

1-Heptanethiol Information Sheet

(CAS Number 1639-09-4)

Background

In January 2010, the New Mexico Environment Department (NMED) modified the Intel-New Mexico facility's air permit to allow emission of the chemical 1-Heptanethiol (NMED 2010). Intel-New Mexico uses 1-Heptanethiol in semiconductor fabrication. Because of community concerns and because of the lack of readily available information about 1-Heptanethiol, ATSDR prepared this information sheet.

Synonyms

- Heptyl mercaptan (Sigma-Aldrich 2008)
- n-Heptanethiol

Uses

1-Heptanethiol is a chemical intermediary in the

- Production of fuels, dyes, pharmaceuticals, and other chemicals (NJDHSS 1999)
- Creation or production of flavor concentrates of all types (The Good Scents Company 2010)

- Production of fuel additives, catalysts, pesticides, perfume, solvents, and synthetic rubber (Lookchem.com 2010)
- Flavoring of baked goods, breakfast cereals, cheese, condiments/relish, confectionary frostings, fats/oils, fish products, frozen dairy, fruit ices, gelatins/puddings, gravies, hard candy, imitation dairy, meat products, milk products, grains, poultry, processed fruits, seasonings/flavors, snack foods, soft candy, soups, and sweet sauces (The Good Scents Company 2010)
- Ink used in micro-contact printing/lithography (Sigma-Aldrich, 2010)

Physical and chemical characteristics

- 1-Heptanethiol is a colorless liquid with a strong odor (NIOSH 2005; IPCS/NIOSH 2006)

See Table 1 below.

Table 1. 1-Heptanethiol Chemical and Physical Characteristics

Characteristic	Value/Description	Reference
Molecular formula:	C ₇ H ₁₆ S/ CH ₃ (CH ₂) ₆ SH	NIOSH 2005 IPCS/NIOSH 2006 NIOSH/RTECS 1997 NIST/CSTL 2008
Reactive group:	Sulfur, Organic	NOAA 2009
Molecular weight:	132.3	NIOSH 2005
	132.29	NIOSH/RTECS 1997
	132.268	NIST/CSTL 2008
Boiling point:	351 °F	NIOSH 2005
	176 °C	IPCS/NIOSH 2006
Melting point:	-43 °C	IPCS/NIOSH 2006
	-41.3 °C	NOAA 2009
Freezing point:	-46 °F	NIOSH 2005
Solubility:	Insoluble	NIOSH 2005
	in water = very poor	IPCS/NIOSH 2006
Specific Gravity (relative	0.84	NIOSH 2005

Characteristic	Value/Description	Reference
density): [water = 1]		IPCS/NIOSH 2006
Flash Point:	115 °F	NIOSH 2005
	46 °C c.c.	IPCS/NIOSH 2006
Vapor pressure, kPa at °C:	0.17	IPCS/NIOSH 2006
Relative vapor density (air = 1):	4.6	IPCS/NIOSH 2006
Relative density of the vapor/air-mixture at 20 °C (air = 1):	1.006	IPCS/NIOSH 2006
Explosive limits, vol% in air:	0.9(lower) to unknown (upper)	IPCS/NIOSH 2006
Octanol/water partition coefficient as log Pow:	3.7	IPCS/NIOSH 2006
Viscosity:	1.24 cp (20 °C)	IPCS/NIOSH 2006
Refractive index:	1.4521 (20 °C)	IPCS/NIOSH 2006
Combustibility:	Class II Combustible Liquid: Flash Point. at or above 100 °F and below 140 °F	NIOSH 2005

Characteristic	Value/Description	Reference
	Explosive vapor/air mixtures may form above 46 °C	IPCS/NIOSH 2006
Incompatibility & Reactivity:	Oxidizers, reducing agents, strong acids & bases, alkali metals	NIOSH 2005 IPCS/NIOSH 2006
	No rapid reaction with air or water	NOAA 2009
	Oxidizing agents, strong acids and strong bases, alkali metals, and nitric acid	NOAA 2009
	Can react with water, steam, or acids to produce toxic and flammable vapors.	NOAA 2009
	Reacts violently with powerful oxidizing agents such as calcium hypochlorite to generate sulfur oxides.	NOAA 2009
	Reacts with hydrides to form flammable H ₂ gas; reacts with halogenated hydrocarbons to yield Hydrogen Halides (e.g., HCl).	NOAA 2009

Characteristic	Value/Description	Reference
	Reacts exothermically with aldehydes.	NOAA 2009
Flammability:	Flammable: gives off irritating or toxic fumes (or gases) in a fire	IPCS/NIOSH 2006

Odor threshold and description

- Given the structural likeness of 1-heptanethiol to 2-heptanethiol, the odor threshold for 2-heptanethiol (10 parts-per-billion) is likely similar to the odor threshold for 1-heptanethiol (Intel 2007).
- Odor description at 0.10 % in propylene glycol: sulfurous onion (The Good Scents Company 2010)

Toxicological information

- Health effects of exposure to 1-Heptanethiol have not been adequately investigated (IPCS/NIOSH 2006).
- **Inhalation risk:** On evaporation of this substance at 20 °C, the rate is unavailable at which a harmful concentration in the air is reached (IPCS/NIOSH 2006).
- Toxicity data have not been evaluated (NIOSH/RTECS 1997).

