SAFETY DATA SHEET

Version 5.8
Revision Date 06/22/2018
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1. PRODUCT AND COMPANY IDENTIFICATION

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

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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
Serious eye damage (Category 1), H318
Respiratory sensitisation (Category 1), H334
Skin sensitisation (Category 1), H317

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)
H302 Harmful if swallowed.
H314 Causes severe skin burns and eye damage.
H317 May cause an allergic skin reaction.
H318 Causes serious eye damage.
H330 Fatal if inhaled.
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.

Precautionary statement(s)
P260 Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.

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 should 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.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	:	1,6-Diisocyanatohexane
Formula	:	$C_8H_{12}N_2O_2$
Molecular weight	:	168.19 g/mol
CAS-No.	:	822-06-0
EC-No.	:	212-485-8
Index-No.	:	615-011-00-1
Registration number	:	01-2119457571-37-XXXX

Hazardous components

Component	Classification	Concentration
Hexamethylene diisocyanate		
	Acute Tox. 4; Acute Tox. 1; Skin Corr. 1C; Eye Dam. 1; Resp. Sens. 1; Skin Sens. 1; H302, H314, H317, H318, H330, H334	90 - 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

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

If inhaled

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

In case of skin contact
Take off contaminated clothing and shoes immediately. 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.Continue rinsing eyes during transport to hospital.

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
No data available

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
No data available

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. Evacuate personnel to safe 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.

6.3 Methods and materials for containment and cleaning up
Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

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.
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. Moisture sensitive.
Storage class (TRGS 510): 6.1B: Non-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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components 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/m3	USA. NIOSH Recommended Exposure Limits
		10 minute ceiling value		
		C	0.02 ppm 0.14 mg/m3	USA. NIOSH Recommended Exposure Limits
		10 minute ceiling value		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
	-	1,6-Hexamethylene diamine	15µg/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift			

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
Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

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)

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, 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 multi-purpose 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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid Colour: clear, colourless
b)	Odour	pungent
c)	Odour Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Freezing point/ range: ca.-66.99 °C (-88.58 °F)
f)	Initial boiling point and boiling range	82 - 85 °C (180 - 185 °F) at 0.1 hPa (0.1 mmHg)
g)	Flash point	135 °C (275 °F) - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapour pressure	0.007 hPa (0.005 mmHg) at 20 °C (68 °F)
l)	Vapour density	5.81 - (Air = 1.0)
m)	Relative density	1.047 g/mL at 20 °C (68 °F)
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Auto-ignition temperature	454 °C (849 °F)
q)	Decomposition temperature	No data available
r)	Viscosity	2.29 mm2/s at 20 °C (68 °F) -
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information

Relative vapour density	5.81 - (Air = 1.0)

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
No data available

10.4 Conditions to avoid
Heat Avoid moisture.

10.5 Incompatible materials
Alcohols, Strong bases, Amines, Strong oxidizing agents, Water

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
LD50 Oral - Rat - male - 746 mg/kg
(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - 0.124 mg/l
(OECD Test Guideline 403)

LD50 Dermal - Rat - male and female - > 7,000 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation
Skin - Rabbit
Result: Corrosive - 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 sensitisation
Maximisation Test - Guinea pig
Result: positive
(OECD Test Guideline 406)

Germ cell mutagenicity
Ames test
Salmonella typhimurium
Result: negative
(IUCLID)

Mutagenicity (mammal cell test):
Chinese hamster ovary cells
Result: negative
(Lit.)

OECD Test Guideline 474
Mouse - male and female - Bone marrow
Result: negative

Carcinogenicity

IARC:	No component 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 component 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

Specific target organ toxicity - single exposure
May cause respiratory irritation. - Respiratory system

Specific target organ toxicity - repeated exposure

Aspiration hazard

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.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to algae	Growth inhibition ErC50 - Desmodesmus subspicatus (green algae) - > 77.4 mg/l - 72 h (OECD Test Guideline 201)
	Growth inhibition NOEC - Desmodesmus subspicatus (green algae) - 11.7 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	Remarks: (IUCLID)

12.2 Persistence and degradability

Biodegradability	Result: 0 % - Not readily eliminated from water. (OECD Test Guideline 302C) aerobic - Exposure time 28 d Result: 42 % - Not readily biodegradable. (OECD Test Guideline 301F)

12.3 Bioaccumulative potential

12.4 Mobility in soil

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

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

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging
Dispose of as unused product.

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

15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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

Pennsylvania Right To Know Components

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

California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

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

Acute Tox.	Acute toxicity
Eye Dam.	Serious eye damage
H302	Harmful if swallowed.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H330	Fatal if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
Resp. Sens.	Respiratory sensitisation
Skin Corr.	Skin corrosion
Skin Sens.	Skin sensitisation

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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

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