

Caffeic Acid SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- * Product Name: Caffeic Acid
- * Catalog Number: S2277
- * CAS Number: 331-39-5
- * IUPAC Name: 2-Propenoic acid, 3-(3,4-dihydroxyphenyl)-

Relevant identified uses and uses advised against

- * Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.
- * Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

- * Company: Selleck Chemicals
- * TollFree: +1 877 796-6397
- * Tel: +1 832 582-8158
- * Fax: +1 832 582-8590

Emergency telephone number

- * Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

- Skin irritation: Category 2. H315
- Serious eye irritation: Category 2. H319
- Specific target organ toxicity (single exposure): Category 3. H335
- Carcinogenicity: Category 2. H351
- Reproductive toxicity: Category 2. H361

2.2 GHS Label elements, including precautionary statements

Hazard 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)

None.

Prevention	P203: Obtain, read and follow all safety instructions before use. P261: Avoid breathing dust/fume/gas/mist/vapors/spray. P264: Wash hands thoroughly after handling. P264+P265: Wash hands thoroughly after handling. Do not touch eyes. P271: Use only outdoors or in a well-ventilated area. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
Response	P302+P352: IF ON SKIN: wash with plenty of water. P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing. P305+P351: IF IN EYES: Rinse cautiously with water for several minutes. P318: if exposed or concerned, get medical advice. P319: Get medical help if you feel unwell. P321: Specific treatment (see information on this label and safety datasheet)). P332+P317: If skin irritation occurs: Get medical help. P337+P317: If eye irritation persists: Get medical help. P338: Remove contact lenses, if present and easy to do. Continue rinsing. P362+P364: Take off contaminated clothing and wash it before reuse.
Storage	P403+P233: Store in a well-ventilated place. Keep container tightly closed. P405: Store locked up.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: Caffeic Acid
 CAS Number: 331-39-5
 PubChem CID: 689043
 Molecular formula: C₉H₈O₄
 Molecular weight: 180.16 g/mol
 IUPAC name: (E)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to t

Skin contact: SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment.

Eye contact: EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.

Ingestion: INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO₂), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

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

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 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/

PRECAUTIONS FOR "CARCINOGENS": There is no universal method of disposal that has been proved satisfactory for all carcinogenic compounds & specific methods of chem destruction ... published have not been tested on all kinds of carcinogen-containing waste. ... summary of avail methods & recommendations ... /given/ must be treated as guide only. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": ... Incineration may be only feasible method for disposal of contaminated laboratory waste from biological expt. However, not all incinerators are suitable for this purpose. The most efficient type ... is probably the gas-fired type, in which a first-stage combustion with a less than stoichiometric air:fuel ratio is followed by a second stage with excess air. Some ... are designed to accept ... aqueous & organic-solvent solutions, otherwise it is necessary ... to absorb soln onto suitable combustible material, such as sawdust. Alternatively, chem destruction may be used, esp when small quantities ... are to be destroyed in laboratory. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": HEPA (high-efficiency particulate arrestor) filters ... can be disposed of by incineration. For spent charcoal filters, the adsorbed material can be stripped off at high temp & carcinogenic wastes generated by this treatment conducted to & burned in an incinerator. ... LIQUID WASTE: ... Disposal should be carried out by incineration at temp that ... ensure complete combustion. SOLID WASTE: Carcasses of lab animals, cage litter & misc solid wastes ... should be disposed of by incineration at temp high enough to ensure destruction of chem carcinogens or their metabolites. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": ... Small quantities of ... some carcinogens can be destroyed using chem reactions ... but no general rules can be given. ... As a general technique ... treatment with sodium dichromate in strong sulfuric acid can be used. The time necessary for destruction ... is seldom known ... but 1-2 days is generally considered sufficient when freshly prepd reagent is used. ... Carcinogens that are easily oxidizable can be destroyed with milder oxidative agents, such as saturated soln of potassium permanganate in acetone, which appears to be a suitable agent for destruction of hydrazines or of compounds containing isolated carbon-carbon double bonds. Conc'n or 50% aqueous sodium hypochlorite can also be used as an oxidizing agent. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": Carcinogens that are alkylating, arylating or acylating agents per se can be destroyed by reaction with appropriate nucleophiles, such as water, hydroxyl ions, ammonia, thiols & thiosulfate. The reactivity of various alkylating agents varies greatly ... & is also influenced by sol of agent in the reaction medium. To facilitate the complete reaction, it is suggested that the agents be dissolved in ethanol or similar solvents. ... No method should be applied ... until it has been thoroughly tested for its effectiveness & safety on material to be inactivated. For example, in case of destruction of alkylating agents, it is possible to detect residual compounds by reaction with 4(4-nitrobenzyl)-pyridine. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": Smoking, drinking, eating, storage of food or of food & beverage containers or utensils, & the application of cosmetics should be prohibited in any laboratory. All personnel should remove gloves, if worn, after completion of procedures in which carcinogens have been used. They should ... wash ... hands, preferably using dispensers of liq detergent, & rinse ... thoroughly. Consideration should be given to appropriate methods for cleaning the skin, depending on nature of the contaminant. No standard procedure can be recommended, but the use of organic solvents should be avoided. Safety pipettes should be used for all pipetting. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": In animal laboratory, personnel should remove their outdoor clothes & wear protective suits (preferably disposable, one-piece & close-fitting at ankles & wrists), gloves, hair covering & overshoes. ... Clothing should be changed daily but ... discarded immediately if obvious contamination occurs ... /also,/ workers should shower immediately. In chemical laboratory, gloves & gowns should always be worn ... however, gloves should not be assumed to provide full protection. Carefully fitted masks or respirators may be necessary when working with particulates or gases, & disposable plastic aprons might provide addnl protection. If

