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SECONDARY VALUES FOR DI-*N*-BUTYL PHTHALATE (CAS No. 84-74-2)

A search was conducted for information on the chemical properties and toxicity of di-*n*-butyl phthalate (synonym dibutyl 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 di-*n*-butyl 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 di-*n*-butyl 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 di-*n*-butyl 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 = 350 µg/L (*Perca flavescens*)

SAV = GMAV/SAF
= 350 µg/L /4.3
= 81.40 µg **/L**

Chronic data for *Daphnia magna* exposed to di-*n*-butyl 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*) = 2,990/1,550 = 1.93
SMACR 2 (default) = 18
SMACR 3 (default) = 18

SACR = geometric mean of 1.93, 18, and 18 = 8.55

SCV = SAV/SACR
= 81.40 µg/L /8.55
= 9.52 µg/L

Warm Water Sportfish

The salmonid category of fish drops out of the database when calculating secondary values for warm water. However, because the lowest GMAV in the cold water database is for yellow perch, and because the only chronic data used to calculate the chronic secondary value is for *Daphnia magna*, the acute and chronic secondary values will be the same for warm water sportfish as for cold water.

Warm Water Forage Fish

All cold water and warm water sport fish drop out of the database for warm water forage fish.

Lowest GMAV = 1,376.50 µg/L (*Pimephales promelas*)

SAV = GMAV/SAF
= 1,376.50 µg/L /4.3
= 320.12 µg **/L**

SCV = SAV/SACR
= 320.12 µg/L /8.55
= 74.45 µg/L

Limited Forage Fish

All cold water, warm water sport fish, and warm water forage fish drop out of the database for limited forage fish. Because fathead minnows remain in the databases, secondary values for limited forage fish will be the same as for warm water forage fish.

Limited Aquatic Life

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

Lowest GMAV = 2,100 µg/L (*Gammarus pseudolimnaeus*)

SAV = GMAV/SAF
= 2,100 µg/L /4.3
= 488.37 µg **/L**

SCV = SAV/SACR
= 488.37 µg/L /8.55
= 57.12 µg/L

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for di-*n*-butyl 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**	**1,600**	**c**	**ECOTOX**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**6,470**	**d**	**ECOTOX**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**2,560**	**d**	**ECOTOX**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**1,480**	**d**	**ECOTOX**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**1,240**	**d**	**ECOTOX**
Species Mean Acute Value (SMAV) = 2,174.65					
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**	**2,910**	**d**	**ECOTOX**
Ictalurus punctatus	**channel catfish**	**96-h/LC50**	**460**	**d**	**ECOTOX**
SMAV = 1,156.98					
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**1,200**	**e**	**ECOTOX**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**480**	**c**	**ECOTOX**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**730**	**d**	**ECOTOX**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**2,100**	**d**	**ECOTOX**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**1,580**	**d**	**ECOTOX**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**2,050**	**d**	**ECOTOX**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**1,550**	**d**	**ECOTOX**
SMAV = 1,237.05					
Perca flavescens	**yellow perch**	**96-h/LC50**	**350**	**d**	**ECOTOX**

3. At least one planktonic crustacean (e.g., cladoceran, copepod).

Daphnia magna	**water flea**	**48-h/EC50**	**3,700**	**b**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/EC50**	**2,990**	**c**	**ECOTOX**

SMAV = 3,326.11

4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).

Gammarus pseudolimnaeus	**scud**	**96-h/LC50**	**2,100**	**d**	**ECOTOX**

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

Chironomus plumosus	**midge**	**48-h/EC50**	**760**	**a**	**ECOTOX**
Chironomus plumosus	**midge**	**48-h/EC50**	**5,400**	**a**	**ECOTOX**
Chironomus plumosus	**midge**	**48-h/EC50**	**4,000**	**a**	**ECOTOX**

SMAV = 2,541.49

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**	**1,100**	**f**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**850**	**f**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**1,540**	**c**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**920**	**c**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**1,300**	**d**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**3,950**	**d**	**ECOTOX**

SMAV = 1,376.50

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.

Paratanytarsus parthenogenetic	**midge**	**96-h/EC50**	**6,290**	**c**	**ECOTOX**

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[a]Streufert, J.M. 1977. Some effects of two phthalic acid esters on the life cycle of the midge (*Chironomus plumosus*). M.S. Thesis., University of Missouri, Columbia.

[b]Call, D.J., L.T. Brooke, N. Ahmad, and J.E. Richter. 1983. Toxicity and metabolism studies with EPA priority pollutants and related chemicals in freshwater organisms. EPA 600/3-83-095, U.S. EPA, Duluth, MN. 120 pp.

