

Chemical Safety Data Sheet MSDS / SDS

Hexa-2,4-dienoic acid 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: Hexa-2,4-dienoic acid

CAS: 110-44-1

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**

Skin irritation, Category 2

Eye irritation, Category 2

Specific target organ toxicity - single exposure, Category 3

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

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

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P271 Use only outdoors or in a well-ventilated area.

Response

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.

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

Continue rinsing.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P319 Get medical help if you feel unwell.

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:	Hexa-2,4-dienoic acid
Common names and synonyms:	Hexa-2,4-dienoic acid
CAS number:	110-44-1
EC number:	203-768-7
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. Rest. Refer for medical attention .

Most important symptoms/effects, acute and delayed

SYMPTOMS: This compound may cause severe irritation. High concentrations are extremely destructive to tissues of the mucous membranes and upper respiratory tract, skin and eyes. The greatest danger from ingestion of large quantities of this compound (2

g/kg) is intestinal obstruction. Aspiration or inhalation could cause chemical pneumonitis. Implantation will cause a foreign body reaction. A case of contact sensitivity has been reported. ACUTE/CHRONIC HAZARDS: This compound is a severe irritant. It is harmful if swallowed or inhaled. High concentrations are extremely destructive to tissues of the mucous membranes and upper respiratory tract, skin and eyes. When heated to decomposition, this compound may emit toxic fumes of carbon monoxide and carbon dioxide. It may produce aldehydes. It may also emit acrid smoke and irritating fumes. (NTP, 1992)

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 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

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Specific hazards arising from the chemical

This chemical is combustible. (NTP, 1992)

Special protective actions for fire-fighters

Use water in large amounts, water spray, foam.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Wash away remainder with plenty of water. Personal protection: P2 filter respirator for harmful particles.

Environmental precautions

Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Wash away remainder with plenty of water. Personal protection: P2 filter respirator for harmful particles.

Methods and materials for containment and cleaning up

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. Environmental precautions: Do not let product enter drains. Methods and materials for containment and cleaning up: Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. Closed system, dust explosion-proof electrical equipment and lighting. Prevent deposition of dust. 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

Well closed. Keep container tightly closed in a dry and well-ventilated place. Recommended storage temperature 2 - 8 deg C. Storage class (TRGS 510): Non Combustible Solids.

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 safety spectacles or eye protection in combination with breathing protection.

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:	Solid. Crystalline.
Colour:	White.
Odour:	Relatively odorless
Melting point/freezing point:	> 120 - < 150 °C. Atm. press.:Ca. 1 013 hPa.
Boiling point or initial boiling point and boiling range:	> 160 - < 260 °C. Atm. press.:Ca. 1 013 hPa. Remarks:A boiling point at atmospheric pressure does not exist.
Flammability:	Combustible.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	127° C
Auto-ignition temperature:	> 402 °C.
Decomposition temperature:	228° C

pH:	no data available
Kinematic viscosity:	no data available
Solubility:	less than 1 mg/mL at 68° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Pow = 1.32. Remarks:20 ± 2 °C.;log Pow = -1.72. Remarks:20 ± 2 °C.
Vapour pressure:	0 hPa. Temperature:20 °C.
Density and/or relative density:	1.201 - 1.203 g/cm ³ . Temperature:20 °C.;1.2. Temperature:20 °C.
Relative vapour density:	3.87 (NTP, 1992) (Relative to Air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

The solution in water is a weak acid.

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

Combustible when exposed to heat or flame. Dust explosion possible if in powder or granular form, mixed with air. SORBIC ACID may discolor on exposure to light. Can react with oxidizing agents. Also incompatible with bases and reducing agents. The dust may become explosive, particularly when mixed with free-radical initiators or oxidizing agents (NTP, 1992).

Conditions to avoid

no data available

Incompatible materials

Incompatible materials: Bases, oxidizing agents, reducing agents.

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and irritating fumes.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - 10 500 mg/kg bw.

Inhalation: no data available

Dermal: LD50 - rat (male) - > 2 000 mg/kg bw.

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, skin and respiratory tract.

STOT-repeated exposure

Repeated or prolonged contact may cause skin sensitization.

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - *Oryzias latipes* - 75 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 70 mg/L - 48 h.

Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - 24.1 mg/L - 72 h.

Toxicity to microorganisms: EC50 - activated sludge of a predominantly domestic sewage - > 100 mg/L - 3 h. Remarks: Respiration rate.

Persistence and degradability

AEROBIC: Sorbic acid is readily degradable in soil(1). Sorbic acid also shows high degradability, 95% within 6 days, in the Zahn-Wellens test(1). 100% degradation of sorbic acid was observed after 3 days incubation in seawater taken from Akashi Beach, Japan and river water taken from the Mino River, Japan, using an initial sorbic acid concentration of 60 ppm(2). Sorbic acid, present at 100 mg/L, reached 83% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test which classified the compound as readily biodegradable(3). Sorbic acid was observed to biodegrade in soil suspensions(4). Sorbic acid (at 2 mg/L) was found to be readily biodegradable in an aerobic BOD test using domestic activated sludge with a 7-day theoretical BOD of 65.5% and a 28-day theoretical BOD of 74.9%(4).

Bioaccumulative potential

An estimated BCF value of 3 was calculated in fish for sorbic acid(SRC), using a log Kow of 1.33(1) and a recommended regression-derived equation(2). According to a classification scheme(3), this BCF value suggests that bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of sorbic acid can be estimated to be 9(SRC). According to a classification scheme(2), this estimated Koc value suggests that sorbic acid is expected to have very high mobility in soil. A Koc of less than 1 was estimated for sorbic using an HPLC method(3). The pKa of sorbic acid is 4.76(4), indicating that this compound will exist almost entirely 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: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (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)

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/>

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