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SECONDARY VALUES FOR 1,4-DIOXANE (CAS # 123-91-1)

A search was conducted for information on the chemical properties and toxicity of 1,4-dioxane (to human health and to fish and aquatic life) using the following databases: ECOTOX (toxicity to fish and aquatic life), IRIS (Integrated Risk Information System; toxicity to human health), CHEMFATE (environmental fate) and ChemFinder (chemical properties and links).

FISH AND AQUATIC LIFE

To calculate an acute toxicity criterion for 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 an extensive search, it was determined that data are available to meet three of the eight requirements. Because there are no acceptable data available for at least one of the three genera in the family Daphnidae (*Ceriodaphnia* sp., *Daphnia* sp., or *Simocephalus* sp.), it is not possible to calculate secondary acute and chronic values for 1,4-dioxane at this time.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for 1,4-dioxane, and corresponding acute toxicity data.

Species Name	Common Name	Duration/ Endpoint	Value µg/L	Reference #	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 warm water species.					
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**>10,000,000**	**2**	**ECOTOX**
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).					
Gammarus pseudolimnaeus	**scud**	**96-h/LC50**	**2,274,000**	**1**	**ECOTOX**
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.					
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**9,872,000**	**1**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**10,800,000**	**3**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**9,850,000**	**3**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**12,326,000**	**1**	**ECOTOX**
Species Mean Acute Value (SMAV) = 10,666,497					
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.					

[1]Brook, L. 1987. Report of the Flow-Through and Static Acute Test Comparisons with Fathead Minnows and Acute Tests with an Amphipod and a Cladoceran. Center for Lake Superior Environ.Stud., Univ.of Wisconsin-Superior, Superior, WI :24 p.

[2]Dawson, G.W., A.L. Jennings, D. Drozdowski, and E. Rider. 1977. The Acute Toxicity of 47 Industrial Chemicals to Fresh and

Saltwater Fishes. J.Hazard.Mater. 1(4):303-318 (OECDG Data File).

[3]Geiger, D.L., L.T. Brooke, and D.J. Call. 1990. Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*). Ctr.for Lake Superior Environ.Stud., Univ.of Wisconsin-Superior, Superior, WI 5:332 p.

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 substance, 1,4-dioxane is currently classified as a B2 carcinogen (probable human carcinogen) by the U.S. EPA (IRIS database, 1990). An oral slope factor is available. No BCFs or BAFs are available, but a BAF can be calculated using the log Kow for this substance. Therefore, it is possible to calculate a human cancer secondary value for 1,4-dioxane.

Oral Reference Dose (RfD)
None available

Carcinogenicity Classification
B2, probable human carcinogen (IRIS; last revised 1990).

Oral Slope Factor (*q1)
1.1×10^{-2} per mg/Kg/day (IRIS; last revised 1990)

Fish Consumption Rate
20 g/d (= 0.02 Kg/d; Ch. NR 105, Wisconsin Administrative Code 1997)

Log K_{ow}
-0.27

K_{ow}
0.5370

There are several steps to calculating a human cancer criterion: 1) calculation of the risk-associated dose (RAD); 2) calculation of the fraction of freely dissolved chemical; 3) calculation of the "baseline BAF"; 4) calculation of the "human health BAF"; and 5) calculation of the human cancer criterion.

1) Calculation of the risk associated dose (RAD)

RAD = (1/*q1)(0.00001)

where

RAD = risk associated dose in milligrams toxicant per kilograms body weight per day (mg/Kg/d)

*q1 = upper 95% confidence limit (one-sided) of the carcinogenic potency factor in milligrams toxicant per kilograms body weight per day (mg/Kg/d) = oral slope factor

0.00001 = incremental risk of human cancer equal to one in 100,000

RAD = (1/0.011 mg/Kg/d)(0.00001)

RAD = 0.0009 mg/Kg/d

2) 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:

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

For 1,4-dioxane, the $K_{ow} = 0.5370$

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(0.5370)]\}$$

$$f_{fd} = 1/1.0000$$

$$f_{fd} = 1.0000$$

3) 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 BCF and a FCM
d) a predicted BAF using a K_{ow} and a FCM

Using the K_{ow} and a FCM:

Baseline BAF = (FCM) (K_{ow})

where
FCM = food chain multiplier, from Table B-1, in 40 CFR Part 132

The FCM will vary depending on whether it is being used for warm water (trophic level 3) or cold water (trophic level 4).

FCM for trophic level 3 = 1.000

FCM for Trophic Level 4 = 1.000

Baseline BAF for warm and cold waters

Baseline BAF = (1.000) (0.5370)

Baseline BAF = 0.5370

4) Calculation of the human health BAF

Because 1,4-dioxane is an organic substance, the appropriate equations for calculating human health BAFs follow.

a) Human health BAF for warm water

Human health BAF_{warm} = {[(baseline BAF_{warm})(0.013)] + 1} (f_{fd})

where

baseline BAF_{warm} = the baseline BAF_{warm} calculated in 3)

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

f_{fd} = fraction freely dissolved

Human health BAF_{warm} = {[(0.5370)(0.013)] + 1} (1.0000)

Human health BAF_{warm} = 1.0070

b) Human health BAF for cold water

Human health BAF_{cold} = {[(baseline BAF_{cold})(0.044)] + 1} (f_{fd})

where

baseline BAF_{cold} = the baseline BAF_{cold} calculated in 3)

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

f_{fd} = fraction freely dissolved

Human health BAF_{cold} = {[(0.5370)(0.044)] + 1} (1.0000)

Human health BAF_{cold} = 1.0236

5) Calculation of the human cancer criterion

Human cancer criterion = (RAD)(70 Kg) / [W_H + (F_H)(BAF)]

where

RAD = risk associated dose in mg/kg/d, as calculated in 1)

70 Kg = average weight of an adult male

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 (warm or cold) human health BAF calculated in 4).

a) Non-Public Water Supply; Limited Aquatic Life

Human cancer criterion = (0.0009)(70 Kg) / [0.01 + (0)]

Note: For limited aquatic life waters, it is assumed that no fish are being caught and consumed.

Human cancer criterion = 6.30 mg/L = 6,300 µg/L

b) Non-Public Water Supply; Warm Water Sport, Warm Water Forage, Limited Forage

Human cancer criterion = (0.0009)(70 Kg) / [0.01 + (0.02)(1.0070)]

Human cancer criterion = 2.0930 mg/L = 2,093 µg/L

c) Non-Public Water Supply; Cold Water

Human cancer criterion = (0.0009)(70 Kg) / [0.01 + (0.02)(1.0236)]

Human cancer criterion = 2.0656 mg/L = 2,066 µg/L

d) Public Water Supply; Warm Water Sport

Human cancer criterion = (0.0009)(70 Kg) / [2 + (0.02)(1.0070)]

Human cancer criterion = 0.0312 mg/L = 31.2 µg/L

e) Public Water Supply; Cold Water

Human cancer criterion = (0.0009)(70 Kg) / [2 + (0.02)(1.0236)]

Human cancer criterion = 0.0312 mg/L = 31.2 μg/L