SUPERFUND CHEMICAL DATA MATRIX

Date: 6/7/2010
Chemical: Tetrahydrothiophene, 1, 1-dioxide
CAS Number: 000126-33-0

TOXICITY

Parameter	Value	Unit	Source
Oral RfD:		mg/kg/day	
Inhal RfD:		mg/kg/day	
Oral Slope:		(mg/kg/day)^-1	
Oral Wt-of-Evid:			
Inhal Slope:		(mg/kg/day)^-1	
Inhal Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Inhal ED10:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:	1.9E+3	mg/kg	RTECS
Dermal LD50:	3.8E+3	mg/kg	RTECS
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE			
Fresh CMC:		µg/L	
Salt CMC:		µg/L	
CHRONIC			
Fresh CCC:		µg/L	
Salt CCC:		µg/L	
Fresh Ecol LC50:	1.4E+5	µg/L	ECOTOX
Salt Ecol LC50:		µg/L	

PERSISTENCE

Parameter	Value	Unit	Source
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	1.0E+2	days	THOMAS
Photolysis:		days	
Biodeg:		days	
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	6.6E+0	days	THOMAS
Photolysis:		days	
Biodeg:		days	
Radio:		days	
Log Kow:	-7.7E-1		CHEMFATE

PHYSICAL CHARACTERISTICS

Parameter	Value	
Metal Contain:	No	
Organic:	Yes	
Gas:	Yes	
Particulate:	Yes	
Radionuclide:	No	
Rad. Element:	No	
Molecular Weight:	1.2E+2	
Density:	1.3E+0	g/mL @ 18.00 C

MOBILITY

Parameter	Value	Unit	Source
Vapor Press:	6.2E-3	Torr	PHYSPROP
Henry's Law:	4.9E-6	atm-m3/mol	PHYSPROP
Water Solub:	3.8E+5	mg/L	CHEMFATE
Distrib Coef:	2.7E-2	ml/g	DITOR_KD
Geo Mean Sol:		mg/L	

BIOACCUMULATION

Parameter	Value	Unit	Source
FOOD CHAIN			
Fresh BCF:			
Salt BCF:			
ENVIRONMENTAL			
Fresh BCF:			
Salt BCF:			
Log Kow:	-7.7E-1		CHEMFATE
Water Solub:	3.8E+5		CHEMFATE
Geo Mean Sol:		mg/L	

OTHER DATA

Melting Point:	2.8E+1	C
Boiling Point:	2.9E+2	C
Formula:	C4 H8 O2 S	

CLASS INFORMATION

Class	Parent Substance

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Chemical: Tetrahydrothiophene, 1, 1-dioxide

CAS Number: 000126-33-0

ASSIGNED FACTOR VALUES

AIR PATHWAY

Parameter	Value
Toxicity:	1
Gas Mobility:	0.2000
Gas Migration:	11

GROUND WATER PATHWAY

Parameter		Value
Toxicity:		1
Water Solub:		3.8E+5
Distrib:		2.7E-2
Geo Mean Sol:		
Mobility:		
Liquid	Karst:	1.0E+0
	Non Karst:	1.0E+0
Non Liq.	Karst:	1.0E+0
	Non Karst:	1.0E+0

SOIL EXPOSURE PATHWAY

Parameter	Value
Toxicity:	1

SURFACE WATER PATHWAY

DRINKING WATER

Parameter	Value
Toxicity:	1
Persistence	
River:	1.0000
Lake:	1.0000

HUMAN FOOD CHAIN

Parameter	Value
Toxicity:	1
Persistence	
River:	1.0000
Lake:	1.0000
Bioaccumulation	
Fresh:	0.5
Salt:	0.5

ENVIRONMENTAL

Parameter	Value
Fresh Tox:	1
Salt Tox:	1
Persistence	
River:	1.0000
Lake:	1.0000
Bioaccumulation	
Fresh:	0.5
Salt:	0.5

BENCHMARKS

AIR PATHWAY

Parameter	Value	Unit
NAAQS/NESHAPS:		µg/m3
Cancer Risk:		mg/m3
Non Cancer Risk:		mg/m3

GROUND WATER PATHWAY

Parameter	Value	Unit
MCL/MCLG:		mg/L
Cancer Risk:		mg/L
Non Cancer Risk:		mg/L

SOIL EXPOSURE PATHWAY

Parameter	Value	Unit
Cancer Risk:		mg/kg
Non Cancer Risk:		mg/kg

RADIONUCLIDE

Parameter	Value	Unit
MCL:		pCi/L
UMTRCA:		pCi/kg
CANCER RISK		
Air:		pCi/m3
DW:		pCi/L
FC:		pCi/kg
Soil Ing:		pCi/kg
Soil Gam:		pCi/kg

