1 Identification

Product identifier

Product name: 1,6-Diisocyanatohexane

Stock number: 43803
CAS Number:
822-06-0
EC number:
212-485-8
Relevant identified uses of the substance or mixture and uses advised against.
Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet
Manufacturer/Supplier:
Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com
Information Department: Health, Safety and Environmental Department
Emergency telephone number:
During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)

GHS06 Skull and crossbones

Acute Tox. 3 H311 Toxic in contact with skin.
Acute Tox. 1 H330 Fatal if inhaled.

GHS08 Health hazard

Resp. Sens. 1 H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.

GHS07

Acute Tox. 4 H302 Harmful if swallowed.
Skin Irrit. 2 H315 Causes skin irritation.
Eye Irrit. 2A H319 Causes serious eye irritation.
Skin Sens. 1 H317 May cause an allergic skin reaction.
STOT SE 3 H335 May cause respiratory irritation.
Hazards not otherwise classified No information known.

Label elements
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)
Hazard pictograms

GHS06 GHS08

Signal word Danger
Hazard statements
H302 Harmful if swallowed.
H311 Toxic in contact with skin.
H330 Fatal if inhaled.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H317 May cause an allergic skin reaction.
H335 May cause respiratory irritation.
Precautionary statements
P260 Do not breathe dust/fume/gas/mist/vapors/spray.
P284 [In case of inadequate ventilation] wear respiratory protection.
P305+P351+P338 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P320 Specific treatment is urgent (see on this label).
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.
WHMIS classification
D1A - Very toxic material causing immediate and serious toxic effects
D2A - Very toxic material causing other toxic effects

Classification system
HMIS ratings (scale 0-4)
(Hazardous Materials Identification System)

Health (acute effects) = 3
Flammability = 1
Physical Hazard = 1

(Contd. on page 2)

Product name: 1,6-Diisocyanatohexane

(Contd. of page 1)

Other hazards
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances
CAS# Description:
822-06-0 1,6-Diisocyanatohexane
Concentration: ≤100%
Identification number(s):
EC number: 212-485-8

4 First-aid measures

Description of first aid measures
General information
Immediately remove any clothing soiled by the product.
Remove breathing apparatus only after contaminated clothing has been completely removed.
In case of irregular breathing or respiratory arrest provide artificial respiration.
After inhalation
Supply fresh air. If required, provide artificial respiration. Keep patient warm.
Seek immediate medical advice.
After skin contact
Immediately wash with water and soap and rinse thoroughly.
Seek immediate medical advice.
After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.
After swallowing Seek medical treatment.
Information for doctor
Most important symptoms and effects, both acute and delayed
Causes skin irritation.
Harmful if swallowed.
Toxic in contact with skin.
Causes serious eye irritation.
Fatal if inhaled.
May cause allergy or asthma symptoms or breathing difficulties if inhaled.
May cause an allergic skin reaction.
Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures

Extinguishing media
Suitable extinguishing agents Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
Special hazards arising from the substance or mixture
If this product is involved in a fire, the following can be released:
Carbon monoxide and carbon dioxide
Nitrogen oxides (NOx)
Advice for firefighters
Protective equipment:
Wear self-contained respirator.
Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures
Wear protective equipment. Keep unprotected persons away.
Ensure adequate ventilation
Environmental precautions: Do not allow product to reach sewage system or any water course.
Methods and material for containment and cleaning up:
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Dispose of contaminated material as waste according to section 13.
Ensure adequate ventilation.
Prevention of secondary hazards: No special measures required.
Reference to other sections
See Section 7 for information on safe handling
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.
Protective Action Criteria for Chemicals
PAC-1: 0.018 ppm
PAC-2: 0.2 ppm
PAC-3: 3 ppm

7 Handling and storage

Handling
Precautions for safe handling
Handle under dry protective gas.
Keep container tightly sealed.
Store in cool, dry place in tightly closed containers.
Ensure good ventilation at the workplace.
Open and handle container with care.
Information about protection against explosions and fires: No information known.

Conditions for safe storage, including any incompatibilities
Storage
Requirements to be met by storerooms and receptacles: No special requirements.
Information about storage in one common storage facility:
Store away from water/moisture.
Store away from oxidizing agents.
Further information about storage conditions:
Store under dry inert gas.
This product is moisture sensitive.
Keep container tightly sealed.
Store in cool, dry conditions in well sealed containers.

