3-Chloro-2-methylpropene CAS No. 563-47-3

Reasonably anticipated to be a human carcinogen First listed in the *Fifth Annual Report on Carcinogens* (1989) Also known as 3-chloro-2-methyl-1-propene

$$CI \xrightarrow{\begin{array}{c} H_2 \\ C \\ C \\ C \\ CH_2 \end{array}} CH_3$$

Carcinogenicity

3-Chloro-2-methylpropene is *reasonably anticipated to be a human carcinogen* based on sufficient evidence of carcinogenicity from studies in experimental animals.

Cancer Studies in Experimental Animals

Oral exposure to 3-chloro-2-methylpropene caused tumors in two rodent species and at several different tissue sites. Administration of 3-chloro-2-methylpropene by stomach tube caused benign or malignant tumors of the forestomach (squamous-cell papilloma or carcinoma) in mice and rats of both sexes; in mice, some of the malignant tumors metastasized to other organs. Kidney and urinary-bladder tumors in male rats may also have been related to 3-chloro-2-methylpropene exposure (NTP 1986).

Since 3-chloro-2-methylpropene was listed in the *Fifth Annual Report on Carcinogens*, an additional study in mice has been identified. Inhalation exposure to 3-chloro-2-methylpropene caused benign forestomach tumors (squamous-cell papilloma) in mice of both sexes and benign Harderian-gland tumors (adenoma) in female mice (Katagiri *et al.* 2000).

Cancer Studies in Humans

No epidemiological studies were identified that evaluated the relationship between human cancer and exposure specifically to 3-chloro-2-methylpropene.

Properties

3-Chloro-2-methylpropene exists at room temperature as a colorless to straw-colored liquid with a sharp, disagreeable odor. It is slightly soluble in water, soluble in acetone, very soluble in chloroform, and miscible with ethanol and diethyl ether. It can polymerize on exposure to light and is explosively flammable. The vapors are heavier than air and may travel from the source and collect in low or confined areas (IARC 1995, Akron 2009, HSDB 2009). Physical and chemical properties of 3-chloro-2-methylpropene are listed in the following table.

Property	Information
Molecular weight	90.6 ^a
Specific gravity	0.92 at 20°C/4°C ^a
Melting point	< -80°Ca
Boiling point	71°C to 72°C ^a
$\log K_{ow}$	2.48 ^b
Water solubility	1.4 g/L at 25°C ^b
Vapor pressure	101.7 mm Hg at 20°C ^a
Vapor density relative to air	3.1 ^a

Sources: aHSDB 2009, bChemIDplus 2009.

Use

3-Chloro-2-methylpropene is used primarily as a chemical intermediate in the production of organic chemicals, including 3-dimethylamino-2-methylpropyl chloride hydrochloride, 2-methyl-

epichlorohydrin, and the pesticides carbofuran, ethalfluralin, and fenbutatin oxide. In 1985, over 97% of its production was used as an intermediate in the production of agricultural chemicals; the remainder was used as a textile or perfume additive or for other purposes. Outside of the United States, 3-chloro-2-methylpropene has been used as an insecticide fumigant for grains, tobacco, and soil; however, it is not registered for use as a pesticide in the United States (NTP 1986, IARC 1995, HSDB 2009).

Production

In 1984, U.S. production of 3-chloro-2-methylpropene was estimated at 12 million to 24 million pounds (NTP 1986). In 2009, 3-chloro-2-methylpropene was produced by one manufacturer worldwide, in China (SRI 2009), and was available from 18 suppliers, including 9 U.S. suppliers (ChemSources 2009). Reports filed in 1986, 1990, 1998, 2002, and 2006 under the U.S. Environmental Protection Agency's Toxic Substances Control Act Inventory Update Rule indicated that U.S. production plus imports of 3-chloro-2-methylpropene totaled 10 million to 50 million pounds; in 1994, the quantity was 1 million to 10 million pounds (EPA 2004, 2009).

