

ALFAAL09659

1-Hexanethiol

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明: Product Description:	1-己硫醇 1-Hexanethiol
Cat No. :	L09659
Synonyms	Hexyl mercaptan
CAS No	111-31-9
Molecular Formula	C6 H14 S
Supplier	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
Emergency Telephone Number	For information US call: 001-800-227-6701 / Europe call: +32 14 57 52 11 Emergency Number US :001-201-796-7100 / Europe : +32 14 57 52 99 CHEMTREC Tel. No. US :001-800-424-9300 / Europe :001-703-527-3887
E-mail address	begel.sdsdesk@thermofisher.com
Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State
Liquid

Appearance
Colorless

Odor
Stench

Emergency Overview

Flammable liquid and vapor. Toxic if inhaled. Causes damage to organs. Harmful if swallowed. Stench.

Classification of the substance or mixture

Flammable liquids.	Category 3
Acute Oral Toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 3
Specific target organ toxicity - (single exposure)	Category 1

Label Elements



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Signal Word**Danger****Hazard Statements**

H226 - Flammable liquid and vapor
H331 - Toxic if inhaled
H370 - Causes damage to organs
H302 - Harmful if swallowed

Precautionary Statements**Prevention**

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
P240 - Ground and bond container and receiving equipment
P241 - Use explosion-proof electrical/ ventilating/ lighting equipment
P242 - Use non-sparking tools
P243 - Take action to prevent static discharges
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P264 - Wash face, hands and any exposed skin thoroughly after handling
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P270 - Do not eat, drink or smoke when using this product
P271 - Use only outdoors or in a well-ventilated area

Response

P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P311 - Call a POISON CENTER or doctor
P330 - Rinse mouth
P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish

Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed
P405 - Store locked up

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Physical and Chemical Hazards

Vapors may cause flash fire or explosion. Flammable liquid.

Health Hazards

Toxic if inhaled. Harmful if inhaled. Causes damage to organs. Harmful if swallowed.

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Is not likely mobile in the environment due its low water solubility. Will likely be mobile in the environment due to its volatility. Spillage unlikely to penetrate soil. The product is insoluble and floats on water. The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces.

Other Hazards

Stench. Toxic to terrestrial vertebrates. This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
1-Hexanethiol	111-31-9	>95

SECTION 4. FIRST AID MEASURES**General Advice**

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

Eye Contact

In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

Skin Contact

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Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.

Inhalation

Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.

Ingestion

Do NOT induce vomiting. Call a physician or poison control center immediately.

Most important symptoms and effects

. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES**Suitable Extinguishing Media**

Carbon dioxide (CO₂). Dry chemical. Water mist may be used to cool closed containers. Chemical foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

Flammable. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Vapors may form explosive mixtures with air.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

SECTION 6. ACCIDENTAL RELEASE MEASURES**Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas. Remove all sources of ignition. Take precautionary measures against static discharges.

Environmental Precautions

Should not be released into the environment.

Methods for Containment and Clean Up

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE**Handling**

Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Keep away from

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open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.

Storage

Keep away from heat, sparks and flame. Flammables area. Keep container tightly closed in a dry and well-ventilated place.

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters

Component	ACGIH TLV	OSHA PEL	NIOSH	The United Kingdom	European Union
1-Hexanethiol			Ceiling: 0.5 ppm Ceiling: 2.7 mg/m ³	-	

Legend

NIOSH: NIOSH - National Institute for Occupational Safety and Health

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Exposure Controls**Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting equipment. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection Long sleeved clothing

Respiratory Protection When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

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Large scale/emergency use	Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387
Small scale/Laboratory use	Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141 When RPE is used a face piece Fit Test should be conducted
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.
Environmental exposure controls	No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	Colorless	
Physical State	Liquid	
Odor	Stench	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	-81 - -80 °C / -113.8 - -112 °F	
Softening Point	No data available	
Boiling Point/Range	150 - 154 °C / 302 - 309.2 °F	@ 760 mmHg
Flash Point	30 °C / 86 °F	Method - No information available
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	Lower 0.5 Upper 5.5	
Vapor Pressure	No data available	
Vapor Density	> 3.0	(Air = 1.0)
Specific Gravity / Density	0.840	
Bulk Density	Not applicable	Liquid
Water Solubility	Insoluble	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
1-Hexanethiol	5.35	
Autoignition Temperature	No data available	
Decomposition Temperature	400 °C	
Viscosity	No data available	
Explosive Properties		explosive air/vapour mixtures possible
Oxidizing Properties	No information available	
Molecular Formula	C6 H14 S	
Molecular Weight	118.24	

SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under normal conditions.
Hazardous Reactions	None under normal processing.
Hazardous Polymerization	Hazardous polymerization does not occur.
Conditions to Avoid	Keep away from open flames, hot surfaces and sources of ignition. Exposure to air. Incompatible products.

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Materials to avoid Bases. Strong oxidizing agents. Metals. Reducing Agent.

Hazardous Decomposition Products Carbon monoxide (CO). Carbon dioxide (CO₂). Sulfur oxides. Sulfides.

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
1-Hexanethiol	LD50 = 1254 mg/kg (Rat)		LC50 = 1080 ppm (Rat) 4 h

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;

Respiratory No data available
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects Do not empty into drains. .

Persistence and Degradability

Persistence Insoluble in water, Persistence is unlikely, based on information available.

Bioaccumulative Potential May have some potential to bioaccumulate

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Component	log Pow	Bioconcentration factor (BCF)
1-Hexanethiol	5.35	No data available

Mobility in soil

Spillage unlikely to penetrate soil The product is insoluble and floats on water The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces Is not likely mobile in the environment due its low water solubility Will likely be mobile in the environment due to its volatility

Endocrine Disruptor Information
Persistent Organic Pollutant
Ozone Depletion Potential

This product does not contain any known or suspected endocrine disruptors
This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13. DISPOSAL CONSIDERATIONS

Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport

UN-No UN3071
Proper Shipping Name Mercaptans, liquid, toxic, flammable, n.o.s.
Technical Shipping Name 1-Hexanethiol
Hazard Class 6.1
Subsidiary Hazard Class 3
Packing Group II

IMDG/IMO

UN-No UN3071
Proper Shipping Name Mercaptans, liquid, toxic, flammable, n.o.s.
Technical Shipping Name 1-Hexanethiol
Hazard Class 6.1
Subsidiary Hazard Class 3
Packing Group II

IATA

UN-No UN3071
Proper Shipping Name Mercaptan mixture, liquid, toxic, flammable, n.o.s.
Technical Shipping Name 1-Hexanethiol
Hazard Class 6.1
Subsidiary Hazard Class 3
Packing Group II

Special Precautions for User

No special precautions required

SECTION 15. REGULATORY INFORMATION

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International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
1-Hexanethiol	X	-	X	X	203-857-0	X	X	X	X	X	X	KE-19793

National Regulations**SECTION 16. OTHER INFORMATION**

Prepared By Health, Safety and Environmental Department
Creation Date 25-Jan-2011
Revision Date 27-Apr-2024
Revision Summary New emergency telephone response service provider.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet