

## SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 10.08.2012

Version 3.5

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

#### 1.1 Product identifier

Catalogue No.	822029
Product name	3,4-Dihydroxycinnamic acid for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

#### 1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal ( <a href="http://www.merck-chemicals.com">www.merck-chemicals.com</a> ).
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#### 1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a>

1.4 Emergency telephone number	Please contact the regional company representation in your country.
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### SECTION 2. Hazards identification

#### 2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Carcinogenicity, Category 2, H351

For the full text of the H-Statements mentioned in this Section, see Section 16.

Classification (67/548/EEC or 1999/45/EC)

Carc.Cat.3    Carcinogenic Category 3    R40

For the full text of the R-phrases mentioned in this Section, see Section 16.

#### 2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

*Hazard pictograms*



*Signal word*  
Warning

*Hazard statements*

H351 Suspected of causing cancer.

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*Precautionary statements*

P281 Use personal protective equipment as required.  
P308 + P313 IF exposed or concerned: Get medical advice/ attention.

CAS-No. 331-39-5

**Labelling (67/548/EEC or 1999/45/EC)**

Symbol(s)  Xn Harmful

R-phrase(s) 40 Limited evidence of a carcinogenic effect.  
S-phrase(s) 36/37 Wear suitable protective clothing and gloves.  
EC-No. 206-361-2

**2.3 Other hazards**

None known.

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**SECTION 3. Composition/information on ingredients**

Formula	(OH) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> CHCHCOOH	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub> (Hill)
CAS-No.	331-39-5	
EC-No.	206-361-2	
Molar mass	180,15 g/mol	

**Hazardous components (REGULATION (EC) No 1272/2008)**

*Chemical Name (Concentration)*

CAS-No.	Registration number	Classification
<i>3,4-dihydroxycinnamic acid (&lt;= 100 % )</i>		
331-39-5	*)	Carcinogenicity, Category 2, H351

\*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

For the full text of the H-Statements mentioned in this Section, see Section 16.

**Hazardous components (1999/45/EC)**

*Chemical Name (Concentration)*

CAS-No.	Classification
<i>3,4-dihydroxycinnamic acid (&lt;= 100 % )</i>	
331-39-5	Carc.Cat.3; R40

For the full text of the R-phrases mentioned in this Section, see Section 16.

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**SECTION 4. First aid measures**

**4.1 Description of first aid measures**

After inhalation: fresh air. Call in physician.

After skin contact: wash off with plenty of water. Remove contaminated clothing. Consult a physician.

After eye contact: rinse out with plenty of water. Call in ophthalmologist.

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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**4.2 Most important symptoms and effects, both acute and delayed**  
irritant effects

**4.3 Indication of any immediate medical attention and special treatment needed**  
No information available.

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**SECTION 5. Firefighting measures**

**5.1 Extinguishing media**

*Suitable extinguishing media*

Water, Carbon dioxide (CO<sub>2</sub>), Foam, Dry powder

*Unsuitable extinguishing media*

For this substance/mixture no limitations of extinguishing agents are given.

**5.2 Special hazards arising from the substance or mixture**

Combustible material

Risk of dust explosion.

Development of hazardous combustion gases or vapours possible in the event of fire.

**5.3 Advice for firefighters**

*Special protective equipment for firefighters*

In the event of fire, wear self-contained breathing apparatus.

*Further information*

Prevent fire extinguishing water from contaminating surface water or the ground water system.

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**SECTION 6. Accidental release measures**

**6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

**6.2 Environmental precautions**

Do not let product enter drains.

**6.3 Methods and materials for containment and cleaning up**

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

**6.4 Reference to other sections**

Indications about waste treatment see section 13.

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**SECTION 7. Handling and storage**

**7.1 Precautions for safe handling**

Work under hood. Do not inhale substance/mixture.

Observe label precautions.

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

Tightly closed. Dry.

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Store at +15°C to +25°C.

