

## SAFETY DATA SHEET

Version 8.3  
Revision Date 01/28/2022  
Print Date 06/01/2022

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

Product name : 1,6-Diisocyanato-2,2,4-trimethylhexane

Product Number : CDS000410

Brand : Aldrich

Index-No. : 615-010-00-6

CAS-No. : 16938-22-0

**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, Inhalation (Category 3), H331  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Respiratory sensitization (Category 1), H334  
Skin sensitization (Category 1), H317  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335  
Long-term (chronic) aquatic hazard (Category 4), H413

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)

H315 Causes skin irritation.  
H317 May cause an allergic skin reaction.  
H319 Causes serious eye irritation.  
H331 Toxic if inhaled.  
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.  
H335 May cause respiratory irritation.  
H413 May cause long lasting harmful effects to aquatic life.

Precautionary statement(s)

P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.  
P264 Wash skin thoroughly after handling.  
P271 Use only outdoors or in a well-ventilated area.  
P272 Contaminated work clothing must not be allowed out of the workplace.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/ eye protection/ face protection.  
P285 In case of inadequate ventilation wear respiratory protection.  
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.  
P304 + P340 + P311 IF INHALED: Remove person to fresh air and keep comfortable for breathing. 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.  
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.  
P337 + P313 If eye irritation persists: Get medical advice/ attention.  
P342 + P311 If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.  
P362 Take off contaminated clothing and wash before reuse.  
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.  
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 : 2,2,4-trimethylhexamethylene-1,6-di-isocyanate  
Molecular weight : 210.27 g/mol  
CAS-No. : 16938-22-0  
EC-No. : 241-001-8  
Index-No. : 615-010-00-6

| Component | Classification | Concentration |
|-----------|----------------|---------------|
|-----------|----------------|---------------|

| <b>1,6-Diisocyanato-2,2,4-trimethylhexane</b> |                                                                                                                                                                                                                                          |          |
|-----------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|
|                                               | Acute Tox. 3; Skin Irrit. 2; Eye Irrit. 2A; Resp. Sens. 1; Skin Sens. 1; STOT SE 3; Aquatic Chronic 4; H331, H315, H319, H334, H317, H335, H413<br>Concentration limits:<br>>= 0.5 %: Resp. Sens. 1, H334; >= 0.5 %: Skin Sens. 1, H317; | <= 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

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. Consult a physician.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. 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>)

Combustible.

Risk of dust explosion.

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**

#### **Advice on safe handling**

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

#### **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): 6.1C: 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

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face 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

required

##### Body Protection

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.

#### 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: liquid      |
| b) Odor                                    | No data available |
| c) Odor Threshold                          | No data available |
| d) pH                                      | No data available |
| e) Melting point/freezing point            | No data available |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point                             | No data available |
| h) Evaporation rate                        | No data available |
| i) Flammability (solid,                    | No data available |

|    |                                              |                                                            |
|----|----------------------------------------------|------------------------------------------------------------|
|    | gas)                                         |                                                            |
| j) | Upper/lower flammability or explosive limits | No data available                                          |
| k) | Vapor pressure                               | No data available                                          |
| l) | Vapor density                                | No data available                                          |
| m) | Density                                      | No data available                                          |
|    | Relative density                             | No data available                                          |
| n) | Water solubility                             | slightly soluble                                           |
| o) | Partition coefficient: n-octanol/water       | log Pow: 4.56 at 25 °C (77 °F) - Potential bioaccumulation |
| 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

No data available

### 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

no information available

### 10.5 Incompatible materials

Strong oxidizing agents

### 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

Oral: No data available

Acute toxicity estimate Inhalation - Expert judgment - 4 h - 5 mg/l - vapor

Dermal: No data available

**Skin corrosion/irritation**

Causes skin irritation. Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**Serious eye damage/eye irritation**

Causes serious eye irritation. Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**Respiratory or skin sensitization**

May cause allergic respiratory and skin reactions Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**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**

Inhalation - May cause respiratory irritation.

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

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

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

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. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14: Transport information

### DOT (US)

UN number: 2810    Class: 6.1    Packing group: III  
Proper shipping name: Toxic, liquids, organic, n.o.s. (1,6-Diisocyanato-2,2,4-trimethylhexane)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 2810    Class: 6.1    Packing group: III    EMS-No: F-A, S-A  
Proper shipping name: TOXIC LIQUID, ORGANIC, N.O.S. (1,6-Diisocyanato-2,2,4-trimethylhexane)

### IATA

UN number: 2810    Class: 6.1    Packing group: III  
Proper shipping name: Toxic liquid, organic, n.o.s. (1,6-Diisocyanato-2,2,4-trimethylhexane)

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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

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

|                                        | CAS-No.    | Revision Date |
|----------------------------------------|------------|---------------|
| 1,6-Diisocyanato-2,2,4-trimethylhexane | 16938-22-0 | 2015-11-23    |

### SARA 311/312 Hazards

Acute Health Hazard

Aldrich - CDS000410

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### Massachusetts Right To Know Components

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

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

### Pennsylvania Right To Know Components

1,6-Diisocyanato-2,2,4-trimethylhexane

CAS-No.  
16938-22-0

Revision Date  
2015-11-23

### New Jersey Right To Know Components

1,6-Diisocyanato-2,2,4-trimethylhexane

CAS-No.  
16938-22-0

Revision Date  
2015-11-23

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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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