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(2)

Excerpt from: National Library of Medicine, TOXNET (Toxicology Data Network), Hazardous Substances Data Bank (HSDB). "1,4-Dioxane." http://toxnet.nlm.nih.gov/, accessed June 11, 2007.

1,4-DIOXANE

CASRN: 123-91-1

Environmental Fate/Exposure Summary:

1,4-**Dioxane**'s production and use as a solvent for cellulose acetate, ethyl cellulose, benzyl cellulose, resins, oils, waxes, spirit-sol dyes, as well as many other organic as well as some inorganic compounds and stabilizer in chlorinated solvents, may result in its release to the environment through various waste streams. If released to the atmosphere, a vapor pressure of 38.1 mm Hg at 25 deg C indicates that 1,4-**dioxane** will exist solely in the vapor phase. Vapor-phase 1,4-**dioxane** is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 35 hours. If released to soil, 1,4-**dioxane** is expected to have very high mobility based upon a Koc of 29. Volatilization from moist soil surfaces is expected to be an important fate process based upon a Henry's Law constant of 4.8X10-6 atm-cu m/mole. 1,4-**Dioxane** may also volatilize from dry soils based upon it vapor pressure. 1,4-**Dioxane** is very slow to biodegrade and is considered recalcitrant in the environment. If released into water, 1,4-**dioxane** is not expected to adsorb to suspended solids and sediment based upon the Koc value. Volatilization from water surfaces is expected to be an important fate process based upon this compound's Henry's Law constant. Estimated volatilization half-lives for a model river and model lake are 5 and 56 days, respectively. BCF values in the range of 0.2-0.7 measured in fish, suggests bioconcentration in aquatic organisms is low. Hydrolysis and photolysis in sunlit surface waters is not expected to be important environmental fate processes for 1,4-**dioxane** since this compound lacks functional groups that hydrolyze or absorb light under environmentally relevant conditions. Occupational exposure to 1,4-**dioxane** may occur through inhalation and dermal contact with this compound at workplaces where 1,4-**dioxane** is produced or used. Monitoring data indicate that the general population may also be exposed to 1,4-**dioxane** via inhalation of ambient air and ingestion of drinking water. (SRC)

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Artificial Pollution Sources:

1,4-**Dioxane**'s production and use as a solvent for cellulose acetate, ethyl cellulose, benzyl cellulose, resins, oils, waxes, spirit-sol dyes, as well as many other organic as well as some inorganic compounds and stabilizer in chlorinated solvents(1), may result in its release to the environment through various waste streams(SRC).

[(1) O'Neil MJ, ed; Merck Index, 13th ed, Whitehouse Station, NJ Merck & Co. p 581 (2001)]**PEER REVIEWED**

Environmental Fate:

TERRESTRIAL FATE: Based on a classification scheme(1), a Koc value of 29 measured in a clay soil(2), indicates that 1,4-**dioxane** is expected to have very high mobility in soil(SRC). Volatilization from moist soil surfaces is expected based upon a Henry's Law constant of 4.8X10-6 atm-cu m/mole(3). The potential for volatilization of 1,4-**dioxane** from dry soil surfaces may exist(SRC) based upon a vapor pressure of 38.1 mm Hg(4). 1,4-**Dioxane** is very

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(2) Alexander M; Biotechnol Bioeng 15: 611-47 (1973) (3) Heukelekian H, Rand MC; J Water Pollut Control Assoc 27: 1040-53 (1955) (4) Fincher EL, Payne WJ; Appl Microbiol 10: 542-7 (1962) (5) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. McGraw-Hill NY p 9-64 (1982) (6) Kawasaki M; Ecotox Environ Safety 4: 444-54 (1980) (7) Chemicals Inspection and Testing Institute. Japan Chemical Industry Ecology - Toxicology and Information Center. ISBN 4-89074-101-1 (1992) (8) Kelley SL et al; Water Res 35: 3791-3800 (2001)]**PEER REVIEWED**

Environmental Abiotic Degradation:

The rate constant for the vapor-phase reaction of 1,4-**dioxane** with photochemically-produced hydroxyl radicals has been measured as 1.09X10-11 cu cm/molecule-sec at 25 deg C(1). This corresponds to an atmospheric half-life of about 35 hours at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(1). 1,4-**Dioxane** is not expected to undergo hydrolysis in the environment due to the lack of hydrolyzable functional groups nor to directly photolyze due to the lack of absorption in the environmental UV spectrum (>290 nm)(2). 1,4-**Dioxane** vapor was mixed with NO at 27 deg C and subjected to UV radiation equal to about 2.6 times the intensity of natural sunlight on a summer day in Freeport, TX. After 3.4 hr, 50% of the 1,4-**dioxane** had degraded(3). 1,4-**Dioxane** is oxidized by aqueous hydroxyl radicals with a half-life of 336 days at pH 7(4).

[(1) Atkinson R; J Phys Chem Ref Data Monograph 1. (1989) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 7-4, 7-5 (1990) (3) Dilling WL et al; Environ Sci Technol 10: 351-6 (1976) (4) Anbar M, Neta P; Int J Appl Radiation Isotopes 18: 493-523 (1967)]**PEER REVIEWED**

Soil Adsorption/Mobility:

The soil adsorption coefficient (Kd) for 1,4-**dioxane** measured in a grey clay soil (45% clay, 43% silt, 10% sand, 0.58% organic carbon) obtained from a landfill site in Ontario, Canada was 0.17(1). Taking into account the fraction of organic carbon, a Koc value of 29 was calculated(SRC). According to a classification scheme(2), this estimated Koc value suggests that 1,4-**dioxane** is expected to have very high mobility in soil(SRC).

[(1) Barone FS et al; J Contam Hydrol 10: 225-250 (1992) (2) Swann RL et al; Res Rev 85: 17-28 (1983)]**PEER REVIEWED**

Molecular Formula:

C4-H8-O2

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Molecular Weight:

88.10

[O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 581]**PEER REVIEWED**

Octanol/Water Partition Coefficient:

log Kow= -0.27

[Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995., p. 8]**PEER REVIEWED**