

## SAFETY DATA SHEET

Version 6.7  
Revision Date 08/27/2023  
Print Date 04/28/2024

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

Product name : 1,6-Dicyanohexane

Product Number : D78008  
Brand : Aldrich  
CAS-No. : 629-40-3

**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)**

Acute toxicity, Oral (Category 3), H301

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 statement(s)  
H301 : Toxic if swallowed.

Precautionary statement(s)	
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
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 - none

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms	: Suberonitrile Octanedinitrile Hexamethylene dicyanide
Formula	: C <sub>8</sub> H <sub>12</sub> N <sub>2</sub>
Molecular weight	: 136.19 g/mol
CAS-No.	: 629-40-3
EC-No.	: 211-089-2

Component	Classification	Concentration
<b>suberic acid dinitrile</b>		
	Acute Tox. 3; H301	<= 100 %

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

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. 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**

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

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**

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. 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**

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): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

### **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.

### **8.2 Exposure controls**

#### **Appropriate engineering controls**

Change contaminated clothing. Preventive skin protection recommended. Wash hands 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**

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Chloroprene

Minimum layer thickness: 0.65 mm

Break through time: 480 min

Material tested: KCL 720 Camapren®

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm  
Break through time: 30 min  
Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

### **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.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

- |   |   |                   |
|---|---|-------------------|
| a) Appearance                                   | Form: clear, liquid<br>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/range: -3.5 °C (25.7 °F) - lit.                     |                   |
| f) Initial boiling point and boiling range      | 185 °C 365 °F at 20 hPa - lit.                                    |                   |
| g) Flash point                                  | 105 °C (221 °F) - closed cup                                      |                   |
| h) Evaporation rate                             | No data available   |                   |
| i) Flammability (solid, gas)                    | No data available   |                   |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 29 %(V)<br>Lower explosion limit: 8.5 %(V) |                   |
| k) Vapor pressure                               | 0.001 hPa at 20 °C (68 °F) - OECD Test Guideline 104              |                   |
| l) Vapor density                                | No data available   |                   |
| m) Density                                      | 0.954 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.                   |                   |
|   | Relative density  | No data available |
| n) Water solubility                             | 11.3 g/l at 20 °C (68 °F) - OECD Test Guideline 105               |                   |
| o) Partition coefficient:                       | log Pow: 0.56 at 25 °C (77 °F) - OECD Test Guideline 107          |                   |

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n-octanol/water

- |    |                           |                   |
|----|---------------------------|-------------------|
| 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      | none              |

## 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.  
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) .

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:  
Bases  
Strong oxidizing agents  
strong reducing agents  
Strong acids

### 10.4 Conditions to avoid

Strong heating.

### 10.5 Incompatible materials

no information 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 - 150 mg/kg

Remarks: (RTECS)

Inhalation: No data available

Dermal: No data available

No data available

**Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation  
(OECD Test Guideline 404)

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation  
(OECD Test Guideline 405)

**Respiratory or skin sensitization**

Local lymph node assay (LLNA) - Mouse

Result: negative  
(OECD Test Guideline 429)

**Germ cell mutagenicity**

No data available

**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: WM2131000

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

After absorption:

We have no description of any toxic symptoms.

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.

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

Toxicity to fish	static test LC50 - <i>Leuciscus idus</i> (Golden orfe) - 383 mg/l - 96 h Remarks: (ECHA)
Toxicity to algae	static test ErC50 - <i>Desmodesmus subspicatus</i> (green algae) - > 320 mg/l - 72 h (OECD Test Guideline 201)

### 12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 90 - 100 % - Readily biodegradable. (OECD Test Guideline 301A)
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### 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

No data available

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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: III  
Proper shipping name: Nitriles, liquid, toxic, n.o.s. (suberic acid dinitrile) (suberic acid dinitrile)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

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**IMDG**

UN number: 3276    Class: 6.1    Packing group: III    EMS-No: F-A, S-A  
Proper shipping name: NITRILES, LIQUID, TOXIC, N.O.S. (suberic acid dinitrile) (suberic acid dinitrile)

**IATA**

UN number: 3276    Class: 6.1    Packing group: III  
Proper shipping name: Nitriles, liquid, toxic, n.o.s. (suberic acid dinitrile) (suberic acid dinitrile)

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

This material does not contain any components with a section 302 EHS TPQ.

**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

**Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

suberic acid dinitrile	CAS-No. 629-40-3	Revision Date 2015-07-08
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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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