SURFACE WATER PATHWAY

DRINKING WATER

Parameter	Value	Unit
MCL/MCLG:		mg/L
Cancer Risk:		mg/L
Non Cancer Risk:		mg/L

HUMAN FOOD CHAIN

Parameter	Value	Unit
FDAAL:		ppm
Cancer Risk:		mg/kg
Non Cancer Risk:		mg/kg

ENVIRONMENTAL

Parameter	Value	Unit
ACUTE		
Fresh CMC:		µg/L
Salt CMC:		µg/L
CHRONIC		
Fresh CCC:		µg/L
Salt CCC:		µg/L

Footnote Code	Footnote Description
A	This recommended water quality criterion was derived from data for arsenic (III), but is applied here to total arsenic, which might imply that arsenic (III) and arsenic (V) are equally toxic to aquatic life and that their toxicities are additive. In the arsenic criteria document (EPA 440/5-84-033, January 1985), Species Mean Acute Values are given for both arsenic (III) and arsenic (V) for five species and the ratios of the SMAVs for each species range from 0.6 to 1.7. Chronic values are available for both arsenic (III) and arsenic (V) for one species; for the fathead minnow, the chronic value for arsenic (V) is 0.29 times the chronic value for arsenic (III). No data are known to be available concerning whether the toxicities of the forms of arsenic to aquatic organisms are additive.
B	This criterion has been revised to reflect The Environmental Protection Agency's q1* or RfD, as contained in the Integrated Risk Information System (IRIS) as of May 17, 2002. The fish tissue bioconcentration factor (BCF) from the 1980 Ambient Water Quality Criteria document was retained in each case.
C	This criterion is based on carcinogenicity of 10^{-6} risk. Alternate risk levels may be obtained by moving the decimal point (e.g., for a risk level of 10^{-5}, move the decimal point in the recommended criterion one place to the right).
D	Freshwater and saltwater criteria for metals are expressed in terms of the dissolved metal in the water column. The recommended water quality criteria value was calculated by using the previous 304(a) aquatic life criteria expressed in terms of total recoverable metal, and multiplying it by a conversion factor (CF). The term "Conversion Factor" (CF) represents the recommended conversion factor for converting a metal criterion expressed as the total recoverable fraction in the water column to a criterion expressed as the dissolved fraction in the water column. (Conversion Factors for saltwater CCCs are not currently available. Conversion factors derived for saltwater CMCs have been used for both saltwater CMCs and CCCs). See "Office of Water Policy and Technical Guidance on Interpretation and Implementation of Aquatic Life Metals Criteria," October 1, 1993, by Martha G. Prothro, Acting Assistant Administrator for Water, available from the Water Resource center, USEPA, 401 M St., SW, mail code RC4100, Washington, DC 20460; and 40CFR§131.36(b)(1). Conversion Factors applied in the table can be found in Appendix A to the Preamble- Conversion Factors for Dissolved Metals (which is attached below).
E	The freshwater criterion for this metal is expressed as a function of hardness (mg/L) in the water column. The value given here corresponds to a hardness of 100 mg/L. Criteria values for other hardness may be calculated from the following: CMC (dissolved) = $\exp\{m_A [\ln(\text{hardness})] + b_A\}$ (CF), or CCC (dissolved) = $\exp\{m_C [\ln(\text{hardness})] + b_C\}$ (CF) and the parameters specified in Appendix B- Parameters for Calculating Freshwater Dissolved Metals Criteria That Are Hardness-Dependent (which is attached below).
