

SAFETY DATA SHEET

Version 6.6
Revision Date 01/10/2024
Print Date 06/15/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : DL-Lactonitrile
Product Number : 69830
Brand : Aldrich
CAS-No. : 78-97-7

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)**

Flammable liquids (Category 4), H227
Corrosive to Metals (Category 1), H290
Acute toxicity, Oral (Category 1), H300
Acute toxicity, Inhalation (Category 1), H330
Acute toxicity, Dermal (Category 1), H310
Carcinogenicity (Category 2), H351
Reproductive toxicity (Category 1B), H360
Specific target organ toxicity - repeated exposure (Category 2), H373
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 3), H412

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 Statements

H227

Combustible liquid.

H290

May be corrosive to metals.

H300 + H310 + H330

Fatal if swallowed, in contact with skin or if inhaled.

H351

Suspected of causing cancer.

H360

May damage fertility or the unborn child.

H373

May cause damage to organs through prolonged or repeated exposure.

H400

Very toxic to aquatic life.

H412

Harmful to aquatic life with long lasting effects.

Precautionary Statements

P201

Obtain special instructions before use.

P202

Do not handle until all safety precautions have been read and understood.

P210

Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.

P234

Keep only in original container.

P260

Do not breathe mist or vapors.

P262

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

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P271

Use only outdoors or in a well-ventilated area.

P273

Avoid release to the environment.

P280

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

P284

Wear respiratory protection.

P301 + P310 + P330

IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.

P302 + P350 + P310

IF ON SKIN: Gently wash with plenty of soap and water. Immediately call a POISON CENTER or doctor/ physician.

P304 + P340 + P310

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.

P308 + P313

IF exposed or concerned: Get medical advice/ attention.

P362

Take off contaminated clothing and wash before reuse.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P390

Absorb spillage to prevent material damage.

P391

Collect spillage.

P403 + P233

Store in a well-ventilated place. Keep container tightly closed.

P403 + P235

Store in a well-ventilated place. Keep cool.

P405

Store locked up.

P406

Store in corrosive resistant container with a resistant inner liner.

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

Synonyms : Acetaldehyde cyanohydrin
2-Hydroxypropionitrile

Formula : C₃H₅NO
Molecular weight : 71.08 g/mol
CAS-No. : 78-97-7
EC-No. : 201-163-2

Component	Classification	Concentration
Lactonitrile		
	Flam. Liq. 4; Acute Tox. 1; Carc. 2; Repr. 1B; STOT RE 2; Aquatic Acute 1; Aquatic Chronic 3; H227, H300, H330, H310, H351, H360, H373, H400, H412 M-Factor - Aquatic Acute: 1	<= 100 %
phosphoric acid		
	Met. Corr. 1; Acute Tox. 4; Skin Corr. 1B; Eye Dam. 1; H290, H302, H314, H318 Concentration limits: >= 1 %: Met. Corr. 1, H290; >= 25 %: Skin Corr. 1B, H314; 10 - < 25 %: Skin Irrit. 2, H315; 10 - < 25 %: Eye Irrit. 2, H319;	>= 1 - < 5 %

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. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

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. Call in ophthalmologist. Remove contact lenses.

If swallowed

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

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**

Water Foam Carbon dioxide (CO₂) 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

Oxides of phosphorus

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

Remove container from danger zone and cool with water. 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. Keep away from heat and sources of ignition. 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 carefully with liquid-absorbent material (e.g. Chemizorb®). 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

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

No metal containers.
Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic 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

Component	CAS-No.	Value	Control parameters	Basis
phosphoric acid	7664-38-2	TWA	1 mg/m ³	USA. ACGIH Threshold Limit Values (TLV)
		STEL	3 mg/m ³	USA. ACGIH Threshold Limit Values (TLV)
		TWA	1 mg/m ³	USA. NIOSH Recommended Exposure Limits
		ST	3 mg/m ³	USA. NIOSH Recommended Exposure Limits
		TWA	1 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	1 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	3 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		TWA	1 mg/m ³	USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)
		STEL	3 mg/m ³	USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)

