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SECONDARY VALUES FOR BUTYLATE (CAS No. 2008-41-5)

A search was conducted for information on the chemical properties and toxicity of butylate 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), BIODEG (degradation), HSDB (Hazardous Substances Data Bank), CCRIS (Chemical Carcinogenesis Research Info System), ATSDR ToxFAQs (Agency for Toxic Substances and Disease Registry chemical fact sheets), and EXTTOXNET (Extension Toxicology Network's pesticide information project). This search yielded some useful information on butylate's properties and toxicity.

Fish and Aquatic Life Secondary Values

To derive an acute toxicity criterion for fish and 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 butylate to fish and other aquatic life, it was determined that data are available to meet six out of the eight requirements. Because data are available for a Daphnid species, it was possible to calculate a secondary acute value for butylate.

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 six out of eight requirements met = 5.2
Lowest GMAV = 2,407.64 µg/L (*Lepomis macrochirus*)

$$\begin{aligned}\text{SAV} &= \text{GMAV}/\text{SAF} \\ &= 2,407.64 \text{ } \mu\text{g/L} / 5.2 \\ &= \mathbf{463.01 \text{ } \mu\text{g/L}}\end{aligned}$$

No chronic data are currently available for butylate which meet acceptability requirements; therefore, a secondary chronic value (SCV) may be calculated using default ratios only.

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

SMACR 1 = 18 (default)
SMACR 2 = 18 (default)

SMACR 3 = 18 (default)

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

$$\begin{aligned}\text{SCV} &= \text{SAV}/\text{SACR} \\ &= 463.01 \text{ } \mu\text{g}/\text{L} / 18 \\ &= \mathbf{25.72 \text{ } \mu\text{g}/\text{L}}\end{aligned}$$

So for cold water designated waters, the secondary acute value is 463 $\mu\text{g}/\text{L}$ and the secondary chronic value is 26 $\mu\text{g}/\text{L}$ for butylate.

Warm Water Sportfish

The salmonid category drops out of the database when calculating secondary values for warm water sportfish designated waters. However, the lowest GMAV left in the database is still the one for *Lepomis macrochirus* (bluegill). Therefore, the secondary values calculated for cold water will also apply to warm water sportfish designated waters.

Warm Water Forage Fish

The cold water (rainbow trout) and warm water game (bluegill and Western mosquitofish) fish species drop out of the database for warm water forage fish designated waters. The lowest GMAV left is for *Gammarus fasciatus* (a scud).

SAF for four out of eight requirements met = 5.2
Lowest GMAV = 11,684.54 $\mu\text{g}/\text{L}$ (*Gammarus fasciatus*)

$$\begin{aligned}\text{SAV} &= \text{GMAV}/\text{SAF} \\ &= 11,684.54 \text{ } \mu\text{g}/\text{L} / 5.2 \\ &= \mathbf{2,247.03 \text{ } \mu\text{g}/\text{L}}\end{aligned}$$

$$\begin{aligned}\text{SCV} &= \text{SAV}/\text{SACR} \\ &= 2,247.03 \text{ } \mu\text{g}/\text{L} / 18 \\ &= \mathbf{124.83 \text{ } \mu\text{g}/\text{L}}\end{aligned}$$

So for warm water forage fish designated waters, the secondary acute value is 2,247 $\mu\text{g}/\text{L}$ and the secondary chronic value is 125 $\mu\text{g}/\text{L}$ for butylate.

Limited Forage Fish and Limited Aquatic Life

Because the lowest GMAV is for an invertebrate (*Gammarus fasciatus*), and because invertebrates will not drop out of the database for any of the remaining water body use

classifications, secondary values calculated for warm water forage fish designated waters will also apply for limited forage fish and limited aquatic life designated waters.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for butylate, 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.					
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	3,600	1	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	23,000	2	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	4,200	2	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	5,200	2	AQUIRE
# <i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	>700,000	2	AQUIRE
# <i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	202,500	2	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	2,100	3	AQUIRE
# - Not used to calculate SMAV because the results were more than 10X the remaining majority of the database. Species Mean Acute Value (SMAV) = 5,198.77					
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warmwater species.					
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	8,000	1	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	5,600	1	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	5,500	1	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	7,500	2	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	6,900	2	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	7,200	2	AQUIRE
# <i>Lepomis macrochirus</i>	bluegill	96-h/LC50	>500,000	2	AQUIRE
# <i>Lepomis macrochirus</i>	bluegill	96-h/LC50	202,500	2	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	300	3	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	210	3	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	470	3	AQUIRE
# - Not used to calculate SMAV because the results were more than 10X the remaining majority of the database.					

