

Chemical Safety Data Sheet MSDS / SDS

DIBROMOACETIC ACID

Revision Date:2025-02-01 Revision Number:1

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

Product name : DIBROMOACETIC ACID
CBnumber : CB6170486
CAS : 631-64-1
EINECS Number : 211-165-5
Synonyms : dibromoacetic acid,Acetic acid, dibromo-

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 4, Oral
Acute toxicity - Category 4, Dermal
Skin corrosion, Sub-category 1B
Acute toxicity - Category 4, Inhalation

Label elements**Pictogram(s)**

☐

Signal word : Danger

Hazard statement(s)

H314 Causes severe skin burns and eye damage
H315 Causes skin irritation

Precautionary statement(s)

P280 Wear protective gloves/protective clothing/eye protection/face protection.
P310 Immediately call a POISON CENTER or doctor/physician.

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

Continuerinsing.

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/...

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.

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P317 Get medical help.

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

P362+P364 Take off contaminated clothing and wash it before reuse.

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.

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

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 | : DIBROMOACETIC ACID |
| Synonyms | : dibromoacetic acid,Acetic acid, dibromo- |
| CAS | : 631-64-1 |
| EC number | : 211-165-5 |
| MF | : C2H2Br2O2 |
| MW | : 217.84 |

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

no data available

Indication of any immediate medical attention and special treatment needed

Absorption, Distribution and Excretion

Dibromoacetic acid (DBA) ... /was/ provided in drinking water in range-finding reproductive/developmental toxicity studies (rats) ... Studies included absorption and biodisposition of DBA ... including passage into placentas, amniotic fluid, fetuses ... or milk . The DBA ... range-finding reproductive/developmental toxicity studies each included 50 Sprague-Dawley rats/sex/group. DBA (0, 125, 250, 500, or 1000 ppm) ... was provided in drinking water 14 days pre-mating through gestation and lactation (63 to 70 days). ... Satellite groups (6 male, 17 female rats/group/study ... were used for bioanalytical sampling. Rats ... had exposure-related reduced water consumption caused by apparent taste aversion to DBA ..., especially in the parental animals at the two highest exposure levels (500 and 1000 ppm DBA . Female rats consumed slightly higher mg/kg/day doses of DBA than male rats, especially during gestation and lactation; weanling rats consumed the highest mg/kg/day doses. DBA produced detectable and quantifiable concentrations in plasma, placentas, amniotic fluid, and milk. Plasma samples confirmed that rats drink predominately during the dark; this drinking pattern, not accumulation, produced detectable plasma concentrations for 18 to 24 hours/day...

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

no data available

Advice for firefighters

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

Sweep up, place in a bag and hold for waste disposal. Avoid raising dust. 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 | Hygroscopic crystals |
| Odour | no data available |
| Melting point/freezing point | 32-38°C(lit.) |
| Boiling point or initial boiling point and boiling range | 128-130°C16 mm Hg(lit.) |
| Flammability | no data available |
| Lower and upper explosion limit/flammability limit | no data available |
| Flash point | >230 °F |
| 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; soluble in diethyl ether |
| Partition coefficient n-octanol/water | log Kow = 0.70 (est) |
| Vapour pressure | 2.3X10 ⁻² mm Hg at 25 deg C (est) |
| Density and/or relative density | 2.382 g/mL at 25°C(lit.) |
| Relative vapour density | no data available |
| Particle characteristics | no data available |

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits toxic vapors of bromide.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral 1737 mg/kg
- 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: LC50; Species: Pimephales promelas (Fathead minnow, standard length 23.0 mm, weight 220 mg); Conditions: freshwater, static, 17.1-17.5 deg C, pH 7.6-8.2, hardness 98-113 mg/L CaCO₃, alkalinity 75-87 mg/L CaCO₃, conductivity 143-178 umhos/cm, dissolved oxygen 6.4-8.8 mg/L; Concentration: 160000 ug/L for 24 hr (95% confidence interval: 138000-1380000 ug/L) /98.9% 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

AEROBIC: Limited data are available regarding the biodegradation of dibromoacetic acid. However, dibromoacetic acid (5 mM) was used as a carbon source by *Xanthobacter autotrophicus* GJ10 as measured by halide production after a period of 10 days at 30 deg C(1).

Bioaccumulative potential

An estimated BCF of 0.17 was calculated for dibromoacetic acid(SRC), using a water solubility of 2.11X10+6 mg/L(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

The Koc of dibromoacetic acid is estimated as 1.5(SRC), using a water solubility of 2.11X10+6 mg/L(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that dibromoacetic acid is expected to have very high mobility in soil. The pKa of dibromoacetic acid is 1.48(4), indicating that this compound will primarily exist in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(5).

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: UN3261 (For reference only, please check.)

IMDG: UN3261 (For reference only, please check.)

IATA: UN3261 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (For reference only, please check.)

IMDG: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (For reference only, please check.)

IATA: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 8 (For reference only, please check.)

IMDG: 8 (For reference only, please check.)

IATA: 8 (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: 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

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

PICCS

Not Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Not 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?pagelD=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/>

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