., 1995	Carlson and Kosian, 1987
118-74-1	Hexachlorobenzene	285		5.9	5.73	*	*	DeBruijn, 1989	DUL
118-74-1	Hexachlorobenzene	285		5.9	5.73	*	*	DeBruijn, 1989	Carlson and Kosian, 1987
CBI	CBI	228	6.5	6.1		*	*		P98-____
CBI	CBI	260	6.8	6.4		*	*		P92-____
CBI	CBI	238	7.5	6.9		*	*		P90-____
Data not used in SAR:									
67-56-1	Methanol	32	-0.76	-0.63	-0.77	<490	<1.18	Hansch & Leo, 1985	DUL
108-10-1	4-Methyl-2-pentanone	100	1.3	1.2	1.31	<56.2	<-0.25	Tanii & Hashimoto, 1986	DUL
994-05-8	tert-Amyl methyl ether	102	1.6	1.9		310	0.48		8FYI-1052; not verified
71-43-2	Benzene	78	2.1	2.0	2.13	<1.6	<-1.69	Hansch & Leo, 1985	DUL
109-64-8	1,3-Dibromopropane	202		2.5	2.37	<0.0831	<-3.4	Hansch et al., 1995	
709-98-8	Propanil	218	3.3	2.9	3.07	0.000484	-5.65	Hansch & Leo, 1985	DUL; excess toxicity
18172-67-3	(is)-(-)-B-Pinene	136	4.1	4.3		0.4	-2.53		CAS-Passino-Reader, 1995;
18172-67-3	(is)-(-)-B-Pinene	136	4.1	4.3		0.16	-2.93		CAS-Passino-Reader, 1995;
4795-86-2	(is)-(-)-trans-Pinane	138	4.7	4.4		0.095	-3.16		CAS-Passino-Reader, 1995;
50-32-8	Benzo[a]pyrene	252	6	6.1	6.13	0.00008	-6.50	DeMaagd et al., 1998	ETFS; excess toxicity
8001-35-2	Toxaphene	414	4.3	6.8		0.0000367	-7.05		ETFS; excess toxicity
CBI	CBI	475	10	9.6	>5.11	*	*	P92-465	P92-____; 56-day test
CBI	CBI	971	11	14		*	*		P89-____; 56-day test
1336-36-3	PCBs					0.0051			ETFS; unspecified structure
						* indicates no effects at saturation			

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DAPHNID ChV

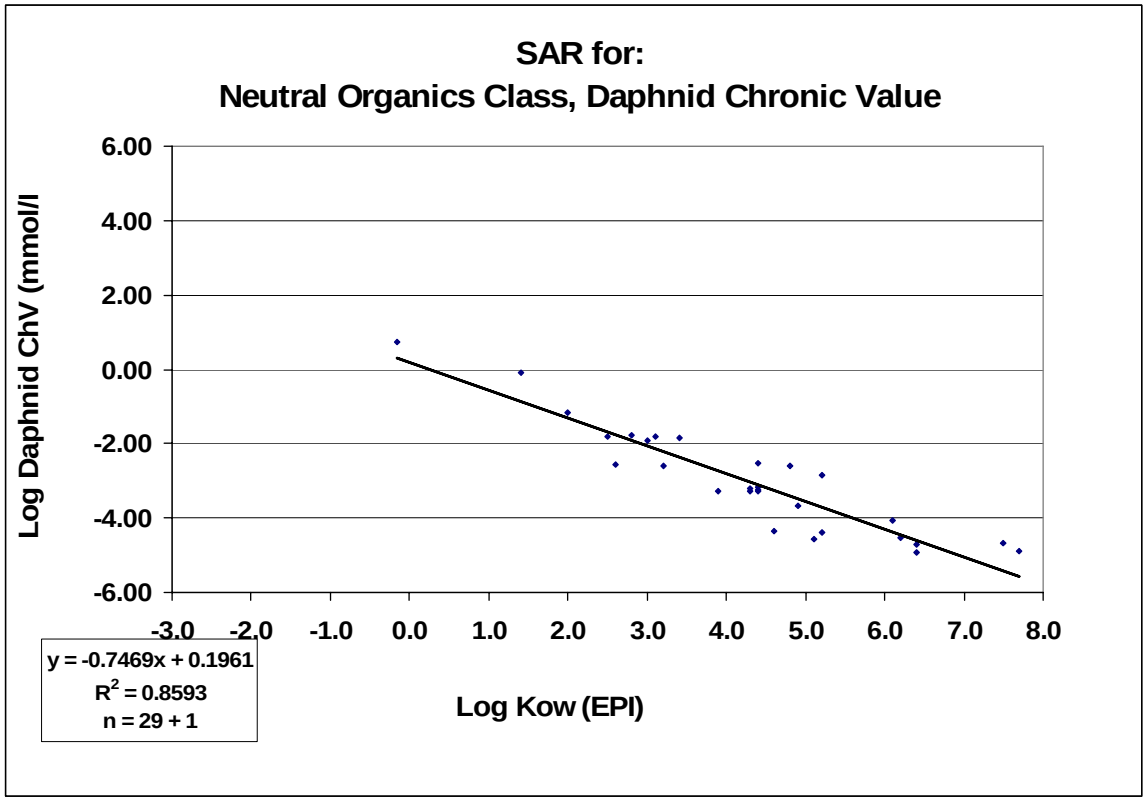
ESTIMATED TOXICITY:
The daphnid ChV values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 16-d ChV (mmol/L) = - 0.7469 log K_{ow} + 0.1961

The ChV is in millimoles per liter (mM/L); N = 29 + 1; and the Coefficient of Determination (R^2) = 0.8593. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

Graph:



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 Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.		M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Daphnid ChV (mg/L)	Log Daphnid ChV (mmol/L)	Reference (Meas. Kow)	Reference (ChV)
75-05-8	Acetonitrile	41	-0.34	-0.15	-0.34	230	0.75	Hansch & Leo, 1985	Tong et al., 1996
1634-04-4	Methyl tert-butyl ether	88	1	1.4	0.94	71	-0.09	Hansch & Leo, 1985	CAS-Wetal, 2001
71-43-2	Benzene	78	2.1	2	2.13	5.2	-1.18	Hansch & Leo, 1985	CAS-Niederlehner et al., 1998
108-88-3	Toluene	92	2.6	2.5	2.73	1.4	-1.82	Hansch & Leo, 1985	CAS-Niederlehner et al., 1998
108-90-7	Monochlorobenzene	113	2.9	2.6	2.84	0.32	-2.55	Sangster, 1994	Hermens et al., 1984
1912-24-9	Atrazine	216	2.4	2.8	2.61	3.5	-1.79	Hansch et al., 1995	Oris et al.
100-41-4	Ethylbenzene	106	3.2	3	3.15	1.3	-1.91	Hansch & Leo, 1985	CAS-Niederlehner et al., 1998
108-38-3	m-Xylene	106	3.1	3.1	3.2	1.7	-1.79	Hansch & Leo, 1985	CAS-Niederlehner et al., 1998
106-43-4	4-Chlorotoluene	127	3.4	3.2	3.33	0.32	-2.60	Hansch & Leo, 1985	Hermens et al., 1984
15972-60-8	Alachlor	270	2.4	3.4	3.52	3.9	-1.84	Hansch & Leo, 1985	Oris et al.
120-82-1	1,2,4-Trichlorobenzene	182	4.2	3.9	4.02	0.1	-3.26	Hansch et al., 1995	Hermens et al., 1984
1836-75-5	Nitrofen	284	5.6	4.3	4.64	0.151	-3.27	Sangster, 1994	Oris et al.
571-58-4	1,4-Dimethylnaphthalene	156	4.3	4.3	4.37	0.1	-3.19	Hansch & Leo, 1985	8(e)-12746
85-01-8	Phenanthrene	178	4.5	4.4	4.46	0.0964	-3.27	Hansch & Leo, 1985	CAS - ETFS
85-01-8	Phenanthrene	178	4.5	4.4	4.46	0.1	-3.25	Hansch & Leo, 1985	CAS-Savino & Tanabe, 1989
4795-86-2	(is)-(-)-trans-Pinane	138	4.7	4.4		0.4	-2.54		CAS-Savino & Tanabe, 1989
4795-86-2	(is)-(-)-trans-Pinane	138	4.7	4.4		0.095	-3.16		CAS-Passino-Reader 1995
634-66-2	1,2,3,4-Tetrachlorobenzene	216	4.6	4.6	4.6	0.01	-4.33	Hansch & Leo, 1985	Hermens et al., 1984
23184-66-9	Butachlor	312	4	4.8	4.5	0.81	-2.59	Hansch et al., 1995	Oris et al.
206-44-0	Fluoranthene	202	5	4.9	5.2	0.043	-3.67	Hansch & Leo, 1985	Oris et al.
556-67-2	Octamethylcyclotetrasiloxar	297	7	5.1	5.1	0.0079	-4.58	TSCATS	8(e)-11820
608-93-5	Pentachlorobenzene	250	5.2	5.2	5.17	0.35	-2.85	Hansch & Leo, 1985	Oris et al.
608-93-5	Pentachlorobenzene	250	5.2	5.2	5.17	0.01	-4.40	Hansch & Leo, 1985	Hermens et al., 1984
CBI	CBI	228	6.5	6.1		0.02	-4.06		P98-____
CBI	CBI	232	6.7	6.2		0.007	-4.52		P90-____, -____, -____, S03-____
CBI	CBI	260	6.8	6.4		0.003	-4.94		P92-____
CBI	CBI	260	6.8	6.4		0.005	-4.72		P92-____
6742-54-7	Alkyl benzene	237	7.9	7.5	8.14	0.005	-4.68	Sherblom et al., 1992	CAS-SIDS
32534-81-9	Pentabromodiphenyl oxide	565	8.3	7.7		0.00755	-4.87		8(e)-14280
SAR data not included in regression equation:									
CBI	CBI	238	7.5	6.9		*	*		P90-____
Data not used in SAR:									
CBI	CBI	73	-1	-0.93		5000	1.84		P94-____; EC100
994-05-8	tert-Amyl methyl ether	102	1.6	1.9		83	-0.09		8FYI-1047; not verified
72-43-5	Methoxychlor	346	5.2	5.7	5.1	0.007	-4.69	Hansch & Leo, 1985	Oris et al.; excess toxicity
8001-35-2	Toxaphene	414	4.3	6.8		0.0000916	-6.66		ETFS; excess toxicity
CBI	CBI	271	8	7.6		0.031	-3.94		P98-____; FLAG per VN
68648-87-3	Benzene, C10-16 alkyl deriv	218	9.1	8.4	9.36	0.017	-4.11	8(e)-9421	8(e)-9421; EC>SH2O
						* indicates no effects 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 anesthetic potency: Acute lethal and sublethal toxicity to *Daphnia magna*. Aquatic Toxicology 5: 143-154.

Niederlehner BR, Cairns J, Smith EP. 1998. Modeling acute and chronic toxicity of nonpolar narcotic chemicals and mixtures to *Ceriodaphnia dubia*. Ecotoxicology and Environmental Safety. 39:136-146.

Oris et al. 1991. Environ. Toxicol. Chem. 10, 217-224.

Savino JF, Tanabe LL. 1989. Sublethal effects of Phenanthrene, Nicotine, and Pinane on Daphnia pulex. Bull. Environ. Contam. Toxicol. 42(5):778-784.

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Tong Z, Huailian Z, Hongjun J. 1996. Chronic toxicity of acrylonitrile and acetonitrile to Daphnia magna in 14-d and 21-d toxicity tests. Bull. Environ. Contam. Toxicol. 57(4)655-659.

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

Wong et al.. 2001. Development of a freshwater aquatic toxicity database for ambient water quality criteria for methyl tertiary-butyl ether. Environmental Toxicology and Chemistry. 20(5):1125-1132.

GREEN ALGAE ChV

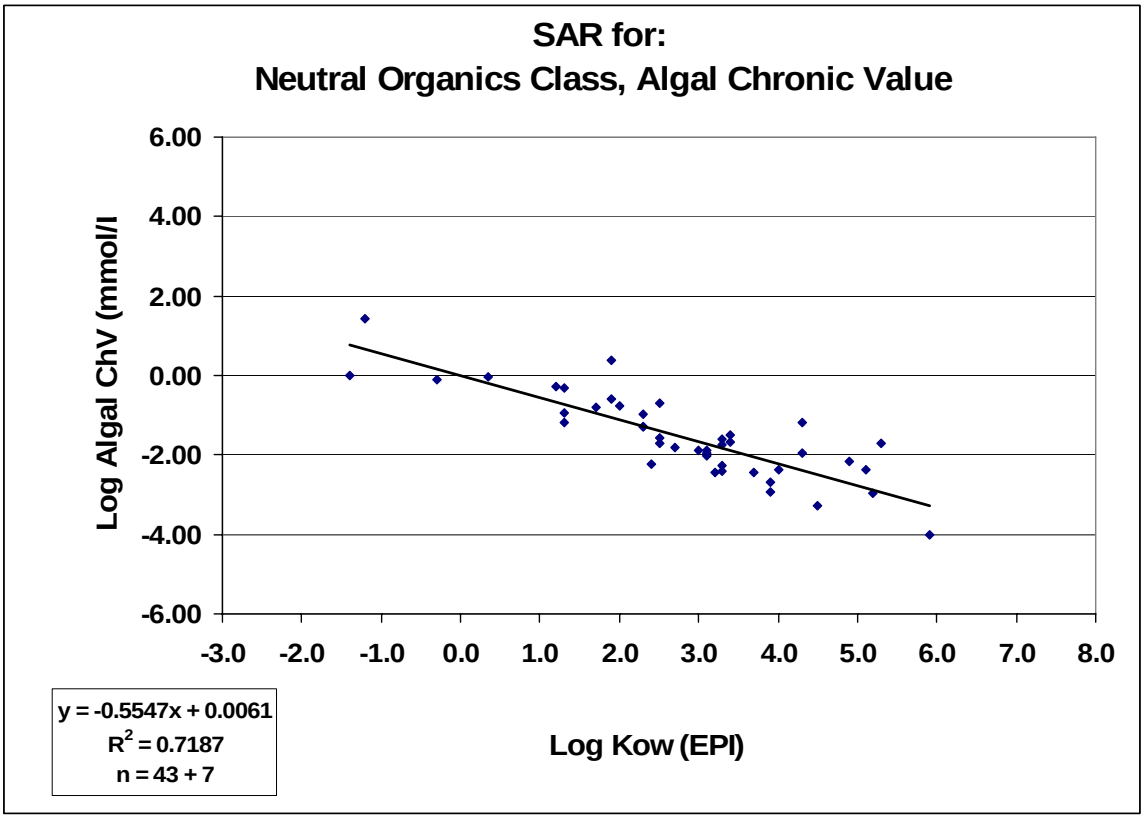
ESTIMATED TOXICITY:
The green algae chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.5547 log K_{ow} + 0.0061

The ChV is in millimoles per liter (mM/L); N = 43 + 7; and the Coefficient of Determination (R^2) = 0.7187. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

Graph:



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 Kow value is greater than 5.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow	log Kow	log Kow (M)	Algal ChV	Log Algal ChV(mmol/L)	Reference (Meas. Kow)	Reference (ChV)
CBI	CBI	355	-2.8	-1.4		360	0.01		P97-____
CBI	CBI	78	-1.4	-1.2	-1.35	2109	1.43	Hansch & Leo, 1985	P92-____
CBI	CBI	116	0	-0.3		90	-0.11		P90-____
111-69-3	1,4-Dicyanobutane	108	-0.42	0.35	-0.32	100	-0.03	Tanii & Hashimoto, 1985	CAS-SIDS
CBI	CBI	190	1.2	1.2		96	-0.30		P93-____
74-85-1	Ethylene	28	1.2	1.3	1.13	13.9	-0.30	Hansch & Leo, 1985	VN sheet/SIDS
CBI	CBI	248	1.9	1.3		15.9	-1.19		P88-____
CBI	CBI	248	1.9	1.3		27.3	-0.96		P88-____
CBI	CBI	172	1.7	1.7		27	-0.80		P94-____
CBI	CBI	271	2.1	1.9		69	-0.59		L96-____
CBI	CBI	102	1.6	1.9	1.55	240	0.37	Datasheet	P98-____
71-43-2	Benzene	78	2.1	2	2.13	13	-0.78	Hansch & Leo, 1985	Herman, 1990
78-87-5	1,2-Dichloropropane	113	2	2.3	1.98	5.7	-1.30	Sangster, 1994	Robert
78-87-5	1,2-Dichloropropane	113	2	2.3	1.98	6	-1.27	Sangster, 1994	Robert
3622-84-2	Benzenesulfonamide, N	213	2.5	2.3	2.1	22	-0.99	PSIDS	SIDS
104-90-5	2-Picoline, 5-ethyl	121	2.5	2.4		0.689	-2.24		CAS-SIDS
108-88-3	Toluene	92	2.6	2.5	2.73	1.8	-1.71	Hansch & Leo, 1985	Herman, 1990
CBI	CBI	303	MF	2.5	2.73	8.2	-1.57	NS	P02-____
CBI	CBI	530	2.7	2.5		103	-0.71		P98-____
104-76-7	2-Ethylhexanol	130	2.8	2.7		2	-1.81		CAS-SIDS
100-41-4	Ethylbenzene	106	3.2	3	3.15	1.4	-1.88	Hansch & Leo, 1985	Herman, 1990
95-47-6	o-Xylene	106	3.1	3.1	3.12	1.4	-1.88	Hansch & Leo, 1985	Herman, 1990
106-42-3	p-Xylene	106	3.1	3.1	3.15	1.2	-1.95	Hansch & Leo, 1985	Herman, 1990
108-38-3	m-Xylene	106	3.1	3.1	3.2	1	-2.03	Hansch & Leo, 1985	Herman, 1990
CBI	CBI	221	3.4	3.2		0.82	-2.43		P92-____
85-02-9	5,6-Benzoquinoline	179	3.2	3.3	3.43	0.98	-2.26	Hansch & Leo, 1985	CAS- van Vlaardingen, 1996
106-46-7	1,4-Dichlorobenzene	147	3.6	3.3	3.44	0.57	-2.41	Hansch et al., 1995	Herman, 1990
229-87-8	Phenanthridine	179	3.2	3.3	3.48	3.15	-1.75	Hansch et al., 1995	CAS- van Vlaardingen, 1996
230-27-3	Benzo[h]quinoline	179	3.2	3.3	3.43	4.47	-1.60	Sangster, 1993	CAS- van Vlaardingen, 1996
CBI	CBI	154	2.4	3.4	2.87	4.8	-1.51	Li & Perdue, 1995	P89-____
4180-23-8	trans-Anethole	148	3.3	3.4		3.09	-1.68		Dul terpene
CBI	CBI	100	4.3	3.7		0.35	-2.46		P02-____
87-61-6	1,2,3-Trichlorobenzene	181	4.3	3.9	4.05	0.22	-2.92	Sangster, 1994	Calamari, 1983
120-82-1	1,2,4-Trichlorobenzene	181	4.3	3.9	4.02	0.37	-2.69	Hansch et al., 1995	Calamari, 1983
CBI	CBI	107	4.9	4	2.76, 5.18	0.46	-2.37	Datasheet	P04-____/P04-____
CBI	CBI	344	2.9	4.3		22	-1.19		P97-____
CBI	CBI	230	3.2	4.3		2.5	-1.96		P00-____
35148-18-6	Z-9-Dodecanol	184	4.5	4.5		0.1	-3.26		8(e)-16211
CBI	CBI	246	MF	4.9		1.7	-2.16		P03-____
CBI	CBI	200	5.1	5.1		0.85	-2.37		P06-____; 8(e)-_____
3081-01-4	N-(1,4-dimethylpentyl)-N'-phenyl-p-phenylenediamine	282	5.9	5.2		0.3	-2.97		8(e)-9170
CBI	CBI	258	4.2	5.3		5.1	-1.70		P00-____
118-74-1	Hexachlorobenzene	285	6.4	5.9	5.73	0.027	-4.02	DeBruijn et al., 1989	Calamari, 1983
SAR data not included in regression equation:									
CBI	CBI	465	9.3	4.9		*	*		L03-____
CBI	CBI	232	6.7	6.2		*	*		P90-____, -____, -____, S03-_
CBI	CBI	260	6.8	6.4		*	*		P92-____
CBI	CBI	525		6.9	5.1	*	*	Rekker	P00-____
CBI	CBI	525	7.2	7.1		*	*		P98-____
CBI	CBI	425	7.5	8.2		*	*		P91-____
CBI	CBI	431	11	10		*	*		L05-____
Data not included in SAR:									
994-05-8	tert-Amyl methyl ether	102	1.6	1.9		0.017	-3.78		8FYI-1050; not verified
CBI	CBI	250	mf	2.4		*	*		P92-____; SRC log Kow too lo
CBI	CBI	290	5.5	5.6		0.012	-4.38		P97-____; VN Flag
CBI	CBI	515	6.8	7	3.26	<0.100		P02-306	P02-____; inequality
							* indicates no effects 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.

