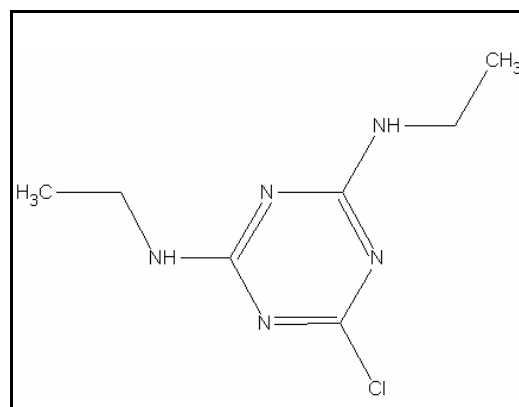




TIER I HUMAN HEALTH NONCANCER CRITERIA

SIMAZINE

CAS RN: 122-34-9
Water Solubility: 0.0005 g/100 mL
Log K_{ow} : 2.087^P
Reference Dose: 0.0052 mg/kg/day
Carcinogenicity Weight-of-Evidence Classification:



Standard

The human health noncancer simazine criterion for drinking water sources is 140 µg/L. The human health noncancer criterion for nondrinking water sources is 3,800 µg/L.

Calculations

Bioaccumulation Factor:

BAF predicted based on Log K_{ow}

Log K_{ow} = 2.087 (CLOGP program), K_{ow} = 122.2

Trophic level 3 FCM = 1.005; trophic level 4 FCM = 1.000

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

$$\text{Baseline BAF}_{T3} = (\text{FCM})(K_{ow}) = (122.2)(1.005) = 122.8$$

$$\text{Baseline BAF}_{T4} = (122.2)(1.000) = 122.2$$

$$\text{Human health BAF}_{T3} = [(122.8)(0.0182)+1](1.0) = 3.235$$

$$\text{Human health BAF}_{T4} = [(122.2)(0.0310)+1](1.0) = 4.788$$

Acceptable Daily Exposure:

From the IRIS database:

Critical Effect: Reduction in weight gain

$$\text{ADE} = \frac{\text{NOAEL}}{\text{UF}} = \frac{0.52 \text{ mg/kg-day}}{100} = 0.0052 \text{ mg/kg/d}$$

Calculation of Criteria:

$$\begin{aligned} \text{Non Drinking Water HNC} &= [(0.0052)(70)(0.8)]/0.01 + [(0.0036)(3.235) + (0.0114)(4.788)] \\ &= \mathbf{3,800 \text{ } \mu\text{g/L}} \end{aligned}$$

$$\begin{aligned} \text{Drinking Water HNC} &= [(0.0052)(70)(0.8)]/2 + [(0.0036)(3.235) + (0.0114)(4.788)] \\ &= \mathbf{140 \text{ } \mu\text{g/L}} \end{aligned}$$

References

1. USEPA 1994. Integrated Risk Information System (IRIS database) chemical file for simazine (CAS # 122-34-9).
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/Abbreviations

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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
UF	Uncertainty factor

Revision History

August 1, 1997 - 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