

# SAFETY DATA SHEET

Version 6.4  
Revision Date 09/13/2023  
Print Date 07/13/2024

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

### 1.1 Product identifiers

Product name : 3-Chloropropionitrile

Product Number : C69101

Brand : Aldrich

CAS-No. : 542-76-7

### 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

Acute toxicity, Oral (Category 2), H300

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

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

Aldrich - C69101

Page 1 of 10

Hazard statement(s)	
H227	Combustible liquid.
H300	Fatal if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
Precautionary statement(s)	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P280	Wear protective gloves/ eye protection/ face protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. 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.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: 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.
P403 + P235	Store in a well-ventilated place. Keep cool.
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

Lachrymator.

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula	: C <sub>3</sub> H <sub>4</sub> CIN
Molecular weight	: 89.52 g/mol
CAS-No.	: 542-76-7
EC-No.	: 208-827-0

Component	Classification	Concentration
<b>3-chloropropiononitrile</b>		
	Flam. Liq. 4; Acute Tox. 2; Skin Irrit. 2; Eye Irrit. 2A; H227, H300, H315, H319	<= 100 %

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**

Show this material 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.

#### **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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### **Suitable extinguishing media**

Water Foam Carbon dioxide (CO<sub>2</sub>) 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

Nitrogen oxides (NO<sub>x</sub>)

Hydrogen chloride gas

Combustible.

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.

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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. 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.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

#### **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**

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

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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.



b)	Odor	No data available
c)	Odor Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Melting point/range: -52 - -50 °C (-62 - -58 °F) - lit.
f)	Initial boiling point and boiling range	174 - 176 °C 345 - 349 °F - lit.
g)	Flash point	No data available
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	No data available
l)	Vapor density	No data available
m)	Density	1.144 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
	Relative density	No data available
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
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

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.

### 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:  
alkalines

Alkali metals

Strong oxidizing agents

strong reducing agents

A risk of explosion and/or of toxic gas formation exists with the following substances:  
acids

#### **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 - 10 mg/kg

Remarks: (RTECS)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Oral: absorption

Symptoms: Possible damages:, mucosal irritations

Dermal: No data available

##### **Skin corrosion/irritation**

No data available

##### **Serious eye damage/eye irritation**

No data available

##### **Respiratory or skin sensitization**

No data available

##### **Germ cell mutagenicity**

Test Type: Ames test

Test system: Salmonella typhimurium

Result: positive

Remarks: (National Toxicology Program)

##### **Carcinogenicity**

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: UG1400000

Cough, Shortness of breath, Headache, Nausea, Vomiting

Other information

The following applies to cyanogen compounds/ nitriles in general: utmost caution! Release of hydrocyanic acid is possible - blockade of cellular respiration. Cardiovascular disorders, dyspnoea, unconsciousness.

Further data:

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**

No data available

**12.2 Persistence and degradability**

No data available

**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**

We have no quantitative data concerning the ecological effects of this product.

Further information on ecology

Discharge into the environment must be avoided.

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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.

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## SECTION 14: Transport information

#### DOT (US)

UN number: 3276 Class: 6.1 Packing group: II  
Proper shipping name: Nitriles, liquid, toxic, n.o.s. (3-chloropropiononitrile) (3-chloropropiononitrile)  
Reportable Quantity (RQ): 1000 lbs  
Poison Inhalation Hazard: No

#### IMDG

UN number: 3276 Class: 6.1 Packing group: II EMS-No: F-A, S-A  
Proper shipping name: NITRILES, LIQUID, TOXIC, N.O.S. (3-chloropropiononitrile) (3-chloropropiononitrile)

#### IATA

UN number: 3276 Class: 6.1 Packing group: II  
Proper shipping name: Nitriles, liquid, toxic, n.o.s. (3-chloropropiononitrile) (3-chloropropiononitrile)

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## SECTION 15: Regulatory information

#### SARA 302 Components

3-chloropropiononitrile	CAS-No. 542-76-7	Revision Date 2007-03-01
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#### SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

3-chloropropiononitrile	CAS-No. 542-76-7	Revision Date 2007-03-01
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#### SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

#### Massachusetts Right To Know Components

3-chloropropiononitrile	CAS-No. 542-76-7	Revision Date 2007-03-01
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#### Pennsylvania Right To Know Components

Aldrich - C69101

Page 9 of 10

The life science business of Merck KGaA, Darmstadt, Germany  
operates as MilliporeSigma in the US and Canada

**Millipore**  
**Sigma**

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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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