[c]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.

[d]Mayer, F.L.J. and M.R. Ellersieck. 1986. Manual of acute toxicity: Interpretation and database for 410 chemicals and 66 species of freshwater animals. Resource Publication No. 160, U.S. Department of the Interior, Fish and Wildlife Service, Washington, D.C. 505 p.

[e]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.

[f]Geiger, D.L., C.E. Northcott, D.J. Call, and L.T. Brooke. 1985. Acute toxicities of organic chemicals to fathead minnows (*Pimephales promelas*), Vol. 2. Center for Lake Superior Environmental Studies, Univ. of WI- Superior. I:326.

Table 2. Requirements for calculation of an chronic toxicity criterion for protection of aquatic life for di-*n*-butyl 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**	**1,550**	**a**	**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.					
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.

Human Health Secondary Values

Di-*n*-butyl-phthalate (CAS RN 84-74-2)

Synonyms: Dibutyl phthalate (among many others)

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). Di-*n*-butyl-phthalate is currently classified as "D", not classifiable, by the U.S. EPA (IRIS, 2004) based on inadequate data from animal bioassays and no human data. The U.S. EPA considers this chemical to be a priority pollutant, and has recommended water quality criteria for the protection of human health. Indiana, Michigan, and Ohio have all calculated human threshold secondary values for di-*n*-butyl phthalate with values of 31, 640, and 31 μg/L for drinking water and 31, 690, and 31 μg/L for non-drinking water, respectively.

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 di-*n*-butyl phthalate, the K_{ow} = 52,500 and log K_{ow} = 4.72 (CHEMFATE database).

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(52{,}500)]\}$$

$$= 1/1.0126$$

$$\mathbf{= 0.9876}$$

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 are available for di-*n*-butyl phthalate. BCF values are available for several invertebrate species which may be used, but only "with caution" under the GLI, since invertebrates may have different mechanisms for metabolism of chemicals, etc. The U.S. EPA really prefers a BCF for fish. The only BCF values available for fish included one for the fathead minnow that was derived in an 11-day (too short) study (ECOTOX database) and one for the sheepshead minnow (a saltwater species; CHEMFATE database). Therefore, a baseline BAF was calculated for di-*n*-butyl phthalate 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 di-*n*-butyl phthalate's log Kow of 4.72, the FCM from the table was interpolated to be 2.2104 for trophic level 3 (warm water), and 1.6806 for trophic level 4 (cold water).

For warm water:

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

= (2.2104)(52,500)

= 116,046.0000

For cold water:

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

= (1.6806)(52,500)

= 88,231.5000

3) Calculation of the human health BAF

Because di-*n*-butyl 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:

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

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

$BAF^{HH}_{TL3} = \{[(116{,}046.0000)(0.013)] + 1\}\ (0.9876)$

= **1,490.8790**

For cold water:

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

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

$BAF^{HH}_{TL4} = \{[(88{,}231.5000)(0.044)] + 1\}\ (0.9876)$

= 3,835.0345

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) = 0.1 mg/Kg/day for di-*n*-butyl 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 = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

$= [(0.1\ mg/Kg/d)(70\ Kg)(0.8)]/[2\ L/d + (0.02\ Kg/d)(1{,}490.8790\ L/Kg)]$

$= 5.6/31.8178$

$= 0.17600\ mg/L$

$= 176.00\ \mu g/L$

Cold water, Public Water Supply

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

$= [(0.1\ mg/Kg/d)(70\ Kg)(0.8)]/[2\ L/d + (0.02\ Kg/d)(3{,}835.0345\ L/Kg)]$

$= 5.6/78.7007$

$= 0.07116\ mg/L$

$= 71.16\ \mu g/L$

Warm Waters, Non-Public Water Supply

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

$= [(0.1\ mg/Kg/d)(70\ Kg)(0.8)]/[0.01\ L/d + (0.02\ Kg/d)(1{,}490.8790\ L/Kg)]$

$= 5.6/29.8276$

$= 0.18776\ mg/L$

$= 187.76\ \mu g/L$

Cold Water, Non-Public Water Supply

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

= $[(0.1\ mg/Kg/d)(70\ Kg)(0.8)]/[0.01\ L/d + (0.02\ Kg/d)(3{,}835.0345\ L/Kg)]$

= 5.6/76.7107

= 0.07300 mg/L

= 73.00 µg/L

Limited Aquatic Life, Non-Public Water Supply

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

= $[(0.1\ mg/Kg/d)(70\ Kg)(0.8)]/[0.01\ L/d]$

= 5.6/0.01

= 560 mg/L

= 560,000 µg/L

References

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