FISH (SW) 96-h LC50

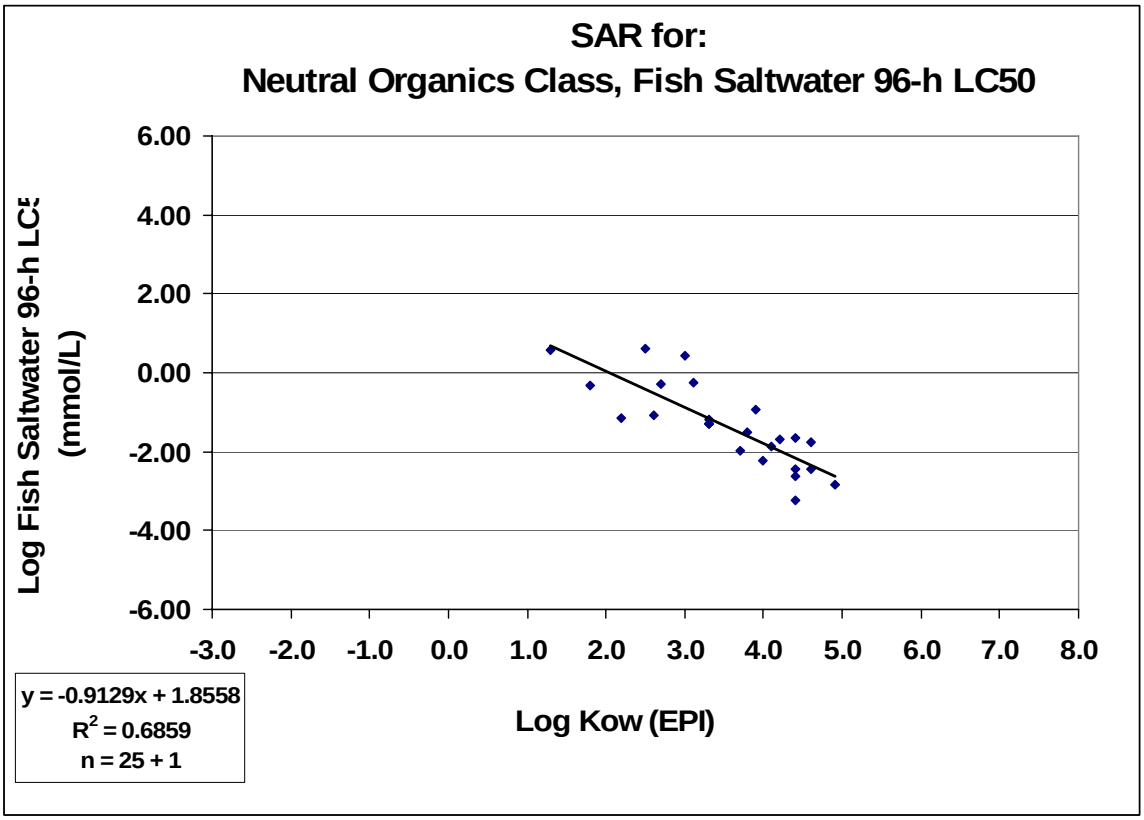
ESTIMATED TOXICITY:
The saltwater fish 96-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h LC50 (mmol/L) = - 0.9129 log K_{ow} + 1.8558

The LC50 is in millimoles per liter (mM/L); N = 25 + 1; and the Coefficient of Determination (R^2) = 0.6859. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 5.0
Maximum MW: 1000

Graph:



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 Kow value is greater than 5.0, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish SW 96-h LC50 (mg/L)	log Fish SW 96-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (LC50)
75-09-2	Methylene chloride	85	1.3	1.3	1.25	322.9	0.58	Hansch & Leo, 1985	Zaroogian et al., 1985
98-95-3	Nitrobenzene	123	1.9	1.8	1.85	58.92	-0.32	Hansch & Leo, 1985	Zaroogian et al., 1985
79-34-5	1,1,2,2-Tetrachloroethane	168	2.6	2.2	2.39	11.883	-1.15	Hansch & Leo, 1985	Zaroogian et al., 1985
108-88-3	Toluene	92	2.6	2.5	2.73	381	0.62	Hansch & Leo, 1985	CAS-ETFS
108-90-7	Chlorobenzene	113	2.9	2.6	2.84	9.804	-1.06	Sangster, 1994	Zaroogian et al., 1985
71-55-6	1,1,1-Trichloroethane	133	2.5	2.7	2.49	70.015	-0.28	Hansch & Leo, 1985	Zaroogian et al., 1985
100-41-4	Ethylbenzene	106	3.2	3	3.15	275	0.41	Hansch & Leo, 1985	CAS-ETFS
76-01-7	1,1,1,2,2-Pentachloroethane	202	3.6	3.11	3.22	113.762	-0.25	Hansch et al., 1995	Zaroogian et al., 1985
95-50-1	1,2-Dichlorobenzene	147	3.5	3.3	3.43	9.491	-1.19	Hansch et al., 1995	Zaroogian et al., 1985
106-46-7	p-Dichlorobenzene	147	3.6	3.3	3.44	7.4	-1.30	Hansch et al., 1995	CAS - ETFS
106-46-7	p-Dichlorobenzene	147	3.6	3.3	3.44	7.2	-1.31	Hansch et al., 1995	Zaroogian et al., 1985
5541-73-1	1,3-Dichlorobenzene	147	3.5	3.3	3.43	7.715	-1.28	Hansch et al., 1995	Zaroogian et al., 1985
132-64-9	Dibenzofuran	168	4.1	3.7	4.12	1.761	-1.98	Hansch & Leo, 1985	Zaroogian et al., 1985
92-52-4	Biphenyl	154	4	3.8	3.98	4.6	-1.52	Sangster, 1993	8(e)-3066
120-82-1	1,2,4-Trichlorobenzene	181	4.2	3.9	4.02	20.833	-0.94	Hansch et al., 1995	Zaroogian et al., 1985
67-72-1	1,1,1,2,2,2-Hexachloroethane	237	4.6	4	4.14	1.38	-2.23	Hansch et al., 1995	Zaroogian et al., 1985
101-84-8	Diphenyl ether	170	4.2	4.1	4.21	2.35	-1.86	Hansch & Leo, 1985	Zaroogian et al., 1985
83-32-9	Acenaphthene	154	3.8	4.2	3.92	3.1	-1.70	Hansch & Leo, 1985	CAS-ETFS
85-01-8	Phenanthrene	178	4.5	4.4	4.46	0.429	-2.62	Hansch & Leo, 1985	CAS - ETFS
85-01-8	Phenanthrene	178	4.5	4.4	4.46	0.108	-3.22	Hansch & Leo, 1985	CAS - ETFS
2051-62-9	4-Chlorobiphenyl	189	4.7	4.4	4.61	0.68	-2.44	Hansch et al., 1995	8(e)-3066
2051-60-7	2-Chlorobiphenyl	189	4.5	4.4	4.53	4.1	-1.66	Hansch et al., 1995	8(e)-3066
95-94-3	1,2,4,5-Tetrachlorobenzene	216	4.8	4.6	4.64	0.784	-2.44	Hansch & Leo, 1985	Zaroogian et al., 1985
634-90-2	1,2,3,5-Tetrachlorobenzene	216	4.8	4.6	4.56	3.666	-1.77	Hansch & Leo, 1985	Zaroogian et al., 1985
143-50-0	Kepone	491	3.5	4.9	5.41	0.693	-2.85	Pomona, 1987	Zaroogian et al., 1985
SAR data not included in regression equation:									
CBI	CBI	519	11	10		*	*		P05-___
Data not used in SAR:									
75-25-2	Bromoform	253	2.4	1.8	2.4	17.893	-1.15	Chem Inspect Test Inst, 1992	Zaroogian et al., 1985; excess tox
101-84-8	Diphenyl ether	170	4.2	4.1	4.21	2.4	-1.85	Hansch & Leo, 1985	LeBlanc, 1984; no duration
58-89-9	Lindane	291	3.7	4.3	3.72	0.801	-2.56	Hansch & Leo, 1985	Zaroogian et al., 1985; excess tox
72-43-5	Methoxychlor	346	5.2	5.7	5.08	0.049	-3.85	Hansch & Leo, 1985	Zaroogian et al., 1985; excess tox
8001-35-2	Toxaphene	414	4.3	6.8		0.000714	-5.76		ETFS; excess toxicity
CBI	CBI					212			P92-___; no structure

References:
U.S. Environmental Protection Agency (USEPA). 1992. Environmental Toxicity Fact Sheet (ETFS). Washington DC: Office of Water, USEPA, 1400 Pennsylvania Avenue NW.

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

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.

MYSID SHRIMP 96-h LC50

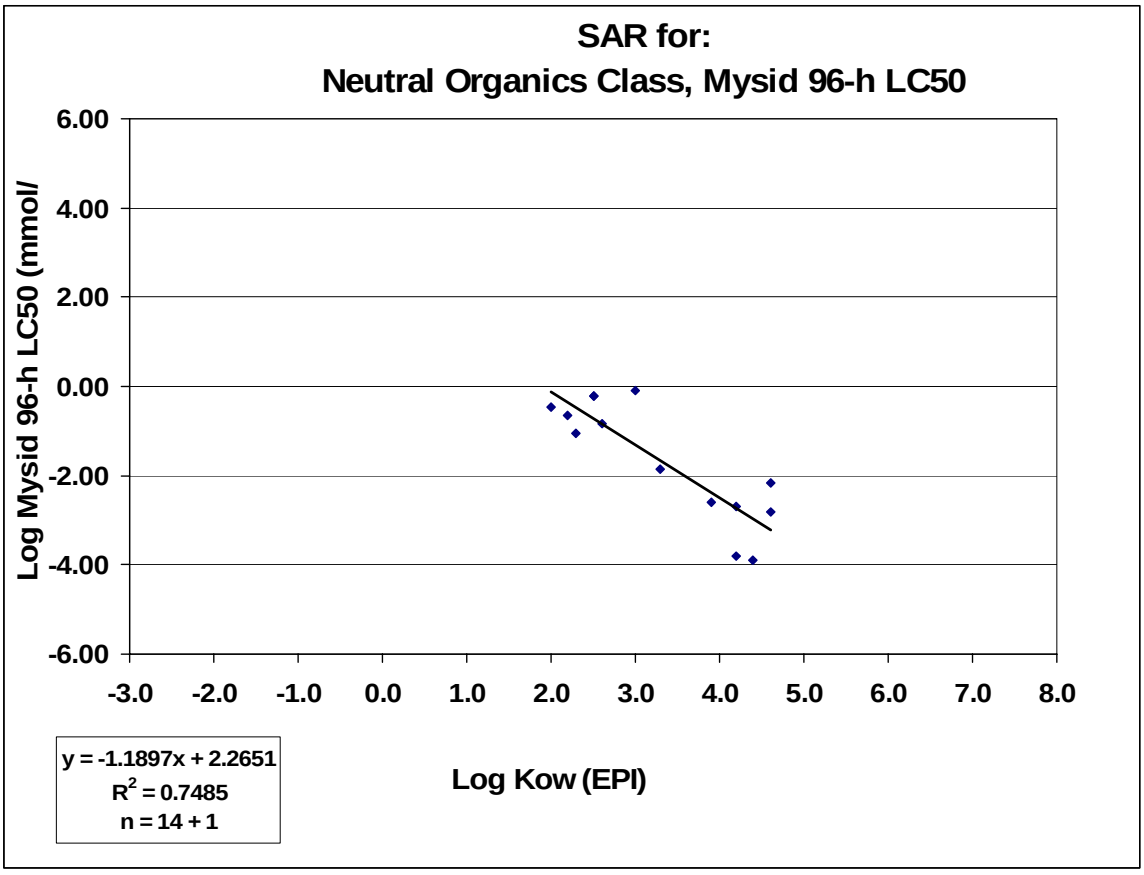
ESTIMATED TOXICITY:
The saltwater mysid shrimp 96-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h LC50 (mmol/L) = - 1.1897 log K_{ow} + 2.2651

The LC50 is in millimoles per liter (mM/L); N = 14 + 1; and the Coefficient of Determination (R^2) = 0.7485. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 5.0
Maximum MW: 1000

Graph:



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 Kow value is greater than 5.0, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Mysid 96-h LC50 (mg/L)	Log Mysid 96-h LC50(mmol/L)	Reference (Meas. Kow)	Reference (LC50)
71-43-2	Benzene	78	2.1	2	2.13	27	-0.46	Hansch & Leo, 1985	CAS-ETFS
CBI	CBI	113	2	2.2		24.79	-0.66		CBI
142-28-9	1,3-Dichloropropane	113	1.7	2.3	2	10.0702	-1.05	Hansch & Leo, 1985	Zaroogian et al., 1985
108-88-3	Toluene	92	2.6	2.5	2.73	56.3	-0.21	Hansch & Leo, 1985	CAS-ETFS
108-88-3	Toluene	92	2.6	2.5	2.73	55.5198	-0.22	Hansch & Leo, 1985	Zaroogian et al., 1985
108-90-7	Chlorobenzene	113	2.9	2.6	2.84	16.2699	-0.84	Sangster, 1994	Zaroogian et al., 1985
100-41-4	Ethylbenzene	106	3.2	3	3.15	87.6	-0.08	Hansch & Leo, 1985	CAS-ETFS
106-46-7	p-Dichlorobenzene	147	3.6	3.3	3.44	1.99	-1.87	Hansch et al, 1995	CAS - ETFS
120-82-1	1,2,4-Trichlorobenzene	181	4.2	3.9	4.02	0.4454	-2.61	Hansch et al., 1995	Zaroogian et al., 1985
83-32-9	Acenaphthene	154	3.8	4.2	3.92	0.3177	-2.69	Hansch & Leo, 1985	CAS-ETFS
83-32-9	Acenaphthene	154	3.8	4.2	3.92	0.025	-3.79	Hansch & Leo, 1985	Zaroogian et al., 1985
85-01-8	Phenanthrene	178	4.5	4.4	4.46	0.0219	-3.91	Hansch & Leo, 1985	CAS - ETFS
95-94-3	1,2,4,5-Tetrachlorobenzene	216	4.8	4.6	4.64	1.4596	-2.17	Hansch & Leo, 1985	Zaroogian et al., 1985
634-90-2	1,2,3,5-Tetrachlorobenzene	216	4.8	4.6	4.56	0.3344	-2.81	Hansch & Leo, 1985	Zaroogian et al., 1985
SAR data not included in regression equation:									
608-93-5	Pentachlorobenzene	250	5.2	5.2	5.17	0.1616	-3.19	Hansch & Leo, 1985	Zaroogian et al., 1985
CBI	CBI	519	11	10		*	*		P05-___
Data not used in SAR:									
994-05-8	tert-Amyl methyl ether	102	1.6	1.9		14	-0.86		8FYI-1056; not verified
101-84-8	Diphenyl ether	170	4.2	4.1	4.21	0.71	-2.38	Hansch & Leo, 1985	LeBlanc, 1984; no duration
58-89-9	Lindane	491	3.7	4.9	3.72	0.0059	-4.92	Hansch & Leo, 1985	Zaroogian et al., 1985; excess toxicity
8001-35-2	Toxaphene	414	4.3	6.8		0.00322	-5.11		ETFS; excess toxicity
53905-38-7	1-(8-Methoxy-4,8-dimethylnd	305	7.8	8		2.83	-2.03		8(e)-9161; not verified

References:
U.S. Environmental Protection Agency (USEPA). 1992. Environmental Toxicity Fact Sheet (ETFS). Washington DC: Office of Water, USEPA, 1400 Pennsylvania Avenue NW.

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

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.

