

Chemical Safety Data Sheet MSDS / SDS

DIBROMOACETONITRILE

Revision Date:2024-12-21 Revision Number:1

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

Product name : DIBROMOACETONITRILE
CBnumber : CB7341454
CAS : 3252-43-5
EINECS Number : 221-843-2
Synonyms : Dibromoacetonitrile,2,2-dibromoacetonitrile

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 : 400-158-6606

SECTION 2: Hazards identification**Classification of the substance or mixture**

Acute toxicity - Category 3, Oral
Eye irritation, Category 2
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

Label elements**Pictogram(s)**

□□□□

Signal word : Danger

Hazard statement(s)

H226 Flammable liquid and vapour
H301 Toxic if swallowed
H314 Causes severe skin burns and eye damage
H318 Causes serious eye damage
H319 Causes serious eye irritation
H351 Suspected of causing cancer

H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

P280 Wear protective gloves/protective clothing/eye protection/face 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.

P405 Store locked up.

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/...

P273 Avoid release to the environment.

Response

P301+P316 IF SWALLOWED: Get emergency medical help immediately.

P321 Specific treatment (see ... on this label).

P330 Rinse mouth.

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

P391 Collect spillage.

Storage

P405 Store locked up.

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

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: DIBROMOACETONITRILE
Synonyms	: Dibromoacetonitrile,2,2-dibromoacetonitrile
CAS	: 3252-43-5
EC number	: 221-843-2
MF	: C2HBr2N
MW	: 198.84

SECTION 4: First aid measures

Description of 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 and effects, both acute and delayed

SYMPTOMS: Symptoms of exposure to this compound include irritation of the eyes, mucous membranes and upper respiratory tract, burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. It is a lachrymator. ACUTE/CHRONIC

HAZARDS: This compound may be fatal by ingestion, inhalation or skin absorption. It is an irritant of the eyes, mucous membranes and upper respiratory tract. It is also a lachrymator. When heated to decomposition it emits highly toxic fumes of carbon monoxide, carbon dioxide, nitrogen oxides, bromine, hydrogen bromide gas and cyanides. (NTP, 1992)

Indication of any immediate medical attention and special treatment needed

Immediate first aid: Remove patient from contact with the material. 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 as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on 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. Cyanide and related compounds

SECTION 5: Firefighting measures

Extinguishing media

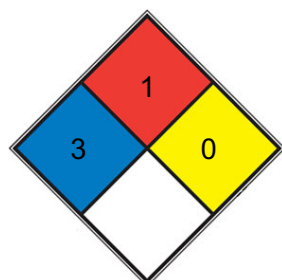
FIREFIGHTING. Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.

Specific Hazards Arising from the Chemical

Literature sources indicate that this compound is nonflammable. (NTP, 1992)

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

NFPA 704

<input checked="" type="checkbox"/>	HEALTH	3	Short exposure could cause serious temporary or moderate residual injury (e.g. liquid hydrogen , sulfuric acid , calcium hypochlorite , hexafluorosilicic acid)
<hr/>			
Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion			
<input checked="" type="checkbox"/>	FIRE	1	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)
<hr/>			
<input checked="" type="checkbox"/>	REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N2)
<hr/>			
<input type="checkbox"/>	SPEC.		
<input type="checkbox"/>	HAZ.		

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

Absorb on sand or vermiculite and place in closed containers for disposal. Ventilate area and wash spill site after material pickup is complete.

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

Keep tightly closed.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure 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

Eye/face protection

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

Skin protection

Wear fire/flammable 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

Information on basic physicochemical properties

Physical state	neat
Colour	Liquid
Odour	no data available
Melting point/freezing point	no data available
Boiling point or initial boiling point and boiling range	163.1°C at 760mmHg
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	31.9°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	5 to 10 mg/mL at 70.7° F (NTP, 1992)
Partition coefficient n-octanol/water	log Kow = 0.47 (est)
Vapour pressure	2 mm Hg at 122° F ; 15 mm Hg at 158° F; 48 mm Hg at 203° F (NTP, 1992)
Density and/or relative density	2.434g/cm ³
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

This chemical may be sensitive to prolonged exposure to air and light. Slightly soluble in water.

Chemical stability

no data available

Possibility of hazardous reactions

DIBROMOACETONITRILE is incompatible with strong acids, strong bases, strong oxidizing agents and strong reducing agents. (NTP, 1992). Nitriles may polymerize in the presence of metals and some metal compounds. They are 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. Acetonitrile and propionitrile are soluble in water, but nitriles higher than propionitrile have low aqueous solubility. They are also insoluble in aqueous acids.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits very toxic fumes of /Nitrogen oxides/, /Hydrogen Bromide/ and /Cyanide/.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Mouse (male) oral 289 mg/kg[Hayes JR et al; Environ Health Perspect 69: 183-202 (1986)] Full text: PMC1474335
- 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

Evaluation: No epidemiological data relevant to the carcinogenicity of dibromoacetonitrile were available. There is inadequate evidence in experimental animals for the carcinogenicity of dibromoacetonitrile. Overall evaluation: Dibromoacetonitrile is not classifiable as to its

carcinogenicity to humans (Group 3).

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: LC50; Species: Pimephales promelas (Fathead minnow, standard length 20.5 mm, weight 150 mg); Conditions: freshwater, static, 16.6-17.0 deg C, pH 7.8-8.3, hardness 98-113 mg/L CaCO₃, alkalinity 75-87 mg/L CaCO₃, dissolved oxygen 8.7-9.6 mg/L;

Concentration: 710 ug/L for 24 hr (95% confidence interval: 650-780 ug/L) /96% purity

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

Dibromoacetonitrile is a by product of water chlorination and hydrolyzes quickly, therefore biodegradation is not expected to be an important fate in the environment. (SRC)

Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for dibromoacetonitrile(SRC), using an estimated log Kow of 0.47(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

Using a structure estimation method based on molecular connectivity indices(1), the Koc of dibromoacetonitrile can be estimated to be 13(SRC). According to a classification scheme(2), this estimated Koc value suggests that dibromoacetonitrile is expected to have 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: UN3275 (For reference only, please check.)

IMDG: UN3275 (For reference only, please check.)

IATA: UN3275 (For reference only, please check.)

UN Proper Shipping Name

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

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

IATA: NITRILES, TOXIC, FLAMMABLE, 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)

Not 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>
Chemical Book

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/>

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