SMA V = 2,407.64

3. At least one planktonic crustacean (e.g., cladoceran, copepod).
Daphnia magna water flea 11,900 2 **AQUIRE**
Daphnia magna water flea 158,600 2 **AQUIRE**
 SMA V = 43,443.53
4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).
Gammarus fasciatus scud 15,000 4 **AQUIRE**
Gammarus fasciatus scud 10,000 4 **AQUIRE**
Gammarus fasciatus scud 11,000 5 **AQUIRE**
Gammarus fasciatus scud 11,000 3 **AQUIRE**
Gammarus fasciatus scud 12,000 3 **AQUIRE**
 SMA V = 11,684.54
5. At least one insect (e.g., mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge).
Chironomus thummi midge 37,000 6 **AQUIRE**
6. At least one fish or amphibian from a family in the phylum Chordata not already represented in one of the other subdivisions.
Gambusia affinis Western mosquitofish 8,500 2 **AQUIRE**
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.

¹Cope, O.B. 1965. Sport fishery investigations. In: Effects of Pesticides on Fish and Wildlife, U.S. Department of Interior, Fish and Wildlife Circular 226:51-63.

²Office of Pesticide Programs. 2000. Environmental Effects Database (EEDB). Environmental Fate and Effects Division, U.S. EPA, Washington, D.C.

³Mayer, F.L.J. and M.R. Ellersieck. 1986. Manual of acute toxicity: Interpretation and data base for 410 chemicals and 66 species of freshwater animals. Resource Publication No. 160. U.S. Department of Interior, U.S. Fish and Wildlife Service, Washington, D.C. 505 pp.

- ⁴Sanders, H.O. 1970. Toxicities of some herbicides to six species of freshwater crustaceans. *Journal of Water Pollution Control Federation* 24(8):1544-1550.
- ⁵Johnson, W.W. and M.T. Finley. 1980. Handbook of acute toxicity of chemicals to fish and aquatic invertebrates. Resource Publication 137, U.S. Department of Interior, U.S. Fish and Wildlife Service, Washington, D.C. 98 pp.
- ⁶Buhl, K.J. and N.L. Faerber. 1989. Acute toxicity of selected herbicides and surfactants to larvae of the midge *Chironomus riparius*. *Archives of Environmental Contamination and Toxicology* 18(4):530-536.

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). Butylate has been classified a Group E chemical, with evidence on non-carcinogenicity for humans (U.S. EPA's IRIS database). Because an oral reference dose and a log octanol water partition coefficient are available, a human threshold secondary value can be calculated for butylate.

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:

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

For butylate, a log K_{ow} of 4.15 (K_{ow} of 14,125.3754) has been published (National Institutes of Health, Hazardous Substance Database).

$$f_{fd} = 1 / \{ 1 + [(0.00000024 \text{ Kg/L})(14,125.3754)] \}$$

$$= 1 / 1.003390$$

$$= \mathbf{0.9966}$$

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 bioconcentration factor (BCF) and a food chain multiplier (FCM)
- d) a predicted BAF using a K_{ow} and a FCM

Currently, there are no BAFs, BSAFs, or BCFs available for butylate; therefore, the baseline BAF was calculated using the K_{ow} and a food chain multiplier (method d above).

Given butylate's log K_{ow} of 4.15 (K_{ow} of 14,125.3754), the FCMs (taken from table B-1 in GLI) are 1.380 for trophic level 3 (warm waters) and 1.130 for trophic level 4 (cold waters).

a) Cold Water

$$\begin{aligned} \text{Baseline BAF} &= (\text{FCM})(K_{ow}) \\ &= (1.130)(14,125.3754) \\ &= \mathbf{15,961.6742} \end{aligned}$$

b) Warm Waters

$$\begin{aligned} \text{Baseline BAF} &= (\text{FCM})(K_{ow}) \\ &= (1.380)(14,125.3754) \\ &= \mathbf{19,493.0180} \end{aligned}$$

