SAFETY DATA SHEET

Version 6.1 Revision Date 07/25/2018 Print Date 10/17/2019

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Acrylonitrile-2-<SP>13</>C

Product Number : 586633 Brand : Aldrich Index-No. : 608-003-00-4

CAS-No. : 89511-33-1

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 Street ST. LOUIS MO 63103 UNITED STATES

Telephone : +1 314 771-5765 Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

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 sensitisation (Category 1), H317

Carcinogenicity (Category 1B), H350

Reproductive toxicity (Category 2), H361

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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Acute aquatic toxicity (Category 2), H401

Pictogram

Chronic aquatic toxicity (Category 2), H411

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

2.2 GHS Label elements, including precautionary statements

Signal word	Danger
Hazard statement(s) H225 H301 + H311 + H331 H315 H317 H318 H335 H350 H361 H411	Highly flammable liquid and vapour. Toxic if swallowed, in contact with skin or if inhaled. Causes skin irritation. May cause an allergic skin reaction. Causes serious eye damage. May cause respiratory irritation. May cause cancer. Suspected of damaging fertility or the unborn child. Toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
P201 P202	Obtain special instructions before use. Do not handle until all safety precautions have been read and understood.
P210 P233 P240	Keep away from heat/sparks/open flames/hot surfaces. No smoking. Keep container tightly closed. Ground/bond container and receiving equipment.
P241 P242	Use explosion-proof electrical/ ventilating/ lighting equipment. Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P264 P270	Wash skin thoroughly after handling. Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P272	Contaminated work clothing should not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face
P301 + P310 + P330	protection. IF SWALLOWED: Immediately call a POISON CENTER/doctor. Rinse mouth.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/doctor.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P333 + P313	If skin irritation or rash occurs: 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.
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 P501	Store locked up. Dispose of contents/ container to an approved waste disposal plant.
1 00 1	Dispesse of contents, container to air approved waste disposal plant.

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2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula : 13_{CC2}H₃N Molecular weight : 54.05 g/mol CAS-No. : 89511-33-1 Index-No. : 608-003-00-4

Hazardous components

Component	Classification Concentration	
Acrylonitrile-2-13C		
	Flam. Liq. 2; Acute Tox. 3; Skin Irrit. 2; Eye Dam. 1; Skin Sens. 1; Carc. 1B; Repr. 2; STOT SE 3; Aquatic Acute 2; Aquatic Chronic 2; H225, H301 + H311 + H331, H315, H317, H318, H335, H350, H361, H411	<= 100 %

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

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 (NOx)

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

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6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. hygroscopic

Recommended storage temperature 2 - 8 °C

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Acrylonitrile-2-13C	89511-33-1	TWA	1.000000 ppm	USA. NIOSH Recommended Exposure Limits
	Remarks	Potential Occupational Carcinogen See Appendix A Potential for dermal absorption 15 minute ceiling value		
		С	10.000000 ppm	USA. NIOSH Recommended Exposure Limits
		Potential Occupational Carcinogen		
		See Appendix A		
		Potential for dermal absorption		
		15 minute ceiling value		
		Substance listed; for more information see OSHA document 1910.1045		
		PEL	2.000000 ppm	OSHA Specifically Regulated Chemicals/Carcinogens
		1910.1045 This section applies to all occupational exposures to acrylonitrile (AN), Chemical Abstracts Service Registry No. 000107131, except		

