

Chemical Safety Data Sheet MSDS / SDS

2,6-dibromo-4-cyanophenyl octanoate 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: 2,6-dibromo-4-cyanophenyl octanoate

CAS: 1689-99-2

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 sensitization, Category 1

Acute toxicity - Category 3, Inhalation
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1
Reproductive toxicity, Category 2

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H302 Harmful if swallowed
H317 May cause an allergic skin reaction
H331 Toxic if inhaled
H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P272 Contaminated work clothing should not be allowed out of the workplace.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.
P203 Obtain, read and follow all safety instructions before use.

Response

P301+P317 IF SWALLOWED: Get medical help.
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P333+P317 If skin irritation or rash occurs: Get medical help.
P321 Specific treatment (see ... on this label).
P362+P364 Take off contaminated clothing and wash it before reuse.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P316 Get emergency medical help immediately.

P391 Collect spillage.
P318 IF exposed or concerned, get medical advice.

Storage

P403+P233 Store in a well-ventilated place. Keep container tightly closed.
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 which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	2,6-dibromo-4-cyanophenyl octanoate
Common names and synonyms:	2,6-dibromo-4-cyanophenyl octanoate
CAS number:	1689-99-2
EC number:	216-885-3
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

Excerpt from ERG Guide 151 [Substances - Toxic (Non-combustible)]: Highly toxic, may be fatal if inhaled, swallowed or absorbed through skin. 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

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if needed. 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 patient can swallow, has a strong gag reflex, and does not drool . Cover skin burns with dry sterile dressings after decontamination . Poison A and B

SECTION 5: Firefighting measures

Suitable extinguishing media

If material on fire or involved in fire: Extinguish fire using agent suitable for type of surrounding fire. (Material itself does not burn or burns with difficulty.) Use water in flooding quantities as fog. Use "alcohol" foam, dry chemical or carbon dioxide.

Specific hazards arising from the chemical

Excerpt from ERG Guide 151 [Substances - Toxic (Non-combustible)]: Non-combustible, substance itself does not burn but may decompose upon heating to produce corrosive and/or toxic fumes. Containers may explode when heated. Runoff may pollute waterways. (ERG, 2016)

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

Environmental considerations: Land spill: Dig a pit, pond, lagoon, holding area to contain liquid or solid material. /SRP: If time permits, pits, ponds, lagoons, soak holes, or holding areas should be sealed with an impermeable flexible membrane liner. / Cover solids with a plastic sheet to prevent dissolving in rain or fire fighting water.

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

Handle carefully ... Do not use or store near heat or open flame. Store at temperature above 3 deg F. If allowed to freeze, remix before using. Do not contaminate water, food or feed by storage or disposal of this chemical.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

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/flare 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:	Bromoxynil octanoate, [solid] is a solid. Used as a selective contact herbicide.
Colour:	Cream, waxy solid
Odour:	Characteristic odor
Melting point/freezing point:	45-46 °C
Boiling point or initial boiling point and boiling range:	424.6 °C at 760 mmHg

Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	210.6 °C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	In water, 0.08 mg/L at 25 deg C
Partition coefficient n-octanol/water:	log Kow = 5.4
Vapour pressure:	2.04E-07mmHg at 25 °C
Density and/or relative density:	1.54g/cm ³
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

No rapid reaction with air. No rapid reaction with water.

Chemical stability

Susceptible to hydrolysis by acids and alkalis.

Possibility of hazardous reactions

BROMOXYNIL OCTANOATE, [SOLID] is an ester. Readily hydrolyzed to bromoxynil and octanoate at pHs exceeding 9.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits toxic fumes of /nitrogen oxide and hydrogen bromide/.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Mouse oral 245 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 *Lepomis macrochirus* (Bluegill) 61 ppb/96 hr (95% confidence interval: 48-79 ppb); static /formulated product

Toxicity to daphnia and other aquatic invertebrates: EC50 *Daphnia magna* (Water flea, varying life stages; intoxication, immobilization) 41-161 ug/L/48 hr; static /formulated product

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

¹⁴C-Labeled bromoxynil octanoate was reported to degrade in sandy loam soil with a half-life of 2 days; the major degradation product was CO₂, which accounted for 64.28% of the applied radioactivity after 90 days(1). In soil photolysis experiments, bromoxynil octanoate was found to degrade with a half-life of 2.6 days when irradiated with a xenon arc lamp; a degradation

half-life of 3.6 days was observed in a dark control(1). Degradation in the dark control suggests that degradation processes in addition to photolysis (e.g., hydrolysis or microbial degradation) were occurring(1). A half-life of <12 hrs was reported when treated sandy loam soil was flooded with pond water and then aerobically incubated; test compound concn was 87% of applied at time zero, declining to undetectable levels in 48 hrs(1). Field dissipation half-lives ranging from 0.5 to 28 days have been reported(2). In degradation experiments using 5 soil types (sandy loam, acid sand, organic silt, sandy loam, and clay) in a soil perfusion apparatus and C14 (cyano) bromoxynil octanoate half-lives ranged from 7 to 22 days(3). In experiments using C14 (ring) bromoxynil octanoate half-life ranged from 10-12 days in clay and sandy loam soils(3). The degradation of bromoxynil octanoate in two soils, a heavy clay and a sandy loam, at 85% of field capacity moisture and at 20 deg C, was studied(4). In both soils bromoxynil octanoate was rapidly degraded to bromoxynil, which was then also rapidly degraded; after 7 days >90% of the original application had disappeared(4). Three pesticides, including bromoxynil octanoate, were applied to two field plots in Saskatchewan; after 10 weeks none of the pesticides could be detected in the top 10 cm of soil(4). Bromoxynil octanoate was reported to degrade with a half-life of 3.7 days in a sandy loam sediment under anaerobic conditions(1). The environmental fate of bromoxynil octanoate was investigated in small ponds in the wetland area of the Delta Waterfowl and Wetlands Research Station in Canada(5). Bromoxynil octanoate, along with bromoxynil butyrate were sprayed on the ponds; sampling showed that bromoxynil octanoate persisted in the surface microlayer (0-1 mm) with half-lives of 0.8-2.5 hours(5). In subsurface waters (10-20 cm depth) the major forms of the pesticides were bromoxynil (phenol) and its monobromo analog(5).

Bioaccumulative potential

A BCF of 230 (whole fish) was reported in bluegill sunfish when continuously exposed to ¹⁴C radiolabeled bromoxynil octanoate at 1.3-4.6 ug/L(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is high, provided the compound is not metabolized by the organism(SRC).

Mobility in soil

The Koc of bromoxynil octanoate is estimated as 21,000(SRC), using a log Kow of 5.4(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that bromoxynil octanoate is expected to be immobile mobility in soil. In an aged soil leaching study, bromoxynil octanoate residues were found to not be mobile in four soils and aquatic sediment(4). A Kd of 7 mL/g (Koc = 1,003) was reported in soils with 1.2% organic matter(4).

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: no data available

IMDG: no data available

IATA: no data available

UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

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: III (For reference only, please check.)

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

IATA: III (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)

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?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/>

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