Date: May 16, 2008
Calculator: James Schmidt (updated based on measured BCF)

SECONDARY VALUES FOR BIS(2-ETHYLHEXYL)PHTHALATE (CAS No. 117-81-7)

A search was conducted for information on the chemical properties and toxicity of bis(2-ethylhexyl)phthalate 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). This search yielded some information on bis(2-ethylhexyl)phthalate's properties and a significant amount of information on its toxicity.

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 bis(2-ethylhexyl)phthalate to fish and other aquatic life, it was determined that data are available to meet seven out of the eight requirements. Because data are available for a Daphnid species, it is possible to calculate a secondary acute value for bis(2-ethylhexyl)phthalate.

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 seven out of eight requirements met = 4.3

Lowest GMAV = 145.88 µg/L (*Daphnia* sp.)

SAV = GMAV/SAF
= 145.88 µg/L /4.3
= 33.92 µg/L

Chronic data for *Daphnia magna* exposed to bis(2-ethylhexyl)phthalate are available which meet suitability requirements and which were collected by some of the same authors as the corresponding acute data (Table 2). Therefore, a secondary chronic value (SCV) may be calculated using some actual chronic data, rather than through default ratios only.

SACR (secondary acute-chronic ratio) = Geometric mean of three species mean acute-chronic ratios (SMACRs).

SMACR 1 (*Daphnia magna*) = 160/110 = 1.4545
SMACR 2 (default) = 18
SMACR 3 (default) = 18

SACR = geometric mean of 1.4545, 18, and 18 = 7.78

SCV = SAV/SACR
= 33.92 µg/L /7.78
= 4.36 µg/L

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

The salmonid category of fish drops out of the database when calculating secondary values for warm water. However, because the lowest GMAV in the entire database is for *Daphnia* sp., and because the only chronic data available are for *Daphnia magna*, the secondary values will be the same for all categories of surface waters.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for bis(2-ethylhexyl)phthalate, 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.					
Oncorhynchus kisutch	**coho salmon**	**96-h/LC50**	**>100,000**	**9**	**ECOTOX**
Oncorhynchus kisutch	**coho salmon**	**96-h/LC50**	**>100,000**	**4**	**ECOTOX**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>139,500**	**2**	**ECOTOX**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>149,200**	**2**	**ECOTOX**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>100,000**	**9**	**ECOTOX**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>320**	**1**	**ECOTOX**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>100,000**	**4**	**ECOTOX**
Gasterosteus aculeatus	**threespine stickleback**	**96-h/EC50**	**>300**	**7**	**ECOTOX**
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warmwater species.					
Ictalurus punctatus	**channel catfish**	**96-h/LC50**	**690**	**2**	**ECOTOX**
Ictalurus punctatus	**channel catfish**	**96-h/LC50**	**>100,000**	**9**	**ECOTOX**
Ictalurus punctatus	**channel catfish**	**96-h/LC50**	**>100,000**	**4**	**ECOTOX**
Ictalurus punctatus	**channel catfish**	**96-h/LC50**	**>200**	**4**	**ECOTOX**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**>770,000**	**8**	**ECOTOX**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**>100,000**	**9**	**ECOTOX**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**>200**	**1**	**ECOTOX**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**>100,000**	**4**	**ECOTOX**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**>200**	**4**	**ECOTOX**

Species Name	Common Name	Duration/ Endpoint	Value µg/L	Reference #	Source
Micropterus salmoides	**largemouth bass**	**96-h/LC50**	**42,100**	**2**	**ECOTOX**
Micropterus salmoides	**largemouth bass**	**96-h/LC50**	**32,900**	**2**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**>160**	**1**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**>670**	**1**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**1,106,200**	**10**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**>1,000**	**4**	**ECOTOX**
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Daphnia magna	**water flea**	**48-h/EC50**	**>160**	**1**	**ECOTOX**
Daphnia pulex	**water flea**	**48-h/EC50**	**133**	**5**	**ECOTOX**
GENUS MEAN ACUTE VALUE (GMAV) = 145.88					
4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).					
Gammarus pseudolimnaeus	**scud**	**96-h/LC50**	**>32,000**	**6**	**ECOTOX**
5. At least one insect (e.g., mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge).					
Chironomus plumosus	**midge**	**48-h/EC50**	**>18,000**	**3**	**ECOTOX**
Chironomus plumosus	**midge**	**48-h/EC50**	**>18,000**	**4**	**ECOTOX**
Chironomus plumosus	**midge**	**48-h/EC50**	**>72,000**	**4**	**ECOTOX**
6. At least one fish or amphibian from a family in the phylum Chordata not already represented in one of the other subdivisions.					
Bufo woodhousei fowleri	**Fowler's toad**	**96-h/LC50**	**3,880**	**2**	**ECOTOX**
Carassius auratus	**goldfish**	**96-h/LC50**	**6,180**	**2**	**ECOTOX**
Carassius auratus	**goldfish**	**96-h/LC50**	**>186,000**	**11**	**ECOTOX**
Carassius auratus	**goldfish**	**96-h/LC50**	**>191,000**	**11**	**ECOTOX**