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as provided in paragraphs (a)(2) and (a)(3) of this section. This section does not apply to exposures which result solely from the processing, use, and handling of the following materials: (i) ABS resins, SAN resins, nitrile barrier resins, solid nitrile elastomers, and acrylic and modacrylic fibers, when these listed materials are in the form of finished polymers, and products fabricated from such finished polymers; (ii) Materials made from and/or containing AN for which objective data is reasonably relied upon to demonstrate that the material is not capable of releasing AN in airborne concentrations in excess of 1 ppm as an eight (8)-hour time-weighted average, under the expected conditions of processing, use, and handling which will cause the greatest possible release; and (iii) Solid materials made from and/or containing AN which will not be heated above 170 °F during handling, use, or processing Acrylonitrile or AN means acrylonitrile monomer, chemical formula CH2=CHCN OSHA specifically regulated carcinogen		
STEL	10.000000 ppm	OSHA Specifically Regulated Chemicals/Carcinogens
1910.1045 This section applies to all occupational exposures to acrylonitrile (AN), Chemical Abstracts Service Registry No. 000107131, except as provided in paragraphs (a)(2) and (a)(3) of this section. This section does not apply to exposures which result solely from the processing, use, and handling of the following materials: (i) ABS resins, SAN resins, nitrile barrier resins, solid nitrile elastomers, and acrylic and modacrylic fibers, when these listed materials are in the form of finished polymers, and products fabricated from such finished polymers; (ii) Materials made from and/or containing AN for which objective data is reasonably relied upon to demonstrate that the material is not capable of releasing AN in airborne concentrations in excess of 1 ppm as an eight (8)-hour time-weighted average, under the expected conditions of processing, use, and handling which will cause the greatest possible release; and (iii) Solid materials made from and/or containing AN which will not be heated above 170 °F during handling, use, or processing Acrylonitrile or AN means acrylonitrile monomer, chemical formula CH2=CHCN OSHA specifically regulated carcinogen PEL 2 ppm California permissible exposure limits for chemical contaminants		
(Title 8, Article 107)		
see Section	Ì	LISA ACCIH Throphold Limit Value
TWA	2 ppm	USA. ACGIH Threshold Limit Values (TLV)
Central Nervous System impairment Lower Respiratory Tract irritation Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption TWA 1 ppm USA. NIOSH Recommended		
Potential Occupational Carcinogen See Appendix A		gen
Potential for C	dermal absorption 10 ppm	USA. NIOSH Recommended Exposure Limits
Potential Occupational Carcinogen See Appendix A Potential for dermal absorption		

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15 minute ceiling value			
PEL	2 ppm	OSHA Specifically Regulated Chemicals/Carcinogens	
1910.1045 This section applies to all occupational exposures to acrylonitrile (AN), Chemical Abstracts Service Registry No. 000107131, except as provided in paragraphs (a)(2) and (a)(3) of this section. This section does not apply to exposures which result solely from the processing, use, and handling of the following materials: (i) ABS resins, SAN resins, nitrile barrier resins, solid nitrile elastomers, and acrylic and modacrylic fibers, when these listed materials are in the form of finished polymers, and products fabricated from such finished polymers; (ii) Materials made from and/or containing AN for which objective data is reasonably relied upon to demonstrate that the material is not capable of releasing AN in airborne concentrations in excess of 1 ppm as an eight (8)-hour time-weighted average, under the expected conditions of processing, use, and handling which will cause the greatest possible release; and (iii) Solid materials made from and/or containing AN which will not be heated above 170 °F during handling, use, or processing Acrylonitrile or AN means acrylonitrile monomer, chemical formula CH2=CHCN OSHA specifically regulated carcinogen			
STEL	10 ppm	OSHA Specifically Regulated Chemicals/Carcinogens	
This section applies to all occupational exposures to acrylonitrile (AN), Chemical Abstracts Service Registry No. 000107131, except as provided in paragraphs (a)(2) and (a)(3) of this section. This section does not apply to exposures which result solely from the processing, use, and handling of the following materials: (i) ABS resins, SAN resins, nitrile barrier resins, solid nitrile elastomers, and acrylic and modacrylic fibers, when these listed materials are in the form of finished polymers, and products fabricated from such finished polymers; (ii) Materials made from and/or containing AN for which objective data is reasonably relied upon to demonstrate that the material is not capable of releasing AN in airborne concentrations in excess of 1 ppm as an eight (8)-hour time-weighted average, under the expected conditions of processing, use, and handling which will cause the greatest possible release; and (iii) Solid materials made from and/or containing AN which will not be heated above 170 °F during handling, use, or processing Acrylonitrile or AN means acrylonitrile monomer, chemical formula CH2=CHCN OSHA specifically regulated carcinogen			
Substance listed; for more information see OSHA document 1910.1045			

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product. **Personal protective equipment**

Eye/face protection

Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

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.

Full contact

Material: butyl-rubber

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Minimum layer thickness: 0.3 mm Break through time: 480 min

Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact Material: Chloroprene

Minimum layer thickness: 0.6 mm Break through time: 30 min

Material tested: Camapren® (KCL 722 / Aldrich Z677493, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an

industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multipurpose 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

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance Form: clear, liquid Odour No data available b) c) Odour Threshold No data available No data available d) рH

Melting point/freezing e)

point

Melting point/range: -83 °C (-117 °F) - lit.

