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SECONDARY VALUES FOR BENTAZON (CAS No. 25057-89-0)

A search was conducted for information on the chemical properties and toxicity of bentazon 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 bentazon'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 bentazon 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 bentazon.

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 = 113,697.45 µg/L (*Oncorhynchus mykiss*)

SAV = GMAV/SAF
= 113,697.45 µg/L / 7.0
= 16,242.49 µg/L

No chronic data are currently available for bentazon which meet acceptability requirements; therefore, a secondary chronic value (SCV) may be calculated using default 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
= 16,242.49 µg/L / 18
= 902.36 µg/L

So for cold water designated waters, the secondary acute value is 16,242 µg/L and the secondary chronic value is 902 µg/L for bentazon.

Warm Water Sportfish

The salmonid category drops out of the database when calculating secondary values for warm water sportfish designated waters.

SAF for four out of eight requirements met = 7.0
Lowest GMAV = 158,740.11 µg/L (*Daphnia magna*)

SAV = GMAV/SAF
= 158,740.11 µg/L / 7.0
= 22,677.16 µg/L

SCV = SAV/SACR
= 22,677.16 µg/L / 18
= 1,259.84 µg/L

So for warm water sportfish designated waters, the secondary acute value is 22,677 µg/L and the secondary chronic value is 1,260 µg/L for bentazon.

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

Because the lowest GMAV 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 sportfish designated waters will also apply for warm water forage fish, 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 bentazon, 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**	**>100,000**	**1**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>100,000**	**1**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>100,000**	**1**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**190,000**	**1**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>100,000**	**1**	**AQUIRE**
Species Mean Acute Value (SMAV) = 113,697.45					
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**	**>100,000**	**1**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**>100,000**	**1**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**610,000**	**1**	**AQUIRE**
SMAV = 182,716.01					
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Daphnia magna	**water flea**	**48-h/EC50**	**64,000**	**1**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**>125,000**	**1**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**>500,000**	**1**	**AQUIRE**
SMAV = 158,740.11					
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.					
Cyprinus carpio	**common carp**	**96-h/LC50**	**978,000**	**2**	**AQUIRE**

Gambusia affinis	**Western mosquitofish**	**96-h/LC50**	**3,874,000**	**3**	**AQUIRE**

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

[2]Sun, F. 1987. Evaluating acute toxicity of pesticides to aquatic organisms: carp, mosquito fish and daphnids. Plant Prot. Bull./Chih Wu Pao Hu Hsueh Hui Hui K'an 29(4):385-396.

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). Bentazon has been classified a Group E chemical, with evidence on non-carcinogenicicty for humans (U.S. EPA's IRIS database). Because an oral reference dose and a log octanol water partition coefficient are available, a human threshold secondary value can be calculated for bentazon.

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:

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

For bentazon, a log K_{ow} of 2.80 (K_{ow} of 630.9573) has been published (National Institutes of Health, Hazardous Substance Database).

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(630.9573)]\}$$

$$= 1/1.000151$$

$$= \mathbf{0.9998}$$

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

Given bentazon's log K_{ow} of 2.80 (K_{ow} of 630.9573), the FCMs (taken from table B-1 in GLI) are interpolated to be 1.021 for trophic level 3 (warm waters) and 1.005 for trophic level 4 (cold waters).

a) Cold Water

Baseline BAF = (FCM)(Kow)

= (1.005)(630.9573)

= 634.1121

b) Warm Waters

Baseline BAF = (FCM)(Kow)

= (1.021)(630.9573)

= 644.2074

3) Calculation of the human health BAF

a) Cold Water

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

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

$BAF^{HH}_{TL4} = \{[(634.1121)(0.044)] + 1\} (0.9998)$

= **28.8951**

b) Warm Waters

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

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} = {[(644.2074)(0.013)] + 1} (0.9998)

= **9.3728**

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; = 0.03 mg/Kg/day for bentazon (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 = human health BAF calculated in 3).

a) Public Water Supply/Cold Water

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

= [(0.03 mg/Kg/d)(70 Kg)(0.8)]/[**2** L/d + (0.02 Kg/d)(28.8951 L/Kg)]

= 0.6517 mg/L

= 651.7 µg/L

b) Public Water Supply/Warm Water Sportfish

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

= [(0.03 mg/Kg/d)(70 Kg)(0.8)]/[**2** L/d + (0.02 Kg/d)(9.3728 L/Kg)]

= 0.7680 mg/L

= 768.0 µg/L

c) Non-Public Water Supply/Cold Water

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

= [(0.03 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0.02 Kg/d)(28.8951 L/Kg)]

= 2.8576 mg/L

= 2,857.6 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 = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.03 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0.02 Kg/d)(9.3728 L/Kg)]

= 8.5106 mg/L

= 8,510.6 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 bentazon through consumption of fish in these areas.

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

= [(0.03 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0)]

= **168** mg/L

= **168,000 µg/L**

Chemical	CAS #	Category	Type of Secondary Value	Water Body Classification	Value (µg/L)
Bentazon	25057-89-0	Fish and Aquatic	Acute	Cold	16,242
Bentazon	25057-89-0	Fish and Aquatic	Chronic	Cold	902
Bentazon	25057-89-0	Fish and Aquatic	Acute	WWSF, WWFF, LFF, LAL	22,677
Bentazon	25057-89-0	Fish and Aquatic	Chronic	WWSF, WWFF, LFF, LAL	1260
Bentazon	25057-89-0	Human Health	Human Threshold	Public Water Supply/Cold	652
Bentazon	25057-89-0	Human Health	Human Threshold	Public Water Supply/WWSF	768
Bentazon	25057-89-0	Human Health	Human Threshold	Non-Public Water Supply/Cold	2,858
Bentazon	25057-89-0	Human Health	Human Threshold	Non-Public Water Supply/WWSF, WWFF, LFF	8,511
Bentazon	25057-89-0	Human Health	Human Threshold	Non-Public Water Supply/LAL	168,000

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)