

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 7.4

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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 : 3-Pentenitrile, predominately *trans*

Product Number : 306118

Brand : Aldrich

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

CAS-No. : 16529-66-1

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

Identified uses : Laboratory chemicals, Manufacture of substances

### 1.3

CHEMIKART

### 1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

Flammable liquids, (Category 3) H226: Flammable liquid and vapor.

Acute toxicity, (Category 4) H302: Harmful if swallowed.

Acute toxicity, (Category 3) H331: Toxic if inhaled.

### 2.2 Label elements

**Labelling according Regulation (EC) No 1272/2008**

Pictogram

|                                |                                                                                                          |
|--------------------------------|----------------------------------------------------------------------------------------------------------|
| Signal Word                    | Danger                                                                                                   |
| Hazard Statements              |                                                                                                          |
| H226                           | Flammable liquid and vapor.                                                                              |
| H302                           | Harmful if swallowed.                                                                                    |
| H331                           | Toxic if inhaled.                                                                                        |
| Precautionary Statements       |                                                                                                          |
| P210                           | Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.           |
| P233                           | Keep container tightly closed.                                                                           |
| P240                           | Ground and bond container and receiving equipment.                                                       |
| P241                           | Use explosion-proof electrical/ ventilating/ lighting/ equipment.                                        |
| P301 + P312                    | IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.                                           |
| P304 + P340 + P311             | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor. |
| Supplemental Hazard Statements | none                                                                                                     |

### Reduced Labeling (<= 125 ml)

Pictogram

|                                |                                                                                                          |
|--------------------------------|----------------------------------------------------------------------------------------------------------|
| Signal Word                    | Danger                                                                                                   |
| Hazard Statements              |                                                                                                          |
| H331                           | Toxic if inhaled.                                                                                        |
| Precautionary Statements       |                                                                                                          |
| P304 + P340 + P311             | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor. |
| 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.

Ecological information:

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.

Toxicological information:

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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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                   |
|------------------|-----------------------------------|
| Formula          | : C <sub>5</sub> H <sub>7</sub> N |
| Molecular weight | : 81,12 g/mol                     |
| CAS-No.          | : 16529-66-1                      |

| Component                     |            | Classification                                                   | Concentration |
|-------------------------------|------------|------------------------------------------------------------------|---------------|
| <b>trans-1-Cyanobut-2-ene</b> |            |                                                                  |               |
| CAS-No.                       | 16529-66-1 | Flam. Liq. 3; Acute Tox. 4;<br>Acute Tox. 3; H226, H302,<br>H331 | <= 100 %      |
| EC-No.                        | 605-402-5  |                                                                  |               |

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

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.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

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 cyanide (hydrocyanic acid)

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

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. 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.

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## **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**

Change contaminated clothing. Preventive skin protection recommended. Wash hands 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 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

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## 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). Safety glasses

##### Skin protection

required

##### Body Protection

Flame retardant antistatic protective clothing.

##### Respiratory protection

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.

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.

##### Control of environmental exposure

Do not let product enter drains. Risk of explosion.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |                                                 |                     |
|-------------------------------------------------|---------------------|
| a) Physical state                               | liquid              |
| b) Color                                        | colorless           |
| c) Odor                                         | No data available   |
| d) Melting point/freezing point                 | No data available   |
| e) Initial boiling point and boiling range      | 144 - 147 °C - lit. |
| f) Flammability (solid, gas)                    | No data available   |
| g) Upper/lower flammability or explosive limits | No data available   |
| h) Flash point                                  | 40 °C - closed cup  |
| i) Autoignition temperature                     | No data available   |

|                                           |                                                                                  |
|-------------------------------------------|----------------------------------------------------------------------------------|
| j) Decomposition temperature              | No data available                                                                |
| k) pH                                     | No data available                                                                |
| l) Viscosity                              | Viscosity, kinematic: No data available<br>Viscosity, dynamic: No data available |
| m) Water solubility                       | No data available                                                                |
| n) Partition coefficient: n-octanol/water | No data available                                                                |
| o) Vapor pressure                         | 33,2 hPa at 50 °C<br>213 hPa at 100 °C                                           |
| p) Density                                | 0,837 g/cm <sup>3</sup> at 25 °C - lit.                                          |
| 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

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Heating.

### 10.5 Incompatible materials

Strong oxidizing agents, Strong bases

### 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

Acute toxicity estimate Oral - 500,1 mg/kg  
(Expert judgment)

Acute toxicity estimate Inhalation - 4 h - 3 mg/l - vapor

(Expert judgment)  
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**

No data available

**Carcinogenicity**

No data available

**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**

**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.

Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. Onset may be delayed 2 to 4 hours or longer.

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

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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**

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.

## 12.7 Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

No data available

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## SECTION 14: Transport information

### 14.1 UN number

ADR/RID: 3275

IMDG: 3275

IATA: 3275

### 14.2 UN proper shipping name

ADR/RID: NITRILES, TOXIC, FLAMMABLE, N.O.S. (trans-1-Cyanobut-2-ene)

IMDG: NITRILES, TOXIC, FLAMMABLE, N.O.S. (trans-1-Cyanobut-2-ene)

IATA: Nitriles, toxic, flammable, n.o.s. (trans-1-Cyanobut-2-ene)

### 14.3 Transport hazard class(es)

ADR/RID: 6.1 (3)

IMDG: 6.1 (3)

IATA: 6.1 (3)

### 14.4 Packaging group

ADR/RID: II

IMDG: II

IATA: II

### 14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

### 14.6 Special precautions for user

Tunnel restriction code : (D/E)

Further information : No data available

### 14.7 Maritime transport in bulk according to IMO instruments

Not applicable for product as supplied.

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## SECTION 15: Regulatory information

### 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture



This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

#### **National legislation**

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

H2 ACUTE TOXIC

P5c FLAMMABLE LIQUIDS

#### **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

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### **SECTION 16: Other information**

#### **Full text of H-Statements**

|      |                             |
|------|-----------------------------|
| H226 | Flammable liquid and vapor. |
| H302 | Harmful if swallowed.       |
| H331 | Toxic if inhaled.           |

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## 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 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](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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