

1 Identification

Product identifier

Product name: 1-Hexanethiol

Stock number: L09659

CAS Number:
111-31-9

EC number:
203-857-0

Relevant identified uses of the substance or mixture and uses advised against.
Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Information Department: Health, Safety and Environmental Department

Emergency telephone number:

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)



GHS02 Flame

Flam. Liq. 3 H226 Flammable liquid and vapour.



GHS06 Skull and crossbones

Acute Tox. 3 H331 Toxic if inhaled.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Hazards not otherwise classified Stench

Label elements

GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms



GHS02 GHS06

Signal word

Danger

Hazard statements

H226 Flammable liquid and vapour.

H302 Harmful if swallowed.

H331 Toxic if inhaled.

Precautionary statements

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P280 Wear protective clothing.

P309 IF exposed or if you feel unwell:

P310 Immediately call a POISON CENTER or doctor/physician.

P403 Store in a well-ventilated place.

WHMIS classification

B2 - Flammable liquid

D1A - Very toxic material causing immediate and serious toxic effects



Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH 3 Health (acute effects) = 3

FIRE 3 Flammability = 3

REACTIVITY 1 Physical Hazard = 1

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances

CAS# Description:

111-31-9 1-Hexanethiol

Concentration: ≤100%

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(Contd. of page 1)

4 First-aid measures
Description of first aid measures
After inhalation
Supply fresh air. If required, provide artificial respiration. Keep patient warm.
Seek immediate medical advice.
After skin contact
Immediately wash with water and soap and rinse thoroughly.
Seek immediate medical advice.
After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.
After swallowing Seek medical treatment.
Information for doctor
Most important symptoms and effects, both acute and delayed
Harmful if swallowed.
Toxic if inhaled.
Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures
Extinguishing media
Suitable extinguishing agents Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
Special hazards arising from the substance or mixture
If this product is involved in a fire, the following can be released:
Carbon monoxide and carbon dioxide
Sulfur oxides (SOx)
Hydrogen sulfide
Advice for firefighters
Protective equipment:
Wear self-contained respirator.
Wear fully protective impervious suit.

6 Accidental release measures
Personal precautions, protective equipment and emergency procedures
Wear protective equipment. Keep unprotected persons away.
Ensure adequate ventilation
Keep away from ignition sources
Environmental precautions: Do not allow material to be released to the environment without proper governmental permits.
Methods and material for containment and cleaning up:
Keep away from ignition sources.
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Dispose of contaminated material as waste according to section 13.
Ensure adequate ventilation.
Prevention of secondary hazards: Keep away from ignition sources.
Reference to other sections
See Section 7 for information on safe handling
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

7 Handling and storage
Handling
Precautions for safe handling
Handle under dry protective gas.
Keep container tightly sealed.
Store in cool, dry place in tightly closed containers.
Ensure good ventilation at the workplace.
Information about protection against explosions and fires:
Protect against electrostatic charges.
Fumes can combine with air to form an explosive mixture.
Keep ignition sources away.
Conditions for safe storage, including any incompatibilities
Storage
Requirements to be met by storerooms and receptacles: No special requirements.
Information about storage in one common storage facility:
Store away from air.
Store away from strong bases.
Store away from oxidizing agents.
Store away from reducing agents.
Store away from alkali metals.
Further information about storage conditions:
Store under dry inert gas.
This product is air sensitive.
Keep container tightly sealed.
Store in cool, dry conditions in well sealed containers.
Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection
Additional information about design of technical systems:
Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.
Control parameters
Components with limit values that require monitoring at the workplace:
111-31-9 1-Hexanethiol (100.0%)

REL (USA)	Ceiling limit value: 2.7* mg/m³, 0.5* ppm *15-min
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Additional information: No data

Product name: 1-Hexanethiol

(Contd. of page 2)

Exposure controls
Personal protective equipment
General protective and hygienic measures
The usual precautionary measures for handling chemicals should be followed.
Keep away from foodstuffs, beverages and feed.
Remove all soiled and contaminated clothing immediately.
Wash hands before breaks and at the end of work.
Do not inhale dust / smoke / mist.
Maintain an ergonomically appropriate working environment.
Breathing equipment: Use suitable respirator when high concentrations are present.
Recommended filter device for short term use:
Use a respirator with multi-purpose combination (US) or type ABEK (EN 14387) as a backup to engineering controls. Risk assessment should be performed to determine if air-purifying respirators are appropriate. Only use equipment tested and approved under appropriate government standards such as NIOSH (USA) or CEN (EU).
Protection of hands:
Impervious gloves
Check protective gloves prior to each use for their proper condition.
The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.
Eye protection: Safety glasses
Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties

General Information

Appearance:

Form: Liquid
Odor: Stench
Odor threshold: Not determined.

pH-value: Not determined.

Change in condition

Melting point/Melting range: -81 °C (-114 °F)
Boiling point/Boiling range: 150-154 °C (302-309 °F)
Sublimation temperature / start: Not determined

Flash point: 30 °C (86 °F)
Flammability (solid, gaseous) Not determined.
Ignition temperature: 247 °C (477 °F)
Decomposition temperature: Not determined
Auto igniting: Not determined.

Danger of explosion: Product is not explosive. However, formation of explosive air/vapor mixtures is possible.

