TIER I HUMAN HEALTH NONCANCER CRITERIA

2-METHYLPHENOL

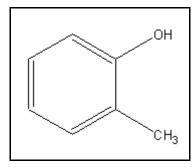
CAS RN: 95-48-7
Water Solubility: 41000 mg/L

 $Log K_{ow}$: 1.97^P

Reference Dose: 0.05 mg/kg/day

Carcinogenicity Weight-of-

Evidence Classification: Class D; Not Classifiable



Standard

The human health noncancer 2-methylphenol criterion for drinking water sources is 1,400 μ g/L. The human health noncancer criterion for nondrinking water sources is 44,000 μ g/L.

Calculations

Bioaccumulation Factor:

BAF predicted based on Log K_{ow} Log $K_{ow} = 1.97$ (CLOGP), $K_{ow} = 93.33$ Trophic level 3 FCM = 1.0; trophic level 4 FCM = 1.0

$$f_{fd} = 1/(1+(0.00000024 \text{ kg/L})(K_{ow})) = 1.00$$

Baseline BAF_{T3} = (FCM)(K_{ow}) = (1.0)(93.33) = 93.33

Baseline $BAF_{T4} = (1.0)(93.33) = 93.33$

Human health $BAF_{T3} = [(93.33)(0.0182)+1](1.00) = 2.698$

Human health BAF_{T4} = [(93.33)(0.0310)+1](1.00) = 3.893

Acceptable Daily Exposure:

From the IRIS database:

Critical Effect: Decreased body weights and neurotoxicity

$$ADE = \frac{NOAEL}{UF} = \frac{50 \text{ mg/kg-day}}{1000} = 0.05 \text{ mg/kg/d}$$

Calculation of Criteria:

Non Drinking Water HNC = [(0.05)(70)(0.8)]/0.01+[(0.0036)(2.698)+(0.0114)(3.893)]

$$= 44,000 \mu g/L$$

Drinking Water HNC =
$$[(0.05)(70)(0.8)]/2+[(0.0036)(4.12)+(2.698)(3.893)]$$

= 1,400 µg/L

References

- 1. USEPA 1990. Integrated Risk Information System (IRIS database) chemical file for 2-methylphenol (95-48-7).
- 2. Leo,A. and D.Weininger 1997. Daylight Software CLogP Version 3.15+ for Unix Pomona Medical Chemistry Project, Pomona College, Claremont, CA. Distributed by Daylight Chemical Information Systems, Inc., 3952 Claremont St., Irving, CA 92714 (Reference for the Log K_{ow}).

Acronyms

| ADE | Acceptable Daily Exposure |
|-----------------|--|
| BAF | Bioaccumulation Factor |
| CAS RN | Chemical Abstract Service Registry Number |
| FCM | Food Chain Multiplier |
| IRIS | Integrated Risk Information System |
| K _{ow} | Octanol-Water Partition Coefficient |
| LOAEL | Lowest observed adverse effect level |
| NOAEL | No observed adverse effect level |
| P (superscript) | Predicted value |
| RPLC | Reverse-phase Liquid Chromatography |
| UF | Uncertainty factor |

Revision History

August 26, 1999 - Criteria first developed April 28, 2000 - Fact sheet updated. No modifications to criteria.

Contact Information

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