Initial boiling point and

77 °C (171 °F) - lit.

boiling range g) Flash point

ca.-4.98 °C (23.04 °F) - closed cup

h) Evaporation rate No data available Flammability (solid, gas) No data available

Upper/lower flammability or

explosive limits

Upper explosion limit: ca.17 %(V) Lower explosion limit: ca.3 %(V)

k) Vapour pressure ca.115 hPa at 20 °C (68 °F)

Vapour density No data available

0.83 g/cm3 at 25 °C (77 °F) m) Relative density

n) Water solubility No data available Partition coefficient: nlog Pow: ca.0.25

octanol/water

p) Auto-ignition No data available

Aldrich- 586633 Page 7 of 11 temperature

q) Decomposition No data available temperature

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

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Vapours may form explosive mixture with air.

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

No data available

Inhalation: No data available Dermal: No data available

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

Carcinogenicity

No data available

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Acrylonitrile-2-13C)

NTP: RAHC - Reasonably anticipated to be a human carcinogen (Acrylonitrile-2-13C)

OSHA: OSHA specifically regulated carcinogen (Acrylonitrile-2-13C)

Reproductive toxicity

No data available

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Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

RTECS: Not available

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated., May be partially metabolized to cyanide in the body., Central nervous system depression, Ataxia., Symptoms may be delayed.

Stomach - Irregularities - Based on Human Evidence Stomach - Irregularities - Based on Human Evidence

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(Acrylonitrile-2-13C)

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal. Toxic to aquatic life with long lasting effects.

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Toxic to aquatic life with long lasting effects.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 1093 Class: 3 (6.1) Packing group: I

Proper shipping name: Acrylonitrile, stabilized Reportable Quantity (RQ) : 100 lbs

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Poison Inhalation Hazard: No

ALL INNER PACKAGINGS MUST BE IN METAL CANS FOR FXG

IMDG

UN number: 1093 Class: 3 (6.1) Packing group: I EMS-No: F-E, S-D

Proper shipping name: ACRYLONITRILE, STABILIZED

Marine pollutant : yes

IATA

UN number: 1093 Class: 3 (6.1) Packing group: I

Proper shipping name: Acrylonitrile, stabilized IATA Passenger: Not permitted for transport

ALL INNER PACKAGINGS MUST BE PACKED WITH ABSORBANT MATERIAL IN TIGHTLY CLOSED METAL OR

RIGID PLASTIC RECEPTACLES, ALL INNER PACKAGINGS MUST BE IN METAL CANS FOR FX AIR

15. REGULATORY INFORMATION

SARA 302 Components

The following components are subject to reporting levels established by SARA Title III, Section 302:

CAS-No. Revision Date 89511-33-1 2008-11-03

Acrylonitrile-2-13C

SARA 313 Components

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

CAS-No. Revision Date 89511-33-1 2008-11-03

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

CAS-No. Revision Date Acrylonitrile-2-13C 89511-33-1 2008-11-03

Pennsylvania Right To Know Components

CAS-No. Revision Date 89511-33-1 2008-11-03

New Jersey Right To Know Components

CAS-No. Revision Date Acrylonitrile-2-13C 89511-33-1 2008-11-03

California Prop. 65 Components

WARNING! This product contains a chemical known to the State of California to cause cancer. CAS-No. Revision Date 2007-09-28

Acrylonitrile-2-13C

16. OTHER INFORMATION

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

H225 Highly flammable liquid and vapour.

H301 Toxic if swallowed.

H301 + H311 + Toxic if swallowed, in contact with skin or if inhaled.

H331

H311 Toxic in contact with skin. H315 Causes skin irritation.

H317 May cause an allergic skin reaction. H318 Causes serious eye damage.

H331 Toxic if inhaled.

H335 May cause respiratory irritation.

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H350 May cause cancer.

H361 Suspected of damaging fertility or the unborn child.

H401 Toxic to aquatic life.

H411 Toxic to aquatic life with long lasting effects.

Further information

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Preparation Information

Sigma-Aldrich Corporation Product Safety – Americas Region 1-800-521-8956

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