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Secondary Values for *p*-Isopropyltoluene (*p*-cymene; CAS # 99-87-6)

A search was conducted for information on the chemical properties and toxicity of *p*-isopropyltoluene (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), BIOLOG (microbial degradation/toxicity), DATALOG (environmental fate bibliography), HSDB (Hazardous Substances Data Bank), CCRIS (Chemical Carcinogenesis Research Info System), GENE-TOX (mutagenicity database), TOXLINE (toxicology bibliography), TERA (Toxicology Excellence for Risk Assessment), and Ingenta (journal article search engine; since 1988). This search yielded some information on *p*-isopropyltoluene's properties (vapor pressure, log octanol/water partition coefficient, Henry's Law, and water solubility), and its biodegradation, but very little information on its toxicity.

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). *p*-Isopropyltoluene is not currently listed in EPA's IRIS database, and no information on its carcinogenicity is available in the CCRIS database. In addition, there is no oral reference dose (RfD; IRIS) and there are no aquatic organism bioaccumulation data (ECOTOX, etc.) available, which are also necessary to calculate a human health criteria or secondary value. Thus, there is insufficient data available at this time to calculate a secondary value for *p*-isopropyltoluene for the protection of human health.

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 one out of the eight requirements. Because data are available for *Daphnia magna*, it is possible to calculate a secondary acute value for *p*-isopropyltoluene. (Data are available for five other species; however, these data either do not meet the quality requirements necessary for use in water quality criteria/secondary value calculations, or they are for saltwater species.)

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for *p*-isopropyltoluene, 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 warmwater species. | | | | | |
| 3. At least one planktonic crustacean (e.g., cladoceran, copepod). | | | | | |
| ***Daphnia magna*** | **water flea** | **48-h/LC50** | **6,500** | **1** | **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]LeBlanc 1980.

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 one out of eight requirements met = 21.9

Lowest GMAV = 6,500 µg/L (*Daphnia magna*)

**SAV** = GMAV/SAF
= 6,500 µg/L /21.9
**= 296.80 µg/L**

There are currently no chronic data for *p*-isopropyltoluene which meet suitability requirements. 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
= 296.80/18
= **16.49 µg/L**

So, for *p*-isopropyltoluene, the **secondary acute value is 297 µg/L** (rounded from 296.80) and the **secondary chronic value is 16 µg/L** (rounded from 16.49).

References

LeBlanc, G.A. 1980. Acute toxicity of priority pollutants to water flea (*Daphnia magna*). Bull. Environ. Contam. Toxicol. 24:684-691.