Chemical Safety Data Sheet MSDS / SDS

Perhydroazepine SDS

Revision Date:2024-04-25 Revision Number:1

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

Product identifier

Product name: Perhydroazepine

CAS: 111-49-9

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.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

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SECTION 2: Hazards identification

Classification of the substance or mixture

Flammable liquids, Category 2
Acute toxicity - Category 4, Oral

Skin corrosion, Sub-category 1C
Serious eye damage, Category 1
Acute toxicity - Category 3, Inhalation
Specific target organ toxicity – single exposure, Category 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H225 Highly flammable liquid and vapour
H302 Harmful if swallowed
H314 Causes severe skin burns and eye damage
H331 Toxic if inhaled
H335 May cause respiratory irritation
H412 Harmful to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.
P242 Use non-sparking tools.
P243 Take action to prevent static discharges.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].
P370+P378 In case of fire: Use ... to extinguish.
P301+P317 IF SWALLOWED: Get medical help.
P330 Rinse mouth.
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P363 Wash contaminated clothing before reuse.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P316 Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P317 Get medical help.
P308+P316 IF exposed or concerned: Get emergency medical help immediately.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	Perhydroazepine
Common names and synonyms:	Perhydroazepine
CAS number:	111-49-9

EC number:	203-875-9
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms/effects, acute and delayed

Inhalation of vapor irritates respiratory tract; high concentrations may cause disturbance of the central nervous system. Ingestion causes burns of mouth and stomach. Contact with concentrated vapor may cause severe eye injury. Contact with liquid causes burns of eyes and skin. (USCG, 1999)

Indication of immediate medical attention and special treatment needed, if necessary

Basic Treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary . Monitor for shock and treat if necessary. Anticipate seizures and treat if necessary. For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patent can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal . Cover skin burns with dry sterile dressings after decontamination . /Organic bases/amines and related compounds/

SECTION 5: Firefighting measures

Suitable extinguishing media

Dry chemical, alcohol foam, carbon dioxide. water may be ineffective.

Specific hazards arising from the chemical

Special Hazards of Combustion Products: Toxic oxides of nitrogen may form in fire. Behavior in Fire: Vapor is heavier than air and may travel to a source of ignition and flash back. (USCG, 1999)

Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours.Avoid contacting with skin and eye. Use personal protective equipment.Wear chemical impermeable gloves. Ensure adequate ventilation.Remove all sources of ignition. Evacuate personnel to safe areas.Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

N-nitrosohexamethylenimine photolysis produced hexamethylenimine which decomp at rate similar to n-nitrosohexamethylenimine. 2-hr lighting of 100 mg n-nitrosohexamethylenimine/l with xeon lamp degraded 90% of n-nitrosohexamethylenimine & raised hexamethylenimine concn to 15% of initial n-nitrosohexamethylenimine concn. during subsequent 24-hr dark incubation, n-nitrosohexamethylenimine disappeared completely & hexamethylenimine level rose to 25% of initial n-nitrosohexamethylenimine concn.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

Component	Perhydroazepine			
CAS No.	111-49-9			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m^3	ppm	mg/m^3
Latvia	?	0,5	?	?
	Remarks			

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Hexamethyleneimine is a colorless liquid with an ammonia-like odor. Flash point 65°F. Toxic by ingestion. Corrosive to metals and tissue. Combustion produces toxic oxides of nitrogen.
Colour:	CLEAR COLORLESS LIQ
Odour:	AMMONIA-LIKE ODOR
Melting point/freezing point:	276°C(lit.)
Boiling point or initial boiling point and boiling range:	138°C
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	1.6%-2.3% (IN AIR)
Flash point:	18°C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available

Solubility:	Very soluble in ethanol and ethyl ether
Partition coefficient n-octanol/water:	no data available
Vapour pressure:	7.4 mm Hg (21.1 °C)
Density and/or relative density:	0.88
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Highly flammable. Soluble in water.

Chemical stability

no data available

Possibility of hazardous reactions

HEXAMETHYLENEIMINE neutralizes acids in exothermic reactions to form salts plus water. May be incompatible with isocyanates, halogenated organics, peroxides, phenols (acidic), epoxides, anhydrides, and acid halides. Flammable gaseous hydrogen is generated in combination with strong reducing agents, such as hydrides.

Conditions to avoid

no data available

Incompatible materials

Reacts vigorously with oxidizers.

Hazardous decomposition products

When heated to decomposition it emits toxic fumes of /nitrogen oxides/.

SECTION 11: Toxicological information

Acute toxicity

Oral: no data available

Inhalation: no data available

Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Hexamethylenimine was degraded in aerobic waste-water microcosms, using acclimated sewage sludge cultures as the test organisms(1). By measuring an increase in cellular proteins, hexamethyleneimine served as the sole carbon and nitrogen source for these organisms. The calculated conversion rate was about 27% over one week(1).

Bioaccumulative potential

no data available

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc for hexamethyleneimine can be estimated to be 170(SRC). According to a classification scheme(2), this estimated Koc value suggests that hexamethyleneimine is expected to have moderate mobility in soil. Furthermore, the pKa of hexamethyleneimine is 11.07(3), indicating that this compound will exist in cation form in the environment and cations generally adsorb to organic carbon and clay more strongly than their neutral counterparts.

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN2493 (For reference only, please check.)
IMDG: UN2493 (For reference only, please check.)
IATA: UN2493 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: HEXAMETHYLENEIMINE (For reference only, please check.)
IMDG: HEXAMETHYLENEIMINE (For reference only, please check.)
IATA: HEXAMETHYLENEIMINE (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)
IMDG: 3 (For reference only, please check.)
IATA: 3 (For reference only, please check.)

Packing group, if applicable

ADR/RID: II (For reference only, please check.)
IMDG: II (For reference only, please check.)
IATA: II (For reference only, please check.)

Environmental hazards

ADR/RID: No
IMDG: No
IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

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

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

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

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

HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

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

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

ECHA - European Chemicals Agency, website: https://echa.europa.eu/