

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.9

Revision Date 20.04.2023

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

Product name : Acrylonitrile-¹⁵N

Product Number : 609587

Brand : Aldrich

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. : 91628-89-6

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

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich (Shanghai) Trading Co.Ltd.
509 Renqing Road
Zhangjiang High Tech East Park, Pudong
SHANGHAI
201201 SHANGHAI
CHINA

Telephone : +86 21 6141-5566
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1.4 Emergency telephone

Emergency Phone # : +86 532 83889090

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****Classification according to Regulation (EC) No 1272/2008**

Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Skin irritation (Category 2), H315
Serious eye damage (Category 1), H318



Skin sensitization (Sub-category 1B), H317
 Carcinogenicity (Category 1B), H350
 Reproductive toxicity (Category 2), H361fd
 Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
 Long-term (chronic) aquatic hazard (Category 2), H411

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

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram



Signal Word

Danger

Hazard statement(s)

H225 Highly flammable liquid and vapor.
 H301 + H311 + H331 Toxic if swallowed, in contact with skin or if inhaled.
 H315 Causes skin irritation.
 H317 May cause an allergic skin reaction.
 H318 Causes serious eye damage.
 H335 May cause respiratory irritation.
 H350 May cause cancer.
 H361fd Suspected of damaging fertility. Suspected of damaging the unborn child.
 H411 Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
 P273 Avoid release to the environment.
 P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
 P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
 P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with 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.

Supplemental Hazard Statements

none

Restricted to professional users.

Reduced Labeling (<= 125 ml)

Pictogram



Signal Word

Danger

Hazard statement(s)

H317 May cause an allergic skin reaction.
 H350 May cause cancer.



H318	Causes serious eye damage.
H361fd	Suspected of damaging fertility. Suspected of damaging the unborn child.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled.
Precautionary statement(s) P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Supplemental Hazard Statements	none

2.3 Other hazards

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.

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula	: C ₃ H ₃ ¹⁵ N
Molecular weight	: 54,05 g/mol
CAS-No.	: 91628-89-6
EC-No.	: 694-108-0

Component		Classification	Concentration
Acrylonitrile-15N			
CAS-No.	91628-89-6	Flam. Liq. 2; Acute Tox. 3; Skin Irrit. 2; Eye Dam. 1; Skin Sens. 1B; Carc. 1B; Repr. 2; STOT SE 3; Aquatic Chronic 2; H225, H301, H331, H311, H315, H318, H317, H350, H361fd, H335, H411	<= 100 %
EC-No.	694-108-0		

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. Immediately 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**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

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. Risk of explosion.

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

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability

Recommended storage temperature
2 - 8 °C

Light sensitive.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

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

8.2 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

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|--|--|
| a) Physical state | clearliquid |
| b) Color | No data available |
| c) Odor | No data available |
| d) Melting point/freezing point | Melting point/range: ca. -83 °C - lit. |
| e) Initial boiling point and boiling range | 77 - 78 °C at 1.025 hPa |
| f) Flammability (solid, gas) | No data available |



- | | |
|---|--|
| g) Upper/lower flammability or explosive limits | Upper explosion limit: ca.17 %(V)
Lower explosion limit: ca.3 %(V) |
| h) Flash point | ca.-4,99 °C |
| i) Autoignition temperature | No data available |
| j) Decomposition temperature | No data available |
| k) pH | No data available |
| l) Viscosity | Viscosity, kinematic: No data available
Viscosity, dynamic: No data available |
| m) Water solubility | No data available |
| n) Partition coefficient: n-octanol/water | log Pow: ca.0,25 - Bioaccumulation is not expected. |
| o) Vapor pressure | ca.110 hPa at 20 °C |
| p) Density | No data available |
| Relative density | No data available |
| q) Relative vapor density | No data available |
| r) Particle characteristics | No data available |
| | |
| s) Explosive properties | No data available |
| t) Oxidizing properties | none |

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heat. May polymerize on exposure to light.
Heat, flames and sparks.
Warming.

