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SECONDARY VALUES FOR 2-METHYLNAPHTHALENE (CAS No. 91-57-6)

A search was conducted for information on the chemical properties and toxicity of 2-methylnaphthalene 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

To derive 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 a search for information on the toxicity of 2-methylnaphthalene to fish and other aquatic life, it was determined that data are available to meet two out of the eight requirements. Because data are available for a Daphnid species, it is possible to calculate a secondary acute value for 2-methylnaphthalene.

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 two out of eight requirements met = 13.0

Lowest GMAV = 1456 µg/L (*Oncorhynchus mykiss*)

**SAV** = GMAV/SAF
= 1456/13
**= 112.0**

There are currently no chronic data for 2-methylnaphthalene. Therefore, a secondary chronic value may be calculated only by using default acute-chronic ratios.

SACR = Geometric mean of 18, 18, and 18 = 18

**SCV** = SAV/SACR
= 112.0/18
= **6.222**

Warm Water Sportfish

The rainbow trout drops out of the database.

Lowest GMAV = 1603 μg/L (*Daphnia magna*)

**SAV** = GMAV/SAF
= 1603/13
**= 123.3 μg/L**

**SCV** = SAV/SACR
= 123.3/18
= **6.850 μg/L**

<u>Warm Water Forage Fish, Limited Forage Fish, Limited Aquatic Life</u>

Because the lowest GMAV in the warm water sportfish database is for *Daphnia magna*, an invertebrate, and because this species will not drop out for any of the other use classifications, secondary values for warm water forage fish, limited forage fish and limited aquatic life waters will be the same as for warm water sportfish waters.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for 2-methylnaphthalene, 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 | 1456 | 3 | AQUIRE |
| 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). | | | | | |
| *Daphnia magna* | water flea | 48-h/EC50 | 13 mmol/m3 = 1848.60 µg/L | 2 | AQUIRE |
| *Daphnia magna* | water flea | 48-h/EC50 | 10.5 mmol/m3 = 1493.10 µg/L | 1 | AQUIRE |
| *Daphnia magna* | water flea | 48-h/EC50 | 10.5 mmol/m3 = 1493.10 µg/L | 1 | AQUIRE |
| Species Mean Acute Value (SMAV; geometric mean of LC50 values for this species): | | | 1603.2709 | | |
| 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. | | | | | |

[1]Abernethy, S., A.M. Bobra, W.Y. Shiu, P.G. Wells and D. MacKay. 1986. Acute lethal toxicity of hydrocarbons and chlorinated

hydrocarbons to two planktonic crustaceans: The key role of organism-water partitioning. Aquatic Toxicology 8(3):163-174.
[2]Bobra, A.M., W.Y. Shiu and D. MacKay. 1983. A predictive correlation for the acute toxicity of hydrocarbons and chlorinated hydrocarbons to the water flea (*Daphnia magna*). Chemosphere 12(9-10):1121-1129.
[3]Kennedy, C.J. 1990. Toxicokinetic studies of chlorinated phenols and polycyclic aromatic hydrocarbons in rainbow trout (*Oncorhynchus mykiss*). Ph.D. Dissertation. Simon Fraser University, Canada. 188 pp. Diss. Abstr. Int. B Sci. Eng. 53(1):18 (1992).

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). 2-Methylnaphthalene has not yet been classified as to its carcinogenicity (IRIS, HSDB, CCRIS). However, because there is an oral RfD available, it is possible to calculate a human threshold secondary value for the protection of human health.

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:

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

For 2-methylnaphthalene, the log $K_{ow}$ = 3.86, $K_{ow}$ = 7,244

$$f_{fd} = 1/\{1 + [(0.00000024 \text{ Kg/L})(7{,}244)]\}$$

$$f_{fd} = 1/1.0017$$

$$f_{fd} = 0.9983$$

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

The baseline BAF for 2-methylnaphthalene was calculated using a $K_{ow}$ and a food chain multiplier:

$$\text{Baseline BAF} = (FCM)\ (K_{ow})$$

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.

Log $K_{ow}$ = 3.86
Kow = 7,244
FCM for trophic level 3 = 1.202
FCM for trophic level 4 = 1.054

For warm water:

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

= (1.202)(7,244)

= 8,707

For cold water:

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

= (1.054)(7,244)

= 7,635

**3) Calculation of the human health BAF**

Because 2-methylnaphthalene 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 2)

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

$f_{fd}$ = fraction freely dissolved

Human health $BAF_{warm}$ = {[(8,707)(0.013)] + 1} (0.9983)

Human health $BAF_{warm}$ = 114.0

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 2)

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

$f_{fd}$ = fraction freely dissolved

Human health $BAF_{cold}$ = {[(7,635)(0.044)] + 1} (0.9983)

Human health $BAF_{cold}$ = 336.4

**4) Calculation of the human threshold criterion**

Human threshold criterion = [(ADE)(70 Kg)(RSC)]/[$W_H$ +($F_H$)(BAF)]

where

ADE = acceptable daily exposure in mg/kg/d (= oral reference dose; = 0.004 for 2-methylnaphthalene)

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 (warm or cold) human health BAF calculated in 3).

**a) Non-Public Water Supply; Limited Aquatic Life**

Human threshold criterion = [(0.004 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d +(0)]

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

Human threshold criterion = 22.4 mg/L = 22,400 µg/L

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

Human threshold criterion = [(0.004 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d +(0.02 Kg/d)(114.0)]

Human threshold criterion = 0.0978 mg/L = 97.8 µg/L

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

Human threshold criterion = [(0.004 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d +(0.02 Kg/d)(336.4)]

Human threshold criterion = 0.0332 mg/L = 33.2 µg/L

**d) Public Water Supply; Warm Water Sport**

Human threshold criterion = [(0.004 mg/Kg/d)(70 Kg)(0.8)]/[2 L/d +(0.02 Kg/d)(114.0)]

Human threshold criterion = 0.0523 mg/L = 52.3 µg/L

**e) Public Water Supply; Cold Water**

Human threshold criterion = [(0.004 mg/Kg/d)(70 Kg)(0.8)]/[2 L/d +(0.02 Kg/d)(336.4)]

Human threshold criterion = 0.0257 mg/L = 25.7 µg/L