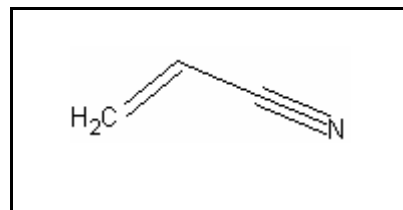




TIER I HUMAN HEALTH CANCER CRITERIA

ACRYLONITRILE

CAS RN:	107-13-1
Water Solubility:	74,500 mg/L
Log K _{ow} :	0.231 ^P
Reference Dose:	0.011 mg/kg/day
Carcinogenicity Weight-of-Evidence Classification:	Class B1; Probable human Carcinogen



Standard

The human health cancer acrylonitrile criterion for drinking water sources is 0.53 µg/L. The human health cancer criterion for nondrinking water sources is 3.0 µg/L.

Calculations

Bioaccumulation Factor:

BAF predicted based on Log K_{ow} and measured BCF (from Stephan 1993)

Log K_{ow} = 0.231 (CLOGP program), K_{ow} = 1.702, BCF = 48, Percent lipid = 4.8

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

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

$$\text{Baseline BAF}_{T3} = (1.0)[(48/1.0)-1](1/0.048) = 979.1671$$

$$\text{Baseline BAF}_{T4} = (1.0)[(48/1.0)-1](1/0.048) = 979.1671$$

$$\text{Human health BAF}_{T3} = [(979.1671)(0.0182)+1](1.0) = 18.82$$

$$\text{Human health BAF}_{T4} = [(979.1671)(0.0310)+1](1.0) = 31.35$$

Acceptable Daily Exposure:

From the IRIS database:

Critical Effect: brain and spinal cord astrocytomas, Zymbal gland carcinomas and stomach papillomas/carcinomas

$$\begin{aligned} \text{RAD} &= 0.00001/\text{q1}^* = 0.00001/0.54 \\ &= 1.8519 \times 10^{-5} \end{aligned}$$

Where:

RAD = Risk Associated Dose (mg/kg/day)
 q1^* = Cancer Slope Factor

Calculation of Criteria:

$$\begin{aligned} \text{Non Drinking Water HCC} &= [(1.8519 \times 10^{-5})(70)]/0.01 + [(0.0036)(18.82) + (0.0114)(31.35)] \\ &= 3.0 \mu\text{g/L} \end{aligned}$$

$$\begin{aligned} \text{Drinking Water HCC} &= [(1.8519 \times 10^{-5})(70)]/2 + [(0.0036)(18.82) + (0.0114)(31.35)] \\ &= 0.53 \mu\text{g/L} \end{aligned}$$

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 acrylonitrile (107-13-1).
3. 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
UF	Uncertainty factor

Revision History

September 17, 1997 - Criteria first developed

March 21, 2000 – Criteria rechecked (no modifications). Fact sheet updated.

Contact Information

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