### 7.3 Specific end uses

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

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## SECTION 8. Exposure controls/personal protection

### 8.1 Control parameters

### 8.2 Exposure controls

#### Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

#### Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

#### *Hygiene measures*

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

#### *Eye/face protection*

Safety glasses

#### *Hand protection*

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet(>,<)> supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

#### *Other protective equipment*

protective clothing

#### *Respiratory protection*

required when dusts are generated.

Recommended Filter type: Filter P 3 (acc. to DIN 3181) for solid and liquid particles of toxic and very toxic substances

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective

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devices are carried out according to the instructions of the producer. These measures have to be properly documented.

**Environmental exposure controls**

Do not let product enter drains.

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**SECTION 9. Physical and chemical properties**

**9.1 Information on basic physical and chemical properties**

Form	powder, finocrystalline
Colour	yellow
Odour	odourless
Odour Threshold	not applicable
pH	No information available.
Melting point	234 - 237 °C (decomposition)
Boiling point	No information available.
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	No information available.
Relative vapour density	No information available.
Relative density	No information available.
Water solubility	at 20 °C slightly soluble
Partition coefficient: n-octanol/water	log Pow: 1,15 (experimental) (Lit.) Bioaccumulation is not expected.
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified als explosive.

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Oxidizing properties none

**9.2 Other data**

none

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**SECTION 10. Stability and reactivity**

**10.1 Reactivity**

Risk of dust explosion.

**10.2 Chemical stability**

The product is chemically stable under standard ambient conditions (room temperature) .

**10.3 Possibility of hazardous reactions**

Violent reactions possible with:

strong alkalis, Strong acids, Strong oxidizing agents

**10.4 Conditions to avoid**

Strong heating (decomposition).

**10.5 Incompatible materials**

no information available

**10.6 Hazardous decomposition products**

no information available

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**SECTION 11. Toxicological information**

**11.1 Information on toxicological effects**

*Skin irritation*

slight irritation

*Eye irritation*

slight irritation

*Genotoxicity in vitro*

Ames test

Result: negative

(National Toxicology Program)

Mutagenicity (mammal cell test): micronucleus.

Result: positive

(National Toxicology Program)

*CMR effects*

Carcinogenicity:

Suspected of causing cancer.

*Specific target organ toxicity - single exposure*

The substance or mixture is not classified as specific target organ toxicant, single exposure.

*Specific target organ toxicity - repeated exposure*

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

*Aspiration hazard*

Based on available data the classification criteria are not met.

**11.2 Further information**

Quantitative data on the toxicity of this product are not available.

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Other dangerous properties can not be excluded.  
This substance should be handled with particular care.

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**SECTION 12. Ecological information**

**12.1 Toxicity**

No information available.

**12.2 Persistence and degradability**

No information available.

**12.3 Bioaccumulative potential**

*Partition coefficient: n-octanol/water*

log Pow: 1,15

(experimental)

(Lit.) Bioaccumulation is not expected.

**12.4 Mobility in soil**

No information available.

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

**12.6 Other adverse effects**

*Additional ecological information*

Discharge into the environment must be avoided.

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**SECTION 13. Disposal considerations**

*Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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**SECTION 14. Transport information**

**Land transport (ADR/RID)**

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

**Inland waterway transport (ADN)**

Not relevant

**Air transport (IATA)**

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

**Sea transport (IMDG)**

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

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

Not relevant

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**SECTION 15. Regulatory information**

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

*EU regulations*

Major Accident Hazard 96/82/EC

Legislation Directive 96/82/EC does not apply

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Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work. Take note of Dir 92/85/EEC on the safety and health at work of pregnant workers.
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*National legislation*

Storage class	10 - 13
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## 15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

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## SECTION 16. Other information

**Full text of H-Statements referred to under sections 2 and 3.**

H351	Suspected of causing cancer.
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**Full text of R-phrases referred to under sections 2 and 3**

R40	Limited evidence of a carcinogenic effect.
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### Training advice

Provide adequate information, instruction and training for operators.

### Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

### Regional representation

This information is given on the authorised Safety Data Sheet for your country.

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*The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.*