Exposure

The primary routes of potential human exposure to 3-chloro-2methylpropene are inhalation, ingestion, and dermal contact. Use as a fumigant would result in the direct release of 3-chloro-2-methylpropene to the environment; however, this use has not been reported in the United States (HSDB 2009). Consumers could be exposed through ingestion of food products that had absorbed 3-chloro-2-methylpropene (NTP 1986). According to EPA's Toxics Release Inventory, environmental releases of 3-chloro-2-methylpropene in 1996 and 1997 totaled 26,000 lb. In 2007, one facility released 6,536 lb to air (TRI 2009). If released to air, 3-chloro-2-methylpropene will exist only in the vapor phase and be degraded by reaction with hydroxyl radicals, with an estimated half-life of 10 hours, and with ozone, with an estimated half-life of 27 hours (HSDB 2009). If released to water, 3-chloro-2-methylpropene will volatilize, with an estimated half-life of 3 hours in a model river and 4 days in a model lake. If released to soil, it is expected to volatilize and to have high mobility. It is not expected to bind to soil or sediments. It is expected to biodegrade under aerobic conditions and to have a low potential for bioaccumulation. Around 1980, 3-chloro-2-methylpropene was detected in the ambient air in an industrial area near Curtis Bay, Maryland, at concentrations of up to $400 \mu g/m^3$ (NTP 1986).

Occupational exposure to 3-chloro-2-methylpropene may occur during its manufacture or use as an intermediate in organic synthesis. No data on occupational exposure were found.

Regulations

Environmental Protection Agency (EPA)

Clean Air Act

New Source Performance Standards: Manufacture of 3-chloro-2-methylpropene is subject to certain provisions for the control of volatile organic compound emissions.

Emergency Planning and Community Right-To-Know Act Toxics Release Inventory: Listed substance subject to reporting requirements.

References

Akron. 2009. *The Chemical Database*. The Department of Chemistry at the University of Akron. http://ull. chemistry.uakron.edu/erd and search on CAS number. Last accessed: 8/11/09.

ChemlDplus. 2009. ChemlDplus Advanced. National Library of Medicine. http://chem.sis.nlm.nih.gov/chemidplus/chemidheavy.jsp and select Registry Number and search on CAS number. Last accessed: 9/11/00

ChemSources. 2009. *Chem Sources - Chemical Search*. Chemical Sources International. http://www.chemsources.com/chemonline.html and search on chloromethylpropene. Last accessed: 8/11/09.

EPA. 2004. Non-confidential IUR Production Volume Information. U.S. Environmental Protection Agency. http://www.epa.gov/oppt/iur/tools/data/2002-vol.html and search on CAS number.

EPA. 2009. Non-confidential 2006 IUR Records by Chemical, Including Manufacturing, Processing and Use Information. U.S. Environmental Protection Agency. http://cfpub.epa.gov/iursearch/2006_iur_companyinfo.cfm?chemid=5037.

HSDB. 2009. Hazardous Substances Data Bank. National Library of Medicine. http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB and search on CAS number. Last accessed: 8/11/09.

IARC. 1995. 3-Chloro-2-methylpropene. In *Dry Cleaning, Some Chlorinated Solvents and Other Industrial Chemicals*. IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Humans, vol. 63. Lyon, France: International Agency for Research on Cancer. pp. 325-333.

Katagiri T, Takeuchi T, Mine T, Noguchi T, Nishizawa T, Yamamoto S, Okudaira M, Matsushima T. 2000. Chronic inhalation toxicity and carcinogenicity studies of 3-chloro-2-methylpropene in BDF_1 mice. Ind Health 38(3): 309-318.

NTP. 1986. Toxicology and Carcinogenesis Studies of 3-Chloro-2-methylpropene (Technical Grade Containing 5% Dimethylvinyl Chloride) (CAS No. 563-47-3) in F344/N Rats and B6C3F, Mice (Gavage Studies). Technical Report Series no. 300. NIH Publication No. 86-2556. Research Triangle Park, NC: National Toxicology Program. 196 pp.

SRI. 2009. *Directory of Chemical Producers*. Menlo Park, CA: SRI Consulting. Database edition. Last accessed: 8/11/09.

TRI. 2009. TRI Explorer Chemical Report. U.S. Environmental Protection Agency. http://www.epa.gov/triexplorer and select 3-Chloro-2-Methyl-1-Propene. Last accessed: 8/11/09.