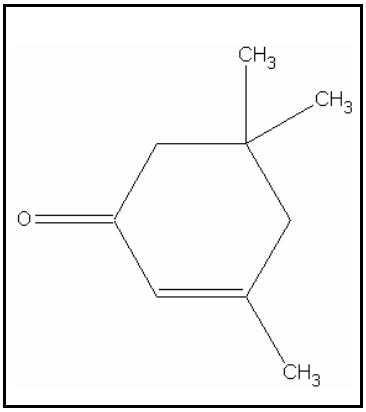
Indiana Department of Environmental Management
Office of Water - Water Quality Standards Section

TIER I HUMAN HEALTH NONCANCER CRITERIA

ISOPHORONE

CAS RN:	78-59-1
Water Solubility:	1.2 g/100 mL
Log K_{ow}:	2.22^{P}
Reference Dose:	0.15 mg/kg/day
Carcinogenicity Weight-of-Evidence Classification:	Class C; Possible human carcinogen



Standard

The human health noncancer isophorone criterion for drinking water sources is 4,100 µg/L. The human health noncancer criterion for nondrinking water sources is 110,000 µg/L.

Calculations

Bioaccumulation Factor:

BAF predicted based on Log K_{ow} and measured BCF (from Stephan 1993)
Log K_{ow} = 2.22 (CLOGP), K_{ow} = 165.96, BCF = 7, Percent lipid = 4.8
Trophic level 3 FCM = 1.005; trophic level 4 FCM = 1.000

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

Baseline $BAF_{T3} = (1.005)[(7/1.00)-1](1/0.048) = 125.63$

Baseline $BAF_{T4} = (1.000)[(7/1.00)-1](1/0.048) = 125.01$

Human health BAF_{T3} = [(125.63)(0.0182)+1](1.00) = 3.286

Human health BAF_{T4} = [(125.01)(0.0310)+1](1.00) = 4.875

Acceptable Daily Exposure:

From the IRIS database:

Critical Effect: No observed effects

$$ADE = \frac{NOAEL}{UF} = \frac{150\ mg/kg\text{-}day}{1000} = 0.15\ mg/kg/d$$

Calculation of Criteria:

Non Drinking Water HNC = [(0.15)(70)(0.8)]/0.01+[(0.0036)(3.286)+(0.0114)(4.875)]
= **110,000 μg/L**

Drinking Water HNC = [(0.1501)(70)(0.8)]/2+[(0.0036)(3.286)+(0.0114)(4.875)]
= **4,100 μg/L**

References

1. Stephen, C.E. 1993. Derivation of Proposed Human Health and Wildlife Bioaccumulation Factors for the Great Lakes Initiative. Environmental Research Laboratory, Office of Research and Development, U.S. EPA, Duluth, MN.

2. USEPA 1991. Integrated Risk Information System (IRIS database) chemical file for isophorone (CAS #78-59-1).

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

July 14, 1999 - Criteria first developed
April 20, 2000 – Fact sheet updated. No modifications to criteria.

Contact Information

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