- **Acute toxicity data and references:** In certain laboratory animals (intra-peritoneal³ mouse), a lethal dose (50 percent kill) is 200 mg/kg (NTIS AD277-689—as cited in NIOSH/RTECS 1997).
- **No Observed Adverse Effect Level (NOAEL):** Most relevant data are from compounds also used as flavoring agents that are structurally related to 1-Heptanethiol. From a 90-day study in male and female rats, 0.56 milligrams (mg/kg) per kilogram of body weight per day of cyclopentanethiol (No. 516)—a flavoring agent and structurally related compound—provides an adequate margin of safety (at least 80 000) in relation to currently estimated intake levels. This NOAEL is also appropriate for two other substances structurally related to 1-Heptanethiol because they are also simple thiols: 1-pentanethiol and 2-heptanethiol. For these substances, the NOAEL of 0.56 mg/kg body weight provides adequate margins of safety (range of >100 000 to >2 million) in relation to the currently estimated intake levels from use as flavoring agents. World Health Organization (WHO) has determined that as a flavoring agent, 1-Heptanethiol is not a safety concern. (WHO 2007; WHO 2008)
- The Expert Panel of the Flavor and Extract Manufacturers Association (FEMA) classified 1-Heptanethiol as “Generally Recognized as Safe” for use as a flavoring ingredient in food (FEMA No. 4259) (WHO 2007; Waddell 2007).

³ Serous membrane lining the abdominopelvic walls

Acute/chronic/signs and exposure symptoms

- **Exposure routes:** Inhalation, ingestion; skin or eye contact or both (NIOSH 2005; IPCS/NIOSH 2006)
- **Irritation:** Eyes, skin, nose, throat (NIOSH 2005; NOAA 2009); redness, pain (IPCS/NIOSH 2006)
- **Inhalation:** Lassitude (weakness, exhaustion), cyanosis (a bluish skin discoloration), increased respiration, nausea, drowsiness, headache, vomiting (NIOSH 2005; IPCS/NIOSH 2006)
- **Target organs:** Eyes, skin, respiratory system, central nervous system, blood (NIOSH 2005)
- **Short-term exposure:** Irritating to the eyes, the skin, and the respiratory tract. Exposure at high levels could cause diminished consciousness (IPCS/NIOSH 2006).

Exposure limits

- **NIOSH Recommended Exposure Limit (REL):** Ceiling Limit: 0.5 parts per million (ppm) (2.7 mg/m³) [15-minute] (NIOSH 2005; NIOSH DHHS #92-100, 1992 as cited in NIOSH/RTECS 1997).

REL Rationale

Both human and animal toxicity data show adverse effects from relatively short-term, 50-ppm thiol inhalation exposure; thiol workplace concentrations should be

kept well below this concentration. But at 0.4-ppm exposure, no effects were observed, and when inhalation exposure stopped altogether, even the minimal effects ceased for that olfactory fatigue and mucosal⁴ irritation observed when persons were exposed to 4-ppm ethanethiol. Because no evidence supports the suggestion that adherence to the 0.5 ppm TLV results in toxicity, NIOSH recommends that for any 15-minute period, the concentration of C1–C12,⁵ C16, C18 alkane thiols, or cyclohexanethiol, or any combination of these thiols in workplace air should not exceed 0.5 ppm as a ceiling concentration. On short-term exposure, the toxic action of thiols is expressed largely by reversible mucosal irritation. Thus NIOSH deems a ceiling concentration limit more appropriate than a TWA concentration limit. The use of a ceiling concentration rather than a TWA effectively increases worker protection about twofold. NIOSH believes that adherence to the proposed ceiling concentration would prevent both irritation and systemic effects arising from occupational exposure to the aliphatic thiols (NIOSH 1978).⁶

⁴ Mucous coat or membrane of various tubular structures

⁵ 1-heptanethiol is C7

⁶ See the following for further details on the individual studies used:

<http://www.cdc.gov/niosh/pdfs/78-213d.pdf>

<http://www.cdc.gov/niosh/pdfs/78-213a.pdf>

- **OSHA Permissible Exposure Limit (PEL):** none (NIOSH 2005)
- **Immediately Dangerous to Life and Health (IDLH):** data unavailable (NOAA 2009)
- Levels approved for use in food: 0.1 to 2.0 ppm (Waddell 2007)

Control/disposal/treatment methods

- **Spillage disposal:** Remove all ignition sources (personal protection: filter respirator for organic gases and vapors); collect leaking liquid in sealable containers and absorb remaining liquid in sand or inert absorbent and remove to safe place. DO NOT wash away into sewer (IPCS/NIOSH 2006) [See NIOSH 2005 for detailed respirator recommendations].
- **Storage:** Fireproof; separated from strong oxidants, strong bases, strong acids (IPCS/NIOSH 2006).
- **Packaging and Labeling:** UN Hazard Class: 3; UN Packing Group: III (IPCS/NIOSH 2006)

Stability/fate and transport in the environment

- The vapor is heavier than air and may travel along the ground; distant ignition is possible (IPCS/NIOSH 2006).
- As 1-Heptanethiol is heated it decomposes, producing toxic and corrosive fumes, including hydrogen sulfide and sulfur oxides (IPCS/NIOSH 2006).

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Glossary of Terms

IDLH - Immediately Dangerous to Life and Health. An atmospheric concentration of any toxic, corrosive, or asphyxiant substance that poses an immediate threat to life or would cause irreversible or delayed adverse health effects or would interfere with a person's ability to escape from a dangerous atmosphere.

NOAEL -No-observed-adverse-effect level. The highest tested dose of a substance that has been reported to have no harmful (adverse) health effects on people or animals.

PEL - Permissible Exposure Limit. PELs are set by the Occupational Safety and Health Administration (OSHA) to protect workers against the health effects of exposure to hazardous substances. PELs are limits on the amount or concentration of a substance in the air based on an 8-hour, time-weighted average (TWA) exposure.

REL – Recommended Exposure Limit. A National Institute for Occupational Safety and Health (NIOSH) time-weighted average concentration for up to a 10-hour work day during a 40-hour work week.