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). Safety glasses

Skin protection

required

Body Protection

protective clothing

Respiratory protection

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. 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: light yellow
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/freezing point: -40 °C (-40 °F)
f) Initial boiling point and boiling range	90 °C 194 °F at 23 hPa - lit.
g) Flash point	77 °C (171 °F) - closed cup
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	11 hPa at 25 °C (77 °F) - OECD Test Guideline 104
l) Vapor density	No data available
m) Density	0.991 g/cm ³ at 20 °C (68 °F) - lit.
Relative density	No data available
n) Water solubility	1,000 g/l at 20 °C (68 °F) - completely miscible
o) Partition coefficient: n-octanol/water	log Pow: -0.32 at 25 °C (77 °F) - OECD Test Guideline 107 - Bioaccumulation is not expected.
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available

- r) Viscosity No data available
- s) Explosive properties No data available
- t) Oxidizing properties No data available

9.2 Other safety information

No data available

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) .
Contains the following stabilizer(s):
phosphoric acid (1 %)

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

Acids, Oxidizing agents, Strong oxidizing agents

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

Acute toxicity estimate Oral - 0.51 mg/kg
(Calculation method)
LD50 Oral - Rat - male - 31 mg/kg
(OECD Test Guideline 401)
Acute toxicity estimate Inhalation - 4 h - 0.051 mg/l - vapor(Calculation method)

Inhalation: No data available

Acute toxicity estimate Dermal - 5.1 mg/kg
(Calculation method)

LD50 Dermal - Rabbit - 20 mg/kg
LD50 Intraperitoneal - Mouse - 15 mg/kg

Remarks: Behavioral:Ataxia.

Lungs, Thorax, or Respiration:Dyspnea.

Nutritional and Gross Metabolic:Changes in:Body temperature decrease.

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster cells

Metabolic activation: with and without metabolic activation

Result: positive

Carcinogenicity

Suspected of causing cancer.

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

May damage the unborn child.

May damage fertility.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

May cause damage to organs through prolonged or repeated exposure.

Aspiration hazard

No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - NOAEL (No observed adverse effect level)
- 6 mg/kg

RTECS: OD8225000

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

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	LC50 - <i>Oryzias latipes</i> - 0.90 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	Immobilization EC50 - <i>Daphnia magna</i> (Water flea) - 17 mg/l - 24 h (OECD Test Guideline 202)
Toxicity to algae	EC50 - <i>Pseudokirchneriella subcapitata</i> - 0.14 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	EC50 - <i>Pseudomonas putida</i> - 0.83 mg/l - 16 h (DIN 38412)
Toxicity to fish(Chronic toxicity)	LC50 - <i>Oryzias latipes</i> (Orange-red killifish) - 0.69 mg/l - 20 d
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	EC50 - <i>Daphnia magna</i> (Water flea) - 0.67 mg/l - 21 d (OECD Test Guideline 211)
	NOEC - <i>Daphnia magna</i> (Water flea) - 0.17 mg/l - 21 d (OECD Test Guideline 211)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 56 - 76 % - Readily biodegradable. (OECD Test Guideline 302)
------------------	---

12.3 Bioaccumulative potential

Bioaccumulation	<i>Cyprinus carpio</i> (Carp) - 6 Weeks at 25 °C(Lactonitrile)
	Bioconcentration factor (BCF): 0.21

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

No data available

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.

SECTION 14: Transport information**DOT (US)**

UN number: 3276 Class: 6.1 Packing group: I
Proper shipping name: Nitriles, liquid, toxic, n.o.s. ((+/-)-Lactonitrile)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 3276 Class: 6.1 Packing group: I EMS-No: F-A, S-A
Proper shipping name: NITRILES, LIQUID, TOXIC, N.O.S. ((+/-)-Lactonitrile)

IATA

UN number: 3276 Class: 6.1 Packing group: I
Proper shipping name: Nitriles, liquid, toxic, n.o.s. ((+/-)-Lactonitrile)

SECTION 15: Regulatory information**SARA 302 Components**

Lactonitrile	CAS-No. 78-97-7	Revision Date 2007-07-01
--------------	--------------------	-----------------------------

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, Chronic Health Hazard

Massachusetts Right To Know Components

Lactonitrile	CAS-No. 78-97-7	Revision Date 2007-07-01
phosphoric acid	7664-38-2	1993-02-16

Pennsylvania Right To Know Components

Lactonitrile	CAS-No. 78-97-7	Revision Date 2007-07-01
--------------	--------------------	-----------------------------

SECTION 16: Other information**Further information**

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 6.6

Revision Date: 01/10/2024

Print Date: 06/15/2024