FISH (SW) ChV

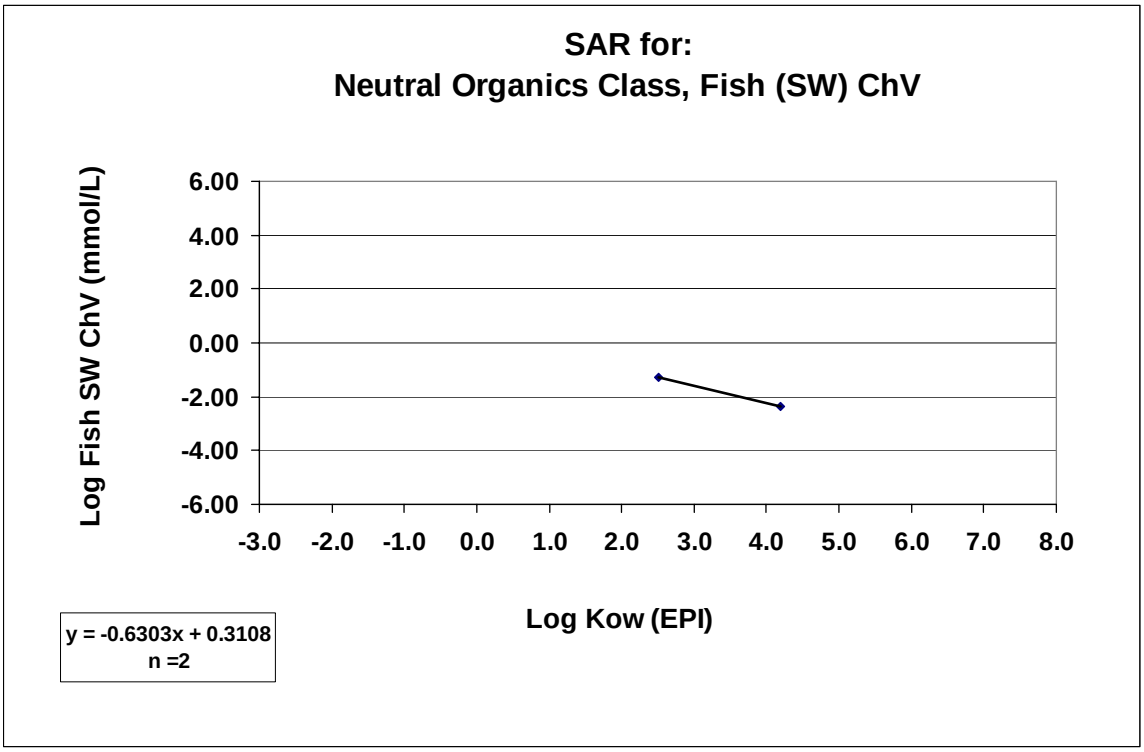
ESTIMATED TOXICITY:
The saltwater fish chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = - 0.6303 log K_{ow} + 0.3108

The ChV is in millimoles per liter (mM/L); and N = 2. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

Graph:



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 Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish SW ChV (mg/L)	Log Fish SW ChV (mmol/L)	Reference (Meas. Kow)	Reference (ChV)
108-88-3	Toluene	92	2.6	2.5	2.73	5	-1.26	Hansch & Leo, 1985	CAS-ETFS
83-32-9	Acenaphthene	154	3.8	4.2	3.92	0.71	-2.34	Hansch & Leo, 1985	CAS-ETFS
Data not used in SAR:									
8001-35-2	Toxaphene	414	4.3	6.8		0.000714	-5.76		ETFS; excess toxicity
72-43-5	Methoxychlor	346	5.2	5.7	5.08	0.017	-4.31	Hansch & Leo, 1985	Hansen & P; excess toxicity

References:
Hansen D.J., and P.R. Parrish. 1977. Suitability of Sheepshead minnows (*Cyprinodon variegates)* for life-cycle toxicity tests. Aquatic Toxicology and Hazard Evaluation, 1st Symposium. ASTM STP 634, Philadelphia, PA: 117-126.

U.S. Environmental Protection Agency (USEPA). 1992. Environmental Toxicity Fact Sheet (ETFS). Washington DC: Office of Water, USEPA, 1400 Pennsylvania Avenue NW.

MYSID (SW) ChV

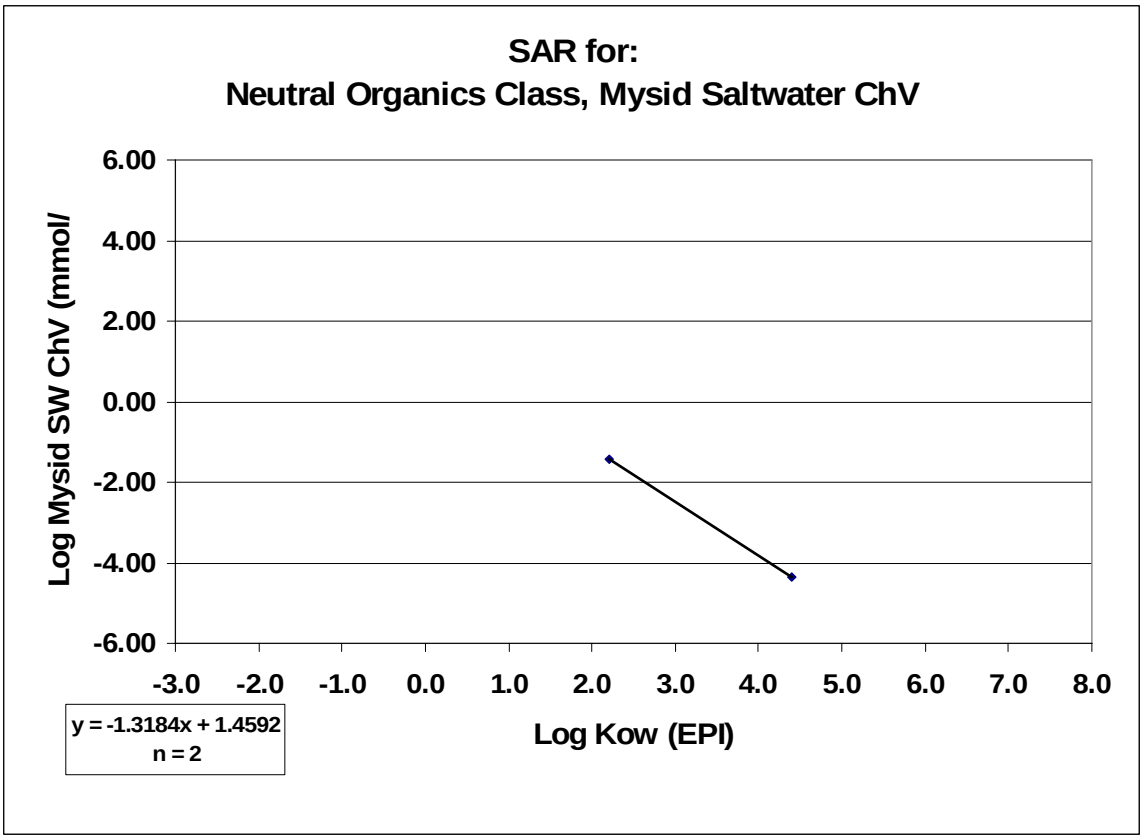
ESTIMATED TOXICITY:
The saltwater mysid ChV values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 16-d ChV (mmol/L) = - 1.3184 log K_{ow} + 1.4592

The ChV is in millimoles per liter (mM/L); and N = 2. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 565

Graph:



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 Kow value is greater than 5.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Mysid SW ChV (mg/L)	Log Mysid SW ChV (mmol/L)	Reference (Meas. Kow)	Reference (ChV)
CBI	CBI	113	2	2.2		4.09	-1.44		CBI
85-01-8	Phenanthrene	178	4.5	4.4	4.46	0.0081	-4.34	Hansch & Leo, 1985	CAS - ETFS
Data not used in SAR:									
8001-35-2	Toxaphene	414	4.3	6.8		0.00179	-5.36		ETFS; excess toxicity

References:
U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

U.S. Environmental Protection Agency (USEPA). 1992. Environmental Toxicity Fact Sheet (ETFS). Washington DC: Office of Water, USEPA, 1400 Pennsylvania Avenue NW.

EARTHWORM 14-d LC50

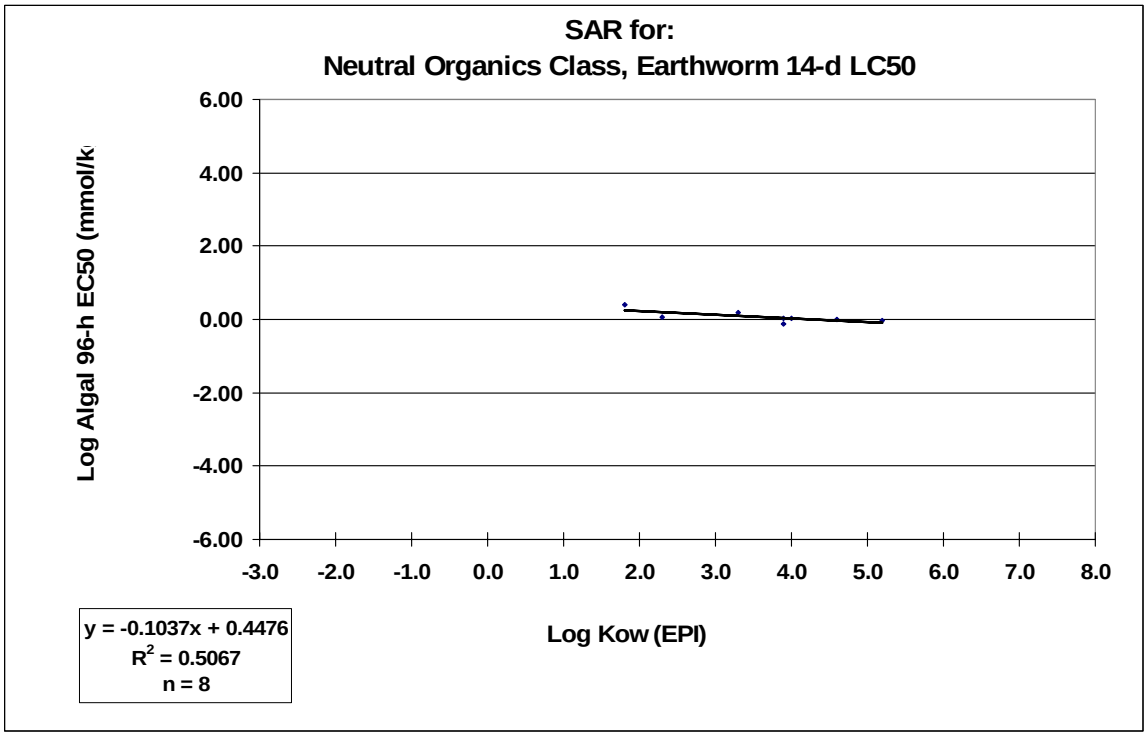
ESTIMATED TOXICITY:
The earthworm 14-d LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 14-d LC50 (mmol/L) = - 0.1037 log K_{ow} + 0.4476

The LC50 is in millimoles per liter (mM/L); N = 8; and the Coefficient of Determination (R^2) = 0.5067. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 6.0
Maximum MW: 1000

Graph:



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:

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Earthworm 14-d LC50 (mg/kg)	Log Earthworm 14-d LC50 (mmol/kg)	Reference (Meas. Kow)	Reference (LC50)
98-95-3	Nitrobenzene	123	1.9	1.8	1.85	319	0.41	Hansch & Leo, 1985	Neuhauser, 1986
78-87-5	1,2-Dichloropropane	113	2.0	2.3	1.98	127	0.05	Sangster, 1994	Neuhauser, 1985
106-46-7	p-Dichlorobenzene	147	3.6	3.3	3.44	229	0.19	Hansch et al., 1995	Van Gestel et al., 1991
120-82-1	1,2,4-Trichlorobenzene	181	4.2	3.9	4.02	197	0.04	Hansch et al., 1995	Neuhauser, 1986
87-61-6	1,2,3-Trichlorobenzene	181	4	3.9	4.05	134	-0.13	Sangster, 1994	Van Gestel et al., 1991
86-73-7	Fluorene	166	4.1	4.0	4.18	173	0.02	Hansch et al., 1995	Neuhauser, 1985
634-66-2	1,2,3,4-Tetrachlorobenze	216	4.6	4.6	4.6	223	0.01	Hansch, C. et al. 1995	Van Gestel et al., 1991
608-93-5	Pentachlorobenzene	250	5.2	5.2	5.17	238	-0.02	Hansch & Leo, 1985	Van Gestel et al., 1991
SAR data not included in regression equation:									
Data not included in SAR:									
						* indicates no effects at saturation			

References:

Belfroid et al.. 1995. Hydrophobic Organic Chemicals in Earthworms. Environ. Sci. & Pollut. Res. 2(1):11 (data from Van Gestel et al., 1991)

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

Neuhauser, E.F., Loehr, R.C., Malecki, M.R., Milligan, D.L. and Durkin, P.R. 1985. The toxicity of selected organic chemicals to the earthworm *Eisenia fetida*. Journal of Environmental Quality 14: 383-388.

FISH 96-h LC50 (Mortality)

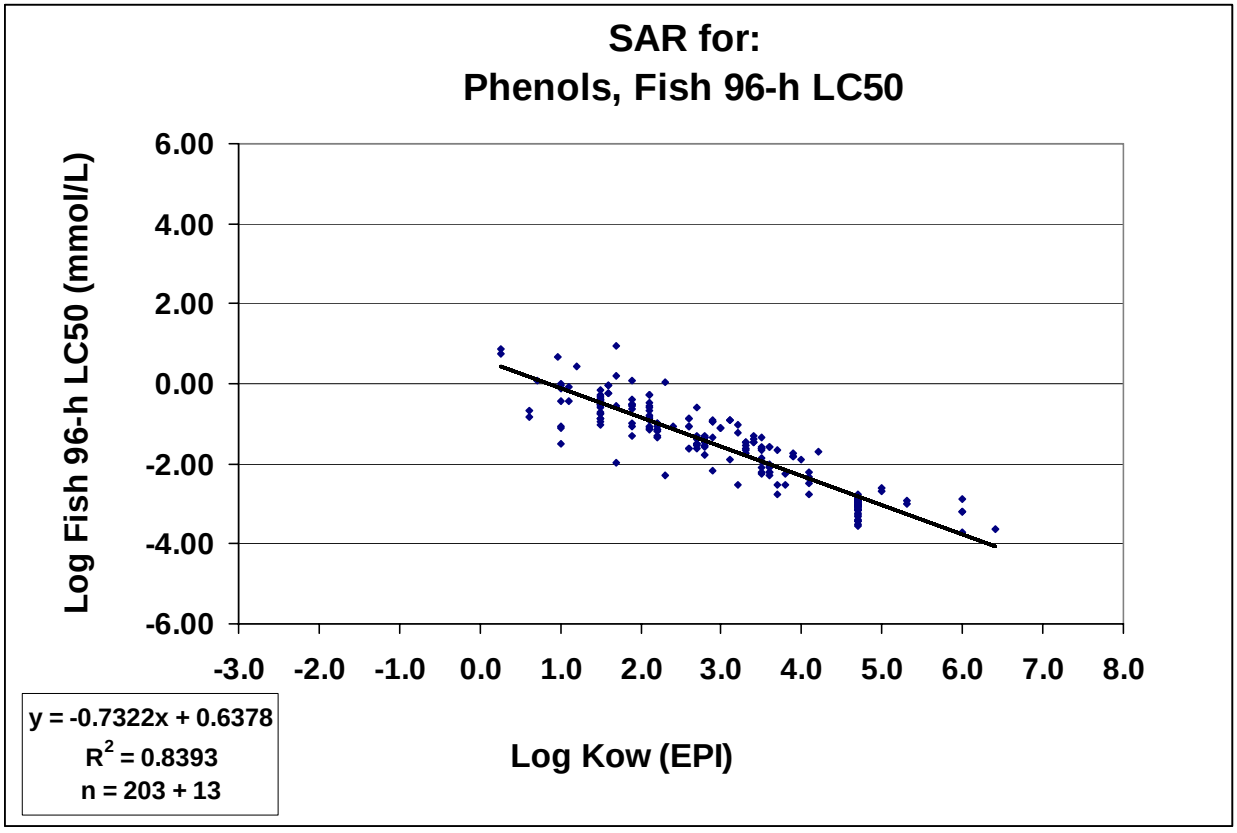
ESTIMATED TOXICITY:
The fish 96-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h LC50 (mmol/L) = -0.7322 (log Kow) + 0.6378

The LC50 is in millimoles per liter (mM/L); N = 203 + 13; and the Coefficient of Determination (R^2) = 0.8393. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 7.0
Maximum MW: 1000

Graph:



Application:
This 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)

