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SECONDARY VALUES FOR PROMETON (CAS No. 1610-18-0)

A search was conducted for information on the chemical properties and toxicity of prometon to human health and to fish and aquatic life using the following databases and search engines: ECOTOX (toxicity to fish and aquatic life), IRIS (Integrated Risk Information System; toxicity to human health), CHEMFATE (environmental fate), BIODEG (degradation), HSDB (Hazardous Substances Data Bank), CCRIS (Chemical Carcinogenesis Research Info System), ATSDR ToxFAQs (Agency for Toxic Substances and Disease Registry chemical fact sheets), and EXTOXNET (Extension Toxicology Network's pesticide information project). This search yielded some useful information on prometon's properties and toxicity.

Fish and Aquatic Life Secondary Values

To derive an acute toxicity criterion for fish and aquatic life, acute toxicity test results are required for at least one species in each of eight different families. Specific requirements and the data available to meet these requirements are found in Table 1. Following a search for information on the toxicity of prometon to fish and other aquatic life, it was determined that data are available to meet four out of the eight requirements. Because data are available for a Daphnid species, it was possible to calculate a secondary acute value for prometon.

Cold Water

To calculate a secondary acute value (SAV), the lowest genus mean acute value (GMAV) in the database is divided by the secondary acute factor (SAF; an adjustment factor corresponding to the number of satisfied requirements).

SAF for four out of eight requirements met = 7.0
Lowest GMAV = 12,000 µg/L (*Poecilia reticulata*)

SAV = GMAV/SAF
= 12,000 µg/L / 7.0
= 1,714.29 µg/L

There are currently no chronic data available for prometon which meet acceptability requirements. Therefore, a secondary chronic value (SCV) may be calculated using default acute-chronic ratios only.

SACR (secondary acute-chronic ratio) = Geometric mean of three species mean acute-chronic ratios (SMACRs).

SMACR 1 = 18
SMACR 2 = 18 (default)

SMACR 3 = 18 (default)

SACR = geometric mean of 18, 18, and 18 = 18

SCV = SAV/SACR
= 1,714.29 µg/L / 18
= 95.24 µg/L

So for cold water-designated waters, the secondary acute value is 1,714 µg/L and the secondary chronic value is 95 µg/L for prometon.

Warm Water Sportfish

Because the lowest GMAV in the cold water database is for *Poecilia reticulata* (guppy), and because this species will not drop out of the databases for warm water sportfish-designated waters, secondary values calculated for cold water designated waters will apply for warm water sportfish-designated waters as well.

Warm Water Forage Fish

Cold water fish and all game fish drop out of the database when calculating secondary values for warm water forage fish-designated waters.

SAF for four out of eight requirements met = 7.0
Lowest GMAV = 38,797.70 µg/L (*Daphnia magna*)

SAV = GMAV/SAF
= 38,797.70 µg/L / 7.0
= 5,542.53 µg/L

SCV = SAV/SACR
= 5,542.53 µg/L / 18
= 307.92 µg/L

So for warm water forage fish-designated waters, the secondary acute value is 5,542 µg/L and the secondary chronic value is 308 µg/L for prometon.

Limited Forage Fish and Limited Aquatic Life

Because the lowest GMAV in the warm water forage fish database is for *Daphnia magna*, and because *Daphnia magna* will not drop out of the database for any of the remaining water body use classifications, secondary values calculated for warm water forage fish-designated waters will also apply for limited forage fish and limited aquatic life-designated waters.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for prometon, and corresponding acute toxicity data.

Species Name	Common Name	Duration/ Endpoint	Value µg/L	Reference #[a]	Source
1. At least one salmonid fish in the family Salmonidae, in the class Osteichthyes.					
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**12,000**	**1**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**12,000**	**2**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**16,000**	**3**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**20,000**	**3**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**19,600**	**3**	**AQUIRE**
Species Mean Acute Value (SMAV) = 15,529.37					
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warmwater species.					
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**40,000**	**1**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**15,500**	**3**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**41,500**	**3**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**>32,000**	**3**	**AQUIRE**
SMAV = 30,122.95					
Ameiurus melas	**black bullhead**	**96-h/LC50**	**20,000**	**2**	**AQUIRE**
SMAV = 20,000					
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Daphnia magna	**water flea**	**48-h/EC50**	**38,000**	**4**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**59,800**	**3**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**25,700**	**3**	**AQUIRE**
SMAV = 38,797.70					
4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).					

