TIER I HUMAN HEALTH NONCANCER CRITERIA

1,3-DICHLOROPROPENE

CAS RN: 542-75-6 Water Solubility: 4,500 mg/L

 $Log K_{ow}: 1.60^{P}$

Reference Dose: 0.034 mg/kg/day

Carcinogenicity Weight-of-

Evidence Classification: Class B2; Probable human carcinogen



Standard

The human health noncancer 1,3-dichloropropene criterion for drinking water sources is 940 μ g/L. The human health noncancer criterion for nondrinking water sources is 46,000 μ g/L.

Calculations

Bioaccumulation Factor:

BAF predicted based on Log K_{ow} Log $K_{ow} = 1.60$ (CLOGP program), $K_{ow} = 39.81$ Trophic level 3 FCM = 1.0; trophic level 4 FCM = 1.0

 $f_{fd} = 1/(1+(0.00000024 \text{ kg/L})(K_{ow})) = 1.0$

Baseline BAF_{T3} = (FCM)(K_{ow}) = (39.81)(1.0) = 39.81

Baseline BAF_{T4} = (39.81)(1.0) = 39.81

Human health BAF_{T3} = [(32.66)(0.0182)+1](1.0) = 1.725

Human health BAF_{T4} = [(32.66)(0.0310)+1](1.0) = 2.234

Acceptable Daily Exposure:

From the IRIS database:

Critical Effect: chronic irritation

$$ADE = \frac{NOAEL}{UF} = \frac{3.4 \text{ mg/kg-day}}{100} = 0.034 \text{ mg/kg/d}$$

Calculation of Criteria:

NonDrinking Water HNC =
$$[(0.034)(70)(0.8)]/0.01+[(0.0036)(1.725)+(0.0114)(2.234)]$$

= 46,000 µg/L

Drinking Water HNC =
$$[(0.034)(70)(0.8)]/2+[(0.0036)(1.725)+(0.0114)(2.234)]$$

= 940 µg/L

References

- 1. USEPA 2000. Integrated Risk Information System (IRIS database) chemical file for 1,3-dichloropropene (CAS # 542-75-6).
- 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

December 1, 1998 - Criteria first developed April 18, 2000 - Fact sheet updated. No modifications to criteria. September 12, 2000 - RfD updated based on new number from EPA. New criteria derrived.

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