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SECONDARY VALUES FOR BUTYL BENZYL PHTHALATE (CAS No. 85-68-7)

A search was conducted for information on the chemical properties and toxicity of butyl benzyl 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 butyl benzyl phthalate's properties, and a significant amount of information on its toxicity.

Fish and Aquatic Life Secondary Values

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 butyl benzyl 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 butyl benzyl 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 = 820 µg/L (*Oncorhynchus mykiss*)

SAV = GMAV/SAF
= 820 µg/L /4.3
= 190.70 µg **/L**

Chronic data for *Daphnia magna* exposed to butyl benzyl 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*) = 2,608.74/514.04 = 5.08
SMACR 2 (default) = 18
SMACR 3 (default) = 18

SACR = geometric mean of 5.08, 18, and 18 = 11.81

SCV = SAV/SACR
= 190.70 µg/L /11.81
= 16.15 µg/L

Warm Water Sportfish

The salmonid category of fish drops out of the database when calculating secondary values for warm water.

Lowest GMAV = 1,394.95 µg/L (*Pimephales promelas*)

SAV = GMAV/SAF
= 1,395.94 µg/L /4.3
= 324.64 µg **/L**

SCV = SAV/SACR
= 324.64 µg/L /11.81
= 27.49 µg/L

Warm Water Forage Fish and Limited Forage Fish

Because the lowest GMAV is the same for warm water sportfish, warm water forage fish, and limited forage fish databases, the secondary values will be the same for these three water body use designations.

Limited Aquatic Life

All fish species drop out of the database for limited aquatic life.

Lowest GMAV = 1,464.24 µg/L (*Chironomus* sp.)

SAV = GMAV/SAF
= 1,464.24 µg/L /4.3
= 340.52 µg **/L**

SCV = SAV/SACR
= 340.52 µg/L /11.81
= 28.83 µg/L

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for butyl benzyl 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 mykiss	**rainbow trout**	**96-h/LC50**	**820**	**d**	**ECOTOX**
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warmwater species.					
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**43,000**	**f**	**ECOTOX**
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Daphnia magna	**water flea**	**48-h/EC50**	**3,700**	**c**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**960**	**d**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**1,600**	**e**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**2,900**	**e**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**4,700**	**e**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**10,000**	**e**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**2,100**	**e**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**4,100**	**e**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**10,000**	**e**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**1,000**	**e**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**1,600**	**e**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**1,800**	**e**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**1,600**	**e**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**2,200**	**e**	**ECOTOX**
Species Mean Acute Value (SMAV) = 2,608.74					
4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).					
Gammarus minus	**scud**	**96-h/LC50**	**8,680**	**b**	**ECOTOX**

5. At least one insect (e.g., mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge).

Chironomus tentans	**midge**	**48-h/EC50**	**1,600**	**a**	**ECOTOX**
Chironomus thummi	**midge**	**48-h/EC50**	**1,340**	**b**	**ECOTOX**

Genus Mean Acute Value (GMAV) = 1,464.24

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**	**2,320**	**c**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**780**	**d**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**1,500**	**d**	**ECOTOX**

SMAV = 1,394.95

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.

Tallaperla maria	**stonefly**	**96-h/LC50**	**7,500**	**b**	**ECOTOX**

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[a]Ziegenfuss, P.S., W.J. Renaudette, and W.J. Adams. 1986. Methodology for assessing the acute toxicity of chemicals sorbed to sediments: Testing the equilibrium partitioning theory. In; T.M. Poston and R. Purdy (Eds.), Aquatic Toxicology and Environmental Fate, 9th Volume, ASTM STP 921, Philadelphia, PA 479-493.

[b]Horne, J.D. and B.R. Oblad. 1983. Aquatic toxicity studies of six priority pollutants. Report No. 4380, NUS Corp., Houston Environmental Center, Houston, TX. 99 p.

[c]Gledhill, W.E., R.G. Kaley, W.J. Adams, O. Hicks, P.R. Michael, V.W. Saeger, and G.A. LeBlanc. 1980. An environmental safety assessment of butyl benzyl phthalate. Environmental Science and Technology 14(3):301-305.

[d] Adams, W.J., G.R. Biddinger, K.A. Robillard, and J.W. Gorsuch. 1995. A summary of the acute toxicity of 14 phthalate esters to representative aquatic organisms. Environmental Toxicology and Chemistry 14(9):1569-1574.

[e]Barera, Y., and W.J. Adams. 1983. Resolving some practical questions about Daphnia acute toxicity tests. In: W.E. Bishop (Ed.), Aquatic Toxicology and Hazard Assessment, 6th Symposium, ASTM STP 802, Philadelphia, PA. 509-518.

[f]Buccafusco, R.J., S.J. Ells, and G.A. LeBlanc. 1981. Acute toxicity of priority pollutants to bluegill (*Lepomis macrichirus*). Bull. Environ. Contam. Toxicol. 26(4):446-452.