If the log Kow value is greater than 7.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish 96-h LC50 (mg/L)	Log Fish 96-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Fish 96-h LC50)
103-90-2	4-Acetamidophenol	151	0.49	0.27	0.46	814	0.73	Sangster, 1994	DUL
621-42-1	3-Acetamidophenol	151	0.49	0.27	0.73	1130	0.87	Hansch & Leo, 1985	DUL
614-80-2	2-Acetamidophenol	151	0.72	0.62	0.72	22.1	-0.83	Hansch & Leo, 1985	DUL
614-80-2	2-Acetamidophenol	151	0.72	0.62	0.72	33	-0.66	Hansch & Leo, 1985	DUL
15128-82-2	3-Hydroxy-2-nitropyridine	140	0.92	0.72		167	0.08		DUL
6636-78-8	2-Chloro-3-pyridinol	130	1.4	0.97		622	0.68		DUL
108-46-3	Resorcinol	110	0.81	1	0.8	40	-0.44	Hansch, C. et al., 1995	Ewell et al., 1986
108-46-3	Resorcinol	110	0.81	1	0.8	100	-0.04	Hansch, C. et al., 1995	Degraeve, 1980
108-46-3	Resorcinol	110	0.81	1	0.8	110	0.00	Hansch, C. et al., 1995	Curtis & Ward, 1981
120-80-9	Catechol	110	0.89	1	0.88	3.5	-1.50	Hansch & Leo, 1985	Datasheet
120-80-9	Catechol	110	0.89	1	0.88	8.9	-1.09	Hansch & Leo, 1985	Degraeve, 1980
120-80-9	Catechol	110	0.89	1	0.88	9.22	-1.08	Hansch & Leo, 1985	DUL
65-45-2	2-Hydroxybenzamide	137	1.3	1	1.28	101	-0.13	Hansch & Leo, 1985	DUL
121-33-5	Vanillin	152	1.4	1.1	1.21; 1.23	57	-0.43	Hansch & Leo, 1985; SIDS	SIDS
121-33-5	Vanillin	152	1.4	1.1	1.21	123	-0.09	Hansch & Leo, 1985	SIDS
6602-32-0	2-Bromo-3-pyridinol	174	1.5	1.2		469	0.43		DUL
108-95-2	Phenol	94	1.5	1.5	1.46	8.9	-1.02	Hansch & Leo, 1985	Degraeve, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	10.2	-0.96	Hansch & Leo, 1985	EPA, 1980
CBI	CBI	94	1.5	1.5	1.46	13	-0.86	Hansch & Leo, 1985	P98-___
CBI	CBI	94	1.5	1.5	1.46	12.31	-0.88	Hansch & Leo, 1985	P05-___
108-95-2	Phenol	94	1.5	1.5	1.46	16.4	-0.76	Hansch & Leo, 1985	EPA, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	16.7	-0.75	Hansch & Leo, 1985	EPA, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	19	-0.69	Hansch & Leo, 1985	EPA, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	24.8	-0.58	Hansch & Leo, 1985	DUL
108-95-2	Phenol	94	1.5	1.5	1.46	26	-0.56	Hansch & Leo, 1985	EPA, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	28.8	-0.51	Hansch & Leo, 1985	DUL
108-95-2	Phenol	94	1.5	1.5	1.46	29.8	-0.50	Hansch & Leo, 1985	Konemann & Musch, 1981
108-95-2	Phenol	94	1.5	1.5	1.46	32	-0.47	Hansch & Leo, 1985	Ewell et al., 1986
108-95-2	Phenol	94	1.5	1.5	1.46	32.4	-0.46	Hansch & Leo, 1985	DUL
108-95-2	Phenol	94	1.5	1.5	1.46	34.9	-0.43	Hansch & Leo, 1985	EPA, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	36	-0.42	Hansch & Leo, 1985	EPA, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	36.3	-0.41	Hansch & Leo, 1985	EPA, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	37	-0.40	Hansch & Leo, 1985	Veith GD & Broderius SJ, 1987
108-95-2	Phenol	94	1.5	1.5	1.46	43	-0.34	Hansch & Leo, 1985	Saarikoski & Viluksela, 1982
108-95-2	Phenol	94	1.5	1.5	1.46	44.5	-0.32	Hansch & Leo, 1985	EPA, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	49.7	-0.28	Hansch & Leo, 1985	DUL
108-95-2	Phenol	94	1.5	1.5	1.46	67.5	-0.14	Hansch & Leo, 1985	Degraeve
150-19-6	3-Methoxyphenol	124	1.6	1.6	1.34	74	-0.22	Hansch & Leo, 1985	DUL
150-19-6	3-Methoxyphenol	124	1.6	1.6	1.34	74	-0.22	Hansch & Leo, 1985	Veith GD & Broderius SJ, 1987
150-76-5	4-Methoxyphenol	124	1.6	1.6	1.58	110	-0.05	Hansch & Leo, 1985	DUL
150-76-5	4-Methoxyphenol	124	1.6	1.6	1.58	110	-0.05	Hansch & Leo, 1985	Veith GD & Broderius SJ, 1987
16879-02-0	6-Chloro-2-pyridinol	130	0.93	1.7		214	0.22		DUL
4214-79-3	5-Chloro-2-pyridinol	130	1.8	1.7		1140	0.94		DUL
2138-22-9	4-Chlorocatechol	145	2	1.7		1.58	-1.96		DUL
CBI	CBI	212	1.6	1.7	1.2	60	-0.55	HPLC	P98-___
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	31.7	-0.64	Hansch & Leo, 1985	Broderius et al., 2005
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	6.93	-1.30	Hansch & Leo, 1985	Marking, 1991
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	14.2	-0.99	Hansch & Leo, 1985	Saarikoski & Viluksela, 1982
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	37.3	-0.57	Hansch & Leo, 1985	DUL
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	41	-0.53	Hansch & Leo, 1985	DUL
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	41	-0.53	Hansch & Leo, 1985	Holcombe, GW et al., 1984
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	58.6	-0.38	Hansch & Leo, 1985	DUL
554-84-7	3-Nitrophenol	139	1.9	1.9	2	11.8	-1.07	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
88-75-5	2-Nitrophenol	139	1.9	1.9	1.8	160	0.06	Hansch & Leo, 1985	DUL
106-44-5	p-Cresol	108	2	2.1	1.95	7.9	-1.14	Hansch & Leo, 1985	Datasheet
106-44-5	4-Methylphenol	108	2	2.1	1.94	16.5	-0.82	Hansch & Leo, 1985	Veith GD & Broderius SJ, 1987
106-44-5	p-Cresol	108	2	2.1	1.95	28.6	-0.58	Hansch & Leo, 1985	Datasheet
108-39-4	m-Cresol	108	2	2.1	1.95	8.9	-1.08	Hansch & Leo, 1985	Datasheet
108-39-4	3-Methylphenol	108	2	2.1	1.96	23.1	-0.67	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982

108-39-4	m-Cresol	108	2	2.1	1.95	55.9	-0.29	Hansch & Leo, 1985	Datasheet
1319-77-3	mixed-Cresol	108	2	2.1	1.95	12.8	-0.93	Hansch & Leo, 1985	DUL
95-48-7	o-Cresol	108	2	2.1	1.95	8.4	-1.11	Hansch & Leo, 1985	Datasheet
95-48-7	o-Cresol	108	2	2.1	1.95	14	-0.89	Hansch & Leo, 1985	DUL
95-48-7	o-Cresol	108	2	2.1	1.95	18.2	-0.77	Hansch & Leo, 1985	Datasheet
552-41-0	2'-Hydroxy-4'-methoxyacetophenone	166	2	2.1		54.9	-0.48		DUL
552-41-0	2'-Hydroxy-4'-methoxyacetophenone	166	2	2.1		87.8	-0.28		DUL
2150-47-2	Methyl, 2,4-dihydroxybenzoate	168	1.9	2.1		45.8	-0.56		DUL
106-48-9	4-Chlorophenol	129	2.5	2.2	2.39	6.11	-1.32	Hansch, C. et al., 1995	DUL
106-48-9	4-Chlorophenol	129	2.5	2.2	2.39	8.5	-1.18	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
108-43-0	3-Chlorophenol	129	2.5	2.2	2.25; 2.5	6.4	-1.30	Hansch, C. et al., 1995; Unkno	Konemann & Musch, 1981
95-57-8	2-Chlorophenol	129	2.2	2.2	2.15	9.41	-1.14	Hansch, C. et al., 1995	DUL
95-57-8	2-Chlorophenol	129	2.2	2.2	2.15	9.41	-1.14	Hansch, C. et al., 1995	Veith GD & Broderius SJ, 1987
95-57-8	2-Chlorophenol	129	2.2	2.2	2.15	11.2	-1.06	Hansch, C. et al., 1995	Konemann & Musch, 1981
95-57-8	2-Chlorophenol	129	2.2	2.2	2.15	13.8	-0.97	Hansch, C. et al., 1995	DUL
95-57-8	2-Chlorophenol	129	2.2	2.2	2.15	13.8	-0.97	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
769-28-8	3-Cyano-4,6-dimethyl-2-hydroxypyridine	148	1.8	2.3		157	0.03		DUL
3428-24-8	4,5-Dichlorocatechol	179	2.7	2.3		0.89	-2.30		DUL
CBI	CBI	120	2.2	2.4		10	-1.08		L96-___
105-67-9	2,4-Dimethylphenol	122	2.5	2.6	2.3	16.6	-0.87	Hansch & Leo, 1985	DUL
105-67-9	2,4-Dimethylphenol	122	2.5	2.6	2.3	16.6	-0.87	Hansch & Leo, 1985	Holcombe, GW et al., 1984
123-07-9	4-Ethylphenol	122	2.5	2.6	2.58	10.4	-1.07	Hansch & Leo, 1985	DUL
123-07-9	4-Ethylphenol	122	2.5	2.6	2.58	10.4	-1.07	Hansch & Leo, 1985	Veith GD & Broderius SJ, 1987
2460-49-3	4,5-Dichloroguaiacol	193	2.9	2.6	3.26	4.47	-1.64	Hansch & Leo, 1985	DUL
2460-49-3	4,5-Dichloro-2-methoxyphenol	193	2.9	2.6	3.26	4.8	-1.60	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
59-50-7	4-Chloro-3-methylphenol	143	3	2.7	3.1	4.05	-1.55	Hansch, C. et al., 1995	DUL
59-50-7	4-Chloro-3-methylphenol	143	3	2.7	3.1	5.72	-1.40	Hansch, C. et al., 1995	Veith GD & Broderius SJ, 1987
59-50-7	4-Chloro-3-methylphenol	143	3	2.7	3.1	7.38	-1.29	Hansch, C. et al., 1995	DUL
6640-27-3	2-Chloro-4-methylphenol	143	2.7	2.7		35.9	-0.60		Veith GD & Broderius SJ, 1987
90-15-3	1-Naphthol	144	2.7	2.7	2.85	3.57	-1.61	Hansch & Leo, 1985	Broderius et al., 2005
90-15-3	1-Naphthol	144	2.7	2.7	2.85	4.63	-1.49	Hansch & Leo, 1985	DUL
90-15-3	1-Naphthol	144	2.7	2.7	2.85	4.63	-1.49	Hansch & Leo, 1985	Veith GD & Broderius SJ, 1987
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	4.2	-1.59	Hansch, C. et al., 1995	Konemann & Musch, 1981
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	5.5	-1.47	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	7.75	-1.32	Hansch, C. et al., 1995	DUL
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	7.75	-1.32	Hansch, C. et al., 1995	Holcombe, GW et al., 1984
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	7.75	-1.32	Hansch, C. et al., 1995	Veith GD & Broderius SJ, 1987
591-35-5	3,5-Dichlorophenol	163	3.3	2.8	3.62	2.7	-1.78	Hansch, C. et al., 1995	Konemann & Musch, 1981
87-65-0	2,6-Dichlorophenol	163	2.6	2.8	2.75	7.8	-1.32	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
17754-90-4	4-(Diethylamino) salicyaldehyde	193	3	2.8		5.36	-1.56		DUL
1745-81-9	2-Allylphenol	134	2.6	2.9		15	-0.95		DUL
1745-81-9	2-Allylphenol	134	2.6	2.9		15	-0.95		Veith GD & Broderius SJ, 1987
1891-95-8	3,5-Dichloro-4-hydroxybenzonitrile	188	2.5	2.9		24.3	-0.89		DUL
1761-61-1	5-Bromosalicylaldehyde	201	2.8	2.9		1.3	-2.19		DUL
88-30-2	3-Trifluoromethyl-4-nitrophenol	207	2.8	2.9		9.14	-1.36		DUL
645-56-7	4-Propylphenol	136	3	3	3.2	11	-1.09	Sangster,1993	DUL
645-56-7	4-Propylphenol	136	3	3	3.2	11	-1.09	Sangster,1993	Veith GD & Broderius SJ, 1987
118-61-6	Ethyl salicylate	166	3	3.1	2.95	19.8	-0.92	Korenman & Danilov, 1990	DUL
118-61-6	Ethyl salicylate	166	3	3.1	2.95	20.7	-0.90	Korenman & Danilov, 1990	DUL
2539-26-6	3,4,5-Trichloro-2,6-dimethoxyphenol	258	2.9	3.1	3.74	3.4	-1.88	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
2416-94-6	2,3,6-Trimethylphenol	136	2.9	3.2	2.67	0.39	-2.54	Sangster, 1993	Saarikoski & Viluksela, 1982
2416-94-6	2,3,6-Trimethylphenol	136	2.9	3.2	2.67	8.2	-1.22	Sangster, 1993	DUL
527-60-6	2,4,6-Trimethylphenol	136	3	3.2	2.73	13	-1.02	Sangster,1993	DUL
88-04-0	4-Chloro-3,5-dimethylphenol	156	3.5	3.3	3.27	3.4	-1.66	Daylight, 1999	Saarikoski & Viluksela, 1982
90-43-7	2-Phenylphenol	170	3.1	3.3	3.09	4.09	-1.62	Pomona, 1987	Broderius et al., 2005
90-43-7	2-Phenylphenol	170	3.1	3.3	3.09	4.79	-1.55	Pomona, 1987	Broderius et al., 2005
90-43-7	2-Phenylphenol	170	3.1	3.3	3.09	6.15	-1.44	Pomona, 1987	DUL
90-43-7	2-Phenylphenol	170	3.1	3.3	3.09	6.15	-1.44	Pomona, 1987	Veith GD & Broderius SJ, 1987
87-17-2	Salicylanilide	213	3.3	3.3	3.27	3.95	-1.73	Hansch & Leo, 1985	DUL
98-54-4	p-tert-Butylphenol	150	3.3	3.4	3.31	5.15	-1.46	Hansch & Leo, 1985	DUL
98-54-4	4-Tert-butylphenol	150	3.3	3.4	3.31	5.15	-1.46	Hansch, C. et al., 1995	Veith GD & Broderius SJ, 1987
1689-84-5	3,5-Dibromo-4-hydroxybenzonitrile	277	2.9	3.4		11.5	-1.38		DUL
1689-84-5	3,5-Dibromo-4-hydroxybenzonitrile	277	2.9	3.4		13.8	-1.30		DUL
89-83-8	Phenol, 5-methyl-2-(1-methylethyl)-	150	3.4	3.5	3.3	3.2	-1.67	Hansch, C. et al., 1995	Ewell et al., 1986
609-19-8	3,4,5-Trichlorophenol	197	3.8	3.5	4.01	1.1	-2.25	Hansch, C. et al., 1995	Konemann & Musch, 1981

88-06-2	2,4,6-Trichlorophenol	197	3.4	3.5	3.69	2.3	-1.93	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
88-06-2	2,4,6-Trichlorophenol	197	3.4	3.5	3.69	2.8	-1.85	Hansch, C. et al., 1995	DUL
88-06-2	2,4,6-Trichlorophenol	197	3.4	3.5	3.69	4.55	-1.64	Hansch, C. et al., 1995	Veith GD & Broderius SJ, 1987
88-06-2	2,4,6-Trichlorophenol	197	3.4	3.5	3.69	4.55	-1.64	Hansch, C. et al., 1995	DUL
88-06-2	2,4,6-Trichlorophenol	197	3.4	3.5	3.69	9.16	-1.33	Hansch, C. et al., 1995	DUL
933-75-5	2,3,6-Trichlorophenol	197	3.2	3.5	3.77	5.1	-1.59	Hansch, C. et al., 1995	Konemann & Musch, 1981
933-78-8	2,3,5-Trichlorophenol	197	3.6	3.5	3.84	1.6	-2.09	Hansch, C. et al., 1995	Konemann & Musch, 1981
95-95-4	2,4,5-Trichlorophenol	197	3.6	3.5	3.72	1.2	-2.22	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
831-82-3	p-Phenoxyphenol	186	3.8	3.6	3.35	4.95	-1.57	Hansch et al., 1995	DUL
831-82-3	4-Phenoxyphenol	186	3.8	3.6	3.35	4.96	-1.57	Hansch, C. et al., 1995	Veith GD & Broderius SJ, 1987
1689-82-3	p-Phenylazophenol	198	4	3.6		1.17	-2.23		DUL
1689-82-3	p-Phenylazophenol	198	4	3.6		1.17	-2.23		Veith GD & Broderius SJ, 1987
1689-82-3	p-Phenylazophenol	198	4	3.6		1.64	-2.08		Broderius et al., 2005
NK	3,4,5-Trichloro-2-methoxyphenol	227	3.3	3.6	3.77	2.1	-2.03	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
1198-55-6	Tetrachlorocatechol	248	3.3	3.6	4.29	1.27	-2.29	Hansch & Leo, 1985	DUL
1198-55-6	3,4,5,6-Tetrachloro-2-hydroxyphenol	248	3.3	3.6	4.3	2.5	-2.00	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
CBI	CBI	207	3.8	3.7		4.4	-1.67		P91-____
88-85-7	2-Sec-butyl-4,6-dinitrophenol	240	3.7	3.7	3.6	0.41	-2.77	Hansch et al., 1995	DUL
88-85-7	2-Sec-butyl-4,6-dinitrophenol	240	3.7	3.7	3.6	0.7	-2.54	Hansch et al., 1995	DUL
118-55-8	Phenyl salicylate	214	4	3.8		1.18	-2.26		DUL
90-59-5	3,5-Dibromosalicylaldehyde	280	3.4	3.8		0.85	-2.52		DUL
80-46-6	p-tert-Pentylphenol	164	3.8	3.9		2.59	-1.80		DUL
80-46-6	4-Tert-pentylphenol	164	3.8	3.9		2.59	-1.80		Veith GD & Broderius SJ, 1987
1689-83-4	3.5-Diiodo-4-hydroxybenzonitrile	371	3.3	3.9	3.43	6.8	-1.74	Comer, J. et al., 1995	DUL
2409-55-4	2-Tert-butyl-4-methylphenol	164	3.8	4		2.1	-1.89		Saarikoski & Viluksela, 1982
4901-51-3	2,3,4,5-Tetrachlorophenol	232	4.1	4.1	4.21	0.41	-2.75	Hansch, C. et al., 1995	DUL
4901-51-3	2,3,4,5-Tetrachlorophenol	232	4.1	4.1	4.21	0.77	-2.48	Hansch, C. et al., 1995	Konemann & Musch, 1981
58-90-2	2,3,4,6-Tetrachlorophenol	232	3.8	4.1	4.45	1.03	-2.35	Hansch, C. et al., 1995	DUL
58-90-2	2,3,4,6-Tetrachlorophenol	232	3.8	4.1	4.45	1.1	-2.32	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
935-95-5	2,3,5,6-Tetrachlorophenol	232	3.8	4.1	3.88	1.4	-2.22	Hansch, C. et al., 1995	Konemann & Musch, 1981
118-79-6	2,4,6-Tribromophenol	331	3.9	4.2	4.13	6.54	-1.70	Hansch & Leo, 1985	DUL
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.0986	-3.43	Hansch, C. et al., 1995	DUL
CBI	CBI	266	4.3	4.7	5.12	0.13	-3.31	Hansch, C. et al., 1995	P02-____
CBI	CBI	266	4.3	4.7	5.12	0.14	-3.28	Hansch, C. et al., 1995	P01-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.15	-3.25	Hansch, C. et al., 1995	P98-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.19	-3.15	Hansch, C. et al., 1995	P98-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.19	-3.15	Hansch, C. et al., 1995	P00-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.19	-3.15	Hansch, C. et al., 1995	P92-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.19	-3.15	Hansch, C. et al., 1995	P92-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.21	-3.10	Hansch, C. et al., 1995	P00-____ Positive Control
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.222	-3.08	Hansch, C. et al., 1995	DUL
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.237	-3.05	Hansch, C. et al., 1995	DUL
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.24	-3.04	Hansch, C. et al., 1995	Veith GD & Broderius SJ, 1987
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.24	-3.04	Hansch, C. et al., 1995	DUL
CBI	CBI	266	4.3	4.7	5.12	0.24	-3.04	Hansch, C. et al., 1995	L92-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.24	-3.04	Hansch, C. et al., 1995	P93-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.24	-3.04	Hansch, C. et al., 1995	P94-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.24	-3.04	Hansch, C. et al., 1995	P94-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.24	-3.04	Hansch, C. et al., 1995	P90-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.24	-3.04	Hansch, C. et al., 1995	P92-____ Positive Control
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.242	-3.04	Hansch, C. et al., 1995	DUL
CBI	CBI	266	4.3	4.7	5.12	0.26	-3.01	Hansch, C. et al., 1995	P94-____ Positive Control
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.261	-3.01	Hansch, C. et al., 1995	DUL
CBI	CBI	266	4.3	4.7	5.12	0.28	-2.98	Hansch, C. et al., 1995	P94-____ Positive Control
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.301	-2.95	Hansch, C. et al., 1995	DUL
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.32	-2.92	Hansch, C. et al., 1995	Ewell et al., 1986
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.32	-2.92	Hansch, C. et al., 1995	Ewell et al., 1986
CBI	CBI	266	4.3	4.7	5.12	0.33	-2.91	Hansch, C. et al., 1995	P95-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.33	-2.91	Hansch, C. et al., 1995	P95-____ Positive Control
CBI	CBI	266	4.3	4.7	5.12	0.34	-2.89	Hansch, C. et al., 1995	P95-____ Positive Control
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.35	-2.88	Hansch, C. et al., 1995	DUL
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.38	-2.85	Hansch, C. et al., 1995	Konemann & Musch, 1981
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.381	-2.84	Hansch, C. et al., 1995	DUL
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.44	-2.78	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
CBI	CBI	288	4.3	4.7		0.081	-3.55		P92-____