F	Freshwater aquatic life values for pentachlorophenol are expressed as a function of pH, and are calculated as follows: CMC = exp(1.005(pH)-4.869); CCC = exp(1.005(pH)-5.134). Values displayed in table correspond to a pH of 7.8.
G	This Criterion is based on 304(a) aquatic life criterion issued in 1980, and was issued in one of the following documents: Aldrin/Dieldrin (EPA 440/5-80-019), Chlordane (EPA 440/5-80-027), DDT (EPA 440/5-80-038), Endosulfan (EPA 440/5-80-046), Endrin (EPA 440/5-80-047), Heptachlor (EPA 440/5- 80-052), Hexachlorocyclohexane (EPA 440/5-80-054), Silver (EPA 440/5-80-071). The Minimum Data Requirements and derivation procedures were different in the 1980 Guidelines than in the 1985 Guidelines. For example, a "CMC" derived using the 1980 Guidelines was derived to be used as an instantaneous maximum. If assessment is to be done using an averaging period, the values given should be divided by 2 to obtain a value that is more comparable to a CMC derived using the 1985 Guidelines.
H	No criterion for protection of human health from consumption of aquatic organisms excluding water was presented in the 1980 criteria document or in the *1986 Quality Criteria for Water*. Nevertheless, sufficient information was presented in the 1980 document to allow the calculation of a criterion, even though the results of such a calculation were not shown in the document.
I	This criterion for asbestos is the Maximum Contaminant Level (MCL) developed under the Safe Drinking Water Act (SDWA).
J	This fish tissue residue criterion for methylmercury is based on a total fish consumption rate of 0.0175 kg/day.
K	This recommended criterion is based on a 304(a) aquatic life criterion that was issued in the *1995 Updates: Water Quality Criteria Documents for the Protection of Aquatic Life in Ambient Water*, (EPA-820-B-96-001, September 1996). This value was derived using the GLI Guidelines (60FR15393-15399, March 23, 1995; 40CFR132 Appendix A); the difference between the 1985 Guidelines and the GLI Guidelines are explained on page iv of the 1995 Updates. None of the decisions concerning the derivation of this criterion were affected by any considerations that are specific to the Great Lakes.
L	The CMC = 1/[(f1/CMC1) + (f2/CMC2)] where f1 and f2 are the fractions of total selenium that are treated as selenite and selenate, respectively, and CMC1 and CMC2 are 185.9 µg/l and 12.82 µg/l, respectively.
M	EPA is currently reassessing the criteria for arsenic.
N	This criterion applies to total pcbs, (e.g., the sum of all congener or all isomer or homolog or Aroclor analyses.)
O	The derivation of the CCC for this pollutant (Endrin) did not consider exposure through the diet, which is probably important for aquatic life occupying upper trophic levels.
P	Although a new RfD is available in IRIS, the surface water criteria will not be revised until the National Primary Drinking Water Regulations: Stage 2 Disinfectants and Disinfection Byproducts Rule (Stage 2 DBPR) is completed, since public comment on the relative source contribution (RSC) for chloroform is anticipated.
Q	This recommended water quality criterion is expressed as µg free cyanide (as CN)/L.
R	This value for selenium was announced (61FR58444-58449, November 14, 1996) as a proposed GLI 303(c) aquatic life criterion. EPA is currently working on this criterion and so this value might change substantially in the near future.
S	This recommended water quality criterion for arsenic refers to the inorganic form only.