(Contd. on page 3)

Product name: 1,6-Diisocyanatohexane

(Contd. of page 2)

Protect from humidity and water.
Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:
Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Control parameters

Components with limit values that require monitoring at the workplace:

822-06-0 1,6-Diisocyanatohexane (100.0%)

REL (USA)	Long-term value: 0.035 mg/m³, 0.005 ppm Ceiling limit value: 0.14* mg/m³, 0.02* ppm *10-min
TLV (USA)	Long-term value: 0.034 mg/m³, 0.005 ppm BEI
EL (Canada)	Long-term value: 0.005 ppm Ceiling limit value: 0.01 ppm S
EV (Canada)	Long-term value: 0.005 ppm Ceiling limit value: 0.02 ppm

Additional information: No data

Exposure controls
Personal protective equipment
General protective and hygienic measures
The usual precautionary measures for handling chemicals should be followed.
Keep away from foodstuffs, beverages and feed.
Remove all soiled and contaminated clothing immediately.
Wash hands before breaks and at the end of work.
Store protective clothing separately.
Avoid contact with the eyes and skin.
Maintain an ergonomically appropriate working environment.
Breathing equipment: Use self-contained respiratory protective device in emergency situations.
Recommended filter device for short term use:
Use a respirator with multi-purpose combination (US) or type ABEK (EN 14387) as a backup to engineering controls. Risk assessment should be performed to determine if air-purifying respirators are appropriate. Only use equipment tested and approved under appropriate government standards such as NIOSH (USA) or CEN (EU).
Protection of hands:
Impervious gloves
Check protective gloves prior to each use for their proper condition.
The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.
Eye protection: Safety glasses with side shields / NIOSH (US) or EN 166(EU)
Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties
General Information

Appearance:	
Form:	Liquid
Odor:	Pungent
Odor threshold:	Not determined.
pH-value:	Not determined.
Change in condition	
Melting point/Melting range:	-67 °C (-89 °F)
Boiling point/Boiling range:	255 °C (491 °F)
Sublimation temperature / start:	Not determined
Flash point:	130 °C (266 °F)
Flammability (solid, gaseous)	Not determined.
Ignition temperature:	454 °C (849 °F)
Decomposition temperature:	Not determined
Auto igniting:	Not determined.
Danger of explosion:	Not determined.
Explosion limits:	
Lower:	0.9 Vol %
Upper:	9.5 Vol %
Vapor pressure at 20 °C (68 °F):	0.007 hPa
Density at 20 °C (68 °F):	1.05 g/cm³ (8.762 lbs/gal)
Relative density	Not determined.
Vapor density	Not determined.
Evaporation rate	Not determined.
Solubility in / Miscibility with	
Water:	Not determined
Partition coefficient (n-octanol/water):	Not determined.
Viscosity:	
dynamic:	Not determined.
kinematic:	Not determined.
Other information	No further relevant information available.

10 Stability and reactivity

Reactivity No information known.
Chemical stability Stable under recommended storage conditions.
Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.
Possibility of hazardous reactions Reacts with strong oxidizing agents
Conditions to avoid No further relevant information available.
Incompatible materials:
Oxidizing agents
Water/moisture

(Contd. on page 4)

Product name: 1,6-Diisocyanatohexane

(Contd. of page 3)

Hazardous decomposition products:
Carbon monoxide and carbon dioxide
Nitrogen oxides

11 Toxicological information

Information on toxicological effects
Acute toxicity:
Harmful if swallowed.
Toxic in contact with skin.
Fatal if inhaled.
Danger through skin absorption.
The Registry of Toxic Effects of Chemical Substances (RTECS) contains acute toxicity data for this substance.

LD/LC50 values that are relevant for classification:

Oral	LD50	745 mg/kg (rat)
Dermal	LD50	599 mg/kg (rabbit)
Inhalative	LC50/4H	124 mg/m3/4H (rat)

Skin irritation or corrosion: May cause irritation
Eye irritation or corrosion: May cause irritation
Sensitization:
May cause allergy or asthma symptoms or breathing difficulties if inhaled.
May cause an allergic skin reaction.
Germ cell mutagenicity: No effects known.
Carcinogenicity: No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.
Reproductive toxicity: No effects known.
Specific target organ system toxicity - repeated exposure: No effects known.
Specific target organ system toxicity - single exposure: May cause respiratory irritation.
Aspiration hazard: No effects known.
Subacute to chronic toxicity: The Registry of Toxic Effects of Chemical Substances (RTECS) contains multiple dose toxicity data for this substance.
Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

Toxicity
Aquatic toxicity: No further relevant information available.
Persistence and degradability No further relevant information available.
Bioaccumulative potential No further relevant information available.
Mobility in soil No further relevant information available.
Additional ecological information:
General notes:
Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.
Avoid transfer into the environment.
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.
Other adverse effects No further relevant information available.

