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SECONDARY VALUES FOR TRIMETHYLBENZENES

Trimethylbenzenes (CAS # 25551-13-7; also written as trimethyl benzenes) is actually a mix of the following isomers: 1,3,5-trimethylbenzene (CAS # 108-67-8), 1,2,4-trimethylbenzene (CAS # 95-63-6); and 1,2,3-trimethylbenzene (CAS # 526-73-8). A search was conducted for information on the chemical properties and toxicity of each of these trimethylbenzenes (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 (physical and chemical properties). This search yielded some chemical property and aquatic toxicity information on 1,2,4-trimethylbenzene and some aquatic toxicity information on 1,3,5-trimethylbenzene.

FISH AND AQUATIC LIFE

1,2,4-trimethylbenzene

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 magna*, it is possible to calculate secondary acute and chronic values for 1,2,4-trimethylbenzene.

1,3,5- trimethylbenzene

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 2. 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 magna*, it is possible to calculate secondary acute and chronic values for 1,3,5-trimethylbenzene.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for **1,2,4-trimethylbenzene**, 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.					
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**7,720**	**1**	**AQUIRE**
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Daphnia magna	**water flea**	**48-h/EC50**	**3,606**	**2**	**AQUIRE**
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.					

[1]Geiger, D.L., S.H. Poirier, L.T. Brooke, and D.J. Call. 1986. Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), Vol. 3. Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI. 328 pp.

[2]Bobra, A.M., W.Y. Shiu, and D. MacKay. 1983. A predictive correlation for the acute toxicity of hydrocarbons and chlorinated hydrocarbons to the water flea (*Daphnia magna*). Chemosphere 12(9-10):1121-1129.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for **1,3,5-trimethylbenzene**, 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.					
Carassius auratus	**goldfish**	**96-h/LC50**	**12,520**	**1**	**AQUIRE**
5. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Daphnia magna	**water flea**	**48-h/EC50**	**6,006**	**2**	**AQUIRE**
6. 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.					

[1]Brenniman, G., R. Hartung, and W.J. Weber, Jr. 1976. A continuous flow bioassay method to evaluate the effects of outboard motor exhausts and selected aromatic toxicants on fish. Water Research 10(2):165-169.
[2]Bobra, A.M., W.Y. Shiu, and D. MacKay. 1983. A predictive correlation for the acute toxicity of hydrocarbons and chlorinated hydrocarbons to the water flea (*Daphnia magna*). Chemosphere 12(9-10):1121-1129.

The Milwaukee River is designated as a warm water sport fish community, non-public water supply. However, it is necessary to calculate secondary values for both cold water and warm water first, for comparative purposes. If the secondary values are lower for warm water than for cold water, then the secondary values for cold water (complete database) will apply for the warm water. If the secondary values for warm water are higher than for cold water, then the secondary values for warm water will apply (and will offer some relief to warm water dischargers).

Cold Water

1,2,4-trimethylbenzene

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 = 3,606 µg/L (*Daphnia magna*)

SAV = GMAV/SAF
= 3,606 µg/L /13.0
= 277.38 µg/L

There are currently no chronic data for 1,2,4-trimethylbenzene. 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
= 277.38/18
= **15.41 µg/L**

So, for 1,2,4-trimethylbenzene, the secondary acute value is 277 µg/L (rounded from 277.38) and the secondary chronic value is 15 µg/L (rounded from 15.41) for cold water.

1,3,5-trimethylbenzene

SAF for two out of eight requirements met = 13.0

Lowest GMAV = 6,009 µg/L (*Daphnia magna*)

SAV = GMAV/SAF
= 6,009 µg/L /13.0
= 462.23 µg/L

There are currently no chronic data for 1,3,5-trimethylbenzene. 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
= 462.23/18
= **25.68 µg/L**

So, for 1,3,5-trimethylbenzene, the secondary acute value is 462 µg/L (rounded from 462.23) and the secondary chronic value is 26 µg/L (rounded from 25.68) for cold water.

Warm Water

Because no species will drop out of the database for either 1,2,4-trimethylbenzene or 1,3,5-trimethylbenzene, the acute and chronic secondary values will be the same for both cold water and warm water.

Because there are no data to suggest which isomer is typically present in higher concentrations, it is suggested that secondary values for 1,2,4-trimethylbenzene (277 µg/L and 15 µg/L) serve as the secondary values for total trimethylbenzenes.

HUMAN HEALTH

A search of the IRIS database and other sources yielded no information on carcinogenicity, oral reference doses, or cancer slope factors for trimethylbenzenes. Thus, it is not possible to calculate a secondary value for human health for any trimethylbenzenes at this time.