

## SAFETY DATA SHEET

Version 6.3  
Revision Date 06/01/2021  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 1-Dodecanethiol

Product Number : 471364  
Brand : Aldrich  
CAS-No. : 112-55-0

**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Skin corrosion (Category 1C), H314  
Serious eye damage (Category 1), H318  
Skin sensitization (Sub-category 1B), H317  
Short-term (acute) aquatic hazard (Category 1), H400  
Long-term (chronic) aquatic hazard (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

**2.2 GHS Label elements, including precautionary statements**

Pictogram



Signal word

Danger

Hazard statement(s)	
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H410	Very toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P272	Contaminated work clothing must not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
P391	Collect spillage.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Stench.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms	: Dodecyl mercaptan Mercaptan C12 Lauryl mercaptan NDM n-Dodecyl mercaptan
Formula	: C <sub>12</sub> H <sub>26</sub> S
Molecular weight	: 202.4 g/mol
CAS-No.	: 112-55-0
EC-No.	: 203-984-1

Component	Classification	Concentration
<b>Dodecane-1-thiol</b>		
	Skin Corr. 1C; Eye Dam. 1; Skin Sens. 1B; Aquatic Acute 1; Aquatic Chronic 1; H314, H318, H317, H400, H410 M-Factor - Aquatic Acute:	<= 100 %

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For the full text of the H-Statements mentioned in this Section, see Section 16.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Call in physician.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

#### If swallowed

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

### 4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Carbon dioxide (CO<sub>2</sub>) Foam Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Sulfur oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

## 5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

### 6.2 Environmental precautions

Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

#### Storage conditions

Tightly closed.

Storage class (TRGS 510): 8A: Combustible, corrosive hazardous materials

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Dodecane-1-thiol	112-55-0	TWA	0.1 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Dermal Sensitization		
		C	0.5 ppm 4.1 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits

### 8.2 Exposure controls

#### Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

## Personal protective equipment

### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

### Body Protection

protective clothing

### Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

### Control of environmental exposure

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |  |   |
|--|---|
| a) Appearance                              | Form: liquid  |
| b) Odor                                    | characteristic  |
| c) Odor Threshold                          | No data available   |
| d) pH                                      | No data available   |
| e) Melting point/freezing point            | Melting point/range: -9 - -7 °C (16 - 19 °F) at 1,013 hPa |
| f) Initial boiling point and boiling range | 266 - 283 °C 511 - 541 °F - lit.                          |

g) Flash point	128 °C (262 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	< 1 hPa at 25 °C (77 °F)
l) Vapor density	7.0
m) Relative density	No data available
n) Water solubility	0.00001 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - partly soluble
o) Partition coefficient: n-octanol/water	log Pow: > 6.5 at 25 °C (77 °F) - Potential bioaccumulation
p) Autoignition temperature	No data available
q) Decomposition temperature	350 °C (662 °F) -
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

## 9.2 Other safety information

Relative vapor density	7.0
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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:  
Strong oxidizing agents  
strong reducing agents  
Alkali metals  
Strong bases

### 10.4 Conditions to avoid

Strong heating.

### 10.5 Incompatible materials

No data available

## 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - > 5,000 mg/kg

(OECD Test Guideline 401)

Remarks: (ECHA)

LC50 Inhalation - Rat - 4.5 h - > 3.1 mg/l

(OECD Test Guideline 403)

LD50 Dermal - Rat - male - > 2,000 mg/kg

(OECD Test Guideline 402)

Remarks: (ECHA)

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: Corrosive

(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: positive

(OECD Test Guideline 429)

#### Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 479

Result: negative

Test Type: Mutagenicity (mammal cell test):

Test system: Mouse lymphoma test

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Micronucleus test

Species: Mouse

Cell type: Bone marrow

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

#### Carcinogenicity

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- IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
- NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
- OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

RTECS: JR3155000

Nausea, Headache, Vomiting

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After uptake:

Headache

The following applies to mercaptans in general: offensive odour.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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**SECTION 12: Ecological information**

**12.1 Toxicity**

Toxicity to fish	semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) - > 100 mg/l - 96 h Remarks: (ECHA)
	semi-static test NOEC - Oncorhynchus mykiss (rainbow trout) - 100 mg/l - 96 h Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 1 - 10 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test EbC50 - Pseudokirchneriella subcapitata (green algae) - 0.25 mg/l - 72 h

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(OECD Test Guideline 201)

static test EC10 - Pseudokirchneriella subcapitata (green algae) - < 0.0145 mg/l - 72 h

(OECD Test Guideline 201)

static test NOEC - Pseudokirchneriella subcapitata (green algae) - < 0.0145 mg/l - 72 h

(OECD Test Guideline 201)

## 12.2 Persistence and degradability

Biodegradability

aerobic - Exposure time 28 d

Result: 0 % - Not readily biodegradable.

(OECD Test Guideline 301D)

Remarks: The value is given in analogy to the following substances: tert-Dodecanethiol

## 12.3 Bioaccumulative potential

No data available

## 12.4 Mobility in soil

No data available

## 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

## 12.6 Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14: Transport information

### DOT (US)

UN number: 1760 Class: 8

Packing group: III

Proper shipping name: Corrosive liquids, n.o.s. (Dodecane-1-thiol)

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

### IMDG

UN number: 1760 Class: 8

Packing group: III

EMS-No: F-A, S-B

Proper shipping name: CORROSIVE LIQUID, N.O.S. (Dodecane-1-thiol)

Marine pollutant : yes

### IATA

UN number: 1760 Class: 8

Packing group: III

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Proper shipping name: Corrosive liquid, n.o.s. (Dodecane-1-thiol)

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## SECTION 15: Regulatory information

### **SARA 302 Components**

This material does not contain any components with a section 302 EHS TPQ.

### **SARA 313 Components**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### **SARA 311/312 Hazards**

Acute Health Hazard

### **Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

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## SECTION 16: Other information

### **Further information**

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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