3) Calculation of the human health BAF

a) Cold Water

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

where

$\text{BAF}_{\text{TL4}}^{\text{HH}}$ = Human health BAF for trophic level 4 (cold water)

baseline BAF = the baseline BAF (for cold waters) calculated in 2)

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

f_{fd} = fraction freely dissolved

$$\begin{aligned} \text{BAF}_{\text{TL4}}^{\text{HH}} &= \{[(15,961.6742)(0.044)] + 1\} (0.9966) \\ &= \mathbf{700.9224} \end{aligned}$$

b) Warm Waters

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

where

BAF^{HH}_{TL3} = Human health BAF for trophic level 3 (warm waters)

baseline BAF = the baseline BAF (for warm waters) calculated in 2)

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

f_{fd} = fraction freely dissolved

$$BAF^{HH}_{TL3} = \{[(19,493.0180)(0.013)] + 1\} (0.9966)$$
$$= 253.5442$$

4) Calculation of the human threshold secondary value

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

where

ADE = acceptable daily exposure (= oral reference dose, or RfD; = 0.05 mg/Kg/day for butylate (IRIS 2003))

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 = human health BAF calculated in 3).

a) Public Water Supply/Cold Water

$$\text{Human Threshold Secondary Value} = [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)]$$
$$= [(0.05 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[2 \text{ L/d} + (0.02 \text{ Kg/d})(700.9224 \text{ L/Kg})]$$
$$= 0.1748 \text{ mg/L}$$
$$= 174.8 \text{ } \mu\text{g/L}$$

b) Public Water Supply/Warm Water Sportfish

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.05 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[2 \text{ L/d} + (0.02 \text{ Kg/d})(253.5442 \text{ L/Kg})] \\ &= 0.3960 \text{ mg/L} \\ &= \mathbf{396.0 \mu\text{g/L}}\end{aligned}$$

c) Non-Public Water Supply/Cold Water

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.05 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0.02 \text{ Kg/d})(700.9224 \text{ L/Kg})] \\ &= \mathbf{0.1996 \text{ mg/L}} \\ &= \mathbf{199.6 \mu\text{g/L}}\end{aligned}$$

d) Non-Public Water Supply/Warm Waters (Warm Water Sportfish, Warm Water Forage Fish, and Limited Forage Fish designated waters)

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.05 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0.02 \text{ Kg/d})(253.5442 \text{ L/Kg})] \\ &= \mathbf{0.5511 \text{ mg/L}} \\ &= \mathbf{551.1 \mu\text{g/L}}\end{aligned}$$

e) Non-Public Water Supply/Limited Aquatic Life

Note: The Limited Aquatic Life classification applies to water bodies with no (or very few) fish present. Therefore, calculation of a human health threshold 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 butylate through consumption of fish in these areas.

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.05 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0)] \\ &= \mathbf{280 \text{ mg/L}} \\ &= \mathbf{280,000 \mu\text{g/L}}\end{aligned}$$

Chemical	CAS #	Category	Type of Secondary Value	Water Body Classification	Value (µg/L)
Butylate	2008-41-5	Fish and Aquatic	Acute	Cold, WWSF	1125
Butylate	2008-41-5	Fish and Aquatic	Chronic	Cold, WWSF	62
Butylate	2008-41-5	Fish and Aquatic	Acute	WWFF, LFF, LAL	2247
Butylate	2008-41-5	Fish and Aquatic	Chronic	WWFF, LFF, LAL	125
Butylate	2008-41-5	Human Health	Human Threshold	Public Water Supply/Cold	175
Butylate	2008-41-5	Human Health	Human Threshold	Public Water Supply/WWSF	396
Butylate	2008-41-5	Human Health	Human Threshold	Non-Public Water Supply/Cold	200
Butylate	2008-41-5	Human Health	Human Threshold	Non-Public Water Supply/WWSF, WWFF, LFF	551
Butylate	2008-41-5	Human Health	Human Threshold	Non-Public Water Supply/LAL	280,000

Cold = cold water designated water bodies

WWSF = warm water sportfish designated water bodies

WWFF = warm water forage fish designated water bodies

LFF = limited forage fish designated water bodies

LAL = limited aquatic life designated water bodies (includes wetlands)