

Chemical Safety Data Sheet MSDS / SDS

3,4-dihydroxycinnamic acid SDS

Revision Date:2024-04-25 Revision Number:1

Section 1	Section 2	Section 3	Section 4	Section 5	Section 6	Section 7	Section 8
Section 9	Section 10	Section 11	Section 12	Section 13	Section 14	Section 15	Section 16

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

Product name: 3,4-dihydroxycinnamic acid

CAS: 331-39-5

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
Carcinogenicity, Category 2
Reproductive toxicity, Category 2

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
H351 Suspected of causing cancer
H361 Suspected of damaging fertility or the unborn child

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.
P203 Obtain, read and follow all safety instructions before use.

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.
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: 3,4-dihydroxycinnamic acid

Common names and synonyms: 3,4-dihydroxycinnamic acid

CAS number: 331-39-5

EC number: 206-361-2

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

ACUTE/CHRONIC HAZARDS: When heated to decomposition this compound emits acrid smoke and fumes. (NTP, 1992)

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 respirations if necessary. 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 . 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. Activated charcoal is not effective . Do not attempt to neutralize because of exothermic reaction. Cover skin burns with dry, sterile dressings after decontamination . Organic acids and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. (NTP, 1992)

Specific hazards arising from the chemical

Flash point data for this chemical are not available; however, it is probably combustible. (NTP, 1992)

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

PRECAUTIONS FOR "CARCINOGENS": A high-efficiency particulate arrestor (HEPA) or charcoal filters can be used to minimize amt of carcinogen in exhausted air ventilated safety cabinets, lab hoods, glove boxes or animal rooms ... Filter housing that is designed so that used filters can be transferred into plastic bag without contaminating maintenance staff is avail commercially. Filters should be placed in plastic bags immediately after removal ... The plastic bag should be sealed immediately ... The sealed bag should be labelled properly ... Waste liquids ... should be placed or collected in proper containers for disposal. The lid should be secured & the bottles properly labelled. Once filled, bottles should be placed in plastic bag, so that outer surface ... is not contaminated ... The plastic bag should also be sealed & labelled. ... Broken glassware ... should be decontaminated by solvent extraction, by chemical destruction, or in specially designed incinerators. Chemical Carcinogens

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

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

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/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 and safety characteristics

Physical state:	PHYSICAL DESCRIPTION: Yellow prisms or plates (from chloroform or ligroin) or pale yellow granules. Alkaline solutions turn from yellow to orange. (NTP, 1992)
Colour:	Yellow crystals from concentrated aqueous solutions. Alkaline solns turn from yellow to orange.
Odour:	no data available
Melting point/freezing point:	210°C(lit.)
Boiling point or initial boiling point and boiling range:	188°C

Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	65°C(lit.)
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	less than 1 mg/mL at 72° F (NTP, 1992)
Partition coefficient n-octanol/water:	no data available
Vapour pressure:	no data available
Density and/or relative density:	1.478 g/cm ³
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

3,4-DIHYDROXYCINNAMIC ACID is a carboxylic acid. Carboxylic acids donate hydrogen ions if a base is present to accept them. They react in this way with all bases, both organic (for example, the amines) and inorganic. Their reactions with bases, called "neutralizations", are accompanied by the evolution of substantial amounts of heat. Neutralization between an acid and a base produces water plus a salt. Insoluble carboxylic acids react rapidly with aqueous solutions containing a chemical base and dissolve as the neutralization generates a soluble salt. Carboxylic acids in aqueous solution and liquid or molten carboxylic acids can react with active metals to form gaseous hydrogen and a metal salt. Such reactions occur in principle for solid carboxylic acids as well, but are slow if the solid acid remains dry. Even "insoluble" carboxylic acids may absorb enough water from the air and dissolve sufficiently in it to corrode or dissolve iron, steel, and aluminum parts and containers. Carboxylic acids, like other acids, react with cyanide salts to generate gaseous hydrogen cyanide. The reaction is slower for dry, solid carboxylic acids. Insoluble carboxylic acids react with solutions of cyanides to cause the release of gaseous hydrogen cyanide. Flammable and/or toxic gases and heat are generated by the reaction of carboxylic acids with diazo compounds, dithiocarbamates, isocyanates, mercaptans, nitrides, and sulfides. Carboxylic acids, especially in aqueous solution, also react with sulfites, nitrites, thiosulfates (to give H₂S and SO₃), dithionites (SO₂), to generate flammable and/or toxic gases and heat. Their reaction with carbonates and bicarbonates generates a harmless gas (carbon dioxide) but still heat. Like other organic compounds, carboxylic acids can be oxidized by strong oxidizing agents and reduced by strong reducing agents. These reactions generate heat. A wide variety of products is possible. Like other acids, carboxylic acids may initiate polymerization reactions; like other acids, they often catalyze (increase the rate of) chemical reactions.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and fumes.

SECTION 11: Toxicological information

Acute toxicity

Oral: no data available

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 data were available on the carcinogenicity of caffeic acid to humans. There is sufficient evidence in experimental animals for the carcinogenicity of caffeic acid. Overall evaluation: Caffeic acid is possibly carcinogenic to humans (Group 2B).

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: no data available

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: C-14 ring-labeled caffeic acid underwent approximately 55 percent mineralization after two weeks in a sandy loam mixed culture indicating the potential for biodegradation in soil(1).

Bioaccumulative potential

An estimated BCF of 3.2 was calculated for caffeic acid(SRC), using a log Kow of 1.15(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 caffeic acid is estimated as 100(SRC), using a log Kow of 1.15(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that caffeic acid is expected to have high mobility in soil. The pKa of caffeic acid is 4.62(4), indicating that this compound will primarily exist in anion form in the environment and anions generally do not adsorb to organic carbon and clay more strongly 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

Not Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

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/>

properties of the product. We as supplier shall not be held liable for any