gowns are of distinctive color, this is a reminder that they should not be worn outside of lab. /Chemical Carcinogens/
PRECAUTIONS FOR "CARCINOGENS": ... Operations connected with synth & purification ... should be carried out under well-ventilated hood. Analytical procedures ... should be carried out with care & vapors evolved during ... procedures should be removed. ... Expert advice should be obtained before existing fume cupboards are used ... & when new fume cupboards are installed. It is desirable that there be means for decreasing the rate of air extraction, so that carcinogenic powders can be handled without ... powder being blown around the hood. Glove boxes should be kept under negative air pressure. Air changes should be adequate, so that concn of vapors of volatile carcinogens will not occur. /Chemical Carcinogens/

PRECAUTIONS FOR "CARCINOGENS": Vertical laminar-flow biological safety cabinets may be used for containment of in vitro procedures ... provided that the exhaust air flow is sufficient to provide an inward air flow at the face opening of the cabinet, & contaminated air plenums that are under positive pressure are leak-tight. Horizontal laminar-flow hoods or safety cabinets, where filtered air is blown across the working area towards the operator, should never be used ... Each cabinet or fume cupboard to be used ... should be tested before work is begun (eg, with fume bomb) & label fixed to it, giving date of test & avg air-flow measured. This test should be repeated periodically & after any structural changes. /Chemical Carcinogens/

For more Preventive Measures (Complete) data for CAFFEIC ACID (9 total), please visit the HSDB record page.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

SMALL SPILLS AND LEAKAGE: Should a spill occur while you are handling this chemical, **FIRST REMOVE ALL SOURCES OF IGNITION**, then you should dampen the solid spill material with 60-70% ethanol and transfer the dampened material to a suitable container. Use absorbent paper dampened with 60-70% ethanol to pick up any remaining material. Seal the absorbent paper, and any of your clothes, which may be contaminated, in a vapor-tight plastic bag for eventual disposal. Solvent wash all contaminated surfaces with 60-70% ethanol followed by washing with a soap and water solution. Do not reenter the contaminated area until the Safety Officer (or other responsible person) has verified that the area has been properly cleaned.

STORAGE PRECAUTIONS: You should store this material under ambient temperatures. (NTP, 1992)

7.2 Conditions for safe storage, including any incompatibilities

Store in a cool, dry, well-ventilated area. Keep container tightly closed.

Store away from incompatible materials (see Section 10).

Protect from light and moisture.

Recommended storage (industry convention for research compounds): -20°C for long-term storage; 2-8°C for short-term use and transport.

[Note: This is a general industry recommendation. Always verify exact storage conditions with the supplier Certificate of Analysis (COA).]

