

Chemical Safety Data Sheet MSDS / SDS

Hexamethylene Diisocyanate

Revision Date:2026-06-27 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifier

Product name : Hexamethylene Diisocyanate
CBnumber : CB4255051
CAS : 822-06-0
EINECS Number : 212-485-8
Synonyms : HDI,HMDI

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P264 Wash hands thoroughly after handling.
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.
P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P307+P311 IF exposed: call a POISON CENTER or doctor/physician.

P342+P311 IF experiencing respiratory symptoms: call a POISON CENTER or doctor/physician.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

P501 Dispose of contents/container to.....

Hazard statements

H302 Harmful if swallowed

H311 Toxic in contact with skin

H314 Causes severe skin burns and eye damage

H315 Causes skin irritation

H317 May cause an allergic skin reaction

H319 Causes serious eye irritation

H330 Fatal if inhaled

H331 Toxic if inhaled

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled

H335 May cause respiratory irritation

H370 Causes damage to organs

H372 Causes damage to organs through prolonged or repeated exposure

SECTION 3: Composition/information on ingredients

Substance

Product name	: Hexamethylene Diisocyanate
Synonyms	: HDI, HMDI
CAS	: 822-06-0
EC number	: 212-485-8
MF	: C ₈ H ₁₂ N ₂ O ₂
MW	: 168.19

SECTION 4: First aid measures

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.

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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media**Suitable extinguishing media**

Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

Foam Water

Special hazards arising from the substance or mixture

Carbon oxides Nitrogen oxides (NO_x) Combustible.

Vapors are heavier than air and may spread along floors. Forms explosive mixtures with air on intense heating.

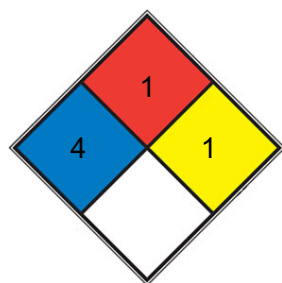
Development of hazardous combustion gases or vapours possible in the event of fire.

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.

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.

NFPA 704

HEALTH 4 Very short exposure could cause death or major residual injury (e.g. hydrogen cyanide, phosgene, methyl isocyanate, [hydrofluoric acid](#))

FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

☒ REACT 1 Normally stable, but can become unstable at elevated temperatures and pressures (e.g. [propene](#))

☐ SPEC.

☐ HAZ.

SECTION 6: Accidental release measures

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.

Environmental precautions

Do not let product enter drains.

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.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

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.

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.

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

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). 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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: 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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: 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 B-(P2)

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.

Exposure limits

TLV-TWA 0.0343 mg/m³ (0.005 ppm) (ACGIH).

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	clear, colorless clear, liquid
Odour	pungent
Odour Threshold	No data available

pH	No data available
Melting point/freezing point	Melting point/freezing point: ca.-67 °C - (ECHA)
Initial boiling point and boiling range	82 - 85 °C at 0,1 hPa
Flash point	130 °C - Pensky-Martens closed cup - DIN 51758
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 9,5 %(V) Lower explosion limit: 0,9 %(V)
Vapour pressure	0,007 hPa at 20 °C
Vapour density	No data available
Relative density	1.05
Water solubility	Hydrolysis
Partition coefficient: n-octanol/water	log Pow: 3,2 at 25 °C - Bioaccumulation is not expected.
Autoignition temperature	454 °C at 1.013,25 hPa
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: 1,68 mm ² /s at 40 °C - OECD Test Guideline 1142,29 mm ² /s at 20 °C - OECD Test Guideline 114 Viscosity, dynamic: 1,73 mPa.s at 40 °C - OECD Test Guideline 1142,4 mPa.s at 20 °C - OECD Test Guideline 114
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

No data available

SECTION 10: Stability and reactivity

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.

Chemical stability

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

Possibility of hazardous reactions

can decompose violently in contact with: Water

Release of:

Carbon dioxide (CO₂) Risk of explosion with:

Alcohols with Bases

Exothermic reaction with:

Alcohols amides Amines

Oxidizing agents

Strong acids and strong bases mercaptans

phenols

Conditions to avoid

Heat. Avoid moisture. Strong heating.

Incompatible materials

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

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

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 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

(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

No data available

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

Toxicity

LD50 orally in Rabbit: 746 mg/kg LD50 dermal Rabbit 570 mg/kg

SECTION 12: Ecological information

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**Persistence and degradability**

Biodegradability aerobic - Exposure time 28 d

Result: 42 % - Not readily biodegradable. (OECD Test Guideline 301F)

Bioaccumulative potential

No data available

Mobility in soil

No data available

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.

Toxics Screening Level

The chronic (long-term) initial threshold screening level (ITSL) for 1,6-hexamethylene diisocyanate (HDI) is 0.2 µg/m³ based on annual averaging time. The short-term ITSL for HDI is 0.3 µg/m³ with an 8-hr averaging time.

Other adverse effects

Stability in water - 5 - 10 min at 20 °C

Remarks: Hydrolyzes on contact with water.

SECTION 13: Disposal considerations

Waste treatment methods**Incompatibilities**

Incompatible with oxidizers; contact may cause fires or explosions. Incompatible with amines, aldehydes, alkali metals, ammonia, carboxylic

acids, capro lactum, alkaline materials, glycols, ketones, mercaptans, hydrides, organotin catalysts, phenols, strong acids, strong bases, strong reducing agents such as hydrides, urethanes, ureas.

Product

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

Waste Disposal

Disposal is by chemical incineration of HDIsolution in a combustible solvent.

SECTION 14: Transport information

UN number

ADR/RID: 2281 IMDG: 2281 IATA: 2281

UN proper shipping name

14.2 ADR/RID: HEXAMETHYLENE DIISOCYANATE IMDG: HEXAMETHYLENE DIISOCYANATE

IATA: Hexamethylene diisocyanate

Transport hazard class(es)

14.3 ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

Packaging group

14.4 ADR/RID: II IMDG: II IATA: II

Environmental hazards

14.5 ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

14.6 No data available

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015: Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC): Listed. website: <https://www.mee.gov.cn/>

EC Inventory: Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS): Listed. website: <https://echa.europa.eu/>

Korea Existing Chemicals List (KECL): Listed. website: <http://ncis.nier.go.kr>

New Zealand Inventory of Chemicals (NZIoC): Listed. website: <https://www.epa.govt.nz/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS): Listed. website: <https://emb.gov.ph/>

United States Toxic Substances Control Act (TSCA) Inventory: Listed. website: <https://www.epa.gov/>

Vietnam National Chemical Inventory: Listed. website: <https://chemicaldata.gov.vn/>

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

References

【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Other Information

The symptoms of asthma often do not become manifest until a few hours have passed and they are aggravated by physical effort. Rest and medical observation are therefore essential. Anyone who has shown symptoms of asthma due to this substance should avoid all further contact. Anyone who has shown skin sensitization due to this substance should avoid all further contact. Workers exposed to this compound may also be sensitized to other isocyanates. The odour warning when the exposure limit value is exceeded is insufficient. Do NOT take working clothes home.

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.