5. At least one insect (e.g., mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge).

6. At least one fish or amphibian from a family in the phylum Chordata not already represented in one of the other subdivisions.

Poecilia reticulata	**guppy**	**96-h/LC50**	**12,000**	**1**	**AQUIRE**
Poecilia reticulata	**guppy**	**96-h/LC50**	**12,000**	**2**	**AQUIRE**

SMAV = 12,000

7. At least one organism from a family in a phylum other than Arthropoda or Chordata (e.g., Rotifera, Annelida, Mollusca).

8. At least one organism from a family in any order of insect or any other phylum not already represented in subdivisions 1 through 7.

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[1]Bathe, R., L. Ullmann, and K. Sachsse. 1973. Determination of pesticide toxicity to fish. Schriftenr. Ver. Wasser-Boden-Lufthyg. Berlin-Dahlem 37:241-256.

[2]Bathe, R., K. Sachsse, L. Ullmann, W.D. Hormann, F. Zak and R. Hess. 1975. The evaluation of fish toxicity in the laboratory. Proc. Eur. Soc. Toxicol. 16:113-124.

[3]Office of Pesticide Programs. 2000. Environmental Effects Database (EEDB). Environmental Fate and Effects Division, U.S. EPA, Washington, D.C.

[4]Marchini, S., L. Passerini, D. Cesareo, and M.L. Tosato. 1988. Herbicidal triazines: Acute toxicity on Daphnia, fish, and plants and analysis of its relationships with structural factors. Ecotoxicology and Environmental Safety 16(2):148-157.

HUMAN HEALTH

To calculate a criteria or secondary value for the protection of human health, it is first necessary to determine if the substance has been shown to be carcinogenic (which will result in the calculation of a human cancer criteria or secondary value) or not (which will result in the calculation of a human threshold criteria or secondary value). The U.S. EPA has not yet classified prometon for its carcinogenicity (EPA's IRIS database). However, because an oral reference dose and a log octanol water partition coefficient are available, a human threshold secondary value can be calculated for prometon.

There are several steps to calculating a human threshold secondary value: 1) calculation of the fraction of freely dissolved chemical; 2) calculation of the "baseline BAF"; 3) calculation of the "human health BAF"; and 4) calculation of the human threshold secondary value.

1) Calculation of the freely-dissolved fraction = f_{fd}

Given a standard dissolved organic carbon (DOC) concentration of 0.000002 Kg/L and a particulate organic carbon (POC) concentration of 0.00000004 Kg/L in water, the equation

$$f_{fd} = 1/\{1 + [(DOC)(K_{ow})/10] + [(POC)(K_{ow})]\}$$

can be reduced to:

$$= 1/\{1 + [(0.00000024\ Kg/L)(K_{ow})]\}$$

A log K_{ow} of 2.99 (K_{ow} of 977.2372) has been published for prometon (National Institutes of Health, Hazardous Substance Database).

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(977.2372)]\}$$

$$= 1/1.000235$$

$$= \mathbf{0.9998}$$

2) Calculation of the baseline BAF

The baseline BAF is calculated according to the equations contained in 40 CFR part 132 (Final Water Quality Guidance for the Great Lakes System), Appendix B, using BAF data that was collected in one of four ways (listed in order of most preferred to least preferred):

a) a measured BAF from a field study
b) a predicted BAF based on field-measured BSAFs
c) a predicted BAF using a laboratory-measured bioconcentration factor (BCF) and a food chain multiplier (FCM)
d) a predicted BAF using a K_{ow} and a FCM

Currently, there are no BAFs, BSAFs, or BCFs available for prometon; therefore, the baseline BAF was calculated using the K_{ow} and a food chain multiplier (method d above).