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

8.1.2 Appropriate engineering controls

Use only in a chemical fume hood or with local exhaust ventilation.

Ensure adequate ventilation to keep airborne concentrations below exposure limits.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear chemical safety goggles.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Use NIOSH-approved dust/mist respirator (N95 or higher) if ventilation is inadequate.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- a) Appearance: 3,4-dihydroxycinnamic acid appears as yellow prisms or plates (from chloroform or ligroin) or pale yellow granules. Alkaline solutions turn from yellow to orange. (NTP, 1992)
- b) Odor: No data available
- c) Odor threshold: No data available
- d) pH: No data available
- e) Melting point/freezing point: 433 to 437 °F (decomposes) (NTP, 1992)
- f) Initial boiling point and boiling range: No data available
- g) Flash point: No data available
- h) Evaporation rate: No data available
- i) Flammability (solid, gas): No data available
- j) Upper/lower flammability or explosive limits: No data available
- k) Vapor pressure: 0.00000025 [mmHg]
- l) Vapor density: No data available
- m) Relative density: No data available
- n) Water solubility: less than 1 mg/mL at 72 °F (NTP, 1992)
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 1.2
- p) Auto-ignition temperature: No data available
- q) Decomposition temperature: No data available
- r) Viscosity: No data available
- s) Explosive properties: No data available
- t) Oxidizing properties: No data available

9.2 Other information

Topological Polar Surface Area (TPSA): 77.8 Å²

Complexity: 212

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

10.5 Incompatible materials

Strong oxidizing agents, strong acids, strong bases.

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO₂).

See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

No acute toxicity data available.

Skin corrosion/irritation:

Causes skin irritation (H315).

Serious eye damage/eye irritation:

Causes serious eye irritation (H319).

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

No data available.

Carcinogenicity:

Suspected of causing cancer (H351).

Reproductive toxicity:

Suspected of damaging fertility or the unborn child (H361).

Specific target organ toxicity (single exposure):

No data available.

Specific target organ toxicity (repeated exposure):

No data available.

Aspiration hazard:

No data available.

11.2 Additional information

Carcinogen classification:

Caffeic acid

Group 2B: Possibly carcinogenic to humans

Volume 56: (1993) Some Naturally Occurring Substances: Food Items and Constituents, Heterocyclic Aromatic Amines and Mycotoxins

1993

1992

2B, possibly carcinogenic to humans. (L135)

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Caffeic acid's production as a laboratory chemical and its use in the development of asthmatic and allergenic drugs may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of 2.5×10^{-7} mm Hg at 25 °C indicates caffeic acid will exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase caffeic acid will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 8.6 hrs. Caffeic acid has been shown to absorb light in the environmental UV spectrum and therefore has the potential for direct photolysis. If released to soil, caffeic acid is expected to have high mobility based upon an estimated Koc of 100. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 1.4×10^{-16} atm-cu m/mole. The pKa of caffeic acid is 4.62, 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. Caffeic acid is not expected to volatilize from dry soil surfaces based upon its vapor pressure. 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. If released into water, ca

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 1.2

Low potential for bioaccumulation (Log P < 3).

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available.

12.6 Other adverse effects

No other adverse ecological effects identified.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same

manner as the product itself.

14. TRANSPORT INFORMATION

14.1 UN number

Not regulated as dangerous goods (research quantities typically exempt).

14.2 UN proper shipping name

Not subject to transport regulations (small quantities for research use).

14.3 Transport hazard class(es)

Not classified as dangerous goods for transport (research quantities).

14.4 Packing group

Not applicable (not regulated as dangerous goods in typical research quantities).

14.5 Environmental hazards

Marine pollutant: No (not classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable.

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

US EPA / TSCA: Subject to EPA TSCA regulations

EU ECHA / REACH: Not available in public databases.

SARA 302 Components:

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components:

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards:

Acute (short-term) health hazard

Chronic (long-term) health hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

California Prop. 65 Components:

This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

Other regulatory listings:

- California Safe Cosmetics Program (CSCP) Reportable Ingredient: Hazard Traits - Carcinogenicity Authoritative List - IARC Carcinogens - 2B; Prop 65 Report - regardless of intended function of ingredient in the product

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/08

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product.

Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.