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SECONDARY VALUES FOR DIBROMOCHLOROMETHANE (CAS No. 124-48-1)

A search was conducted for information on the chemical properties and toxicity of dibromochloromethane 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), and CHEMFATE (environmental fate).

Fish and Aquatic Life Secondary Values

Only 15 records were found in the ECOTOX database, and none of them were for one of the species necessary for calculation of a secondary acute value for fish and aquatic life. Therefore, at this time, it is not possible to calculate acute or chronic secondary values for dibromochloromethane.

Human Health Secondary Values

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). Dibromochloromethane is currently classified as "C", a possible human carcinogen, by the U.S. EPA (IRIS, 2004). The U.S. EPA considers this chemical to be a priority pollutant, and has recommended water quality criteria for the protection of human health. An oral slope factor (IRIS, 2004) is available, and it is possible to calculate a predicted baseline bioaccumulation factor (BAF); therefore, a human cancer secondary value may be calculated for this substance.

There are several steps to calculating a human cancer secondary value: 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 secondary value.

1) Calculation of the Risk Associated Dose (RAD):

$RAD = (1/q_1^*)(0.00001)$

where

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

q_1^* = upper 95% confidence limit (one-sided) of the carcinogenic potency factor in milligrams toxicant per kilograms body weight per day (mg/Kg/day)

= Cancer slope factor

For dibromochloromethane, q_1^* = 0.084 mg/Kg/day (IRIS 2004)

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

RAD = (1/0.084)(0.00001)

= 0.0001 mg/Kg/day

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

For dibromochloromethane, the K_{ow} = 169.8244 and log K_{ow} = 2.23.

$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(169.8244)]\}$

$= 1/1.0000$

= 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; GLI), 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

No field-measured BAFs or BSAFs are available for dibromochloromethane. Therefore, at this time, the baseline BAF will be calculated using a K_{ow} and a food chain multiplier.

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

The FCM is at trophic level 3 for a discharge to a water body classified as warm water, and the FCM is at trophic level 4 for a discharge to a water body classified as cold water. Given dibromochloromethane's log K_{ow} of 2.23, the FCM from the table is 1.005 for trophic level 3 (warm water), and 1.000 for trophic level 4 (cold water).

For warm water:

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

= (1.005)(169.8244)

= 170.6735

For cold water:

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

= (1.000) (169.8244)

= 169.8244

4) Calculation of the Human Health BAF:

Because dibromochloromethane is an organic substance, the equations to use are the following:

For warm water:

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

where

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

baseline BAF = the baseline BAF calculated in 3) for warm water (using the octanol-water partition coefficient method)

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

f_{fd} = fraction freely dissolved

BAF^{HH}_{TL3} = {[(170.6735)(0.013)] + 1} (1.0000)

= 3.2188

For 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 calculated in 3) for cold water (using the octanol-water partition coefficient method)

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

f_{fd} = fraction freely dissolved

BAF^{HH}_{TL4} = {[(169.8244)(0.044)] + 1} (1.0000)

= 8.4723

5) Calculation of the Human Cancer Secondary Value:

Human Cancer Secondary Value = (RAD)(70 Kg)/[W_H + (F_H)(BAF)]

where

RAD = risk associated dose in mg/Kg/day, as calculated in 1)

70 Kg = average weight of an adult

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 DNR (= 0.02 Kg/d)

BAF = human health BAF calculated in 4).

Cold Water, Public Water Supply

Human Cancer Secondary Value = (RAD)(70 Kg)/[W_H + (F_H)(BAF)]

= (0.0001 mg/Kg/d)(70 Kg)/[2 L/d + (0.02 Kg/d)(8.4723 L/Kg)]

= 0.0070/2.1694

= 0.0032 mg/L

= 3.2 μg/L

Warm Waters, Public Water Supply

Human Cancer Secondary Value = (RAD)(70 Kg)/[W_H + (F_H)(BAF)]

= (0.0001 mg/Kg/d)(70 Kg)/[2 L/d + (0.02 Kg/d)(3.2188 L/Kg)]

= 0.0070/2.0644

= 0.0034 mg/L

= 3.4 μg/L

Cold Water, Non-Public Water Supply

Human Cancer Secondary Value = (RAD)(70 Kg)/[W_H + (F_H)(BAF)]

= (0.0001 mg/Kg/d)(70 Kg)/[0.01 L/d + (0.02 Kg/d)(8.4723 L/Kg)]

= 0.0070/0.1794

= 0.0390 mg/L

= 39 μg/L

Warm Water, Non-Public Water Supply

Human Cancer Secondary Value = (RAD)(70 Kg)/[W_H + (F_H)(BAF)]

= (0.0001 mg/Kg/d)(70 Kg)/[0.01 L/d + (0.02 Kg/d)(3.2188 L/Kg)]

= 0.0070/0.0744

= 0.0941 mg/L

= 94.1 μg/L

Limited Aquatic Life, Non-Public Water Supply

Human Cancer Secondary Value = $(RAD)(70\ Kg)/[W_H + (F_H)(BAF)]$

$= (0.0001\ mg/Kg/d)(70\ Kg) / 0.01\ L/d$

$= 0.0070/0.01$

$= 0.7000\ mg/L$

$= 700\ \mu g/L$