

# Safety Data Sheet

acc. to OSHA HCS

Printing date 05/13/2024

Reviewed on 05/13/2024

## 1 Identification

- **Product identifier**
- **Trade name:** Hexanethiol 96%  
1-hexanethiol
- **Article number:** H1975
- **CAS Number:**  
111-31-9
- **EC number:**  
203-857-0
- **Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**  
Aqua Solutions, Inc.  
6913 Highway 225  
DEER PARK, TX 77536  
USA  
800-256-2586
- **Information department:**  
Technical Coordinator  
Sherman Nelson [shermann@aquasolutions.org](mailto:shermann@aquasolutions.org)
- **Emergency telephone number:**  
Chemtrec: 800-424-9300  
Canutec: 613-996-6666



## 2 Hazard(s) identification

- **Classification of the substance or mixture**



GHS02 Flame

Flammable Liquids 3

H226 Flammable liquid and vapor.



GHS06 Skull and crossbones

Acute Toxicity - Inhalation 3 H331 Toxic if inhaled.



GHS07

Acute Toxicity - Oral 4

H302 Harmful if swallowed.

- **Label elements**

- **GHS label elements** The substance is classified and labeled according to the Globally Harmonized System (GHS).

- **Hazard pictograms**



GHS02



GHS06

- **Signal word** Danger

- **Hazard statements**

Flammable liquid and vapor.

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*Harmful if swallowed.**Toxic if inhaled.***· Precautionary statements***Keep away from heat/sparks/open flames/hot surfaces. - No smoking.**Ground/bond container and receiving equipment.**Use explosion-proof electrical/ventilating/lighting/equipment.**Use only non-sparking tools.**Take precautionary measures against static discharge.**Avoid breathing dust/fume/gas/mist/vapors/spray**Wash thoroughly after handling.**Do not eat, drink or smoke when using this product.**Use only outdoors or in a well-ventilated area.**Wear protective gloves/protective clothing/eye protection/face protection.**If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.**IF INHALED: Remove person to fresh air and keep comfortable for breathing.**Call a poison center.**Rinse mouth.**In case of fire: Use CO2, sand, extinguishing powder to extinguish.**Store in a well-ventilated place. Keep container tightly closed.**Store in a well-ventilated place. Keep cool.**Store locked up.**Dispose of contents/container in accordance with local/regional/national/international regulations.***· Classification system:****· NFPA ratings (scale 0 - 4)**

Health = 3

Fire = 2

Reactivity = 0

**· HMIS-ratings (scale 0 - 4)**

Health = 3

Fire = 2

Reactivity = 0

**· Other hazards****· Results of PBT and vPvB assessment****· PBT:** Not applicable.**· vPvB:** Not applicable.

## 3 Composition/information on ingredients

**· Chemical characterization: Substances****· CAS No. Description**

CAS: 111-31-9 Hexanethiol 96%

**· Identification number(s)****· EC number:** 203-857-0

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## 4 First-aid measures

- **Description of first aid measures**
- **General information:**  
Immediately remove any clothing soiled by the product.  
Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.  
Remove breathing apparatus only after contaminated clothing have been completely removed.  
In case of irregular breathing or respiratory arrest provide artificial respiration.
- **After inhalation:**  
Supply fresh air or oxygen; call for doctor.  
In case of unconsciousness place patient stably in side position for transportation.
- **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
- **After eye contact:** Rinse opened eye for several minutes under running water. Then consult a doctor.
- **After swallowing:** Immediately call a doctor.
- **Information for doctor:**  
· **Most important symptoms and effects, both acute and delayed** No further relevant information available.  
· **Indication of any immediate medical attention and special treatment needed**  
No further relevant information available.

## 5 Fire-fighting measures

- **Extinguishing media**
- **Suitable extinguishing agents:**  
CO<sub>2</sub>, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
- **Special hazards arising from the substance or mixture** No further relevant information available.
- **Advice for firefighters**
- **Protective equipment:** Mouth respiratory protective device.

## 6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures**  
Wear protective equipment. Keep unprotected persons away.
- **Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:**  
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).  
Dispose contaminated material as waste according to section 13.  
Ensure adequate ventilation.
- **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.
- **Protective Action Criteria for Chemicals**
- **PAC-1:** 0.045 ppm
- **PAC-2:** 0.5 ppm
- **PAC-3:** 48 ppm

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### 7 Handling and storage

- **Handling:**
- **Precautions for safe handling**  
Ensure good ventilation/exhaustion at the workplace.  
Open and handle receptacle with care.
- **Information about protection against explosions and fires:**  
Keep ignition sources away - Do not smoke.  
Protect against electrostatic charges.  
Keep respiratory protective device available.
- **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:** Not required.
- **Further information about storage conditions:** Keep receptacle tightly sealed.
- **Specific end use(s)** No further relevant information available.