CBI	CBI	288	4.3	4.7		0.088	-3.51		P92-____
CBI	CBI	288	4.3	4.7		0.103	-3.45		P93-____ Positive Control
CBI	CBI	288	4.3	4.7		0.12	-3.38		P94-____ Positive Control
CBI	CBI	288	4.3	4.7		0.24	-3.08		P94-____
CBI	CBI	288	4.3	4.7		0.4	-2.86		P01-____ Positive Control
CBI	CBI	270	5.1	5		0.54	-2.70		8(e)-____
609-23-4	2,4,6-Triiodophenol	472	4.6	5		1.21	-2.59		DUL
140-66-9	4-(Tert-octyl) phenol	206	5.2	5.3		0.21	-2.99		TSCA 8(e) Triage Data Summary
140-66-9	4-(Tert-octyl) phenol	206	5.2	5.3		0.25	-2.92		8(e)-2453
104-40-5	Nonylphenol	220	6.2	6	5.76	0.14	-3.20	Itokawa et al., 1989	DUL
104-40-5	4-Nonylphenol	220	6.2	6	5.76	0.14	-3.20		Veith GD & Broderius SJ, 1987
25154-52-2	p-Nonylphenol	220	6.6	6	5.76	0.3	-2.87	Itokawa, H. et al., 1989	8(e)-10001
608-71-9	Pentabromophenol	489	4.9	6		0.093	-3.72		DUL
732-26-3	2,4,6-Tri-tert-butylphenol	262	7	6.4	6.06	0.0609	-3.63	Chem Inspect Test Inst., 1992	DUL
SAR Data Not Included in Regression Equation:									
CBI	CBI	355	4.5	3.8	4.5@ pH 6.3	*		Unknown	P92-____
CBI	CBI	355	4.5	3.8	7.3; >4.3	*		HPLC; shake flask	P01-____
CBI	CBI	353	5.9	4.9		*			P88-
CBI	CBI	316	7.2	5.6		*			P94-____
CBI	CBI	426	7.2	6.4		*			P94-____
CBI	CBI	371	5.1	6.9		*2.5	*-2.17		P94-____
CBI	CBI	262	7	7		*0.6	*-2.64		P01-____
CBI	CBI	553	8	7.6		*			P91-____
CBI	CBI	438	8.9	7.8		*			P90-____
CBI	CBI	531	7.9	8.9		*1.9	*-2.45		P95-____
CBI	CBI	451	10	9		*			P91-____/8(e)-____
CBI	CBI	347	11	10		*			P94-____
CBI	CBI	644	9.3	12		*			P90-____
Data Not Included in SAR:									
1987-50-4	4-Heptylphenol	192	5.1	5		0.2 to 0.3	-2.98 to -2.81		Knut-Erik T. et al., 1995
						* indicates no effects at saturation			

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U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

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FISH 14-d LC50 (Mortality)

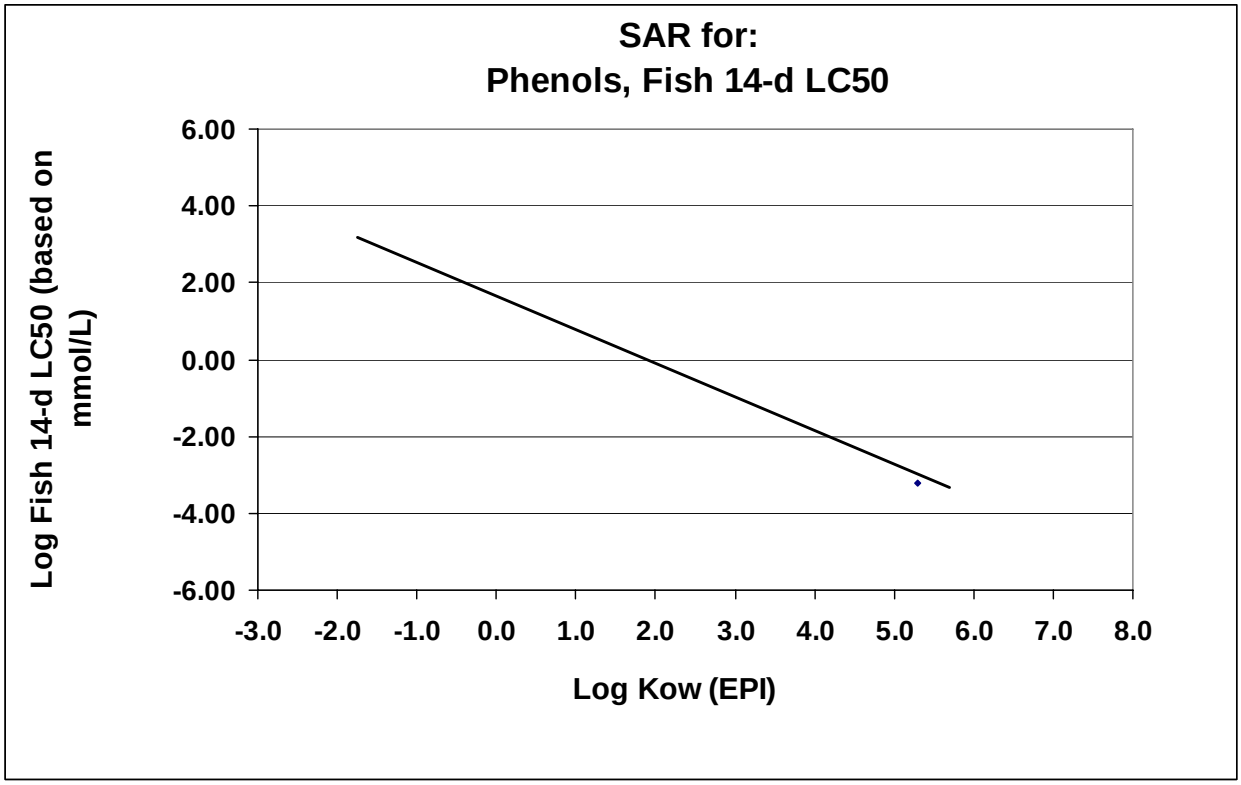
ESTIMATED TOXICITY:
No adequate data were available for the phenols SAR fish 14-d LC50 endpoint. Predictions for this endpoint are based on SARs for neutral organics. The neutral organic SAR equation used to estimate toxicity is:

Log LC50 (mmol/L) = -0.8729 log Kow + 1.6375

To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 6.4
Maximum MW: 1000

Graph:



Application:
This 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)

If the log Kow value is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish 14-d LC50 (mg/L)	Log Fish 14-d LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Fish 14-d LC50)
140-66-9	4-(1,1,3,3-Tetramethylbutyl)-phenol	206	5.2	5.3		0.12	-3.23		8(e)-9729
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
						* indicates no effects at saturation			

References:

DAPHNID 48-h LC50 (Mortality)

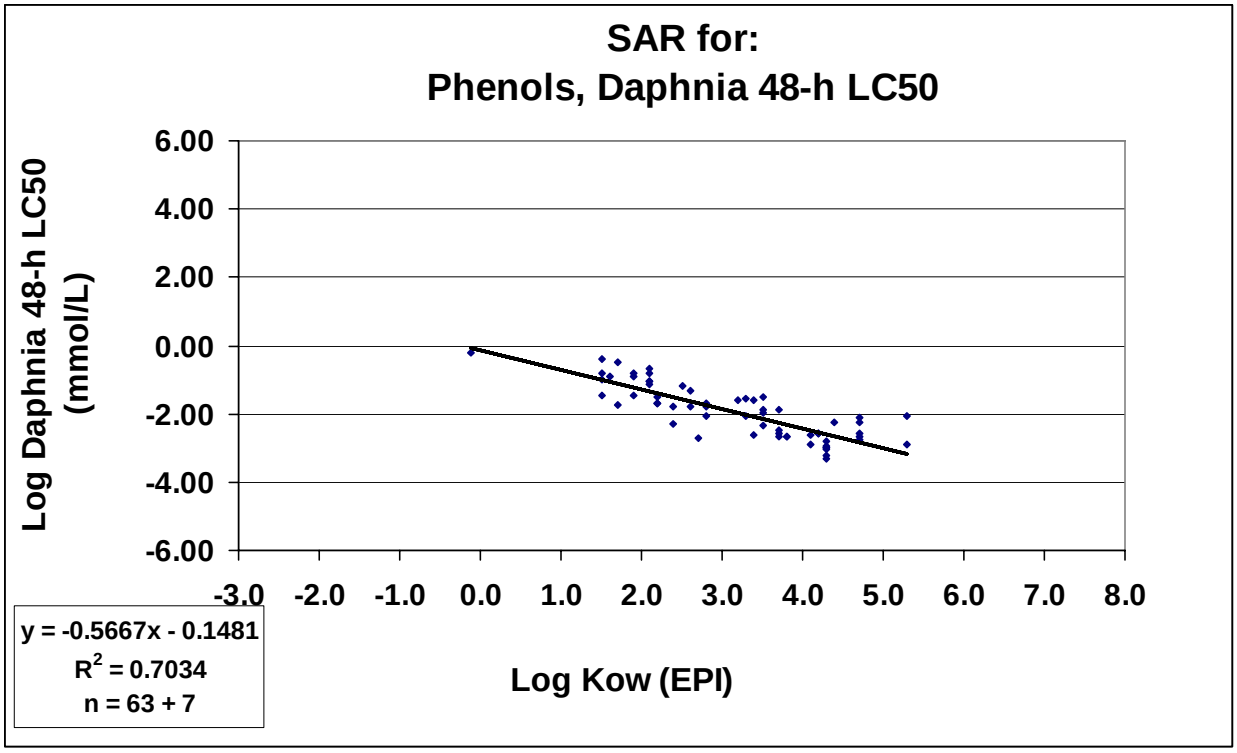
ESTIMATED TOXICITY:
The daphnid 48-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 48-h LC50 (mmol/L) = - 0.5667 (log Kow) - 0.1481

The LC50 is in millimoles per liter (mM/L); N = 63 + 7; and the Coefficient of Determination (R^2) = 0.7034.
To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 7
Maximum MW: 1000

Graph:



Application:
This 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)

If the log Kow value is greater than 5.5, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Daphnia 48-h LC50 (mg/L)	Log Daphnia 48-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Daphnia 48-h LC50)
701-82-6	3-Hydroxyphenylurea	152	0.18	-0.12		93	-0.21		Kuhn, R. et al., 1989
108-95-2	Phenol	94	1.5	1.5	1.46	3.1	-1.48	Hansch & Leo, 1985	Oris, 1991
108-95-2	Phenol	94	1.5	1.5	1.46	10	-0.97	Hansch & Leo, 1985	Kuhn, R. et al., 1989
108-95-2	Phenol	94	1.5	1.5	1.46	14	-0.83	Hansch & Leo, 1985	EPA, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	36.39	-0.41	Hansch & Leo, 1985	EPA, 1980
767-00-0	4-Hydroxybenzonitrile	119	1.6	1.6	1.6	15	-0.90	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
500-99-2	3,5-Dimethoxyphenol	154	1.6	1.7	1.64	2.7	-1.76	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
CBI	CBI	212	1.6	1.7	1.2	71	-0.48	HPLC	P98-___
100-02-7	P-Nitrophenol	139	1.9	1.9	1.91	4.7	-1.47	Hansch & Leo, 1985	Kuhn, R. et al., 1989
88-75-5	O-Nitrophenol	139	1.9	1.9	1.8	17	-0.91	Hansch & Leo, 1985	Kuhn, R. et al., 1989
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	22	-0.80	Hansch & Leo, 1985	Le Blanc, G., 1980
106-44-5	p-Cresol	108	2	2.1	1.95	7.7	-1.15	Hansch & Leo, 1985	Kuhn, R. et al., 1989
95-48-7	o-Cresol	108	2	2.1	1.95	9.5	-1.06	Hansch & Leo, 1985	Sloof, 1983
95-48-7	o-Cresol	108	2	2.1	1.95	9.6	-1.05	Hansch & Leo, 1985	Sloof, 1983
95-48-7	o-Cresol	108	2	2.1	1.95	16.4	-0.82	Hansch & Leo, 1985	Sloof, 1983
106-44-5	p-Cresol	108	2	2.1	1.95	22.7	-0.68	Hansch & Leo, 1985	DeGraeve
106-48-9	p-Chlorophenol	129	2.5	2.2	2.39	2.5	-1.71	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
95-57-8	2-Chlorophenol	129	2.2	2.2	2.15	2.6	-1.70	Hansch, C. et al., 1995	Le Blanc, G., 1980
106-48-9	4-Chlorophenol	129	2.5	2.2	2.39	4.1	-1.50	Hansch, C. et al., 1995	Le Blanc, G., 1980
CBI	CBI	120	2.2	2.4		1.9	-1.80		L96-___
95-56-7	o-Bromophenol	173	2.4	2.4	2.35	0.9	-2.28	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
98-17-9	3-(Trifluoromethyl)phenol	162	2.9	2.5	2.95	11	-1.17	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
105-67-9	2,4-Dimethylphenol	122	2.5	2.6	2.3	2.1	-1.76	Hansch & Leo, 1985	Le Blanc, G., 1980
123-07-9	p-Ethylphenol	122	2.5	2.6	2.58	5.7	-1.33	Hansch & Leo, 1985	Kuhn, R. et al., 1989
6640-27-3	4-Chloro-6-methylphenol	143	3	2.7	2.63	0.29	-2.69	Hansch, C. et al., 1995	Le Blanc, G., 1980
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	1.4	-2.07	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	2.6	-1.80	Hansch, C. et al., 1995	Le Blanc, G., 1980
576-24-9	2,3-Dichlorophenol	163	2.8	2.8	2.84	3.1	-1.72		Kuhn, R. et al., 1989
87-65-0	2,6-Dichlorophenol	163	2.6	2.8	2.75	3.4	-1.68	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
527-60-6	2,4,6-Trimethylphenol	136	3	3.2	2.73	3.3	-1.62	Sangster,1993	Kuhn, R. et al., 1989
88-04-0	4-Chloro-3,5-dimethylphenol	156	3.5	3.3	3.27	4.5	-1.54	Daylight, 1999	Kuhn, R. et al., 1989
90-43-7	o-Phenylphenol	170	3.1	3.3	3.09	1.5	-2.05	Pomona, 1987	Kuhn, R. et al., 1989
98-54-4	4-tert-Butylphenol	150	3.3	3.4	3.31	3.9	-1.59	Hansch & Leo, 1985	Kuhn, R. et al., 1989
1570-65-6	2,4-Dichloro-6-methylphenol	177	3.5	3.4		0.43	-2.61		Le Blanc, G., 1980
95-95-4	2,4,5-Trichlorophenol	197	3.6	3.5	3.72	0.9	-2.34	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
88-06-2	2,4,6-Trichlorophenol	197	3.4	3.5	3.69	2.2	-1.95	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
95-95-4	2,4,5-Trichlorophenol	197	3.6	3.5	3.72	2.7	-1.86	Hansch, C. et al., 1995	Le Blanc, G., 1980
88-06-2	2,4,6-Trichlorophenol	197	3.4	3.5	3.69	6	-1.52	Hansch, C. et al., 1995	Le Blanc, G., 1980
CBI	CBI	207	3.8	3.7		2.7	-1.88		P91-___
Nk	2'-Methyl-2-hydroxy-3-nitrobenzanilide	272	3.5	3.7		0.947	-2.46		Dai & Wang, 2000
Nk	2'-Ethoxy-2-hydroxy-5-nitrobenzanilide	302	3.4	3.7		0.653	-2.67		Dai & Wang, 2000
Nk	2'-Ethoxy-2-hydroxy-3-nitrobenzanilide	302	3.4	3.7		0.836	-2.56		Dai & Wang, 2000
Nk	4'-Methoxy-2-hydroxy-5-nitrobenzanilide	288	3.5	3.8		0.637	-2.66		Dai & Wang, 2000
Nk	4'-Methoxy-2-hydroxy-3-nitrobenzanilide	288	3.5	3.8		0.654	-2.64		Dai & Wang, 2000
58-90-2	2,3,4,6-Tetrachlorophenol	232	3.8	4.1	4.45	0.29	-2.90	Hansch, C. et al., 1995	Le Blanc, G., 1980
935-95-5	2,3,5,6-Tetrachlorophenol	232	3.8	4.1	3.88	0.57	-2.61	Hansch, C. et al., 1995	Le Blanc, G., 1980
Nk	4'-Methyl-2-hydroxy-3-	272	4	4.2		0.735	-2.57		Dai & Wang, 2000
Nk	4'-Methyl-2-hydroxy-5-	272	4	4.2		0.753	-2.56		Dai & Wang, 2000
NK	4'-Chloro-2-hydroxy-5-nitrobenzanilide	293	4.3	4.3		0.137	-3.33		Dai & Wang, 2000
NK	4'-Chloro-2-hydroxy-3-nitrobenzanilide	293	4.3	4.3		0.17	-3.24		Dai & Wang, 2000
Nk	4'-Ethoxy-2-hydroxy-3-nitrobenzanilide	302	4	4.3		0.483	-2.80		Dai & Wang, 2000
NK	2'-Methyl-3'-chloro-2-hydroxy-5-nitrobenzanilide	307	4.3	4.3		0.288	-3.03		Dai & Wang, 2000
NK	2'-Methyl-5'-chloro-2-hydroxy-5-nitrobenzanilide	307	4.3	4.3		0.301	-3.01		Dai & Wang, 2000
NK	2'-Methyl-3'-chloro-2-hydroxy-3-nitrobenzanilide	307	4.3	4.3		0.327	-2.97		Dai & Wang, 2000
NK	2'-Methyl-5'-chloro-2-hydroxy-3-nitrobenzanilide	307	4.3	4.3		0.36	-2.93		Dai & Wang, 2000
CBI	CBI	366	MF	4.4		2	-2.26		P94-___
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.48	-2.74	Hansch, C. et al., 1995	Sloof, 1983
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.55	-2.68	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.68	-2.59	Hansch, C. et al., 1995	Le Blanc, G., 1980
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	1.5	-2.25	Hansch, C. et al., 1995	Sloof, 1983
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	2	-2.12	Hansch, C. et al., 1995	Sloof, 1983
140-66-9	4-(Tert-octyl) phenol	206	5.2	5.3		0.27	-2.88		8(e)-2454
1138-52-9	3,5-Di-tert-butylphenol	206	5.1	5.3		1.7	-2.08		Kuhn, R. et al., 1989

