

MICHIGAN DEPARTMENT OF ENVIRONMENTAL QUALITY

INTEROFFICE COMMUNICATION

TO: File for 1-Propanethiol (CAS# 107-03-9)

FROM: Doreen Lehner, Toxics Unit, Air Quality Division

SUBJECT: Screening Level Determination for 1-Propanethiol

DATE: June 6, 2013

The Initial Threshold Screening Level for 1-propanethiol is 16 $\mu\text{g}/\text{m}^3$ with a 1-hour averaging time.

1-Propanethiol (CAS# 107-03-9) also known as n-propyl mercaptan is an alkyl thiol with a molecular weight of 76.16 g/mol. 1-Propanethiol (water density = 0.843 g/cm³; odor threshold is 0.75 ppb and is a clear, colorless liquid with a strong offensive rotten cabbage-like odor and is less dense than water, which means that it will float on the water's surface. In gaseous form, 1-propanethiol (relative vapor density = 2.63) is also more dense than air and may travel along the ground (NIOSH, 2008; Haug, 1993). 1-Propanethiol is used as a chemical intermediate in the manufacture of herbicides, pesticides, and pharmaceuticals; as a polymer additive; as a flavoring agent; and as odorants in commercial applications (ex. propane and natural gas). 1-Propanethiol is released from crushed onions and other bulbs in the *Allium* plant family. It can be produced as a degradation product of some pesticides (ex. Ethoprop), and may also be formed during waste decomposition (OECD, 2010).



Figure 1. 1-Propanethiol Structure

A literature review was conducted to attempt to derive an initial threshold screening level (ITSL) for 1-propanethiol. The following references and databases were searched: Chemical Criteria Database (CCD), United States Environmental Protection Agency (US EPA) Integrated Risk Information System (IRIS), National Institute for Occupational Safety and Health (NIOSH), American Conference of Governmental Industrial Hygienists (ACGIH) Threshold Limit Values and Biological Exposure Indices (TLV/BEI) 2012 guide, National Toxicology Program (NTP) Study Database, International Agency for Research on Cancer (IARC), Acute Database, Chemical Abstract Service (CAS) Online (searched 9/20/12), National Library of Medicine (NLM)-online, EPA Aggregated

Computational Toxicology Resource (ACToR) Database, US EPA TSCATS database, and Hazardous Substances Data Bank (HSDB).

Not many studies on 1-propanethiol have been performed, but of the inhalation studies, all were acute toxicity studies. Fairchild, et. al., (1958) studied 1-propanethiol on both rats and mice. "Male Wistar rats (6/group) were exposed (whole body) to n-propyl mercaptan for four hours at analytical concentrations of 3,050, 4,500, 8,340, or 11,260 ppm (9.5, 14.0, 26.0, or 35.1 mg/L)...All animals survived the exposure to 3,050 and 4,500 ppm. At 8,340 ppm, four of the five animals died; three died by 4 hours, and one by 24 hours. All 5 animals died within 4 hours following exposure to 11,260 ppm. Increased respiration, restlessness, uncoordinated movement, staggering gait, muscular weakness, cyanosis, and sedation were seen at higher concentrations, including those causing mortality. Irritation of the mucous membrane was evidenced by rubbing of the eyes and nose, eye closure, watering of the eyes, cortical opacities and retracting of the head were the major clinical signs. The 4-hour LC₅₀ was 7,300 ppm (22.8 mg/L)." (OECD, 2010)

Fairchild, et. al., (1958) exposed male Swiss mice via whole body to 1-propanethiol "for 4 hours at concentrations of 3,050, 4,500, 8,340, or 11,260 ppm (9.51, 14.03, 26.01, or 35.11 mg/L). All animals survived exposure at 3,050 ppm. At 4,500 ppm, 14 of the 20 animals died by 15 days. All animals died within 4 hours following exposure to 8,340 and 11,260 ppm...The 4-hour LC₅₀ was 4,010 ppm (12.5 mg/L)." (OECD, 2010) The clinical signs of exposure in the mice were the same as listed above for rats.

The Fairchild et al., (1958) study does not address the irritancy effects of this compound. NIOSH has established a recommended exposure limit (REL) of 0.5 ppm (1.6 mg/m³) [15-minute ceiling level] to be protective against acute irritation effects which appear to be the most sensitive endpoints identified by available data. According to Rule 232(1)(c) an ITSL can be determined using the NIOSH REL using the equation below:

$$ITSL = \frac{\text{occupational exposure level}}{100} = \frac{1.6 \text{ mg}/\text{m}^3}{100} = 0.016 \text{ mg}/\text{m}^3 = 16 \mu\text{g}/\text{m}^3$$

The Initial Threshold Screening Level for 1-propanethiol is 16 µg/m³ with a 1-hour averaging time, but the odor threshold for this compound should be taken into consideration when developing permit conditions since it is 0.75 (2.3 µg/m³) (Haug, 1993).

References:

Act 451 of 1994. Natural Resources and Environmental Protection Act and Air Pollution Control Rules, Michigan Department of Environmental Quality.

Fairchild, E.J. and Stockinger, H.E. 1958. Toxicologic studies on organic sulfur compounds. 1. Acute toxicity of some aliphatic and aromatic thiols. Am. Ind. Hyg. Assoc. J. 19:171-189.

Haug, RT. 1993. Odor Management 1 – Quantifying and Treating. Table 16.4. The Variation in Odor Recognition Threshold for Organic Sulfur Compounds. In The Practical Handbook of Compost Engineering. Lewis Publishers, CRC Press LLC. ISBN: 0-87371-373-7. Pp. 553.

NIOSH. 2008. International Chemical Safety Card for 1-Propanethiol. Available online at: <http://www.cdc.gov/niosh/ipcsneng/neng1492.html>

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OECD. 2010. SIDS Dossier. OECD HPV Chemical Programme, SIDS Dossier approved at SIAM 30 (20-22 April 2010).

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