

Chemical Safety Data Sheet MSDS / SDS

2-bromo-2-(bromomethyl)pentanedinitrile 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: 2-bromo-2-(bromomethyl)pentanedinitrile

CAS: 35691-65-7

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

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SECTION 2: Hazards identification**Classification of the substance or mixture**Acute toxicity - Category 4, Oral
Skin irritation, Category 2

Skin sensitization, Category 1
Serious eye damage, Category 1
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H302 Harmful if swallowed
H315 Causes skin irritation
H317 May cause an allergic skin reaction
H318 Causes serious eye damage
H400 Very toxic to aquatic life

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P272 Contaminated work clothing should not be allowed out of the workplace.
P273 Avoid release to the environment.

Response

P301+P317 IF SWALLOWED: Get medical help.
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P321 Specific treatment (see ... on this label).
P332+P317 If skin irritation occurs: Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P333+P317 If skin irritation or rash occurs: Get medical help.
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.

P391 Collect spillage.

Storage

none

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: 2-bromo-2-(bromomethyl)pentanedinitrile

Common names and synonyms: 2-bromo-2-(bromomethyl)pentanedinitrile

CAS number: 35691-65-7

EC number: 252-681-0

Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Give one or two glasses of water to drink. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]: TOXIC; inhalation, ingestion or skin contact with material may cause severe injury or death. Contact with molten substance may cause severe burns to skin and eyes. Avoid any skin contact. Effects of contact or inhalation may be delayed. Fire may produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause pollution. (ERG, 2016)

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

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Poisons A and B

SECTION 5: Firefighting measures

Suitable extinguishing media

Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]: SMALL FIRE: Dry chemical, CO₂ or water spray. LARGE FIRE: Dry chemical, CO₂, alcohol-resistant foam or water spray. Move containers from fire area if you can do it without risk. Dike fire-control water for later disposal; do not scatter the material. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Do not get water inside containers. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. (ERG, 2016)

Specific hazards arising from the chemical

Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]: Non-combustible, substance itself does not burn but may decompose upon heating to produce corrosive and/or toxic fumes. Some are oxidizers and may ignite combustibles (wood, paper, oil, clothing, etc.). Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated. For electric vehicles or equipment, ERG Guide 147 (lithium ion batteries) or ERG Guide 138 (sodium batteries) should also be consulted. (ERG, 2016)

Special protective actions for fire-fighters

Use water spray, powder, foam, carbon dioxide.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. 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

MAK sensitization of skin (SH)

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 safety goggles.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Crystals with a pungent odor. Insoluble in water. Used as a preservative in latex paint, adhesives, etc.
Colour:	Yellowish-white granular solid
Odour:	Slightly sweet odor

Melting point/freezing point:	51 - 52 °C
Boiling point or initial boiling point and boiling range:	338.6 °C at 760 mmHg
Flammability:	Combustible. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	158.6 °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 chloroform, ethyl acetate. Soluble in methanol, ethanol, ether.
Partition coefficient n-octanol/water:	log Kow = 1.63 (est)
Vapour pressure:	6.7E-3 Pascal /SRC: 5.025X10-5 mm Hg/ at 25 deg C
Density and/or relative density:	1.889 g/cm ³
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on burning. This produces toxic fumes.

Chemical stability

The chemical was found to be stable when subjected to Al, Sn, Ni, Fe, thermal and photosensitivity tests. One year storage at room temperature did not produce any significant change regarding purity, color, specific gravity, and refractive index.

Possibility of hazardous reactions

1-BROMO-1-(BROMOMETHYL)-1,3-PROPANEDICARBONITRILE may polymerize in the presence of metals and some metal compounds. Incompatible with acids; mixing nitriles with strong oxidizing acids can lead to extremely violent reactions. Nitriles are generally incompatible with other oxidizing agents such as peroxides and epoxides. The combination of bases and nitriles can produce hydrogen cyanide. Nitriles are hydrolyzed in both aqueous acid and base to give carboxylic acids (or salts of carboxylic acids). These reactions generate heat. Peroxides convert nitriles to amides. Nitriles can react vigorously with reducing agents.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Rat (male) oral 0.77 g/kg /Technical 99.9%/ from table

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

The substance is irritating to the eyes and skin.

STOT-repeated exposure

Repeated or prolonged contact may cause skin sensitization.

Aspiration hazard

A harmful concentration of airborne particles can be reached quickly.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50; Species: *Lepomis macrochirus* (Bluegill); Conditions: freshwater, static; Concentration: 29000 µg/L for 96 hr (95% confidence interval: 27000-31000 µg/L) /10% purity

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water flea) age <24 hr; Conditions: freshwater, static; Concentration: 2200 ug/L for 48 hr (95% confidence interval: 1600-3200 ug/L); Effect: intoxication, immobilization /98% purity

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

no data available

Bioaccumulative potential

An estimated BCF of five was calculated in fish for 1,2-dibromo-2,4-dicyanobutane(SRC), using an estimated log Kow of 1.63(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

At concentrations of 0.1 to 1.0 ug/mL, 1,2-dibromo-2,4-dicyanobutane exhibited Koc values of 528 in sand, 87.8 in sandy loam soil, 72.9 in clay loam, and 33.4 in silt loam soil, corresponding to Freundlich coefficients of 0.264, 0.351, 0.474, and 0.701, respectively(1). According to a classification scheme(2), this Koc range suggests that 1,2-dibromo-2,4-dicyanobutane is expected to have moderate to very high mobility in soil.

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: UN3439 (For reference only, please check.)

IMDG: UN3439 (For reference only, please check.)

IATA: UN3439 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: NITRILES, SOLID, TOXIC, N.O.S. (For reference only, please check.)

IMDG: NITRILES, SOLID, TOXIC, N.O.S. (For reference only, please check.)

IATA: NITRILES, SOLID, TOXIC, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (For reference only, please check.)

Environmental hazards

ADR/RID: Yes

IMDG: Yes

IATA: Yes

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

Not 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/>

Other Information

Do NOT take working clothes home.

Disclaimer: 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. We as supplier shall not be held liable for any