SAR Data Not Included in Regression Equation:									
CBI	CBI	355	4.5	3.8	4.5 @ pH 6.3	*		Unknown	P92-____
CBI	CBI	316	7.2	5.6		*			P94-____
CBI	CBI	426	7.2	6.4		*			P94-____
CBI	CBI	553	8	7.6		*			P91-____
CBI	CBI	531	7.9	8.9		*3.3	*-2.21		P95-____
CBI	CBI	451	10	9		*			P91-____/8(e)-____
CBI	CBI	644	9.3	12		*			P90-____
Data Not Included in SAR:									
						* indicates no effects at saturation			

References:
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Kuhns RM, Pattard KD, Pernak, Winter A. 1989. Results of the harmful effects of selected water pollutants (Anilines, Phenols, Aliphatic Compounds) to *Daphnia magna*. Water Res. 23(4):495-499.

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

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U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

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).

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.).

GREEN ALGAE 96-h EC50 (Growth)

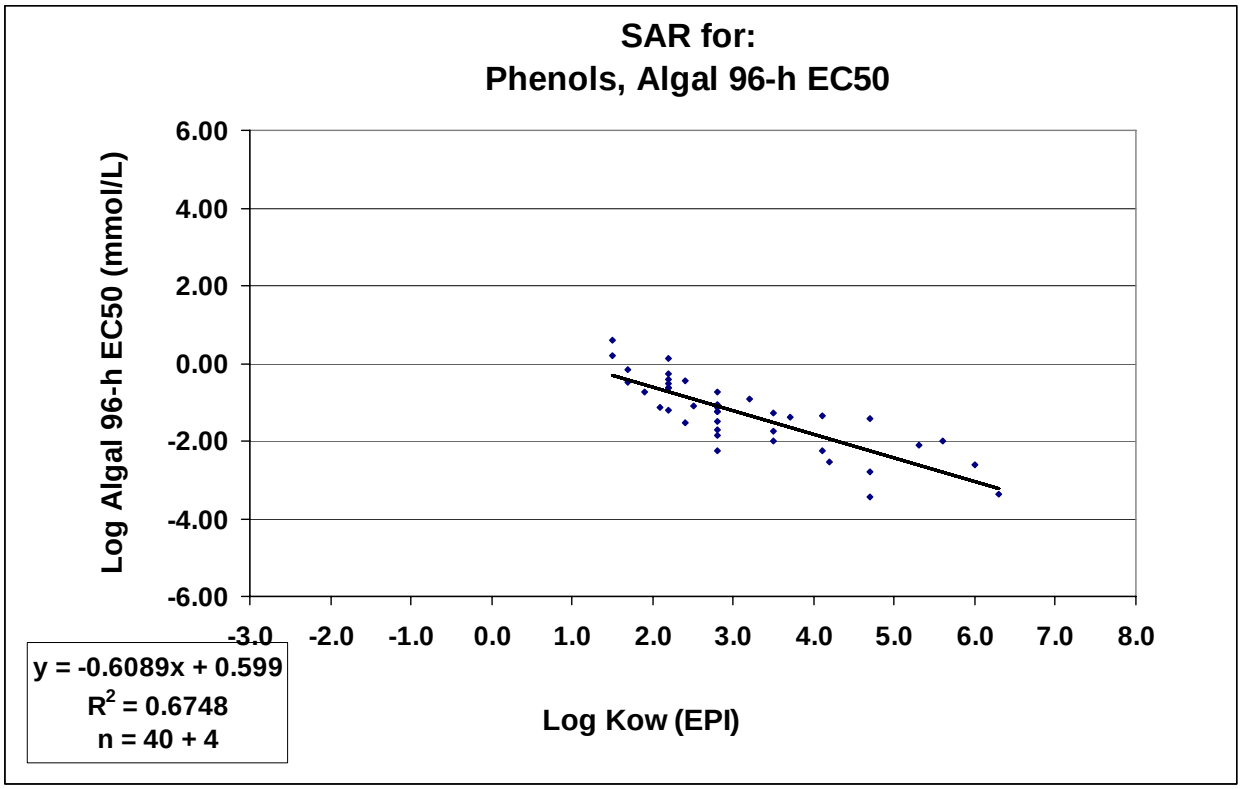
ESTIMATED TOXICITY:
The green algae 96-h EC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h EC50 (mmol/L) = -0.6089 (log Kow) + 0.599

The EC50 is in millimoles per liter (mM/L); N = 40 + 4; and the Coefficient of Determination (R^2) = 0.6748. To convert the EC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 7
Maximum MW: 1000

Graph:



Application:
This 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)

If the log Kow value is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Algal 96-h EC50 (mg/L)	Log Algal 96-h EC50 (mmol/L)	Reference (Meas. Kow)	Reference (Algal 96-h EC50)
108-95-2	Phenol	94	1.5	1.5	1.46	150	0.20	Hansch & Leo, 1985	Shigeoka, 1988
108-95-2	Phenol	94	1.5	1.5	1.46	370	0.60	Hansch & Leo, 1985	Shigeoka, 1988
500-99-2	3,5-Dimethoxy phenol	154	1.6	1.7	1.64	110	-0.15	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
CBI	CBI	212	1.6	1.7	1.2	68	-0.49	HPLC	P98-____
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	26	-0.73	Hansch & Leo, 1985	Kuhn & Pattard, 1990
106-44-5	p-Cresol	108	2	2.1	1.95	7.8	-1.14	Hansch & Leo, 1985	Kuhn & Pattard, 1990
106-48-9	4-Chlorophenol	129	2.5	2.2	2.39	8	-1.21	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
108-43-0	3-Chlorophenol	129	2.5	2.2	2.25; 2.5	29	-0.65	Hansch, C. et al., 1995; Unkno	Shigeoka, 1988
106-48-9	4-Chlorophenol	129	2.5	2.2	2.39	29	-0.65	Hansch, C. et al., 1995	Shigeoka, 1988
106-48-9	4-Chlorophenol	129	2.5	2.2	2.39	38	-0.53	Hansch, C. et al., 1995	Shigeoka, 1988
95-57-8	2-Chlorophenol	129	2.2	2.2	2.15	50	-0.41	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
95-57-8	2-Chlorophenol	129	2.2	2.2	2.15	70	-0.27	Hansch, C. et al., 1995	Shigeoka, 1988
95-57-8	2-Chlorophenol	129	2.2	2.2	2.15	170	0.12	Hansch, C. et al., 1995	Shigeoka, 1988
CBI	CBI	120	2.2	2.4		3.5	-1.54		L96-____
95-56-7	2-Bromophenol	173	2.4	2.4	2.35	60	-0.46	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
12167-20-3	Nitrocresol	153	2.4	2.5	2.37	12	-1.11	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
591-35-5	3,5-Dichlorophenol	163	3.3	2.8	3.62	0.89	-2.26	Hansch, C. et al., 1995	Comber et al., 1995
591-35-5	3,5-Dichlorophenol	163	3.3	2.8	3.62	2.3	-1.85	Hansch, C. et al., 1995	Shigeoka, 1988
95-77-2	3,4-Dichlorophenol	163	3.2	2.8	3.3	3.2	-1.71	Hansch, C. et al., 1995	Shigeoka, 1988
576-24-9	2,3-Dichlorophenol	163	2.8	2.8	2.84	5	-1.51		Shigeoka, 1988
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	9.2	-1.25	Hansch, C. et al., 1995	Shigeoka, 1988
87-65-0	2,6-Dichlorophenol	163	2.6	2.8	2.75	9.7	-1.23	Hansch, C. et al., 1995	Shigeoka, 1988
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	11.5	-1.15	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	14	-1.07	Hansch, C. et al., 1995	Shigeoka, 1988
87-65-0	2,6-Dichlorophenol	163	2.6	2.8	2.75	29	-0.75	Hansch, C. et al., 1995	Shigeoka, 1988
527-60-6	2,4,6-Trimethylphenol	136	3	3.2	2.73	17	-0.90	Sangster,1993	Kuhn & Pattard, 1990
15950-66-0	2,3,4-Trichlorophenol	197	3.5	3.5	3.8	2	-1.99	Hansch, C. et al., 1995	Shigeoka, 1988
88-06-2	2,4,6-Trichlorophenol	197	3.4	3.5	3.69	3.5	-1.75	Hansch, C. et al., 1995	Shigeoka, 1988
88-06-2	2,4,6-Trichlorophenol	197	3.4	3.5	3.69	10	-1.29	Hansch, C. et al., 1995	Shigeoka, 1988
CBI	CBI	207	3.8	3.7		8.4	-1.39		P91-____
58-90-2	2,3,4,6-Tetrachlorophenol	232	3.8	4.1	4.45	1.3	-2.25	Hansch, C. et al., 1995	Shigeoka, 1988
58-90-2	2,3,4,6-Tetrachlorophenol	232	3.8	4.1	4.45	10.1	-1.36	Hansch, C. et al., 1995	Shigeoka, 1988
3516-95-8	1-(2-Hydroxyphenyl)-3-phenyl-1-propanone	226	4.2	4.2		0.64	-2.55		8(e)-15485
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.1	-3.42	Hansch, C. et al., 1995	Graff, L. et al., 2003
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.42	-2.80	Hansch, C. et al., 1995	Shigeoka, 1988
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	10.3	-1.41	Hansch, C. et al., 1995	Shigeoka, 1988
140-66-9	4-(Tert-octyl) phenol	206	5.2	5.3		1.6	-2.11		8(e)-2453
CBI	CBI	316	7.2	5.6		3.16	-2.00		P94-____
104-40-5	Nonylphenol	220	6.2	6	5.76	0.53	-2.62	Itokawa et al., 1989	Graff, L. et al., 2003
CBI	CBI	277	6.4	6.3		0.12	-3.36		P01-____
SAR Data Not Included in Regression Equation:									
CBI	CBI	355	4.5	3.8	4.5 @ pH 6.3	*		Unknown	P92-____
CBI	CBI	355	4.5	3.8	7.3; >4.3	*		HPLC; shake flask	P01-____
CBI	CBI	426	7.2	6.4		*			P94-____
CBI	CBI	531	7.9	8.9		*12	*-1.645		P95-____
Data Not Included in SAR:									
59-50-7	4-Chloro-3-methylphenol	143	3	2.7	3.1	>10	>-1.16	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
						* indicates no effects at saturation			

References:

Comber MHI, Smyth DV, Thompson RS. 1995. Assessment of the toxicity to algae of colored substances. Bull. Environ. Contam. Toxicol. 55:922-928.

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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.

Shigeoka T, Sato Y, Takeda Y, Yoshida K, Yamauchi F. 1988. Acute toxicity of chlorophenols to green algae, Selenastrum capricornutum and Chlorella vulgaris, and quantitative structure-activity relationships. Environmental Toxicology and Chemistry ETOCDK 7(10):847-857.

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).

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

FISH 30-d ChV

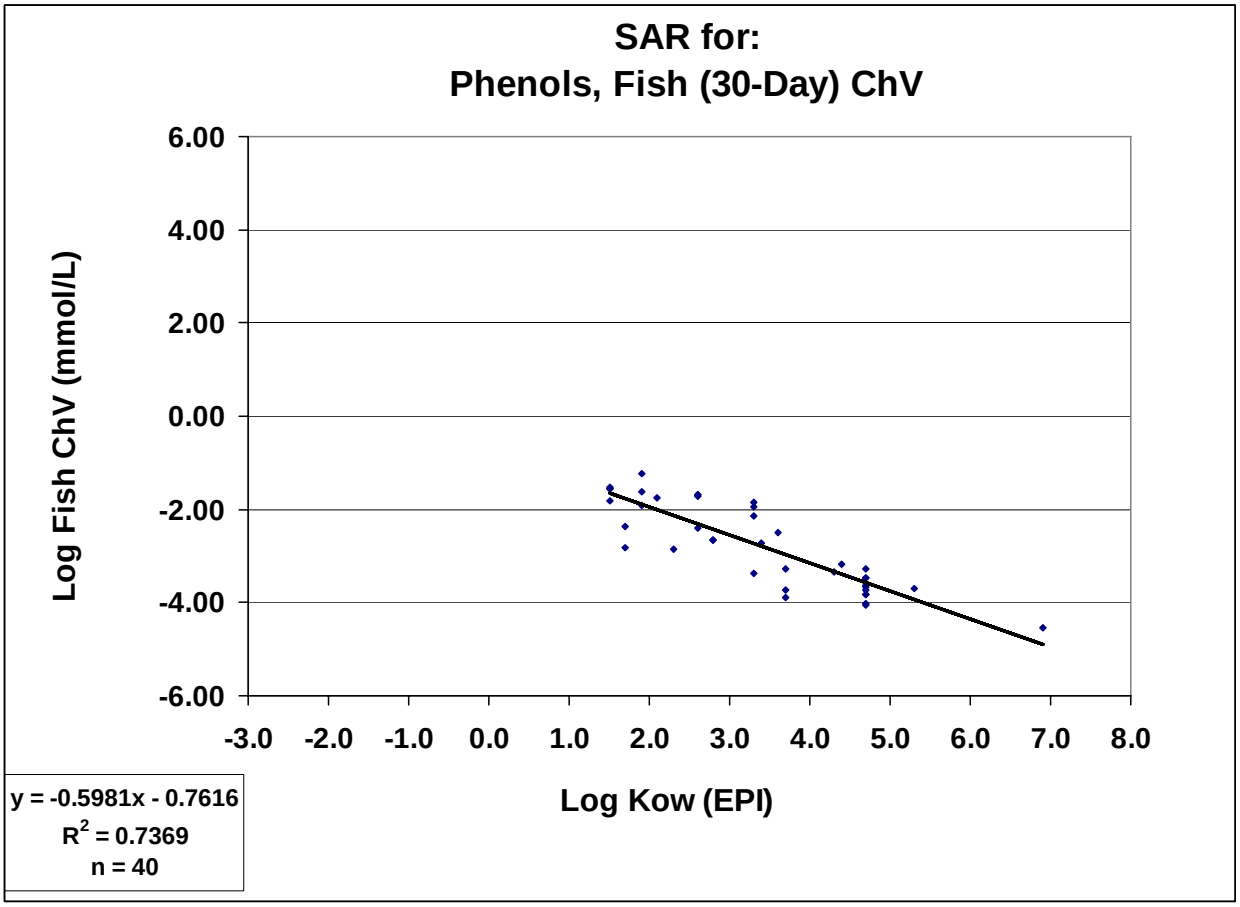
ESTIMATED TOXICITY:
The fish 30-d chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.5981 (log Kow) - 0.7616

The ChV is in millimoles per liter (mM/L); N = 40; and the Coefficient of Determination (R^2) = 0.7369. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

Graph:



Application:
This 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)