Footnote Code	Footnote Description
T	This recommended water quality criterion for selenium is expressed in terms of total recoverable metal in the water column. It is scientifically acceptable to use the conversion factor (0.996- CMC or 0.922- CCC) that was used in the GLI to convert this to a value that is expressed in terms of dissolved metal.
U	The organoleptic effect criterion is more stringent than the value for priority toxic pollutants.
V	This value was derived from data for heptachlor and the criteria document provides insufficient data to estimate the relative toxicities of heptachlor and heptachlor epoxide.
W	Although EPA has not published a completed criteria document for butylbenzyl phthalate it is EPA's understanding that sufficient data exist to allow calculation of aquatic criteria. It is anticipated that industry intends to publish in the peer reviewed literature draft aquatic life criteria generated in accordance with EPA Guidelines. EPA will review such criteria for possible issuance as national WQC.
X	There is a full set of aquatic life toxicity data that show that DEHP is not toxic to aquatic organisms at or below its solubility limit.
Y	This value was derived from data for endosulfan and is most appropriately applied to the sum of alpha-endosulfan and beta-endosulfan.
Z	A more stringent MCL has been issued by EPA. Refer to drinking water regulations (40 CFR 141) or Safe Drinking Water Hotline (1-800-426-4791) for values.
aa	This criterion is based on a 304(a) aquatic life criterion issued in 1980 or 1986, and was issued in one of the following documents: Aldrin/Dieldrin (EPA 440/5-80-019), Chlordane (EPA 440/5-80-027), DDT (EPA 440/5-80- 038), Endrin (EPA 440/5-80-047), Heptachlor (EPA 440/5-80-052), Polychlorinated biphenyls (EPA 440/5-80-068), Toxaphene (EPA 440/5-86-006). This CCC is currently based on the Final Residue Value (FRV) procedure. Since the publication of the Great Lakes Aquatic Life Criteria Guidelines in 1995 (60FR15393-15399, March 23, 1995), the Agency no longer uses the Final Residue Value procedure for deriving CCCs for new or revised 304(a) aquatic life criteria. Therefore, the Agency anticipates that future revisions of this CCC will not be based on the FRV procedure.
bb	This water quality criterion is based on a 304(a) aquatic life criterion that was derived using the 1985 Guidelines (*Guidelines for Deriving Numerical National Water Quality Criteria for the Protection of Aquatic Organisms and Their Uses*, PB85-227049, January 1985) and was issued in one of the following criteria documents: Arsenic (EPA 440/5-84-033), Cadmium (EPA 882-R-01-001), Chromium (EPA 440/5-84-029), Copper (EPA 440/5-84-031), Cyanide (EPA 440/5- 84-028), Lead (EPA 440/5-84-027), Nickel (EPA 440/5-86-004), Pentachlorophenol (EPA 440/5-86-009), Toxaphene, (EPA 440/5-86-006), Zinc (EPA 440/5-87- 003).
cc	When the concentration of dissolved organic carbon is elevated, copper is substantially less toxic and use of Water-Effect Ratios might be appropriate.
dd	The selenium criteria document (EPA 440/5-87-006, September 1987) provides that if selenium is as toxic to saltwater fishes in the field as it is to freshwater fishes in the field, the status of the fish community should be monitored whenever the concentration of selenium exceeds 5.0 µg/L in salt water because the saltwater CCC does not take into account uptake via the food chain.
ee	This recommended water quality criterion was derived on page 43 of the mercury criteria document (EPA 440/5- 84-026, January 1985). The saltwater CCC of 0.025 ug/L given on page 23 of the criteria document is based on the Final Residue Value procedure in the 1985 Guidelines. Since the publication of the Great Lakes Aquatic Life Criteria Guidelines in 1995 (60FR15393-15399, March 23, 1995), the Agency no longer uses the Final Residue Value procedure for deriving CCCs for new or revised 304(a) aquatic life criteria.
ff	This recommended water quality criterion was derived in *Ambient Water Quality Criteria Saltwater Copper Addendum* (Draft, April 14, 1995) and was promulgated in the Interim final National Toxics Rule (60FR22228- 222237, May 4, 1995).
gg	EPA is actively working on this criterion and so this recommended water quality criterion may change substantially in the near future.
hh	This recommended water quality criterion was derived from data for inorganic mercury (II), but is applied here to total mercury. If a substantial portion of the mercury in the water column is methylmercury, this criterion will probably be under protective. In addition, even though inorganic mercury is converted to methylmercury and methylmercury bioaccumulates to a great extent, this criterion does not account for uptake via the food chain because sufficient data were not available when the criterion was derived.
ii	This criterion applies to DDT and its metabolites (i.e., the total concentration of DDT and its metabolites should not exceed this value).
F2	The derivation of this value is presented in the Red Book (EPA 440/9-76-023, July, 1976).
G2	This value is based on a 304(a) aquatic life criterion that was derived using the 1985 Guidelines (*Guidelines for Deriving Numerical National Water Quality Criteria for the Protection of Aquatic Organisms and Their Uses*, PB85-227049, January 1985) and was issued in one of the following criteria documents: Aluminum (EPA 440/5-86-008); Chloride (EPA 440/5-88-001); Chloropyrifos (EPA 440/5-86-005).
I2	This value for aluminum is expressed in terms of total recoverable metal in the water column.
L2	There are three major reasons why the use of Water-Effect Ratios might be appropriate. (1) The value of 87 µg/l is based on a toxicity test with the striped bass in water with pH= 6.5-6.6 and hardness <10 mg/L. Data in "Aluminum Water-Effect Ratio for the 3M Plant Effluent Discharge, Middleway, West Virginia" (May 1994) indicate that aluminum is substantially less toxic at higher pH and hardness, but the effects of pH and hardness are not well quantified at this time. (2) In tests with the brook trout at low pH and hardness, effects increased with increasing concentrations of total aluminum even though the concentration of dissolved aluminum was constant, indicating that total recoverable is a more appropriate measurement than dissolved, at least when particulate aluminum is primarily aluminum hydroxide particles. In surface waters, however, the total recoverable procedure might measure aluminum associated with clay particles, which might be less toxic than aluminum associated with aluminum hydroxide. (3) EPA is aware of field data indicating that many high quality waters in the U.S. contain more than 87 µg aluminum/L, when either total recoverable or dissolved is measured.