Explosion limits:

Lower: 1 Vol %
Upper: 8.4 Vol %
Vapor pressure at 25 °C (77 °F): 6 hPa (5 mm Hg)
Density at 20 °C (68 °F): 0.838 g/cm³ (6.993 lbs/gal)
Relative density Not determined.
Vapor density Not determined.
Evaporation rate Not determined.
Solubility in / Miscibility with
Water: Not miscible or difficult to mix
Partition coefficient (n-octanol/water): Not determined.
Viscosity:
dynamic at 20 °C (68 °F): 0.813 mPas
kinematic: Not determined.
Other information No further relevant information available.

10 Stability and reactivity

Reactivity No information known.
Chemical stability Stable under recommended storage conditions.
Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.
Possibility of hazardous reactions Reacts with strong oxidizing agents
Conditions to avoid No further relevant information available.
Incompatible materials:
Air
Oxidizing agents
Bases
Reducing agents
Alkali metals
Hazardous decomposition products:
Carbon monoxide and carbon dioxide
Sulfur oxides (SOx)
Hydrogen sulfide

11 Toxicological information

Information on toxicological effects

Acute toxicity:

Harmful if swallowed.
Toxic if inhaled.
The Registry of Toxic Effects of Chemical Substances (RTECS) contains acute toxicity data for this substance.

LD/LC50 values that are relevant for classification:

Oral	LD50	1254 mg/kg (rat)
Inhalative	LC50/4H	1080 ppm/4H (rat)

Skin irritation or corrosion: May cause irritation

Eye irritation or corrosion: May cause irritation

Sensitization: No sensitizing effects known.

Germ cell mutagenicity: No effects known.

Carcinogenicity: No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.

Reproductive toxicity: No effects known.

(Contd. on page 4)
USA

Product name: 1-Hexanethiol

(Contd. of page 3)

Specific target organ system toxicity - repeated exposure: No effects known.
Specific target organ system toxicity - single exposure: No effects known.
Aspiration hazard: No effects known.
Subacute to chronic toxicity: No effects known.
Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.
Carcinogenic categories
OSHA-Ca (Occupational Safety & Health Administration) Substance is not listed.

12 Ecological information

Toxicity
Aquatic toxicity: No further relevant information available.
Persistence and degradability No further relevant information available.
Bioaccumulative potential No further relevant information available.
Mobility in soil No further relevant information available.
Additional ecological information:
General notes:
Do not allow material to be released to the environment without proper governmental permits.
Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.
Avoid transfer into the environment.
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.
Other adverse effects No further relevant information available.

13 Disposal considerations

Waste treatment methods
Recommendation Consult state, local or national regulations to ensure proper disposal.
Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.

14 Transport information

UN-Number DOT, IMDG, IATA	UN3071
UN proper shipping name DOT IMDG, IATA	Mercaptans, liquid, toxic, flammable, n.o.s. (1-Hexanethiol) MERCAPTANS, LIQUID, TOXIC, FLAMMABLE, N.O.S. (1-Hexanethiol)
Transport hazard class(es) DOT  Class Label Class Label IMDG, IATA  Class Label	6.1 Toxic substances. 6.1+3 6.1 (TF1) Toxic substances 6.1+3 6.1 Toxic substances. 6.1+3
Packing group DOT, IMDG, IATA	II
Environmental hazards:	Not applicable.
Special precautions for user EMS Number:	Warning: Toxic substances F-E,S-D
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code Not applicable.	
Transport/Additional information:	
DOT Marine Pollutant (DOT):	No
UN "Model Regulation":	UN3071, Mercaptans, liquid, toxic, flammable, n.o.s. (1-Hexanethiol), 6.1 (3), II

15 Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)
Hazard pictograms



GHS02 GHS06
Signal word Danger
Hazard statements
H226 Flammable liquid and vapour.
H302 Harmful if swallowed.
H331 Toxic if inhaled.
Precautionary statements
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P280 Wear protective clothing.
P309 IF exposed or if you feel unwell:
P310 Immediately call a POISON CENTER or doctor/physician.

(Contd. on page 5)
USA

Product name: **1-Hexanethiol**

(Contd. of page 4)

P403 Store in a well-ventilated place.

National regulations

All components of this product are listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical substance Inventory.
All components of this product are listed on the Canadian Domestic Substances List (DSL).

SARA Section 313 (specific toxic chemical listings) Substance is not listed.

California Proposition 65

Prop 65 - Chemicals known to cause cancer Substance is not listed.

Prop 65 - Developmental toxicity Substance is not listed.

Prop 65 - Developmental toxicity, female Substance is not listed.

Prop 65 - Developmental toxicity, male Substance is not listed.

Information about limitation of use: For use only by technically qualified individuals.

Other regulations, limitations and prohibitive regulations

Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.

The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.

Substance is not listed.

Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.

Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department

Date of preparation / last revision 01/17/2017 / -

Abbreviations and acronyms:

RID: Règlement International concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)

IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)

ICAO: International Civil Aviation Organization

ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

EINECS: European Inventory of Existing Commercial Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

HMS: Hazardous Materials Identification System (USA)

WHMIS: Workplace Hazardous Materials Information System (Canada)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

vPvB: very Persistent and very Bioaccumulative

ACGIH: American Conference of Governmental Industrial Hygienists (USA)

OSHA: Occupational Safety and Health Administration (USA)

NTP: National Toxicology Program (USA)

IARC: International Agency for Research on Cancer

EPA: Environmental Protection Agency (USA)

Flam. Liq. 3: Flammable liquids, Hazard Category 3

Acute Tox. 4: Acute toxicity, Hazard Category 4

Acute Tox. 3: Acute toxicity, Hazard Category 3