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## SECONDARY VALUES FOR PENDIMETHALIN (CAS No. 40487-42-1)

A search was conducted for information on the chemical properties and toxicity of pendimethalin 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 pendimethalin'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 pendimethalin to fish and other aquatic life, it was determined that data are available to meet five out of the eight requirements. Because data are available for a Daphnid species, it was possible to calculate a secondary acute value for pendimethalin.

### 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 five out of eight requirements met = 6.1  
Lowest GMAV = 178.14 µg/L (*Oncorhynchus mykiss*)

$$\begin{aligned}\text{SAV} &= \text{GMAV}/\text{SAF} \\ &= 178.14 \text{ µg/L} / 6.1 \\ &= \mathbf{29.20 \text{ µg/L}}\end{aligned}$$

There are currently no chronic data available for pendimethalin 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).

$$\begin{aligned}\text{SMACR 1} &= 18 \\ \text{SMACR 2} &= 18 \text{ (default)}\end{aligned}$$

SMACR 3 = 18 (default)

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

$$\begin{aligned}\text{SCV} &= \text{SAV}/\text{SACR} \\ &= 29.20 \mu\text{g/L} / 18 \\ &= \mathbf{1.62 \mu\text{g/L}}\end{aligned}$$

**So for cold water-designated waters, the secondary acute value is 29  $\mu\text{g/L}$  and the secondary chronic value is 1.6  $\mu\text{g/L}$  for pendimethalin.**

### Warm Water Sportfish

Cold water fish drop out of the database when calculating secondary values for warm water sportfish-designated waters.

SAF for five out of eight requirements met = 6.1  
Lowest GMAV = 575.30  $\mu\text{g/L}$  (*Lepomis macrochirus*)

$$\begin{aligned}\text{SAV} &= \text{GMAV}/\text{SAF} \\ &= 575.30 \mu\text{g/L} / 6.1 \\ &= \mathbf{94.31 \mu\text{g/L}}\end{aligned}$$

$$\begin{aligned}\text{SCV} &= \text{SAV}/\text{SACR} \\ &= 94.31 \mu\text{g/L} / 18 \\ &= \mathbf{5.24 \mu\text{g/L}}\end{aligned}$$

**So for warm water sportfish-designated waters, the secondary acute value is 94  $\mu\text{g/L}$  and the secondary chronic value is 5.2  $\mu\text{g/L}$  for pendimethalin.**

### 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 five out of eight requirements met = 6.1  
Lowest GMAV = 1,000  $\mu\text{g/L}$  (*Procambarus simulans*)

$$\begin{aligned}\text{SAV} &= \text{GMAV}/\text{SAF} \\ &= 1,000 \mu\text{g/L} / 6.1 \\ &= \mathbf{163.93 \mu\text{g/L}}\end{aligned}$$

$$\begin{aligned}\text{SCV} &= \text{SAV}/\text{SACR} \\ &= 163.93 \mu\text{g/L} / 18 \\ &= \mathbf{9.11 \mu\text{g/L}}\end{aligned}$$

**So for warm water forage fish-designated waters, the secondary acute value is 164 µg/L and the secondary chronic value is 9.1 µg/L for pendimethalin.**

Limited Forage Fish and Limited Aquatic Life

**Because the lowest GMAV in the warm water forage fish database is for *Procambarus simulans*, and because *Procambarus simulans* 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 pendimethalin, 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.					
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	>50	1	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	>50	1	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	138	2	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	1,000	2	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	520	2	AQUIRE
All LC50s were used because even though they varied by over 10X, the two lowest had “greater than” signs, suggesting they weren’t as low as 50 ug/L although that’s the number used in calculating the SMAV.					
Species Mean Acute Value (SMAV) = 178.14					
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warmwater species.					
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	199	2	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	1,040	2	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	920	2	AQUIRE
SMAV = 575.30					
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
<i>Daphnia magna</i>	water flea	48-h/EC50	280	2	AQUIRE
<i>Daphnia magna</i>	water flea	48-h/EC50	5,100	2	AQUIRE
Unclear which end of the range is representative, so both values were used to calculate SMAV.					
SMAV = 1,194.99					
4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).					
<i>Procambarus simulans</i>	crayfish	96-h/LC50	>1,000	2	AQUIRE
SMAV = 1,000					

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.  
*Ictalurus punctatus*      **channel catfish**      **96-h/LC50**      **1,900**      **2**      **AQUIRE**  
SMAV = 1,900
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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<sup>1</sup>Kikuchi, M., T. Miyagaki and M. Wakabayashi. 1996. Evaluation of pesticides used in golf links be acute toxicity test on rainbow trout. Bull. Jpn. Soc. Sci. Fish. (Nippon Suisan Gakkaishi) 62(3):414-419.

