

## Chemical Safety Data Sheet MSDS / SDS

## Caffeic Acid-13C3

Revision Date:2026-05-31 Revision Number:1

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

**Product identifier**

Product name : Caffeic Acid-13C3  
CBnumber : CB91565682  
CAS : 1185245-82-2  
Synonyms : 3-(3,4-Dihydroxyphenyl)-2-propenoic Acid-13C3

**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 : 010-86108875

## SECTION 2: Hazards identification

**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

**Precautionary statements**

P201 Obtain special instructions before use.  
P202 Do not handle until all safety precautions have been read and understood.  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P264 Wash skin thoroughly after handling.  
P271 Use only outdoors or in a well-ventilated area.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P302+P352 IF ON SKIN: wash with plenty of soap and water.  
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P308+P313 IF exposed or concerned: Get medical advice/attention.

P312 Call a POISON CENTER or doctor/physician if you feel unwell.  
P321 Specific treatment (see ... on this label).  
P332+P313 IF SKIN irritation occurs: Get medical advice/attention.  
P337+P313 IF eye irritation persists: Get medical advice/attention.  
P403+P233 Store in a well-ventilated place. Keep container tightly closed.  
P405 Store locked up.  
P501 Dispose of contents/container to.....

#### **Hazard statements**

H315 Causes skin irritation  
H319 Causes serious eye irritation  
H351 Suspected of causing cancer  
H361 Suspected of damaging fertility or the unborn child  
H335 May cause respiratory irritation

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name : Caffeic Acid-13C3  
Synonyms : 3-(3,4-Dihydroxyphenyl)-2-propenoic Acid-13C3  
CAS : 1185245-82-2  
MF : C613C3H8O4  
MW : 183

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## SECTION 4: First aid measures

### **Description of first aid measures**

#### **After inhalation**

In case of unconsciousness place patient stably in side position for transportation.

#### **After skin contact**

Immediately wash with water and soap and rinse thoroughly.

#### **After eye contact**

Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.

#### **After swallowing**

If symptoms persist consult doctor.

### **Most important symptoms and effects, both acute and delayed**

No further relevant information available.

### **Indication of any immediate medical attention and special treatment needed**

No further relevant information available.

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing agents

Use fire fighting measures that suit the environment.

A solid water stream may be inefficient.

#### Special hazards arising from the substance or mixture

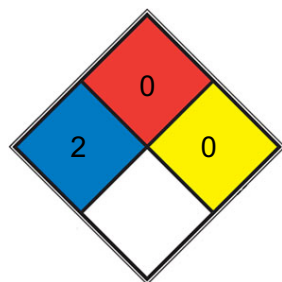
No further relevant information available.

#### Advice for firefighters

#### Protective equipment

No special measures required.

#### NFPA 704



HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

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FIRE 0 Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes.(e.g. Carbon tetrachloride)

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REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,[N2](#))

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SPEC.  
 HAZ.

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## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Not required.

### Environmental precautions

Do not allow to enter sewers/ surface or ground water.

## **Methods and material for containment and cleaning up**

Dispose contaminated material as waste according to section 13.

Ensure adequate ventilation.

## **Protective Action Criteria for Chemicals**

### **PAC-1**

Substance is not listed.

### **PAC-2**

Substance is not listed.

### **PAC-3**

Substance is not listed.

## **Reference to other sections**

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

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# **SECTION 7: Handling and storage**

## **Precautions for safe handling**

No special precautions are necessary if used correctly.

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

Avoid prolonged or repeated exposure.

Keep away from sources of ignition.

Take precautionary measures against static discharge.

## **Information about protection against explosions and fires**

No special measures required.

## **Conditions for safe storage, including any incompatibilities**

### **Storage**

Store in accordance with information listed on the product insert.

## **Requirements to be met by storerooms and receptacles**

No special requirements.

## **Information about storage in one common storage facility**

Not required.

## **Further information about storage conditions**

Keep receptacle tightly sealed.

### **Specific end use(s)**

No further relevant information available.

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## **SECTION 8: Exposure controls/personal protection**

### **Control parameters**

#### **Components with limit values that require monitoring at the workplace**

Not required.

#### **Additional information**

The lists that were valid during the creation were used as basis.

### **Exposure controls**

#### **Appropriate engineering controls**

No further data; see section 7.

#### **Personal protective equipment**

#### **General protective and hygienic measures**

Keep away from foodstuffs, beverages and feed.

Immediately remove all soiled and contaminated clothing.

Wash hands before breaks and at the end of work.

Avoid contact with the eyes and skin.

#### **Breathing equipment**

In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.

#### **Protection of hands**

Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

#### **Material of gloves**

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

#### **Penetration time of glove material**

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

## Eye protection

Tightly sealed goggles

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# SECTION 9: Physical and chemical properties

## Information on basic physicochemical properties

### Physical State

Solid

### Color

Grey

### Odor

Characteristic

### Structural Formula

C6[13C]3H8O4

### Molecular Weight

183.1 g/mol

### Storage Buffer

### Odor Threshold

Not determined.

### Formulation

### Melting point/Melting range

Undetermined.

### Boiling point/Boiling range

Undetermined.