### 8 Exposure controls/personal protection

- **Additional information about design of technical systems:** No further data; see section 7.
- **Control parameters**

· **Components with limit values that require monitoring at the workplace:**

**CAS: 111-31-9 Hexanethiol 96%**

REL	Ceiling limit value: 2.7* mg/m <sup>3</sup> , 0.5* ppm *15-min
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- **Additional information:** The lists that were valid during the creation were used as basis.
- **Exposure controls**
- **Personal protective equipment:**
- **General protective and hygienic measures:**  
Keep away from foodstuffs, beverages and feed.  
Immediately remove all soiled and contaminated clothing.  
Wash hands before breaks and at the end of work.  
Store protective clothing separately.
- **Breathing equipment:**  
In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.
- **Protection of hands:**  
The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.  
Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.  
Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation
- **Material of gloves**  
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.
- **Penetration time of glove material**  
The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

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· **Eye protection:**

Tightly sealed goggles

· **Body protection:** Protective work clothing

## 9 Physical and chemical properties

· **Information on basic physical and chemical properties**· **General Information**· **Appearance:**

· <b>Form:</b>	Liquid
· <b>Color:</b>	Clear
· <b>Odor:</b>	Stench
· <b>Odor threshold:</b>	Not determined.

· **pH-value:** Not determined.· **Change in condition**

· <b>Melting point/Melting range:</b>	-81--80 °C (-113.8--112 °F)
· <b>Boiling point/Boiling range:</b>	150-154 °C (302-309.2 °F)

· **Flash point:** 30 °C (86 °F)· **Flammability (solid, gaseous):** Flammable.· **Decomposition temperature:** Not determined.· **Ignition temperature:** Not determined.· **Danger of explosion:** Product is not explosive. However, formation of explosive air/vapor mixtures are possible.· **Explosion limits:**

· <b>Lower:</b>	Not determined.
· <b>Upper:</b>	Not determined.

· **Vapor pressure at 20 °C (68 °F):** >3 hPa (>2.3 mm Hg)· **Density at 20 °C (68 °F):** 0.838 g/cm<sup>3</sup> (6.99311 lbs/gal)· **Relative density** Not determined.· **Vapor density** Not determined.· **Evaporation rate** Not determined.· **Solubility in / Miscibility with**· **Water:** Not determined.· **Partition coefficient (n-octanol/water):** Not determined.· **Viscosity:**

· <b>Dynamic:</b>	Not determined.
· <b>Kinematic:</b>	Not determined.

· **Other information** No further relevant information available.

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### 10 Stability and reactivity

- **Reactivity** No further relevant information available.
- **Chemical stability**
- **Thermal decomposition / conditions to be avoided:** No decomposition if used according to specifications.
- **Possibility of hazardous reactions** No dangerous reactions known.
- **Conditions to avoid** No further relevant information available.
- **Incompatible materials:** No further relevant information available.
- **Hazardous decomposition products:** No dangerous decomposition products known.

### 11 Toxicological information

- **Information on toxicological effects**
- **Acute toxicity:**

· **LD/LC50 values that are relevant for classification:**

Oral	LD50	500 mg/kg (ATE)
Inhalative	LC50/4h	3 mg/l (ATE)

- **Primary irritant effect:**
- **on the skin:** No irritant effect.
- **on the eye:** No irritating effect.
- **Sensitization:** No sensitizing effects known.
- **Additional toxicological information:**
- **Carcinogenic categories**
- **IARC (International Agency for Research on Cancer)** Substance is not listed.
- **NTP (National Toxicology Program)** Substance is not listed.
- **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.
- **Behavior in environmental systems:**
- **Bioaccumulative potential** No further relevant information available.
- **Mobility in soil** No further relevant information available.
- **Additional ecological information:**
- **General notes:**
- **Water hazard class 3 (Assessment by list):** extremely hazardous for water  
Do not allow product to reach ground water, water course or sewage system, even in small quantities.  
Danger to drinking water if even extremely small quantities leak into the ground.
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.
- **Other adverse effects** No further relevant information available.

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## 13 Disposal considerations

- **Waste treatment methods**
- **Recommendation:**  
Must not be disposed of together with household garbage. Do not allow product to reach sewage system.
- **Uncleaned packagings:**
- **Recommendation:** Disposal must be made according to official regulations.

## 14 Transport information

<ul style="list-style-type: none"> <li>· <b>UN-Number</b></li> <li>· <b>DOT, IMDG, IATA</b></li> </ul>	UN3071
<ul style="list-style-type: none"> <li>· <b>UN proper shipping name</b></li> <li>· <b>DOT</b></li> <li>· <b>IMDG, IATA</b></li> </ul>	Mercaptans, liquid, toxic, flammable, n.o.s. MERCAPTANS, LIQUID, TOXIC, FLAMMABLE, N.O.S. (Hexanethiol 96%)
<ul style="list-style-type: none"> <li>· <b>Transport hazard class(es)</b></li> <li>· <b>DOT</b></li> </ul>	<div style="display: flex; align-items: center; gap: 10px;"> </div>
<ul style="list-style-type: none"> <li>· <b>Class</b></li> <li>· <b>Label</b></li> </ul>	6.1 Toxic substances 6.1, 3
<ul style="list-style-type: none"> <li>· <b>IMDG</b></li> </ul>	<div style="display: flex; align-items: center; gap: 10px;"> </div>
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<ul style="list-style-type: none"> <li>· <b>Class</b></li> <li>· <b>Label</b></li> </ul>	6.1 Toxic substances 6.1 (3)
<ul style="list-style-type: none"> <li>· <b>Packing group</b></li> <li>· <b>DOT, IMDG, IATA</b></li> </ul>	II
<ul style="list-style-type: none"> <li>· <b>Environmental hazards:</b></li> <li>· <b>Marine pollutant:</b></li> </ul>	No
<ul style="list-style-type: none"> <li>· <b>Special precautions for user</b></li> <li>· <b>Hazard identification number (Kemler code):</b></li> <li>· <b>EMS Number:</b></li> </ul>	Warning: Toxic substances 63 F-E,S-D