13 Disposal considerations

Waste treatment methods
Recommendation Consult state, local or national regulations to ensure proper disposal.
Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.

14 Transport information

UN-Number	
DOT, IMDG, IATA	UN2281
UN proper shipping name	
DOT	Hexamethylene diisocyanate
ADR	2281 Hexamethylene diisocyanate
IMDG, IATA	HEXAMETHYLENE DIISOCYANATE
Transport hazard class(es)	
DOT	

Class	6.1 Toxic substances
Label	6.1
ADR	

Class	6.1 (T1) Toxic substances
Label	6.1
IMDG, IATA	

Class	6.1 Toxic substances
Label	6.1
Packing group	
DOT, ADR, IMDG, IATA	II

(Contd. on page 5)

Product name: 1,6-Diisocyanatohexane

(Contd. of page 4)

Environmental hazards:	Not applicable.
Special precautions for user	Warning: Toxic substances
EMS Number:	F-A,S-A
Stowage Category	E
Stowage Code	SW2 Clear of living quarters.
Handling Code	H1 Keep as dry as reasonably practicable
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information:	
DOT	
Quantity limitations	On passenger aircraft/rail: 5 L On cargo aircraft only: 60 L
Hazardous substance:	100 lbs, 45.4 kg
Marine Pollutant (DOT):	No
IMDG	
Limited quantities (LQ)	100 ml
Excepted quantities (EQ)	Code: E4 Maximum net quantity per inner packaging: 1 ml Maximum net quantity per outer packaging: 500 ml
UN "Model Regulation":	UN 2281 HEXAMETHYLENE DIISOCYANATE, 6.1, II

15 Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)
Hazard pictograms

GHS06 GHS08

Signal word Danger
Hazard statements
H302 Harmful if swallowed.
H311 Toxic in contact with skin.
H330 Fatal if inhaled.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H317 May cause an allergic skin reaction.
H335 May cause respiratory irritation.
Precautionary statements
P260 Do not breathe dust/fume/gas/mist/vapors/spray.
P284 [In case of inadequate ventilation] wear respiratory protection.
P305+P351+P338 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P320 Specific treatment is urgent (see on this label).
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.
National regulations
All components of this product are listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical substance Inventory.
All components of this product are listed on the Canadian Domestic Substances List (DSL).

SARA Section 313 (specific toxic chemical listings)

822-06-0	1,6-Diisocyanatohexane

California Proposition 65
Prop 65 - Chemicals known to cause cancer Substance is not listed.
Prop 65 - Developmental toxicity Substance is not listed.
Prop 65 - Developmental toxicity, female Substance is not listed.
Prop 65 - Developmental toxicity, male Substance is not listed.
Information about limitation of use: For use only by technically qualified individuals.
Other regulations, limitations and prohibitive regulations
Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.
The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.
Substance is not listed.
Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.
Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department
Date of preparation/Revision: Print date, revision date and version number are in the header of each page.
Abbreviations and acronyms:
ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
EINECS: European Inventory of Existing Commercial Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
HMIS: Hazardous Materials Identification System (USA)
WHMIS: Workplace Hazardous Materials Information System (Canada)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
PBT: Persistent, Bioaccumulative and Toxic
SVHC: Substances of Very High Concern
vPvB: very Persistent and very Bioaccumulative
ACGIH: American Conference of Governmental Industrial Hygienists (USA)
OSHA: Occupational Safety and Health Administration (USA)
NTP: National Toxicology Program (USA)
IARC: International Agency for Research on Cancer
EPA: Environmental Protection Agency (USA)
Acute Tox. 4: Acute toxicity – Category 4

(Contd. on page 6)

Product name: 1,6-Diisocyanatohexane

(Contd. of page 5)

Acute Tox. 3: Acute toxicity – Category 3
Acute Tox. 1: Acute toxicity – Category 1
Skin Irrit. 2: Skin corrosion/irritation – Category 2
Eye Irrit. 2A: Serious eye damage/eye irritation – Category 2A
Resp. Sens. 1: Respiratory sensitisation – Category 1
Skin Sens. 1: Skin sensitisation – Category 1
STOT SE 3: Specific target organ toxicity (single exposure) – Category 3