### Flammability

Product is not flammable.

### Explosion limits

Lower: Not determined.

Upper: Not determined.

### Flash point

Not applicable.

**Decomposition temperature**

Not determined.

**pH**

Not applicable.

**Viscosity****Kinematic**

Not applicable.

**SOLUBILITY**

DMSO: Slightly; Methanol: Very Slightly

**Dynamic**

Not applicable.

**Solubility in / Miscibility with**

DMSO (Sparingly), Methanol (Slightly)

**Water**

Not determined.

**Partition coefficient (n-octanol/water)**

Not determined.

**Vapor Pressure**

Not applicable.

**Density**

Not determined.

**Relative Density**

Not determined.

**Vapor Density**

Not applicable.

**Particle characteristics**

Not determined.

**Other information****Appearance****Form**

Solid

**Important information on protection of health and environment, and on safety.**

**Ignition temperature**

Not determined.

**Danger of explosion**

Product does not present an explosion hazard.

**Change in condition**

**Evaporation Rate**

Not applicable.

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**SECTION 10: Stability and reactivity**

**Reactivity**

No further relevant information available.

**Chemical stability**

**Thermal decomposition / conditions to be avoided**

No decomposition if used according to specifications.

**Possibility of hazardous reactions**

No dangerous reactions known.

**Conditions to avoid**

No further relevant information available.

**Incompatible materials**

Strong acids. Strong bases. Strong oxidizing agents

**Hazardous decomposition products**

carbon dioxide, carbon monoxide

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**SECTION 11: Toxicological information**

**RTECS Number**

GD8950000 (Unlabeled Cas No. 331-39-5)

**Information on toxicological effects**

**Acute toxicity**

LD/LC50 values that are relevant for classification:

Route	Endpoint	Value
Oral	TDLO	50 mg/kg (guinea pig) 200 mg/kg (rat)

### **Primary irritant effect**

#### **on the skin**

Irritant to skin and mucous membranes.

#### **on the eye**

Irritating effect.

### **Sensitization**

No sensitizing effects known.

### **Additional toxicological information**

#### **Interactive effects**

No interactive effects between components are known.

### **Carcinogenic categories**

#### **IARC (International Agency for Research on Cancer)**

Substance is not listed.

#### **NTP (National Toxicology Program)**

Substance is not listed.

#### **OSHA-Ca (Occupational Safety & Health Administration)**

Substance is not listed.

### **Alternative sources for toxicological information**

No non-standard sources for toxicological information where used.

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## SECTION 12: Ecological information

### **Toxicity**

#### **Aquatic toxicity**

No further relevant information available.

#### **Persistence and degradability**

No further relevant information available.

#### **Bioaccumulative potential**



Class: 6.1 Toxic substances

Label: 6.1

**IMDG, IATA**

Class: 6.1 Toxic substances

Label: 6.1

**Packing group**

DOT, IMDG, IATA II

**Environmental hazards**

Not applicable.

**Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code**

Not applicable.

**Transport/Additional information**

**DOT:**

**Quantity limitations**

On passenger aircraft/rail: 25 kg

On cargo aircraft only: 100 kg

**IMDG:**

**Limited quantities (LQ)**

500 g

**Excepted quantities (EQ)**

Code: E4

Maximum net quantity per inner packaging: 1 g

Maximum net quantity per outer packaging: 500 g

**Special precautions for user**

Warning: Toxic substances

**Hazard identification number (Kemler code)**

60

**EMS Number**

F-A, S-A

**Stowage Category**

B

**UN "Model Regulation"**

UN 2811 TOXIC SOLID, ORGANIC, N.O.S. (CAFFEIC

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## SECTION 15: Regulatory information

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

No further relevant information available.

#### Sara

Section 355 (extremely hazardous substances):	Substance is not listed.
Section 313 (Specific toxic chemical listings):	Substance is not listed.
TSCA (Toxic Substances Control Act):	Substance is not listed.
Hazardous Air Pollutants:	Substance is not listed.
Chemicals known to cause cancer:	Substance is not listed.
Chemicals known to cause reproductive toxicity for females:	Substance is not listed.
Chemicals known to cause reproductive toxicity for males:	Substance is not listed.
Chemicals known to cause developmental toxicity:	Substance is not listed.

#### Carcinogenic categories

EPA (Environmental Protection Agency):	Substance is not listed.
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#### TLV (Threshold Limit Value)

Substance is not listed.

#### NIOSH-Ca (National Institute for Occupational Safety and Health)

Substance is not listed.

#### Chemical safety assessment

A Chemical Safety Assessment has not been carried out.

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## SECTION 16: Other information

### Abbreviations and acronyms

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMS: Hazardous Materials Identification System (USA)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety & Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

Skin irritation 2: Skin corrosion/irritation – Category 2

Eye irritation 2A: Serious eye damage/eye irritation – Category 2A

Carcinogenicity 2: Carcinogenicity – Category 2

Reproductive toxicity 2: Reproductive toxicity – Category 2

Specific target organ toxicity (single exposure) 3: Specific target organ toxicity (single exposure) – Category 3

**Disclaimer:**

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.