Species Name	Common Name	Duration/ Endpoint	Value µg/L	Reference #	Source
Rana pipiens	**leopard frog**	**96-h/LC50**	**4440**	**2**	**ECOTOX**

7. At least one organism from a family in a phylum other than Arthropoda or Chordata (e.g., Rotifera, Annelida, Mollusca).

Americamysis bahia	**opossum shrimp**	**96-h/EC50**	**>370**	**1**	**ECOTOX**

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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[11]Birge, W.J., J.A. Black, and D.M. Bruser. 1979. Toxicity of organic chemicals to embryo-larval stages of fish. EPA-560/11-79-007, U.S. EPA, Washington, D.C. 60 p.

Table 2. Requirements for calculation of a chronic toxicity criterion for protection of aquatic life for bis(2-ethylhexyl)phthalate, and corresponding chronic 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 warmwater species.					
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Daphnia magna	**water flea**	**21-d/MATC**	**110**	**1**	**ECOTOX**
GENUS MEAN CHRONIC VALUE (GMCV) = 110					
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.					

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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). Bis(2-ethylhexyl) phthalate is currently classified as "B2", probable human carcinogen, by the U.S. EPA (IRIS, 2004) based on studies which produced dose-response relationships for the endpoint of liver tumor incidence. 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 bis(2-ethylhexyl) phthalate, $q_1^* = 0.014$ mg/Kg/day (IRIS 2004)

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

RAD = (1/0.014)(0.00001)

= 0.000714 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 bis(2-ethylhexyl) phthalate, the K_{ow} = 28,379,190 and log K_{ow} = 7.453 (Brooke et al. 1990; slow stir method).

$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(28,379,190)]\}$

$= 1/7.811006$

= 0.1280

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

Using a K_{ow} and a measured BCF:

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

From the testing done on this substance, the measured BCF was 114 L/kg, log K_{ow} was 7.6 (from Illinois' calculation), and the fraction of the tissue that was lipid in the test was 0.0355 (3.55%).

FCM = 16.749 (coldwater) and 11.708 (warmwater)

Baseline BAF coldwater = [16.749] [(114/0.128) – 1] [1/0.0355] = 419481
Baseline BAF warmwater = [11.708] [(114/0.128) – 1] [1/0.0355] = 293472

4) Calculation of the Human Health BAF:

Because bis(2-ethylhexyl) phthalate 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} = {[(293472)(0.013)] + 1} (0.1280)

= 488.47

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)

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

f_{fd} = fraction freely dissolved

BAF^{HH}_{TL4} = {[(419481)(0.044)] + 1} (0.1280)

= 2362.64

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)]

= (0.000714 mg/Kg/d)(70 Kg)/[2 L/d + (0.02 Kg/d)(2362.64 L/Kg)]

= 0.05/49.253

= 0.001015 mg/L

= 1.015 µg/L

Warm Waters, Public Water Supply

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

= (0.000714 mg/Kg/d)(70 Kg)/[2 L/d + (0.02 Kg/d)(488.47 L/Kg)]

= 0.05/11.7694

= 0.004248 mg/L

= 4.25 µg/L

Cold Water, Non-Public Water Supply

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

= (0.000714 mg/Kg/d)(70 Kg)/[0.01 L/d + (0.02 Kg/d)(2362.64 L/Kg)]

= 0.05/47.263

= 0.001058 mg/L

= 1.058 µg/L

= 0.74 ng/L

Warm Water, Non-Public Water Supply

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

= (0.000714 mg/Kg/d)(70 Kg)/[0.01 L/d + (0.02 Kg/d)(488.47 L/Kg)]

= 0.05/9.7794

= 0.005113 mg/L

= 5.11 μg/L

Limited Aquatic Life, Non-Public Water Supply

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

= (0.000714 mg/Kg/d)(70 Kg) / 0.01 L/d

= 0.05/0.01

= 5 mg/L

= 5000 μg/L

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