

Chemical Safety Data Sheet MSDS / SDS

1-Dodecanethiol

Revision Date:2025-01-11 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifier

Product name : 1-Dodecanethiol
CBnumber : CB9363948
CAS : 112-55-0
EINECS Number : 203-984-1
Synonyms : 1-dodecanethiol,ndm

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P501 Dispose of contents/container to.....

P405 Store locked up.

P391 Collect spillage. Hazardous to the aquatic environment

P310 Immediately call a POISON CENTER or doctor/physician.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P273 Avoid release to the environment.

P272 Contaminated work clothing should not be allowed out of the workplace.

P264 Wash skin thoroughly after handling.

P264 Wash hands thoroughly after handling.

P262 Do not get in eyes, on skin, or on clothing.

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

Hazard statements

H412 Harmful to aquatic life with long lasting effects

H410 Very toxic to aquatic life with long lasting effects

H402 Harmful to aquatic life

H335 May cause respiratory irritation

H319 Causes serious eye irritation

H317 May cause an allergic skin reaction

H315 Causes skin irritation

H314 Causes severe skin burns and eye damage

SECTION 3: Composition/information on ingredients

Substance

| | |
|--------------|-----------------------|
| Product name | : 1-Dodecanethiol |
| Synonyms | : 1-dodecanethiol,ndm |
| CAS | : 112-55-0 |
| EC number | : 203-984-1 |
| MF | : C12H26S |
| MW | : 202.4 |

SECTION 4: First aid measures

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.

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

Indication of any immediate medical attention and special treatment needed

SECTION 5: Firefighting measures

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.

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.

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.

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.

NFPA 704



HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N₂](#))

SPEC.

HAZ.

SECTION 6: Accidental release measures

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.

Environmental precautions

Do not let product enter drains.

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. Chemizorb?). Dispose of properly. Clean up affected area.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

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.

Recommended Filter type: Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

| | |
|--|--|
| Appearance | liquid |
| Odour | characteristic |
| Odour Threshold | No data available |
| pH | No data available |
| Melting point/freezing point | Melting point/range: -9 - -7 °C at 1.013 hPa |
| Initial boiling point and boiling range | 266 - 283 °C - lit. |
| Flash point | 128 °C - closed cup - Regulation (EC) No. 440/2008, Annex, A.9 |
| Evaporation rate | No data available |
| Flammability (solid, gas) | No data available |
| Upper/lower flammability or explosive limits | No data available |
| Vapour pressure | < 1 hPa at 25 °C |
| Vapour density | 7,0 |
| Relative density | 0,845 g/cm ³ at 25 °C - lit. No data available |
| Water solubility | 0,00001 g/l at 20 °C - OECD Test Guideline 105- partly soluble |
| Partition coefficient: n-octanol/water | log Pow: >6,5 at 25 °C - Potential bioaccumulation |
| Autoignition temperature | No data available |

| | |
|---------------------------|---|
| Decomposition temperature | 350 °C - |
| Viscosity | Viscosity, kinematic: No data available Viscosity, dynamic: 3,24 mPa.s at 20 °C |
| Explosive properties | No data available |
| Oxidizing properties | No data available |
| λ_{max} | 205nm(lit.) |

Other safety information

Relative vapor density

7,0

SECTION 10: Stability and reactivity

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.

Chemical stability

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

Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents strong reducing agents Alkali metals

Strong bases

Conditions to avoid

Strong heating.

Incompatible materials

No data available

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

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)

Skin corrosion/irritation

Skin - Rabbit Result: Corrosive

(OECD Test Guideline 404)

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

(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

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

Toxicity

LD50 orally in Rabbit: > 2000 mg/kg

SECTION 12: Ecological information

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

(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)

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

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Toxics Screening Level

The Initial threshold Screening Level (ITSL) is µg/m³ with an 8-hour average.

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

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

UN number

ADR/RID: 1760 IMDG: 1760 IATA: 1760

UN proper shipping name

ADR/RID: CORROSIVE LIQUID, N.O.S. (Dodecane-1-thiol) IMDG: CORROSIVE LIQUID, N.O.S. (Dodecane-1-thiol)

IATA: Corrosive liquid, n.o.s. (Dodecane-1-thiol)

Transport hazard class(es)

ADR/RID: 8 IMDG: 8 IATA: 8

Packaging group

ADR/RID: III IMDG: III IATA: III

Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

EC Inventory:Listed.

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Other Information

Do NOT take working clothes home.

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.