Table 2. Requirements for calculation of a chronic toxicity criterion for protection of aquatic life for butyl benzyl 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**	**630**	**a**	**ECOTOX**
Daphnia magna	**water flea**	**21-d/MATC**	**440**	**b**	**ECOTOX**
Daphnia magna	**water flea**	**21-d/MATC**	**490**	**b**	**ECOTOX**
Species Mean Chronic Value = 514.04					
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.					

[a]Rhodes, J.E., W.J. Adams, G.R. Biddinger, K.A. Robillard, and J.W. Gorsuch. 1995. Chronic toxicity of 14 phthalate esters to *Daphnia magna* and rainbow trout (*Oncorhynchus mykiss*). Environmental Toxicology and Chemistry 14(11):1967-1976.

[b]Adams, W.J. and B.B. Heidolph. 1985. Short-cut chronic toxicity estimates using *Daphnia magna*. In: R.D. Cardwell, R. Purdy and R.C. Bahner (Eds.), Aquatic Toxicology and Hazard Assessment, 7th Symposium, ASTM STP 854, Philadelphia, PA. 87-103.

Human Health Secondary Values

Butyl Benzyl Phthalate (CAS RN 85-68-7)

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). Butyl benzyl phthalate is currently classified as "C", a possible human carcinogen, by the U.S. EPA (IRIS, 2004). However, there is no quantitative estimate of carcinogenic risk from oral exposure (oral slope factor) available. An oral reference dose (RfD; IRIS, 2004) is available, and it is possible to calculate a predicted baseline bioaccumulation factor (BAF); therefore, a human threshold secondary value may be calculated for this substance.

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:

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

For butyl benzyl phthalate, the K_{ow} = 81,283 and log K_{ow} = 4.91 (CHEMFATE database).

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(81,283)]\}$$

$$= 1/1.0195$$

$$\mathbf{= 0.9809}$$

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 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

No field-measured BAFs or BSAFs or usable lab-measured BCFs are available for butyl benzyl phthalate. Therefore, a baseline BAF was calculated using a K_{ow} and a FCM.

The FCM will be for trophic level 3 for a discharge to a water body classified as warm water, and the FCM will be for trophic level 4 for a discharge to a water body classified as cold water. Given butyl benzyl phthalate's log Kow of 4.91, the FCM from the table is 2.780 for trophic level 3 (warm water), and 2.193 for trophic level 4 (cold water).

For warm water:

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

= (2.780)(81,283)

= 225,967

For cold water:

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

= (2.193)(81,283)

= 178,254

3) Calculation of the human health BAF

Because butyl benzyl phthalate is an organic substance, the equations to use are as follows (depending on whether the discharge is to a water body classified as warm water or cold water):

For warm water:

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

where

baseline BAF = the baseline BAF calculated in 2)

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

f_{fd} = fraction freely dissolved

BAF^{HH}_{TL3} = {[(225,967)(0.013)] + 1} (0.9809)

= **2,882.4443**

For cold water:

BAF^{HH}_{TL4} = {[(baseline BAF)(0.044)] + 1} (f_{fd})

where

baseline BAF = the baseline BAF calculated in 2)

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

f_{fd} = fraction freely dissolved

BAF^{HH}_{TL4} = {[(178,254)(0.044)] + 1} (0.9809)

= 7,694.3522

4) Calculation of the human threshold secondary value

Human Threshold Secondary Value = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

where

ADE = acceptable daily exposure (= oral reference dose, or RfD)
= 0.2 mg/Kg/day for butyl benzyl phthalate (IRIS 2004)

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 DNR (= 0.02 Kg/d)

BAF = human health BAF calculated in 3).

Warm Waters, Public Water Supply

Human Threshold Secondary Value = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.2 mg/Kg/d)(70 Kg)(0.8)]/[2 L/d + (0.02 Kg/d)(2,882 L/Kg)]

= 11.2/59.64

= 0.1878 mg/L

= 187.8 μg/L

Cold Water, Public Water Supply

Human Threshold Secondary Value = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.2 mg/Kg/d)(70 Kg)(0.8)]/[2 L/d + (0.02 Kg/d)(7,694 L/Kg)]

= 11.2/155.88

= 0.0719 mg/L

= 71.9 μg/L

Warm Waters, Non-Public Water Supply

Human Threshold Secondary Value = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.2 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d + (0.02 Kg/d)(2,882 L/Kg)]

= 11.2/57.65

= 0.1943 mg/L

= 194.3 μg/L

Cold Water, Non-Public Water Supply

Human Threshold Secondary Value = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.2 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d + (0.02 Kg/d)(7,694 L/Kg)]

= 11.2/153.89

= 0.0728 mg/L

= 72.8 μg/L

Limited Aquatic Life, Non-Public Water Supply

Human Threshold Secondary Value = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.2 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d]

= 11.2/0.01

= 1,120 mg/L

= 1,120,000 μg/L

References

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Syracuse Research Corporation. CHEMFATE database. http://esc.syrres.com/efdb.htm

U.S. EPA. Aquatic Toxicity Information Retrieval (AQUIRE) database. http://www.epa.gov/med/databases.html

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