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SECONDARY VALUES FOR BENZO[A]PYRENE (CAS # 50-32-8)

A search was conducted for information on the chemical properties and toxicity of benzo[a]pyrene (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), and ChemFinder (chemical properties). This search yielded some information on benzo[a]pyrene's properties (vapor pressure, log octanol/water partition coefficient, Henry's Law, and water solubility), its biodegradation, and some information on its toxicity.

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 only two out of the eight requirements. Because there are data available for *Daphnia pulex*, it is possible to calculate secondary acute and chronic values for benzo[a]pyrene.

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 = 5 µg/L (*Daphnia pulex*)

SAV = GMAV/SAF
= 5 µg/L /13.0
= 0.3846 µg/L

There are currently no chronic toxicity data for benzo[a]pyrene which meet suitability requirements. 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
= 0.3846/18
= **0.0214 µg/L**

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

Because no species will drop out of the cold water database for any of the other use designations, the acute and chronic secondary values will be the same for all use designations.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for benzo[a]pyrene, 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.					
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Daphnia pulex	**water flea**	**96-h/LC50**	**5**	**1**	**ECOTOX**
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.					
Xenopus laevis	**clawed toad**	**96-h/EC50**	**8,700**	**2**	**ECOTOX**
Xenopus laevis	**clawed toad**	**96-h/EC50**	**9,600**	**2**	**ECOTOX**
SMAV = 9,138.93					
GMAV = 9,138.93					
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]Trucco, R.G., F.R. Engelhardt and B. Stacey. 1983. Toxicity, accumulation and clearance of aromatic hydrocarbons in *Daphnia pulex*. Environ. Pollut. Ser. A Ecol. Biol. 31(3):191-202.

[2]Propst, T.L., D.J. Fort and E.L. Stover. 1997. Evaluation of the developmental toxicity of benzo[a]pyrene and 2-acetylaminofluorine using *Xenopus*: Modes of biotransformation. Drug Chem. Toxicol. 20(1/2):45-61.

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). Benzo[a]pyrene is currently classified in Group B2, a probable human carcinogen, in EPA's IRIS database. A cancer oral slope factor is available; therefore, it is possible to calculate a human cancer secondary value for the protection of human health.

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/d) = Cancer slope factor

RAD = (1/7.3 mg/Kg/d)(0.00001)

= 1.37E-6

= 0.00000137 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:

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

For benzo[a]pyrene, the K_{ow} = 933,254 and log K_{ow} = 5.97 (CHEMFATE database).

f_{fd} = 1/{1 + [(0.00000024 Kg/L)(933,254)]}

= 1/1.22398

= 0.8170

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 measured BAF from a field study
-a predicted BAF based on field-measured BSAFs
-a predicted BAF using a laboratory-measured bioconcentration factor (BCF) and a food chain multiplier (FCM)
-a predicted BAF using a K_{ow} and a FCM

A BAF of 1,000 L/kg was measured, and the lipid tissue fraction (f_l) was 0.05.

Baseline BAF = [(Measured BAF / f_{fd}) – 1] [1/f_l]

= [(1000/0.817)-1] / 0.05

= 24460 (rounded)

4) Calculation of the human health BAF

a) Human Health BAF for Cold Waters

BAF^{HH}_{cold} = {[(baseline BAF_{cold})(0.044)] + 1} (f_{fd})

where

baseline BAF = the baseline BAF calculated in 3)

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

f_{fd} = fraction freely dissolved

BAF^{HH}_{cold} = {[(baseline BAF_{cold})(0.044)] + 1} (f_{fd})

= {[(24,460)(0.044)] + 1} (0.8170)

= 880.1

b) Human Health BAF for Warm Waters

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

where

baseline BAF = the baseline BAF calculated in 3)

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

f_{fd} = fraction freely dissolved

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

$= \{[(24{,}460)(0.013)] + 1\} (0.8170)$

$= 260.6$

5) Calculation of the human cancer secondary value

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

where

RAD = risk associated dose in milligrams toxicant per kilogram body weight per day (mg/Kg/d) that is associated with a lifetime incremental cancer risk equal to one in 100,000 as derived in 1) (above).

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 = human health BAF calculated in 4) (above).

a) Non-Public Water Supply; Limited Aquatic Life

$\text{Human Cancer Criterion} = [(RAD)(70\ Kg)]/[W_H + (F_H)(BAF)]$

$= [(0.00000137\ mg/Kg/d)(70\ Kg)]/[0.01\ L/d + (0)]$

$= 0.0096\ mg/L = 9{,}6\ \mu g/L$

Note: The limited aquatic life classification applies to water bodies with no (or very few) fish present. Therefore, calculation of a human cancer 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 contaminants through consumption of fish in these areas.

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

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

= [(0.00000137 mg/Kg/d)(70 Kg)]/[0.01 L/d + (0.02)(260.6)]

= 1.84E-5 mg/L = 18.4 ng/L

c) Non-Public Water Supply; Cold Water

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

= [(0.00000137 mg/Kg/d)(70 Kg)]/[0.01 L/d + (0.02)(880.1)]

= 5.45E-06 mg/L = 5.45 ng/L

d) Public Water Supply; Warm Water Sport

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

= [(0.00000137 mg/Kg/d)(70 Kg)]/[2 L/d + (0.02)(260.6)]

= 1.33E-5 mg/L = 13.3 ng/L

e) Public Water Supply; Cold Water

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

= [0.00000137 mg/Kg/d ()(70 Kg)]/[2 L/d + (0.02)(880.1)]

= 4.90E-6 mg/L = 4.9 ng/L