Given prometon's log K_{ow} of 2.99 (K_{ow} of 977.2372), the FCMs (taken from table B-1 in GLI) are 1.028 for trophic level 3 (warm waters) and 1.007 for trophic level 4 (cold waters).

a) Cold Water

Baseline BAF = (FCM)(Kow)

= (1.007)(977.2372)

= **984.0779**

b) Warm Waters

Baseline BAF = (FCM)(Kow)

= (1.028)(977.2372)

= 1,004.5998

3) Calculation of the human health BAF

a) Cold Water

BAF^{HH}_{TL4} = {[(baseline BAF)(0.044)] + 1} (f_{fd})

where

BAF^{HH}_{TL4} = Human health BAF for trophic level 4 (cold water)

baseline BAF = the baseline BAF (for cold waters) calculated in 2)

0.044 = fraction lipid value for cold water fish and aquatic life communities

f_{fd} = fraction freely dissolved

BAF^{HH}_{TL4} = {[(**984.0779)**(0.044)] + 1} (0.9998)

= **44.2906**

b) Warm Waters

BAF^{HH}_{TL3} = {[(baseline BAF)(0.013)] + 1} (f_{fd})

where

BAF^{HH}_{TL3} = Human health BAF for trophic level 3 (warm waters)

baseline BAF = the baseline BAF (for warm waters) calculated in 2)

0.013 = fraction lipid value for warm water fish and aquatic life communities

f_{fd} = fraction freely dissolved

BAF^{HH}_{TL3} = {[(**1,004.5998**)(0.013)] + 1} (0.9998)

= **14.0570**

4) Calculation of the human threshold secondary value

Human Threshold Secondary Value = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

where

ADE = acceptable daily exposure (= oral reference dose, or RfD; = 0.015 mg/Kg/day for prometon (IRIS 2003))

70 Kg = average weight of an adult

RSC = relative source contribution to account for other routes of exposure (= 0.8 in the absence of other data)

W_H = average per capita daily water consumption (= 2 L/d for public water supplies, and 0.01 L/d for non-public water supplies)

F_H = average consumption of sport-caught fish in Wisconsin (= 0.02 Kg/d)

BAF = appropriate (cold or warm) human health BAF calculated in 3).

a) Public Water Supply/Cold Water

Human Threshold Secondary Value = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.015 mg/Kg/d)(70 Kg)(0.8)]/[**2** L/d + (0.02 Kg/d)(44.2906 L/Kg)]

= 0.2911 mg/L

= 291.1 µg/L

b) Public Water Supply/Warm Water Sportfish

Human Threshold Secondary Value = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.015 mg/Kg/d)(70 Kg)(0.8)]/[**2** L/d + (0.02 Kg/d)(14.0570 L/Kg)]

= 0.3682 mg/L

= 368.2 µg/L

c) Non-Public Water Supply/Cold Water

Human Threshold Secondary Value = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.015 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0.02 Kg/d)(44.2906 L/Kg)]

= 0.9377 mg/L

= 937.7 µg/L

d) Non-Public Water Supply/Warm Waters (Warm Water Sportfish, Warm Water Forage Fish, and Limited Forage Fish designated waters)

Human Threshold Secondary Value = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.015 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0.02 Kg/d)(14.0570 L/Kg)]

= 2.8856 mg/L

= 2,885.6 µg/L

e) Non-Public Water Supply/Limited Aquatic Life

Note: The Limited Aquatic Life classification applies to water bodies with no (or very few) fish present. Therefore, calculation of a human health threshold value for water bodies with this classification does not include a human health BAF since it is assumed that humans will not be exposed to prometon through consumption of fish in these areas.

Human Threshold Secondary Value = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.015 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0)]

= **84** mg/L

= **84,000 µg/L**

Chemical	CAS #	Category	Type of Secondary Value	Water Body Classification	Value (µg/L)
Prometon	1610-18-0	Fish and Aquatic	Acute	Cold/WWSF	1,714
Prometon	1610-18-0	Fish and Aquatic	Chronic	Cold/WWSF	95
Prometon	1610-18-0	Fish and Aquatic	Acute	WWFF, LFF, LAL	5,542
Prometon	1610-18-0	Fish and Aquatic	Chronic	WWFF, LFF, LAL	308
Prometon	1610-18-0	Human Health	Human Threshold	Public Water Supply/Cold	291
Prometon	1610-18-0	Human Health	Human Threshold	Public Water Supply/WWSF	368
Prometon	1610-18-0	Human Health	Human Threshold	Non-Public Water Supply/Cold	938
Prometon	1610-18-0	Human Health	Human Threshold	Non-Public Water Supply/WWSF, WWFF, LFF	2,886
Prometon	1610-18-0	Human Health	Human Threshold	Non-Public Water Supply/LAL	84,000

Cold = cold water designated water bodies
WWSF = warm water sportfish designated water bodies
WWFF = warm water forage fish designated water bodies
LFF = limited forage fish designated water bodies
LAL = limited aquatic life designated water bodies (includes wetlands)