

# SAFETY DATA SHEET

Version 6.6 Revision Date 11/06/2025 Print Date 11/07/2025

#### **SECTION 1. IDENTIFICATION**

#### 1.1 Product identifiers

Product name :  $(\pm)$ -a-Lipoic acid

Product Number : 62320 Brand : Sigma CAS-No. : 1077-28-7

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption

(40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by

MilliporeSigma.

# 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 number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-

527-3887 CHEMTREC (International) 24

Hours/day; 7 Days/week

## **SECTION 2. HAZARDS IDENTIFICATION**

# GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

# Hazards for the product as supplied

Acute toxicity (Oral) : Category 4

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Skin irritation : Category 2

Eye irritation : Category 2A

Skin sensitisation : Category 1

Short-term (acute)

aquatic hazard

: Category 2

Long-term (chronic)

aquatic hazard

Category 2

#### Other hazards

None known.

#### **GHS label elements**

Hazard pictograms





Signal word : Warning

Hazard statements : H302 Harmful if swallowed.

H315 Causes skin irritation.

H317 May cause an allergic skin reaction.

H319 Causes serious eye irritation.

H411 Toxic to aquatic life with long lasting effects.

# Precautionary statements:

## **Prevention:**

P261 Avoid breathing dust.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this

product.

P272 Contaminated work clothing must not be allowed

out of the workplace.

P273 Avoid release to the environment.

P280 Wear protective gloves/ eye protection/ face

protection.

#### Response:

P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.

P302 + P352 IF ON SKIN: Wash with plenty of soap and

water.

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

present and easy to do. Continue rinsing.

P333 + P313 If skin irritation or rash occurs: Get

medical advice/ attention.

P337 + P313 If eye irritation persists: Get medical

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advice/ attention.

P362 Take off contaminated clothing and wash before

reuse.

P391 Collect spillage.

#### Disposal:

P501 Dispose of contents/ container to an approved

waste disposal plant.

# **SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Substance / Mixture : Substance

CAS-No. : 1077-28-7

## Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
5-(dithiolan-3-yl)valeric acid	1077-28-7*	>= 90 - <= 100	-

 $<sup>\</sup>ensuremath{^{*}}$  Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

#### **SECTION 4. FIRST AID MEASURES**

General advice : Show this safety data sheet to the doctor in

attendance.

If inhaled : After inhalation: fresh air.

In case of skin contact : In case of skin contact: Take off immediately all

contaminated clothing. Rinse skin with water/ shower.

Consult a physician.

In case of eye contact : After eye contact: rinse out with plenty of water.

Call in ophthalmologist. Remove contact lenses.

If swallowed : After swallowing: immediately make victim drink

water (two glasses at most).

Consult a physician.

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

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

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#### **SECTION 5. FIREFIGHTING MEASURES**

Suitable extinguishing

media

: Water Foam

Carbon dioxide (CO2)

Dry powder

Unsuitable extinguishing

media

: For this substance/mixture no limitations of

extinguishing agents are given.

Specific hazards during

fire fighting

: Combustible.

Development of hazardous combustion gases or

vapours possible in the event of fire.

Hazardous combustion

products

: Carbon oxides

Sulphur oxides

Specific extinguishing

methods

: No data available

Further information : Suppress (knock down) gases/vapours/mists with a

water spray jet.

Prevent fire extinguishing water from contaminating

surface water or the ground water system.

Special protective equipment for fire-

fighters

: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe

distance or by wearing suitable protective clothing.

# **SECTION 6. ACCIDENTAL RELEASE MEASURES**

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:

Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation.

Evacuate the danger area, observe emergency

procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.

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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 dry. Dispose of properly. Clean up affected

area. Avoid generation of dusts.

#### **SECTION 7. HANDLING AND STORAGE**

For precautions see section 2.2.

Further information on storage conditions

: Tightly closed.

Dry.

Storage class : 11, Combustible Solids

Recommended storage

temperature

: 36 - 46 °F / 2 - 8 °C

## **SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**

# Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

# **Personal protective equipment**

Respiratory protection : required when dusts 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 P2

The entrepeneur 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.

Hand protection

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Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Full contact

Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Splash contact

Manufacturer : KCL 741 Dermatril® L

Remarks : 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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-

36124 Eichenzell, Internet: www.kcl.de).

Eye protection : Use equipment for eye protection tested and

approved under appropriate government standards

such as NIOSH (US) or EN 166(EU).

Safety glasses

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply

preventive skin protection. Wash hands and face

after working with substance.

#### **SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

Appearance : powder

Color : No data available

Odor : No data available

Odor Threshold : No data available pH : No data available

Melting point/ range : 140 - 144 °F / 60 - 62 °C

Boiling point/boiling range : 547 °F / 286 °C (ca. 1,013 hPa)

Decomposition: yes

Method: Regulation (EC) No. 440/2008, Annex, A.2

Decomposes below the boiling point.

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Flash point : No data available

: No data available Evaporation rate

Flammability (solid, gas) : No data available

Flammability (liquids) : No data available

Burning rate : No data available

Upper explosion limit /

Upper flammability limit

: No data available

: No data available

: No data available

Lower explosion limit / Lower flammability limit

Relative vapour density : No data available

Relative density : No data available

Density : ca. 1.4 g/cm3 (73 °F / 23 °C)

Method: OECD Test Guideline 109

Solubility(ies)

Vapor pressure

Water solubility : ca. 0.87 g/l (72 °F / 22 °C)

Method: OECD Test Guideline 105

GLP: yes

Solubility in other

solvents

: 50 g/l (68 °F / 20 °C)

Solvent: Ethanol

Partition coefficient: n-

octanol/water

: log Pow: 2.53 (77 °F / 25 °C)

Method: (calculated)

Bioaccumulation is not expected.

