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## SECONDARY VALUES FOR PROPAZINE (CAS No. 139-40-2)

A search was conducted for information on the chemical properties and toxicity of propazine 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 EXTTOXNET (Extension Toxicology Network's pesticide information project). This search yielded some useful information on propazine'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 propazine to fish and other aquatic life, it was determined that data are available to meet only one out of the eight requirements. However, because data are available for a Daphnid species, it was still possible to calculate a secondary acute value for propazine.

### 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 one out of eight requirements met = 21.9  
Lowest GMAV = 7,649.84 µg/L (*Daphnia magna*)

$$\begin{aligned}\text{SAV} &= \text{GMAV}/\text{SAF} \\ &= 7,649.84 \text{ µg/L} / 21.9 \\ &= \mathbf{349.31 \text{ µg/L}}\end{aligned}$$

There are currently no chronic data available for propazine 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 (default)

SMACR 2 = 18 (default)

SMACR 3 = 18 (default)

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

**SCV** = SAV/SACR

= 349.31 µg/L / 18

= **19.41 µg/L**

**So for cold water-designated waters, the secondary acute value is 349 µg/L and the secondary chronic value is 19 µg/L for propazine.**

Warm Water Sportfish, Warm Water Forage Fish, Limited Forage Fish, and Limited Aquatic Life

Because the lowest (and the only) GMAV in the cold water database is for *Daphnia magna*, an invertebrate species that will not drop out of the database for any of the remaining water body use designations, secondary values calculated for cold water designated waters will apply for warm water sportfish, warm water forage fish, limited forage fish and limited aquatic life-designated waters as well.

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

Species Name	Common Name	Duration/ Endpoint	Value µg/L	Reference # <sup>a</sup>	Source
1. At least one salmonid fish in the family Salmonidae, in the class Osteichthyes.					
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warmwater species.					
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
<i>Daphnia magna</i>	<b>water flea</b>	<b>48-h/EC50</b>	<b>11,000</b>	<b>1</b>	<b>AQUIRE</b>
<i>Daphnia magna</i> SMAV = 7,649.84	<b>water flea</b>	<b>48-h/EC50</b>	<b>&gt;5,320</b>	<b>2</b>	<b>AQUIRE</b>
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.					
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.					

<sup>1</sup>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.

<sup>2</sup>Office of Pesticide Programs. 2000. Environmental Effects Database (EEDB). Environmental Fate and Effects Division, U.S. EPA, Washington, D.C.

## 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 classified propazine as a class C carcinogen (possible human carcinogen) (EXTOXNET database); however it has not yet established a cancer slope factor (IRIS database). Because an oral reference dose and a log octanol water partition coefficient are available, however, it is possible to calculate a secondary threshold value for propazine.

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:

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

A log  $K_{ow}$  of 2.93 ( $K_{ow}$  of 851.1380) has been published for propazine (National Institutes of Health, Hazardous Substance Database).

$$f_{fd} = 1 / \{ 1 + [(0.00000024 \text{ Kg/L})(851.1380)] \}$$

$$= 1 / 1.000204$$

$$= \mathbf{0.9998}$$

### **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 propazine; therefore, the baseline BAF was calculated using the  $K_{ow}$  and a food chain multiplier (method d above).

Given propazine's log  $K_{ow}$  of 2.93 ( $K_{ow}$  of 851.1380), 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

$$\begin{aligned} \text{Baseline BAF} &= (\text{FCM})(K_{ow}) \\ &= (1.007)(851.1380) \\ &= \mathbf{857.0960} \end{aligned}$$

b) Warm Waters

$$\begin{aligned} \text{Baseline BAF} &= (\text{FCM})(K_{ow}) \\ &= (1.028)(851.1380) \\ &= \mathbf{874.9699} \end{aligned}$$

### 3) Calculation of the human health BAF

a) Cold Water

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

where

$\text{BAF}_{\text{TL4}}^{\text{HH}}$  = 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

$f_{\text{fd}}$  = fraction freely dissolved

$$\begin{aligned} \text{BAF}_{\text{TL4}}^{\text{HH}} &= \{[(\mathbf{857.0960})(0.044)] + 1\} (0.9998) \\ &= \mathbf{38.7045} \end{aligned}$$

b) Warm Waters

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

where

$BAF_{TL3}^{HH}$  = 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

$$BAF_{TL3}^{HH} = \{[(874.9699)(0.013)] + 1\} (0.9998)$$
$$= \mathbf{12.3721}$$

#### 4) Calculation of the human threshold secondary value

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

where

ADE = acceptable daily exposure (= oral reference dose, or RfD; = 0.02 mg/Kg/day for propazine (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

$$\text{Human Threshold Secondary Value} = [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)]$$
$$= [(0.02 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[2 \text{ L/d} + (0.02 \text{ Kg/d})(38.7045 \text{ L/Kg})]$$
$$= 0.4037 \text{ mg/L}$$
$$= \mathbf{403.7 \mu\text{g/L}}$$

**b) Public Water Supply/Warm Water Sportfish**

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.02 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[2 \text{ L/d} + (0.02 \text{ Kg/d})(12.3721 \text{ L/Kg})] \\ &= 0.4983 \text{ mg/L} \\ &= \mathbf{498.3 \text{ }\mu\text{g/L}}\end{aligned}$$

**c) Non-Public Water Supply/Cold Water**

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.02 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0.02 \text{ Kg/d})(38.7045 \text{ L/Kg})] \\ &= \mathbf{1.4284 \text{ mg/L}} \\ &= \mathbf{1,428.4 \text{ }\mu\text{g/L}}\end{aligned}$$

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

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.02 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0.02 \text{ Kg/d})(12.3721 \text{ L/Kg})] \\ &= \mathbf{4.3512 \text{ mg/L}} \\ &= \mathbf{4,351.2 \text{ }\mu\text{g/L}}\end{aligned}$$

**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 propazine through consumption of fish in these areas.

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.02 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0)]\end{aligned}$$

= **112 mg/L**

= **112,000 µg/L**



<b>Chemical</b>	<b>CAS #</b>	<b>Category</b>	<b>Type of Secondary Value</b>	<b>Water Body Classification</b>	<b>Value (µg/L)</b>
Propazine	139-40-2	Fish and Aquatic	Acute	Cold/WWSF/WWFF/ LFF/LAL	349
Propazine	139-40-2	Fish and Aquatic	Chronic	Cold/WWSF/WWFF/ LFF/LAL	19
Propazine	139-40-2	Human Health	Human Threshold*	Public Water Supply/Cold	404
Propazine	139-40-2	Human Health	Human Threshold*	Public Water Supply/WWSF	498
Propazine	139-40-2	Human Health	Human Threshold*	Non-Public Water Supply/Cold	1,428
Propazine	139-40-2	Human Health	Human Threshold*	Non-Public Water Supply/WWSF, WWFF, LFF	4,351
Propazine	139-40-2	Human Health	Human Threshold*	Non-Public Water Supply/LAL	112,000

\*This substance has been classified as a Class C carcinogen (possible human carcinogen) by the U.S. EPA.

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)