If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted. A test duration of more than 30 days may result in a lower chronic toxicity; at 60 days the toxicity will be 20x lower than predicted by this SAR for phenols with a log Kow of 1.5 and 4x lower for phenols with a log Kow of 5.3. For an exposure of 60 days, a separate SAR has been developed.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish (30 Day) ChV (mg/L)	Log Fish (30 Day) ChV (mmol/L)	Reference (Meas. Kow)	Reference (Fish (30 Day) ChV)
108-95-2	Phenol	94	1.5	1.5	1.46	1.4	-1.83	Hansch & Leo, 1985	Degraeve, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	2.56	-1.56	Hansch & Leo, 1985	US EPA, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	2.56	-1.56	Hansch & Leo, 1985	Holcomb, 1982
108-95-2	Phenol	94	1.5	1.5	1.46	2.87	-1.52	Hansch & Leo, 1985	DUL
51-28-5	2,4-Dinitro-phenol	184	1.8	1.7	1.67	0.272	-2.83	Hansch, C. et al., 1995	DUL
51-28-5	2,4-Dinitro-phenol	184	1.8	1.7	1.67	0.79	-2.37	Hansch, C. et al., 1995	Call et al., 1989
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	8.29	-1.22	Hansch & Leo, 1985	Broderius et al., 2005
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	1.65	-1.93	Hansch & Leo, 1985	DUL
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	3.38	-1.61	Hansch & Leo, 1985	Marking, 1991
106-44-5	p-Cresol	108	2	2.1	1.95	1.86	-1.76	Hansch & Leo, 1985	DUL
534-52-1	4,6-Dinitro-o-cresol	198	2.3	2.3	2.12	0.27	-2.87	Hansch, C. et al., 1995	DUL
105-67-9	2,4-Dimethylphenol	122	2.5	2.6	2.3	0.491	-2.40	Hansch & Leo, 1985	DUL
105-67-9	2,4-Dimethylphenol	122	2.5	2.6	2.3	2.41	-1.70	Hansch & Leo, 1985	DUL
105-67-9	2,4-Dimethylphenol	122	2.5	2.6	2.3	2.5	-1.69	Hansch & Leo, 1985	Holcomb, 1982
105-67-9	2,4-Dimethylphenol	122	2.5	2.6	2.3	2.5	-1.69	Hansch & Leo, 1985	DUL
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	0.353	-2.66	Hansch, C. et al., 1995	DUL
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	0.37	-2.64	Hansch, C. et al., 1995	Holcomb, 1982
90-43-7	2-Phenylphenol	170	3.1	3.3	3.09	1.21	-2.15	Pomona, 1987	DUL
90-43-7	2-Phenylphenol	170	3.1	3.3	3.09	1.9	-1.95	Pomona, 1987	Broderius et al., 2005
90-43-7	2-Phenylphenol	170	3.1	3.3	3.09	2.33	-1.86	Pomona, 1987	Broderius et al., 2005
87-17-2	Salicylanilide	213	3.3	3.3	3.27	0.0878	-3.38	Hansch & Leo, 1985	DUL
1689-84-5	3,5-Dibromo-4-hydroxybenzonitrile	277	2.9	3.4		0.504	-2.74		DUL
1689-82-3	p-Phenylazophenol	198	4	3.6		0.645	-2.49		Broderius et al., 2005
88-85-7	2-Sec-butyl-4,6-dinitrophenol (Dinoseb)	240	3.7	3.7	3.6	0.03	-3.90	Hansch et al., 1995	Call et al., 1989
88-85-7	2-Sec-butyl-4,6-dinitrophenol (Dinoseb)	240	3.7	3.7	3.6	0.0458	-3.72	Hansch et al., 1995	DUL
88-85-7	2-Sec-butyl-4,6-dinitrophenol (Dinoseb)	240	3.7	3.7	3.56	0.13	-3.27	Hansch, C. et al., 1995	Call et al., 1989
97-23-4	2,2-Methylene-bis-(4-chlorophenol)	269	4.9	4.3	4.26	0.122	-3.34	Hansch, C. et al., 1995	DUL
CBI	CBI	366	MF	4.4		0.25	-3.17		P94-___
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.024	-4.04	Hansch, C. et al., 1995	Spehar,1985
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.0244	-4.04	Hansch, C. et al., 1995	DUL
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.04	-3.82	Hansch, C. et al., 1995	Spehar,1985
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.0404	-3.82	Hansch, C. et al., 1995	DUL
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.049	-3.73	Hansch, C. et al., 1995	Spehar,1985
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.057	-3.67	Hansch, C. et al., 1995	Holcomb, 1982
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.0636	-3.62	Hansch, C. et al., 1995	DUL
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.089	-3.48	Hansch, C. et al., 1995	Spehar,1985
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.0892	-3.47	Hansch, C. et al., 1995	DUL
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.144	-3.27	Hansch, C. et al., 1995	Hedtke, 1986
140-66-9	4-(Tert-octyl) phenol	206	5.2	5.3		0.04	-3.71		Datasheet
70-30-4	2,2-Methylene-bis-(3,4,6-trichlorophenol) (hexachlorophene	407	7.1	6.9	7.54	0.012	-4.53	Hansch, C. et al., 1995	Call et al., 1989
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
108-46-3	Resorcinol	110	0.81	1	0.8	<3.16	<-1.54	Hansch, C. et al., 1995	Degraeve, 1980
108-95-2	Phenol	94	1.5	1.5	1.46	<3.26	<-1.46	Hansch & Leo, 1985	DUL
95-48-7	o-Cresol	108	2	2.1	1.95	<1.33	<-1.91	Hansch & Leo, 1985	DUL
534-52-1	4,6-Dinitro-o-cresol	198	2.3	2.3	2.12	<0.183	<-3.03	Hansch, C. et al., 1995	DUL
95-95-4	2,4,5-Trichlorophenol	197	3.6	3.5	3.72	<0.0788	<-3.4	Hansch, C. et al., 1995	Saarikoski & Viluksela, 1982
1689-82-3	4-Phenyl azo phenol	198	4	3.6		<0.219	<-2.96		Veith GD & Broderius SJ, 1987/ DUL
70-30-4	2,2-Methylene-bis-(3,4,6-trichlorophenol) (hexachlorophene	407	7.1	6.9	7.54	<0.00289	<-5.15	Hansch, C. et al., 1995	DUL
						* indicates no effects at saturation			

References:
Broderius et al.. 2005. Toxicity of mixtures to the fathead minnow. Environ. Toxicol. Chem. 24: p.3121

Call DJ, Poirier SH, Lindberg CA, Harting SL, Markee TP, Brooke LT, Zarvan N, Northcott CE. 1989. Toxicity of selected uncoupling and Acetylcholinesterase-inhibiting pesticides to the Fathead minnow (*Pimephales promelas*). Proc. Natl. Res. Conf., Virginia Polytechnic Inst. and State Univ., Blacksburg, VA:317-336.

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.

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.

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

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Spehar RL, Nelson HP, Swanson MJ, and Renos JW. 1985. Pentachlorophenol toxicity 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).

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

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

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.

FISH 60-d ChV

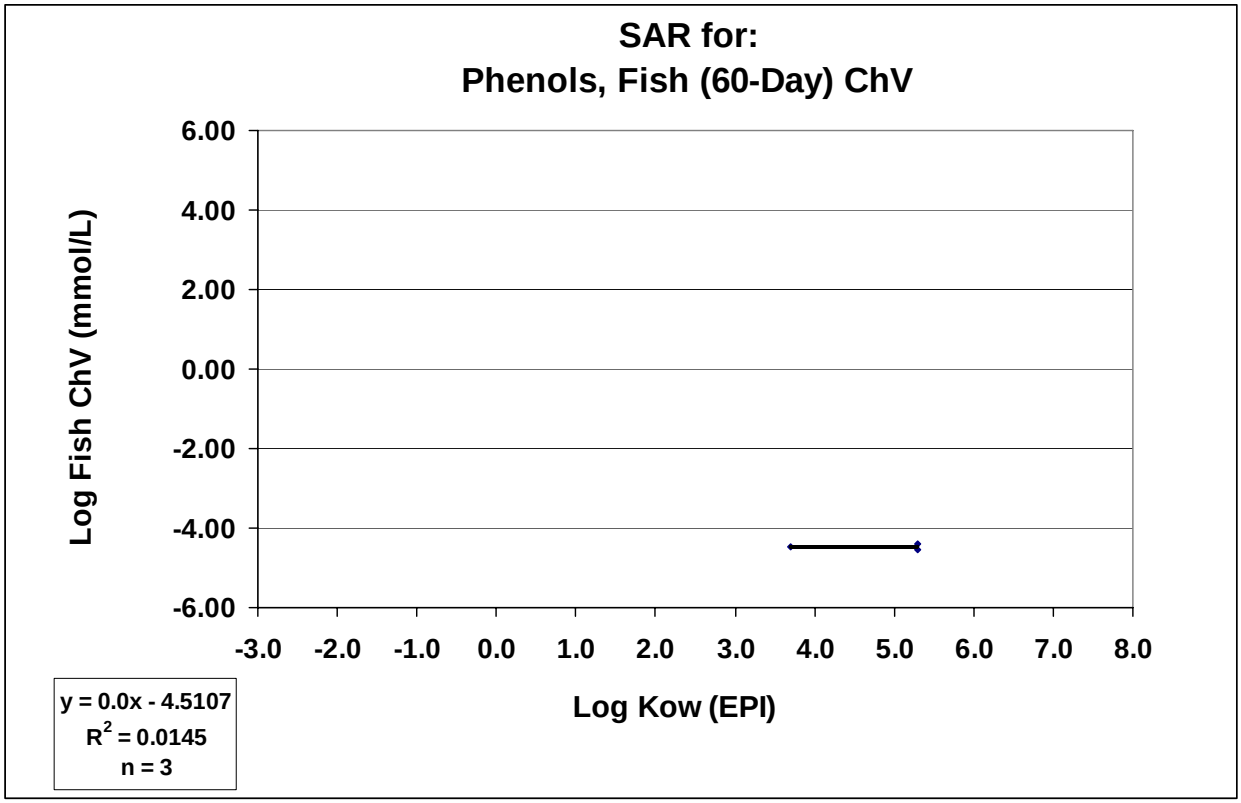
ESTIMATED TOXICITY:
The fish 60-d chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = 0.0077 (log Kow) - 4.5107

The ChV is in millimoles per liter (mM/L); N = 3; and the Coefficient of Determination (R^2) = 0.0145. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

Graph:



Application:
This 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)

If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted. A test duration of more or less then 60-days may results in greater then or less then estimated toxicity.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish (60-d) ChV (mg/L)	Log Fish (60-d) ChV (mmol/L)	Reference (Meas. Kow)	Reference (Fish (60-d) ChV)
88-85-7	2-Sec-butyl-4,6-dinitrophenol	240	3.7	3.7	3.6	0.00791	-4.48	Hansch et al., 1995	DUL
140-66-9	4-(1,1,3,3-Tetramethylbutyl)-phenol	206	5.2	5.3		0.0061	-4.53		8(e)-9765
140-66-9	4-(1,1,3,3-Tetramethylbutyl)-phenol	206	5.2	5.3		0.008	-4.41		U.S. EPA, 1984
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
108-95-2	Phenol	94	1.5	1.5	1.46	<0.2	<-2.67	Hansch & Leo, 1985	Degraeve, 1980
						* indicates no effects at saturation			

References:

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.

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).

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

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

DAPHNID 21-d ChV

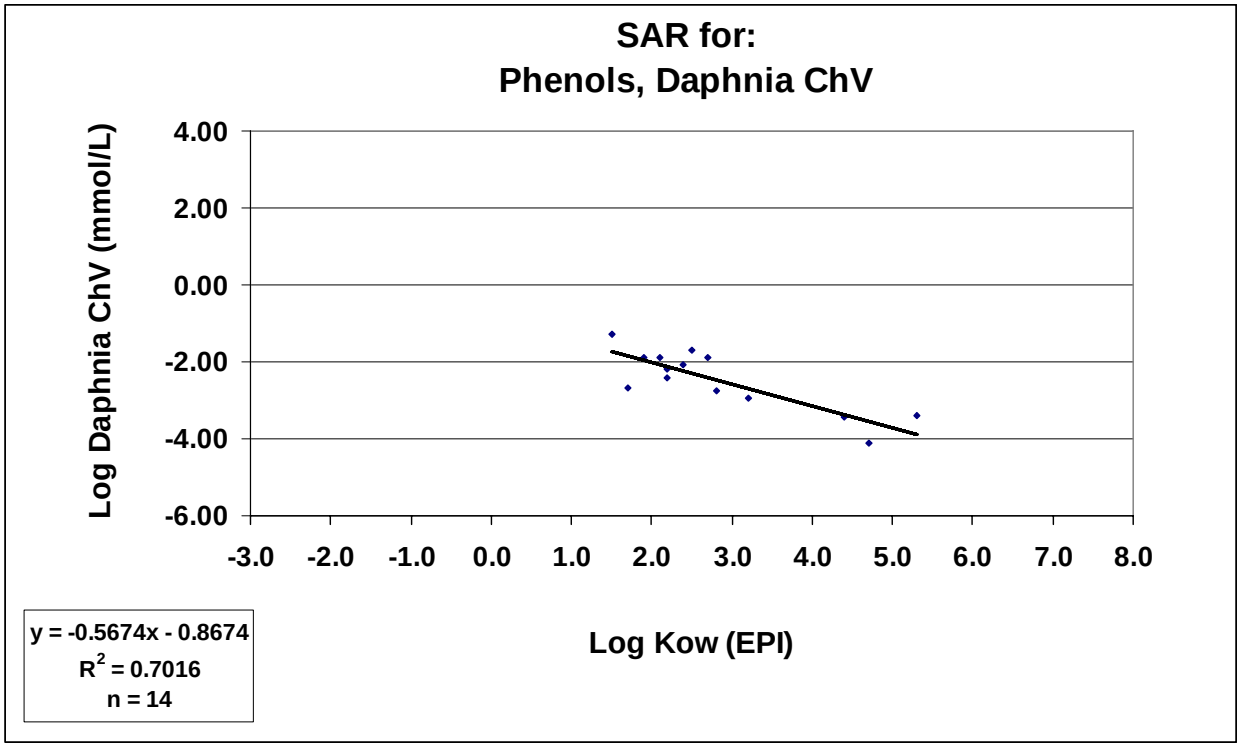
ESTIMATED TOXICITY:
The daphnid chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.5674 (log Kow) - 0.8674

The ChV is in millimoles per liter (mM/L); N = 14; and the Coefficient of Determination (R^2) = 0.7016. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

Graph:



Application:
This 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)

3,5-Dimethoxyphenol has an excess toxicity of 18x that predicted by this SAR.

If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Daphnia ChV (mg/L)	Log Daphnia ChV (mmol/L)	Reference (Meas. Kow)	Reference (Daphnia ChV)
108-95-2	Phenol	94	1.5	1.5	1.46	4.9	-1.28	Hansch & Leo, 1985	Oris et al., 1991
500-99-2	3,5-Dimethoxyphenol	154	1.6	1.7	1.64	0.32	-2.68	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	1.8	-1.89	Hansch & Leo, 1985	Kuhn, R. et al., 1989
106-44-5	4-Methylphenol	108	2	2.1	1.94	1.4	-1.89	Hansch & Leo, 1985	Kuhn, R. et al., 1989
95-57-8	2-Chlorophenol	129	2.2	2.2	2.15	0.5	-2.41	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
106-48-9	4-Chlorophenol	129	2.5	2.2	2.39	0.84	-2.19	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
95-56-7	2-Bromophenol	173	2.4	2.4	2.35	1.5	-2.06	Hansch et al., 1995	Kuhn, R. et al., 1989
12167-20-3	2-Nitro-para-cresol	153	2.4	2.5	2.37	3.2	-1.68	Hansch et al., 1995	Kuhn, R. et al., 1989
59-50-7	4-Chloro-3-methylphenol	143	3	2.7	3.1	1.8	-1.90	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	0.29	-2.75	Hansch, C. et al., 1995	Kuhn, R. et al., 1989
527-60-6	2,4,6-Trimethylphenol	136	3	3.2	2.73	0.16	-2.93	Sangster,1993	Kuhn, R. et al., 1989
CBI	CBI	366	MF	4.4		0.13	-3.45		P94-____
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.02	-4.12	Hansch, C. et al., 1995	Stephenson, 1991
140-66-9	4-(Tert-octyl) phenol	206	5.2	5.3		0.086	-3.38		U.S. EPA, 1984
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	<0.01	<-4.42	Hansch, C. et al., 1995	Stephenson, 1991
140-66-9	4-(Tert-octyl) phenol	206	5.2	5.3		<0.037	<-3.75		8(e)-9766
						* indicates no effects at saturation			

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.

Stephenson GL, Kaushik NK, Solomon KR. 1991 Acute toxicity of pure pentachlorophenol and a technical formulation to three species of Daphnia. Arch. Environ. Contam. Toxicol. 20(1):73-80.

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).

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from data submitted under the “Toxic Substance Control Act” (TSCA). Public Law 94-469, 90 Stat. 2003, October 11, 1976. Washington DC: OPPT, USEPA, 1400 Pennsylvania Ave., N.W.

GREEN ALGAE ChV

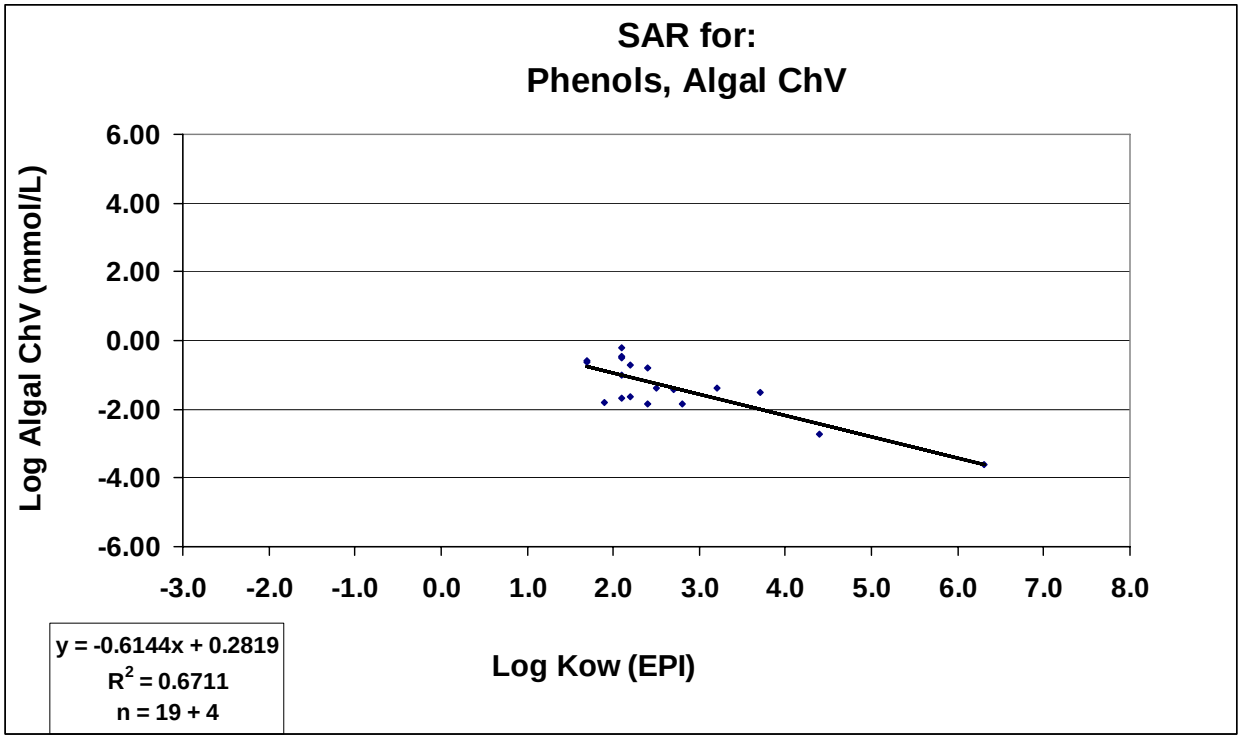
ESTIMATED TOXICITY:
The green algae chronic values (ChV) used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log ChV (mmol/L) = -0.6144 (log Kow) + 0.2819

