

## SAFETY DATA SHEET

Version 6.6  
Revision Date 03/04/2024  
Print Date 05/12/2024

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

Product name : Hexamethylene diisocyanate

Product Number : 52649

Brand : Sigma

Index-No. : 615-011-00-1

CAS-No. : 822-06-0

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

**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 4), H302

Acute toxicity, Inhalation (Category 1), H330

Skin corrosion (Category 1C), H314

Sigma - 52649

Page 1 of 12

Serious eye damage (Category 1), H318  
 Respiratory sensitization (Category 1), H334  
 Skin sensitization (Category 1), H317  
 Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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 Statements

H302	Harmful if swallowed.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H330	Fatal if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H335	May cause respiratory irritation.

Precautionary Statements

P260	Do not breathe mist or vapors.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P272	Contaminated work clothing must not be allowed out of the workplace.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P284	Wear respiratory protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately 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.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P342 + P311	If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.
P363	Wash contaminated clothing 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

Lachrymator., Rapidly absorbed through skin.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms	:	1,6-Diisocyanatohexane
Formula	:	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Molecular weight	:	168.19 g/mol
CAS-No.	:	822-06-0
EC-No.	:	212-485-8
Index-No.	:	615-011-00-1

Component	Classification	Concentration
<b>hexamethylene diisocyanate</b>		
	Acute Tox. 4; Acute Tox. 1; Skin Corr. 1C; Eye Dam. 1; Resp. Sens. 1; Skin Sens. 1; STOT SE 3; H302, H330, H314, H318, H334, H317, H335 Concentration limits: >= 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.

## 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

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Pulmonary failure possible after aspiration of vomit. Call a physician immediately. Do not attempt to neutralise.

#### **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**

Carbon dioxide (CO<sub>2</sub>) Dry powder

##### **Unsuitable extinguishing media**

Foam Water

#### **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.

---

### **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.

---

## 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.

Store under inert gas. Moisture sensitive.

#### Storage class

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

### 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

Component	CAS-No.	Value	Control parameters	Basis
hexamethylene diisocyanate	822-06-0	TWA	0.0050 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Upper Respiratory Tract irritation Respiratory sensitization		
		TWA	0.0050 ppm 0.035 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		10 minute ceiling value		
		C	0.02 ppm 0.14 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		10 minute ceiling value		

#### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
-----------	---------	------------	-------	---------------------	-------

hexamethylene diisocyanate	822-06-0	1,6-Hexamethylene diamine	15µg/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift			

## 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). Tightly fitting safety goggles

#### 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: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

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 A-(P3)

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.

---

### SECTION 9: Physical and chemical properties

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

a) Appearance	Form: clear, liquid Color: clear, colorless
b) Odor	pungent
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/freezing point: ca.-67 °C (ca.-89 °F) - (ECHA)
f) Initial boiling point and boiling range	82 - 85 °C 180 - 185 °F at 0.1 hPa
g) Flash point	130 °C (266 °F) - Pensky-Martens closed cup - DIN 51758
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 9.5 %(V) Lower explosion limit: 0.9 %(V)
k) Vapor pressure	0.007 hPa at 20 °C (68 °F)
l) Vapor density	No data available
m) Density	1.047 g/mL at 20 °C (68 °F) - lit.
Relative density	No data available
n) Water solubility	Hydrolysis
o) Partition coefficient: n-octanol/water	log Pow: 3.2 at 25 °C (77 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	454 °C (849 °F) at 1,013.25 hPa
q) Decomposition temperature	No data available
r) Viscosity	1.68 mm <sup>2</sup> /s at 40 °C (104 °F) - OECD Test Guideline 114 - 2.29 mm <sup>2</sup> /s at 20 °C (68 °F) - OECD Test Guideline 114 -
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**

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**

can decompose violently in contact with:

Water

Release of:

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

Risk of explosion with:

Alcohols

with

Bases

Exothermic reaction with:

Alcohols

amides

Amines

Oxidizing agents

Strong acids and strong bases

mercaptans

phenols

### **10.4 Conditions to avoid**

Heat. Avoid moisture.

Strong heating.

### **10.5 Incompatible materials**

nonferrous metals, Copper, Copper alloys, Mild steel, Zinc

### **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**

LD<sub>50</sub> Oral - Rat - male - 746 mg/kg

(OECD Test Guideline 401)

LC<sub>50</sub> Inhalation - Rat - male and female - 4 h - 0.124 mg/l - vapor

(OECD Test Guideline 403)

LD<sub>50</sub> Dermal - Rat - male and female - > 7,000 mg/kg

(OECD Test Guideline 402)

No data available

Sigma - 52649

Page 8 of 12



**Skin corrosion/irritation**

Skin - Rabbit

Result: Corrosive after 1 to 4 hours of exposure - 4 h  
(OECD Test Guideline 404)

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Causes serious eye damage.  
(OECD Test Guideline 405)

**Respiratory or skin sensitization**

Maximization Test - Guinea pig

Result: positive

(OECD Test Guideline 406)

Sensitisation test: - Guinea pig

Result: positive

**Germ cell mutagenicity**

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

Test Type: Micronucleus test

Species: Mouse

Cell type: Bone marrow

Application Route: inhalation (vapor)

Method: OECD Test Guideline 474

Result: negative

**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. - Respiratory system

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

RTECS: MO1740000

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

---

**SECTION 12: Ecological information****12.1 Toxicity**

No data available

Toxicity to algae                      static test ErC50 - *Desmodesmus subspicatus* (green algae) - > 77.4 mg/l - 72 h  
(OECD Test Guideline 201)

Toxicity to bacteria

**12.2 Persistence and degradability**

Biodegradability                      aerobic - Exposure time 28 d  
Result: 42 % - Not readily biodegradable.  
(OECD Test Guideline 301F)

**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**

Stability in water                      - 5 - 10 min at 20 °C  
Remarks: Hydrolyzes on contact with water.

---

## 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.

---

## SECTION 14: Transport information

#### DOT (US)

UN number: 2281    Class: 6.1    Packing group: II  
Proper shipping name: Hexamethylene diisocyanate  
Reportable Quantity (RQ): 100 lbs  
Poison Inhalation Hazard: No

#### IMDG

UN number: 2281    Class: 6.1    Packing group: II    EMS-No: F-A, S-A  
Proper shipping name: HEXAMETHYLENE DIISOCYANATE

#### IATA

UN number: 2281    Class: 6.1    Packing group: II  
Proper shipping name: Hexamethylene diisocyanate

---

## 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
hexamethylene diisocyanate	822-06-0	1993-02-16

#### SARA 311/312 Hazards

Acute Health Hazard

#### Massachusetts Right To Know Components

	CAS-No.	Revision Date
hexamethylene diisocyanate	822-06-0	1993-02-16

---

## SECTION 16: Other information

### 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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 6.6

Revision Date: 03/04/2024

Print Date: 05/12/2024