Autoignition temperature : No data available

Decomposition

temperature

: No data available

Viscosity, dynamic : No data available

Viscosity, kinematic : No data available

Flow time : No data available

Explosive properties : Not classified as explosive.

Oxidizing properties : none

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Molecular weight : 206.33 g/mol

Particle characteristics

Particle size : No data available

#### **SECTION 10. STABILITY AND REACTIVITY**

Reactivity : The following applies in general to flammable organic

substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion

potential may generally be assumed.

Chemical stability : The product is chemically stable under standard

ambient conditions (room temperature) .

Possibility of hazardous

reactions

: Violent reactions possible with:

Strong oxidizing agents

Conditions to avoid : no information available

Incompatible materials : No data available

Hazardous decomposition : In the event of fire: see section 5

products

## **SECTION 11. TOXICOLOGICAL INFORMATION**

# 11.1 Information on toxicological effects

## **Acute toxicity**

LD50 Oral - Rat - male - 1,190 mg/kg

Remarks: (ECHA)

Inhalation: No data available Dermal: No data available

## Skin corrosion/irritation

Skin - In vitro study Result: non-corrosive

(OECD Test Guideline 431)

Skin - In vitro study Result: positive

(OECD Test Guideline 439)

# Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

Sensitisation test: Result: positive

(OECD Test Guideline 442C)

In vitro study

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Millipore SigMa Result: positive Remarks: (ECHA)

# 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: Chromosome aberration test in vitro Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Micronucleus test

Species: Mouse

Application Route: Oral

Method: Mutagenicity (micronucleus test)

Result: negative

# Carcinogenicity

IARC: No component 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 component 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: JP1192000

irritant effects, depressed respiration, Convulsions, Tiredness

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#### **SECTION 12. ECOLOGICAL INFORMATION**

# **Ecotoxicity**

#### **Components:**

# 5-(dithiolan-3-yl)valeric acid:

Toxicity to fish : LC50 (Danio rerio (zebra fish)): 43 - 96 mg/l

Exposure time: 96 h Test Type: static test

Method: OECD Test Guideline 203

GLP: yes

Toxicity to daphnia and

other aquatic invertebrates

: EC50 (Daphnia magna (Water flea)): ca. 15.1 mg/l

Exposure time: 48 h Test Type: static test Analytical monitoring: yes

Method: OECD Test Guideline 202

GLP: yes

Toxicity to algae/aquatic

plants

: ErC50 (Pseudokirchneriella subcapitata (green

algae)): ca. 5.51 mg/l Exposure time: 72 h Test Type: static test

Method: OECD Test Guideline 201

GLP: yes

EC10 (Pseudokirchneriella subcapitata (green algae)):

ca. 0.583 mg/l Exposure time: 72 h Test Type: static test

Method: OECD Test Guideline 201

GLP: yes

# Persistence and degradability

# **Components:**

## 5-(dithiolan-3-yl)valeric acid:

Biodegradability : aerobic

Concentration: 1,000 mg/l Result: Not readily biodegradable.

Biodegradation: ca. 26 % Exposure time: 28 d

Method: OECD Test Guideline 301A

GLP: yes

## **Bioaccumulative potential**

## **Components:**

## 5-(dithiolan-3-yl)valeric acid:

Bioaccumulation : Remarks: No data available

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Partition coefficient: n-

: log Pow: 2.53 (77 °F / 25 °C)

octanol/water

Method: (calculated)

Remarks: Bioaccumulation is not expected.

# Mobility in soil

# **Components:**

# 5-(dithiolan-3-yl)valeric acid:

Stability in soil : Remarks: No data available

# Other adverse effects

#### Components:

# 5-(dithiolan-3-yl)valeric acid:

Additional ecological

information

: No data available

#### **SECTION 13. DISPOSAL CONSIDERATIONS**

# **Disposal methods**

Waste from residues : 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.

## **SECTION 14. TRANSPORT INFORMATION**

## **International Regulations**

# **IATA-DGR**

UN/ID No. : UN 3077

: Environmentally hazardous substance, solid, n.o.s. Proper shipping name

(5-(dithiolan-3-yl)valeric acid)

9 Class Packing group : III

Labels : Class 9 - Miscellaneous dangerous substances and

articles

Packing instruction (cargo: 956

aircraft)

Packing instruction

(passenger aircraft)

: 956

IMDG-Code

UN number : UN 3077

Proper shipping name : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID,

(5-(dithiolan-3-yl)valeric acid)

Sigma - 62320 Page 11 of 14 Class : 9 Packing group : III Labels : 9

EmS Code : F-A, S-F Marine pollutant : yes

# Transport in bulk according to IMO instruments

Not applicable for product as supplied.

# **National Regulations**

#### 49 CFR Road

Not regulated as a dangerous good

Poison Inhalation Hazard : No

# Special precautions for user

Remarks : EHS-Mark required (ADR 2.2.9.1.10, IMDG code

2.10.3) for single packagings and combination packagings containing inner packagings with

Dangerous Goods > 5L for liquids or > 5kg for solids. Packages smaller than or equal to 5 kg / L , not

dangerous goods of Class 9

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

## **SECTION 15. REGULATORY INFORMATION**

## **CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

## **SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

## SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

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

SARA 311/312

Hazards

: Acute Health Hazard

**SARA 313** : 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.

# **US State Regulations**

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

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

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# **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

## **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

# **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

#### The components of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA

inventory.

#### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

#### **SECTION 16. OTHER INFORMATION**

#### Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN -Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx -Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA -International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO -International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO -International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA -Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation,

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Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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