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· <b>Stowage Category</b>	C
· <b>Stowage Code</b>	SW2 Clear of living quarters.
· <b>Segregation Code</b>	SG57 Stow "separated from" odour-absorbing cargoes
· <b>Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</b>	Not applicable.
· <b>Transport/Additional information:</b>	
· <b>DOT</b>	
· <b>Quantity limitations</b>	On passenger aircraft/rail: 5 L On cargo aircraft only: 60 L
· <b>IMDG</b>	
· <b>Limited quantities (LQ)</b>	1L
· <b>Excepted quantities (EQ)</b>	Code: E2 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 500 ml
· <b>UN "Model Regulation":</b>	UN 3071 MERCAPTANS, LIQUID, TOXIC, FLAMMABLE, N.O.S. (HEXANETHIOL 96%), 6.1 (3), II

## 15 Regulatory information

- **Safety, health and environmental regulations/legislation specific for the substance or mixture**  
No further relevant information available.
- **Sara**
- **Section 355 (extremely hazardous substances):** Substance is not listed.
- **Section 313 (Specific toxic chemical listings):** Substance is not listed.
- **TSCA (Toxic Substances Control Act):** ACTIVE
- **Hazardous Air Pollutants** Substance is not listed.
- **Proposition 65**
- **Chemicals known to cause cancer:** Substance is not listed.
- **Chemicals known to cause reproductive toxicity for females:** Substance is not listed.
- **Chemicals known to cause reproductive toxicity for males:** Substance is not listed.
- **Chemicals known to cause developmental toxicity:** Substance is not listed.
- **Carcinogenic categories**
- **EPA (Environmental Protection Agency)** Substance is not listed.
- **TLV (Threshold Limit Value)** Substance is not listed.
- **NIOSH-Ca (National Institute for Occupational Safety and Health)** Substance is not listed.
- **GHS label elements** The substance is classified and labeled according to the Globally Harmonized System (GHS).
- **Hazard pictograms**



GHS02 GHS06

- **Signal word** Danger
- **Hazard statements**  
Flammable liquid and vapor.  
Harmful if swallowed.  
Toxic if inhaled.

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· **Precautionary statements**

- Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
- Ground/bond container and receiving equipment.
- Use explosion-proof electrical/ventilating/lighting/equipment.
- Use only non-sparking tools.
- Take precautionary measures against static discharge.
- Avoid breathing dust/fume/gas/mist/vapors/spray
- Wash thoroughly after handling.
- Do not eat, drink or smoke when using this product.
- Use only outdoors or in a well-ventilated area.
- Wear protective gloves/protective clothing/eye protection/face protection.
- If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
- IF INHALED: Remove person to fresh air and keep comfortable for breathing.
- Call a poison center.
- Rinse mouth.
- In case of fire: Use CO<sub>2</sub>, sand, extinguishing powder to extinguish.
- Store in a well-ventilated place. Keep container tightly closed.
- Store in a well-ventilated place. Keep cool.
- Store locked up.
- Dispose of contents/container in accordance with local/regional/national/international regulations.
- **Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

\* **16 Other information**

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

- **Department issuing SDS:** Environment protection department.
- **Contact:**  
Date of Preparation / Last Revision:
- **Date of preparation / last revision**  
Revision 1.2, 05/13/2024: Reviewed SDS for accuracy. MH/STN  
Creation date for SDS 10-21-2014. STN  
05/13/2024
- **Abbreviations and acronyms:**  
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)  
NFPA: National Fire Protection Association (USA)  
HMIS: Hazardous Materials Identification System (USA)  
LC50: Lethal concentration, 50 percent  
LD50: Lethal dose, 50 percent  
PBT: Persistent, Bioaccumulative and Toxic  
vPvB: very Persistent and very Bioaccumulative  
NIOSH: National Institute for Occupational Safety  
OSHA: Occupational Safety & Health  
TLV: Threshold Limit Value  
PEL: Permissible Exposure Limit  
REL: Recommended Exposure Limit  
Flammable Liquids 3: Flammable liquids – Category 3  
Acute Toxicity - Oral 4: Acute toxicity – Category 4  
Acute Toxicity - Inhalation 3: Acute toxicity – Category 3
- **\* Data compared to the previous version altered.**