<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 is currently reviewing carcinogenicity data for pendimethalin (EXTOXNET). However, because an oral reference dose and a log octanol water partition coefficient are available, a human threshold secondary value can be calculated for pendimethalin.

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 5.18 ( $K_{ow}$  of 151,356.1248) has been published for pendimethalin (National Institutes of Health, Hazardous Substance Database).

$$f_{fd} = 1 / \{ 1 + [(0.00000024 \text{ Kg/L})(151,356.1248)] \}$$

$$= 1/1.036325$$

$$= \mathbf{0.9649}$$

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

Given pendimethalin's log  $K_{ow}$  of 5.18 ( $K_{ow}$  of 151,356.1248), the FCMs (taken from table B-1 in GLI) are 4.188 for trophic level 3 (warm waters) and 3.873 for trophic level 4 (cold waters).

a) Cold Water

$$\begin{aligned} \text{Baseline BAF} &= (\text{FCM})(K_{ow}) \\ &= (3.873)(151,356.1248) \\ &= \mathbf{586,202.2713} \end{aligned}$$

b) Warm Waters

$$\begin{aligned} \text{Baseline BAF} &= (\text{FCM})(K_{ow}) \\ &= (4.188)(151,356.1248) \\ &= \mathbf{633,879.4507} \end{aligned}$$

### 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

$$\begin{aligned} \text{BAF}_{\text{TL4}}^{\text{HH}} &= \{[(\mathbf{586,202.2713})(0.044)] + 1\} (0.9649) \\ &= \mathbf{24,888.5340} \end{aligned}$$

b) Warm Waters

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



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

$$\begin{aligned} BAF^{HH}_{TL3} &= \{[(633,879.4507)(0.013)] + 1\} (0.9649) \\ &= 7,952.1586 \end{aligned}$$

#### 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; = 0.04 mg/Kg/day for pendimethalin (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

$$\begin{aligned} \text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.04 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[2 \text{ L/d} + (0.02 \text{ Kg/d})(24,888.5340 \text{ L/Kg})] \\ &= 0.0045 \text{ mg/L} \\ &= 4.5 \text{ } \mu\text{g/L} \end{aligned}$$

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

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.04 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[2 \text{ L/d} + (0.02 \text{ Kg/d})(7,952.1586 \text{ L/Kg})] \\ &= 0.0139 \text{ mg/L} \\ &= \mathbf{13.9 \mu\text{g/L}}\end{aligned}$$

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

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.04 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0.02 \text{ Kg/d})(24,888.5340 \text{ L/Kg})] \\ &= \mathbf{0.0045 \text{ mg/L}} \\ &= \mathbf{4.5 \mu\text{g/L}}\end{aligned}$$

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

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.04 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0.02 \text{ Kg/d})(7,952.1586 \text{ L/Kg})] \\ &= \mathbf{0.0141 \text{ mg/L}} \\ &= \mathbf{14.1 \mu\text{g/L}}\end{aligned}$$

**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 pendimethalin through consumption of fish in these areas.

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

$$= [(0.04 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0)]$$

$$= 224 \text{ mg/L}$$

$$= 224,000 \text{ } \mu\text{g/L}$$

Chemical	CAS #	Category	Type of Secondary Value	Water Body Classification	Value (µg/L)
Pendimethalin	40487-42-1	Fish and Aquatic	Acute	Cold	29
Pendimethalin	40487-42-1	Fish and Aquatic	Chronic	Cold	1.6
Pendimethalin	40487-42-1	Fish and Aquatic	Acute	WWSF	94
Pendimethalin	40487-42-1	Fish and Aquatic	Chronic	WWSF	5.2
Pendimethalin	40487-42-1	Fish and Aquatic	Acute	WWFF, LFF, LAL	164
Pendimethalin	40487-42-1	Fish and Aquatic	Chronic	WWFF, LFF, LAL	9.1
Pendimethalin	40487-42-1	Human Health	Human Threshold	Public Water Supply/Cold	4.5
Pendimethalin	40487-42-1	Human Health	Human Threshold	Public Water Supply/WWSF	13.9
Pendimethalin	40487-42-1	Human Health	Human Threshold	Non-Public Water Supply/Cold	4.5
Pendimethalin	40487-42-1	Human Health	Human Threshold	Non-Public Water Supply/WWSF, WWFF, LFF	14.1
Pendimethalin	40487-42-1	Human Health	Human Threshold	Non-Public Water Supply/LAL	224,000

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)