10.5 Incompatible materials

Copper, Strong oxidizing agents

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The life science business of Merck operates as MilliporeSigma in the US and Canada



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 - female - 95,1 mg/kg

Remarks: (ECHA)

The value is given in analogy to the following substances: acrylonitrile

LC50 Inhalation - Rat - female - 4 h - 2,05 mg/l - vapor

(OECD Test Guideline 403)

The value is given in analogy to the following substances: acrylonitrile

LD50 Dermal - Rabbit - 250 mg/kg

Remarks: (IUCLID)

The value is given in analogy to the following substances: acrylonitrile

Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 24 h

(OECD Test Guideline 404)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

The value is given in analogy to the following substances: acrylonitrile

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Risk of serious damage to eyes.

(OECD Test Guideline 405)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

The value is given in analogy to the following substances: acrylonitrile

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: positive

(OECD Test Guideline 406)

The value is given in analogy to the following substances: acrylonitrile

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: Metabolic activation

Method: OECD Test Guideline 471

Result: positive

The value is given in analogy to the following substances: acrylonitrile

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation

Result: positive

Remarks: (ECHA)

The value is given in analogy to the following substances: acrylonitrile

Test Type: In vitro mammalian cell gene mutation test



Test system: mouse lymphoma cells
Metabolic activation: without metabolic activation
Method: OECD Test Guideline 476
Result: positive

The value is given in analogy to the following substances: acrylonitrile
Carcinogenicity
Presumed to have carcinogenic potential for humans

Reproductive toxicity

Suspected of damaging fertility.
Suspected of damaging the unborn child.

Specific target organ toxicity - single exposure

May cause respiratory irritation.

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
The value is given in analogy to the following substances: acrylonitrile

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Endocrine disrupting properties

Product:

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea, and vomiting., Skin contact or inhalation may result in:., spasm, inflammation and edema of the larynx, May be partially metabolized to cyanide in the body., Ataxia.

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

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	semi-static test LC50 - <i>Oryzias latipes</i> - 5,1 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - 2,5 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> - 10 mg/l - 72 h (OECD Test Guideline 201)



Toxicity to bacteria	EC5 - Pseudomonas putida - 53 mg/l - 16 h Remarks: (Lit.) (maximum permissible toxic concentration) The value is given in analogy to the following substances: acrylonitrile
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Pimephales promelas (fathead minnow) - 0,17 mg/l - 30 d Remarks: (ECHA) The value is given in analogy to the following substances: acrylonitrile
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	NOEC - Daphnia magna (Water flea) - 2 mg/l - 21 d Remarks: (ECOTOX Database) The value is given in analogy to the following substances: acrylonitrile
	LOEC - Daphnia magna (Water flea) - > 4 mg/l - 21 d Remarks: (ECOTOX Database) The value is given in analogy to the following substances: acrylonitrile

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 14 d Result: 100 % - Inherently biodegradable. (OECD Test Guideline 302C)
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12.3 Bioaccumulative potential

Bioaccumulation	Lepomis macrochirus - 14 d - 9,94 µg/l(Acrylonitrile-15N)
	Bioconcentration factor (BCF): 48

12.4 Mobility in soil

No data available

12.5 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.

12.6 Endocrine disrupting properties

Product:

Assessment	: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.
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12.7 Other adverse effects

Toxic to aquatic life with long lasting effects.



Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3.

H225	Highly flammable liquid and vapor.
H301	Toxic if swallowed.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled.
H311	Toxic in contact with skin.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H318	Highly flammable liquid and vapor.
H331	Toxic if swallowed, in contact with skin or if inhaled.
H335	Causes skin irritation.
H350	May cause an allergic skin reaction.
H361fd	Causes serious eye damage.
H411	May cause respiratory irritation.



Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; 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; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; 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 Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; 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; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization 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; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; 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

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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