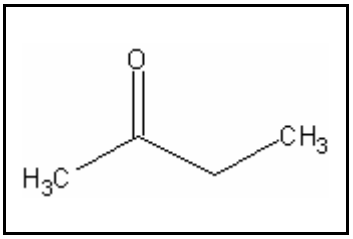
Indiana Department of Environmental Management
Office of Water - Water Quality Standards Section

TIER I HUMAN HEALTH NONCANCER CRITERIA

2-BUTANONE

CAS RN:	78-93-3
Water Solubility:	256,000 mg/L
Log K_{ow}:	0.32^{P}
Reference Dose:	0.59 mg/kg/day
Carcinogenicity Weight-of-Evidence Classification:	Class D; Not Classifiable



Standard

The human health noncancer 2-butanone (methyl ethyl ketone) criterion for drinking water sources is 16 µg/L. The human health noncancer criterion for nondrinking water sources is 1,300 µg/L.

Calculations

Bioaccumulation Factor:

BAF predicted based on Log K_{ow}

Log K_{ow} = 0.32 (CLOGP program), K_{ow} = 2.094

Trophic level 3 FCM = 1.0; trophic level 4 FCM = 1.0

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

Baseline $BAF_{T3} = (FCM)(K_{ow}) = (2.094)(1.0) = 2.094$

Baseline $BAF_{T4} = (2.094)(1.0) = 2.094$

Human health BAF_{T3} = [(2.094)(0.0182)+1](1.0) = 1.038

Human health BAF_{T4} = [(2.094)(0.0310)+1](1.0) = 1.065

Acceptable Daily Exposure:

From the IRIS database:

Critical Effect: decreased fetal birth weight

$$ADE = \frac{NOAEL}{UF} = \frac{1771 \text{ mg/kg-day}}{3000} = 0.5903 \text{ mg/kg/d}$$

Calculation of Criteria:

Non Drinking Water HNC = [(0.5903)(70)(0.8)]/0.01+[(0.0036)(1.038)+(0.0114)(1.065)]

= **1300 μg/L**

Drinking Water HNC = [(0.5903)(70)(0.8)]/2+[(0.0036)(1.038)+(0.0114)(1.065)]

= **16 μg/L**

References

1. USEPA 1993. Integrated Risk Information System (IRIS database) chemical file for 2-butanone (methyl ethyl ketone) (CAS # 78-93-3).

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

July 13, 1998 - Criteria first developed

Contact Information

David B. Kallander
Water Quality Standards Section
Indiana Department of Environmental Management
100 North Senate Ave., P.O. Box 6015
Indianapolis, IN 46206-6015
(317) 233-2472
Email: dkalland@dem.state.in.us