Footnote Code	Footnote Description
jj	Freshwater criteria are pH, temperature, and life stage dependent. See calculation of freshwater ammonia criterion listed below. Also, see: http://www.epa.gov/ostwater/criteria/ammonia/technical.html.
kk	Saltwater criteria are pH and temperature dependent. See table below. See: http://www.epa.gov/ostwater/criteria/ammonia/technical.html
ll	The ambient aquatic water quality criteria for tributyltin oxide was obtained by dividing the ambient aquatic water criteria for tributyltin by 0.9477 to reflect the percent tributyltin in tributyltin oxide. See the *Ambient Aquatic Life Water Quality Criteria for Tributyltin (TBT) - Final* (EPA, December 2003, EPA 822-R-03-031).
nn	See below for asbestos air migration pathway cancer risk screening concentration calculation.

Conversion Factors for Dissolved Metals				
Metal	**Conversion Factor Freshwater CMC**	**Conversion Factor Freshwater CCC**	**Conversion Factor Saltwater CMC**	**Conversion Factor Saltwater CMC**
Arsenic	1.000	1.000	1.000	1.000
Cadmium	1.136672-[(ln hardness)(0.041838)]	1.101672-[(ln hardness)(0.041838)]	0.994	0.994
ChromiumIII	0.316	0.860	--	--
Chromium VI	0.982	0.962	0.993	0.993
Copper	0.960	0.960	0.83	0.83
Lead	1.46203-[(ln hardness)(0.145712)]	1.46203-[ln hardness)(0.145712)]	0.951	0.951
Mercury	0.85	0.85	0.85	0.85
Nickel	0.998	0.997	0.990	0.990
Selenium	--	--	0.998	0.998
Silver	0.85	--	0.85	--
Zinc	0.978	0.986	0.946	0.946

Parameters for Calculating Freshwater Dissolved Metals That are Hardness Dependent						
					Conversion Factors (CF)	
Chemical	m_A	b_A	m_C	b_C	**CMC**	**CCC**
Cadmium	1.0166	-3.924	0.7409	-4.719	1.136672-[(ln hardness)(0.041838)]	1.101672-[(ln hardness)(0.041838)]
Chromium III	0.8190	3.7256	0.8190	0.6848	0.316	0.860
Copper	0.9422	-1.700	0.8545	-1.702	0.960	0.960
Lead	1.273	-1.460	1.273	-4.705	1.46203-[(ln hardness)(0.145712)]	1.46203-[(ln hardness)(0.145712)]
Nickel	0.8460	2.255	0.8460	0.0584	0.998	0.997
Silver	1.72	-6.59	--	--	0.85	--
Zinc	0.8473	0.884	0.8473	0.884	0.978	0.986

Hardness-dependent metals' criteria may be calculated from the following:

CMC (dissolved) = exp $\{m_A [\ln(\text{hardness})] + b_A\}$ (CF)

CCC (dissolved) = exp $\{m_C [\ln(\text{hardness})] + b_C\}$ (CF)

Calculation of Freshwater Ammonia Criterion

1. The one-hour average concentration of total ammonia nitrogen (in mg N/L) does not exceed, more than once every three years on the average, the CMC (acute criterion) calculated using the following equations:

Where salmonid fish are present:

CMC = (0.275/(1 + 107.204-pH)) + (39.0/(1 + 10pH-7.204))

Or where salmonid fish are not present:

CMC = (0.411/(1 + 107.204-pH)) + (58.4/(1 + 10pH-7.204))

2A. The thirty-day average concentration of total ammonia nitrogen (in mg N/L) does not exceed, more than once every three years on theaverage, the CCC (chronic criterion) calculated using the following equations:

When fish early life stages are present:

CCC = ((0.0577/(1 + 107.688-pH)) + (2.487/(1 + 10pH-7.688))) x MIN (2.85, 1.45·100.028·(25-T))

When fish early life stages are absent:

CCC = ((0.0577/(1 + 107.688-pH)) + (2.487/(1 + 10pH-7.688))) x 1.45·100.028·(25-MAX(T,7))

2B. In addition, the highest four-day average within the 30-day period should not exceed 2.5 times the CCC.

Asbestos Air Migration Pathway Cancer Risk Screening Concentration Calculation:

$$\text{Action Level for Asbestos in Air (f/cc)} = \frac{\text{Target Risk}}{[\text{IUR} \bullet \text{TWF}]}$$

$$\text{Action Level for Asbestos in Air (f/cc)} = 1\text{x}10^{-6} \div [0.23\ (\text{f/cc})^{-1} \text{ x } 0.96]$$
$$= 0.0000045 \text{ f/cc or} \sim 4.5 \text{ x } 10^{-6} \text{ f/cc}$$

Where:
Target Risk = 10^{-6}
IUR = Inhalation Unit Risk = 0.23
TWF = Time Weighting Factor = 350/365 = 0.96
f/cc = fibers per cubic centimeter