The ChV is in millimoles per liter (mM/L); N = 19 + 4; and the Coefficient of Determination (R^2) = 0.6711. To convert the ChV from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 8.0
Maximum MW: 1000

Graph:



Application:
This 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)

If the log Kow value is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Algal ChV (mg/L)	Log Algal ChV (mmol/L)	Reference (Meas. Kow)	Reference (Algal ChV)
500-99-2	3,5-Dimethoxyphenol	154	1.6	1.7	1.64	40	-0.59	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
CBI	CBI	212	1.6	1.7	1.2	50	-0.63	HPLC	P98-____
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	2.1	-1.82	Hansch & Leo, 1985	Kuhn & Pattard, 1990
106-44-5	p-Cresol	108	2	2.1	1.95	2.3	-1.67	Hansch & Leo, 1985	Kuhn & Pattard, 1990
95-48-7	o-Cresol	108	2	2.1	1.95	11	-0.99	Hansch & Leo, 1985	Sloof,1983
95-48-7	o-Cresol	108	2	2.1	1.95	34	-0.50	Hansch & Leo, 1985	Sloof,1983
95-48-7	o-Cresol	108	2	2.1	1.95	36	-0.48	Hansch & Leo, 1985	Sloof,1983
95-48-7	o-Cresol	108	2	2.1	1.95	65	-0.22	Hansch & Leo, 1985	Sloof,1983
106-48-9	4-Chlorophenol	129	2.5	2.2	2.39	3	-1.63	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
95-57-8	2-Chlorophenol	129	2.2	2.2	2.15	24	-0.73	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
CBI	CBI	120	2.2	2.4		1.79	-1.83		L96-____
95-56-7	2-Bromophenol	173	2.4	2.4	2.35	28	-0.79	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
12167-20-3	Nitrocresol	153	2.4	2.5	2.37	6.3	-1.39	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
59-50-7	4-Chloro-3-methylphenol	143	3	2.7	3.1	5.2	-1.44	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	2.4	-1.83	Hansch, C. et al., 1995	Kuhn & Pattard, 1990
527-60-6	2,4,6-Trimethylphenol	136	3	3.2	2.73	5.8	-1.37	Sangster,1993	Kuhn & Pattard, 1990
CBI	CBI	207	3.8	3.7		6.4	-1.51		P91-____
CBI	CBI	366	MF	4.4		0.7	-2.72		P94-____
CBI	CBI	277	6.4	6.3		0.07	-3.60		P01-____
SAR Data Not Included in Regression Equation:									
CBI	CBI	355	4.5	3.8	4.5 @ pH 6.3	*		Unknown	P92-____
CBI	CBI	355	4.5	3.8	7.3; >4.3	*		HPLC; shake flask	P01-____
CBI	CBI	426	7.2	6.4		*			P94-____
CBI	CBI	531	7.9	8.9		*7.2	*-1.868		P95-____
Data Not Included in SAR:									
140-66-9	4-(Tert-octyl) phenol	206	5.2	5.3		<0.86	<-2.38		US EPA, 1984
						* indicates no effects at saturation			

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 (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).

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

FISH (SW) 96-h LC50 (Mortality)

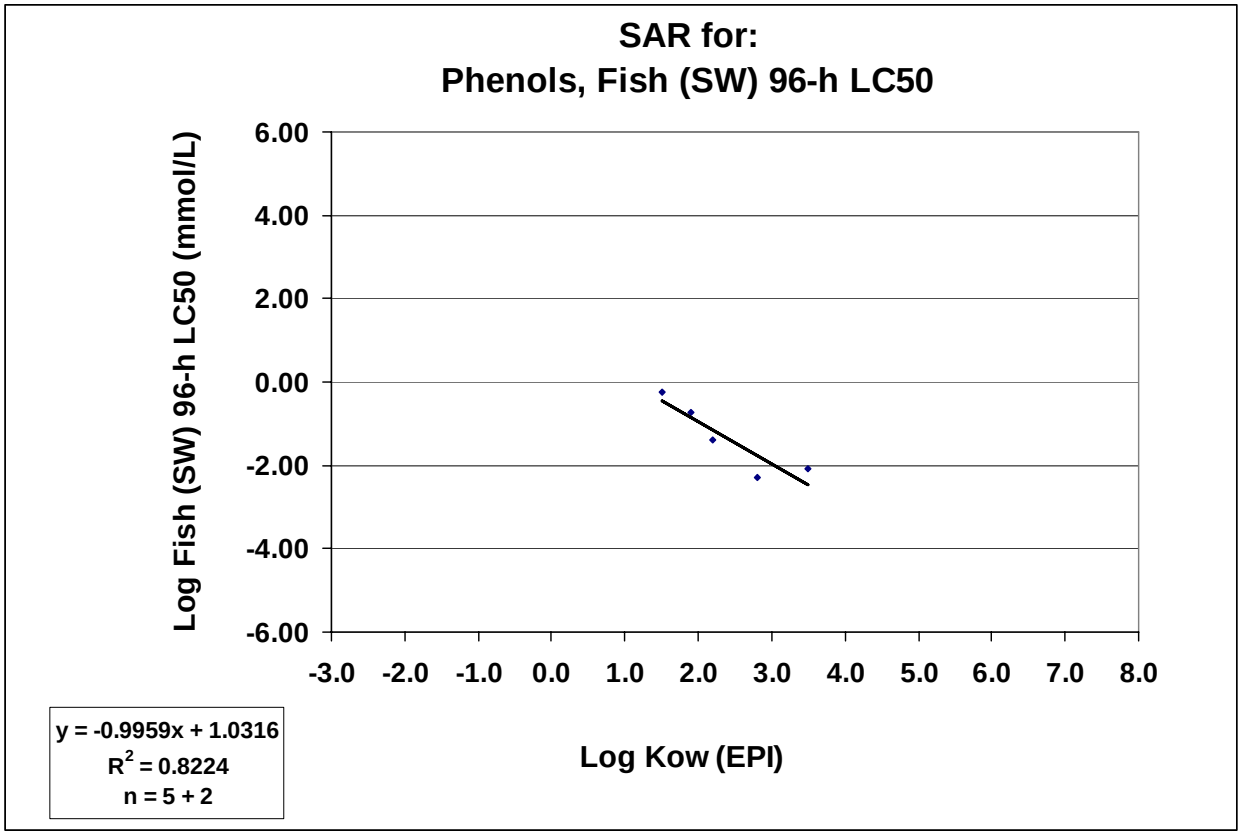
ESTIMATED TOXICITY:
The fish (sw) 96-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h LC50 (mmol/L) = -0.9959 (log Kow) + 1.0316

The LC50 is in millimoles per liter (mM/L); N = 5 + 2; and the Coefficient of Determination (R^2) = 0.8224.
To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 5.0
Maximum MW: 1000

Graph:



Application:
This 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)

If the log Kow value is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Fish (SW) 96-h LC50 (mg/L)	Log Fish (SW) 96-h LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Fish (SW) 96-h LC50)
88-89-1	2,4,6-Trinitrophenol	229	1.6	1.5	1.33	128.838	-0.25	Sangster, 1994	Zaroogian et al., 1985
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	26.507	-0.72	Hansch & Leo, 1985	Zaroogian et al., 1985
106-48-9	4-Chlorophenol	129	2.5	2.2	2.39	5.359	-1.38	Hansch, C. et al., 1995	Zaroogian et al., 1985
CBI	CBI	163	3.3	2.8	3.62	0.87	-2.27	Hansch, C. et al., 1995	CBI
95-95-4	2,4,5-Trichlorophenol	197	3.6	3.5	3.72	1.681	-2.07	Hansch, C. et al., 1995	Zaroogian et al., 1985
SAR Data Not Included in Regression Equation:									
104-40-5	Nonylphenol	220	6.2	6	5.76	*70	*-0.5	Itokawa et al., 1989	Lussier, SM et al., 2000
104-40-5	Nonylphenol	220	6.2	6	5.76	*142	*-0.19	Itokawa et al., 1989	Lussier, SM et al., 2000
Data Not Included in SAR:									
						* indicates no effects at saturation			

References:
Lussier SM, Champlin D, LiVolsi J, Poucher S, and Pruell RJ. Acute toxicity of para-nonylphenol to saltwater animals. Environmental toxicology and chemistry, Vol. 19, No. 3, pp. 617-621.

U.S. Environmental Protection Agency (USEPA). 2006. Database of environmental toxicity data from Premanufacture Notifications (PMN). Washington DC: Risk Assessment Division (RAD), OPPT, USEPA, 1400 Pennsylvania Ave., N.W. (Unpublished test data.)

Zarogian 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.

EARTHWORM 14-d LC50 (Mortality)

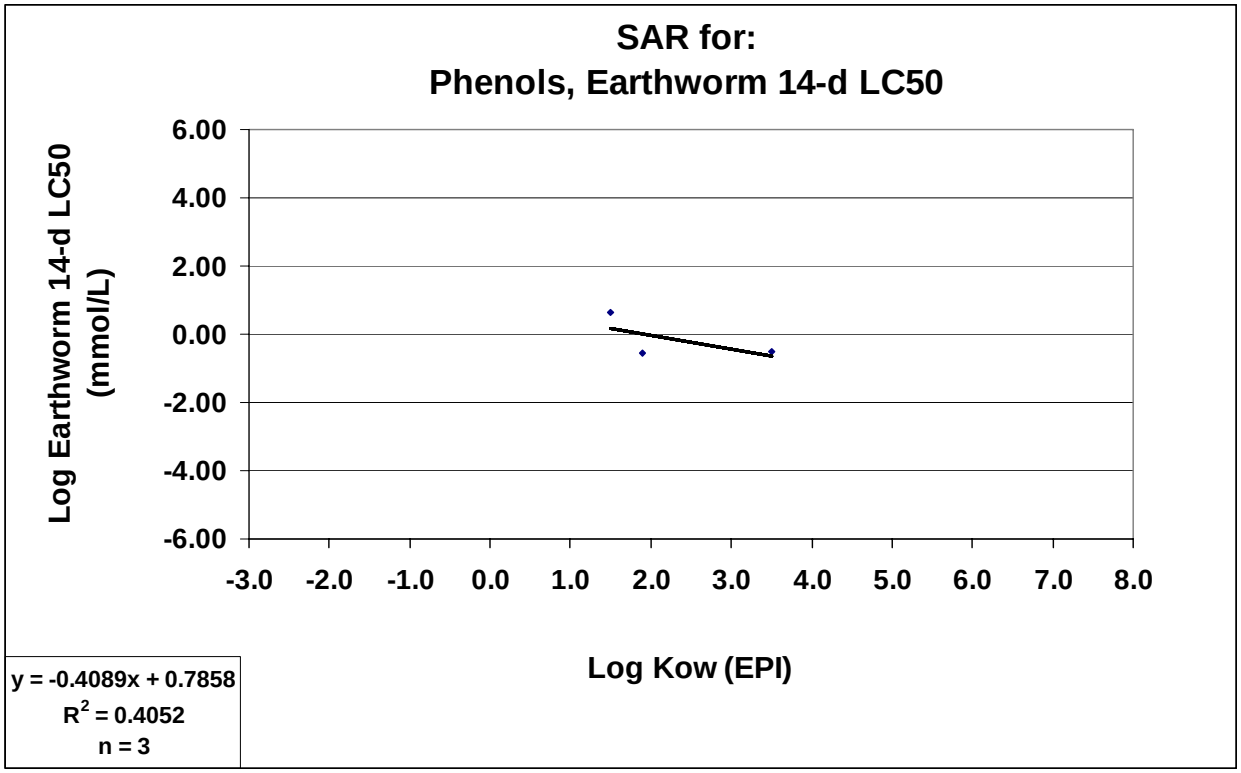
ESTIMATED TOXICITY:
The earthworm 14-d-h LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h EC50 (mmol/L) = -0.4089 (log Kow) + 0.7858

The LC50 is in millimoles per liter (mM/L); N = 3; and the Coefficient of Determination (R^2) = 0.4052. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 6.4
Maximum MW: 1000

Graph:



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

Limitations:
If the log Kow value is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	Earthworm 14-d LC50 (mg/L)	Log Earthworm 14 d LC50 (mmol/L)	Reference (Meas. Kow)	Reference (Earthworm 14-d LC50)
108-95-2	Phenol	94	1.5	1.5	1.46	401	0.63	Hansch & Leo, 1985	Neuhauser et al., 1985
100-02-7	4-Nitrophenol	139	1.9	1.9	1.91	38	-0.56	Hansch & Leo, 1985	Neuhauser et al., 1985
88-06-2	2,4,6-Trichlorophenol	197	3.4	3.5	3.69	58	-0.53	Hansch, C. et al., 1995	Neuhauser et al., 1985
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
						* indicates no effects at saturation			

References:

Neuhauser, E.F., Loehr, R.C., Malecki, M.R., Milligan, D.L. and Durkin, P.R. 1985. The toxicity of selected organic chemicals to the earthworm *Eisenia fetida.* Journal of Environmental Quality 14: 383-388.

LEMNA GIBBA 7-d EC50

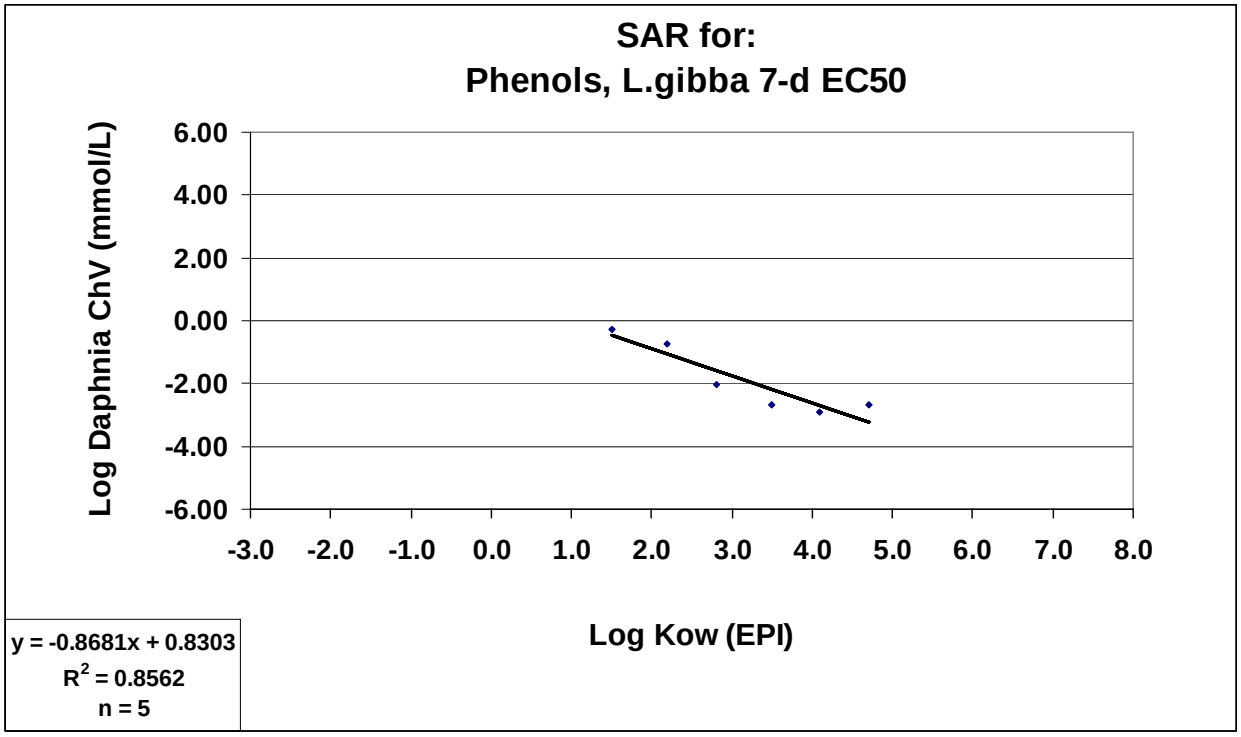
ESTIMATED TOXICITY:
The *lemna gibba* 7-d LC50 values used to develop this SAR were measured and the octanol water partition coefficients (Kow) were calculated using the computer program, KOWWIN (Version 1.67). The SAR equation used to estimate toxicity is:

Log 96-h EC50 (mmol/L) = -0.8681 (log Kow) + 0.8303

The LC50 is in millimoles per liter (mM/L); N = 5; and the Coefficient of Determination (R^2) = 0.8562. To convert the LC50 from mM/L to mg/L, multiply by the molecular weight of the compound.

Maximum K_{ow}: 6.4
Maximum MW: 1000

Graph:



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

Limitations:
If the log Kow value is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted.

Data:

CAS No.	Chemical Name	M.W.	log Kow (CLogP)	log Kow (EPI)	log Kow (M)	L.gibba 7-d EC50 (mg/L)	Log L.gibba 7-d EC50 (mmol/L)	Reference (Meas. Kow)	Reference (L.gibba 7-d EC50)
108-95-2	Phenol	94	1.5	1.5	1.46	50.82	-0.27	Hansch & Leo, 1985	Sharma et al., 1997
106-48-9	4-Chlorophenol	129	2.5	2.2	2.39	23.5	-0.74	Hansch, C. et al., 1995	Sharma et al., 1997
120-83-2	2,4-Dichlorophenol	163	3	2.8	3.06	1.4995	-2.04	Hansch, C. et al., 1995	Sharma et al., 1997
95-95-4	2,4,5-Trichlorophenol	197	3.6	3.5	3.72	0.4146	-2.68	Hansch, C. et al., 1995	Sharma et al., 1997
58-90-2	2,4,5,6-Tetrachlorophenol	232	3.8	4.1	4.45	0.2783	-2.92	Hansch, C. et al., 1995	Sharma et al., 1997
87-86-5	Pentachlorophenol	266	4.3	4.7	5.12	0.5326	-2.70	Hansch, C. et al., 1995	Sharma et al., 1997
SAR Data Not Included in Regression Equation:									
Data Not Included in SAR:									
						* indicates no effects at saturation			

References:

Sharma HA, Barber JT, Ensley HE, and Polito MA. 1997. A comparison of the toxicity and metabolism of phenol and chlorinated phenols by *Lemna gibba*, with special reference to 2,4,5-Trichlorophenol. Environmental Toxicology and Chemistry, Vol. 16, No. 2, pp. 346-350.