

1,4-DITHIANE

PROFILE OF DRINKING WATER CONTAMINANTS FOR EMERGENCY RESPONSE

GENERAL INFORMATION

1,4-Dithiane (diethylene disulfide) exists as a volatile, white, monoclinic, crystalline solid at room temperature. Although there is no known mechanism for 1,4-dithiane formation, mustard gas is thought to undergo polymerization and dealkylation reactions during storage to produce 1,4-dithiane.

1,4-Dithiane has been found in groundwater near Denver, Colorado, at concentrations of 3,600 to 9,678 μ g/L, and in Maryland at concentrations of 1,000 μ g/L (1 ppm).

There are few data on the environmental fate of 1,4-dithiane. However, it easily photo-oxides to sulfoxides and sulfones and readily forms metal halide-addition compounds. No studies of the fate of 1,4-dithiane in aqueous media are available.

PHARMACOKINETICS

No quantitative data on the absorption of 1,4-dithiane from oral, inhalation, or dermal exposure have been found in the available literature. One study, however, provided evidence that 1,4-dithiane is systemically absorbed following oral gavage.

HEALTH EFFECTS

Humans

No studies on the health effects of 1,4-dithiane to humans were found in the literature.

HEALTH EFFECTS

Experimental Animals

Rats given an acute oral dose of 1,4-dithiane developed central nervous system problems, tearing and crusty eyes, lethargy, and crusty noses, as well as gastrointestinal disturbances.

In a 90-day oral study with rats, the most significant finding was the presence of anisotropic crystals of an undetermined composition in the nasal olfactory mucosa of both sexes.

Morphologic lesions also occurred in female liver and male kidney, and these changes were associated with increased absolute weights of these organs.

No lifetime, reproductive, developmental, or carcinogenicity studies were available.

It has been determined that 1,4-dithiane is nonmutagenic in *Salmonella typhimurium* with and without metabolic activation. No other mutagenicity studies are available.

OTHER CRITERIA, ANALYSES, AND TREATMENT TECHNOLOGIES

No Threshold Limit Value, Short-Term-Exposure Limit, or Permissible-Exposure-Limit for 1,4-dithiane has been designated.

Gas chromatography and mass spectrometry are the most widely applied methods for analyzing 1,4-dithiane. Nuclear magnetic resonance spectroscopy has been used to analyze the chemical structure of 1,4-dithiane.

No specific information on the treatment of 1,4-dithiane in water is available.

Physical and Chemical Properties

Empirical Formula

C₄H₈S₂

Synonyms

Diethylene disulfide; Diethylene sulfide; p-Dithiane; 1,4-Dithiacyclohexane;

Tetrahydro-1,4-Dithiin: Triethylene trisulfide (early 1920s misnomer):

Tetramethylene 1,4-disulfide (German equivalent)

CAS Number

505-29-3

Physical State

White, monoclinic crystals at 25°C; moderately clear,

prism shaped crystals

Molecular Weight

120.23

Melting Point Boiling Point

111-112°C (ranging from 108-113°C)

Vapor Pressure

119-200°C (1 atm, 769 mm Hg)

Solubility

0.8 mm Hg at 25°C (estimated); 51.4 mm Hg at 111°C, over liquid (estimated);

11.88 g/L in water at 25°C.

Health Effects Data and Advisory Values

Genotoxicity

1,4-Dithiane was not mutagenic in the Ames Salmonella/Mamalian

Microsome Mutagenicity Assay.

Reproductive and Developmental Effects

No studies were available for evaluating potential reproductive and develop-

mental effects.

Cancer Classification

EPA Group D: Not classifiable as to human carcinogenicity.

Reference Dose (RfD)

0.01 mg/kg/day

Drinking Water

0.4 mg/L

Equivalent Level (DWEL)

Health Advisory Values

One-Day

0.4 mg/L

Ten-Day

0.4 mg/L

Longer-Term (child)

0.4 mg/L

Longer-Term (adult)

1.0 mg/L

Lifetime

0.08 mg/L

This summary was developed using information from the Drinking Water Health Advisory.

A copy of the Health Advisory is available from the National Technical Information Service at (703) 487-4650.

The order number for the 1,4-Dithiane Health Advisory is PB93-117026.

For further information contact EPA's Office of Science and Technology at (202) 260-7571.

Office of Science and Technology
Office of Water
U.S. Environmental Protection Agency
401 M Street, SW
Washington, DC 20460

January 18, 1993



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