

SAFETY DATA SHEET

Version 8.5
Revision Date 16.02.2023
Print Date 23.05.2023**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 1-Dodecanethiol for synthesis

Product Number : 8.20544
Catalogue No. : 820544
Brand : Millipore
CAS-No. : 112-55-0

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

Identified uses : Chemical for synthesis

1.3 Details of the supplier of the safety data sheet

Company : SIGMA-ALDRICH CANADA LTD.
2149 WINSTON PARK DRIVE
OAKVILLE ON L6H 6J8
CANADA

Telephone : +1 905 829-9500
Fax : +1 905 829-9292

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 Hazardous Products Regulations (HPR) (SOR/2015-17)**

Skin corrosion (Category 1C), H314
Serious eye damage (Category 1), H318
Skin sensitization (Sub-category 1A), 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 mist or vapors.
P264	Wash skin thoroughly after handling.
P272	Contaminated work clothing should 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.
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.
P362 + P364	Take off contaminated clothing and wash it 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

- none

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula	:	C ₁₂ H ₂₆ S
Molecular weight	:	202.39 g/mol
CAS-No.	:	112-55-0
EC-No.	:	203-984-1

Component	Classification	Concentration *
Dodecane-1-thiol	Skin Corr. 1C; Eye Dam. 1; Skin Sens. 1A; Aquatic Acute 1; Aquatic Chronic 1; H314, H318, H317, H400, H410 M-Factor - Aquatic Acute: 10 - Aquatic Chronic: 10	<= 100 %
* Weight %		

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

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂) 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.

Fire may cause evolution of:

Sulfur oxides

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.

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.

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.

Recommended storage temperature see product label.

Storage class

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Components	CAS-No.	Value	Control parameters	Basis
Dodecane-1-thiol	112-55-0	TWA	0.1 ppm	Canada. British Columbia OEL
Remarks	Substance with specific evidence of sensitization by dermal route			

		TWA	0.1 ppm 0.8 mg/m ³	Canada. Alberta, Occupational Health and Safety Code (table 2: OEL)
	Occupational exposure limit is based on irritation effects and its adjustment to compensate for unusual work schedules is not required			
		TWA	0.1 ppm	USA. ACGIH Threshold Limit Values (TLV)

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).

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).

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.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid Color: colorless
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 at 1,013 hPa
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) Density	0.845 g/cm ³ at 20 °C (68 °F)
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	none

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

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - \geq 5,000 mg/kg
(OECD Test Guideline 401)
LC50 Inhalation - Rat - 4.5 h - $>$ 3.1 mg/l - vapor

(OECD Test Guideline 403)
LD50 Dermal - Rat - male - \geq 2,000 mg/kg
(OECD Test Guideline 402)

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: *S. 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

No data available

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

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.

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)
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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 - Raphidocelis subcapitata (freshwater green alga) - < 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
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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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

Discharge into the environment must be avoided.

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 for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

TDG

UN number: 1760 Class: 8 Packing group: III
 Proper shipping name: CORROSIVE LIQUID, N.O.S. (Dodecane-1-thiol)
 Labels: 8
 ERG Code: 154
 Marine pollutant: 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

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

SECTION 15: Regulatory information

This product has been classified in accordance with the hazard criteria of the Hazardous Products Regulations (HPR) and the SDS contains all the information required by the HPR.

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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