

MATERIAL SAFETY DATA SHEET



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1 . IDENTIFICATION OF THE SUBSTANCE / MIXTURE AND OF THE COMPANY

1.1 Product identifiers

Product name : [3,5-Di-O-caffeoyl quinic acid](#)
Catalogue number : 4946 S
CAS NUMBER : 2450-53-5 **EC Number** : -

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

Reagent for research use only.

1.3 Details of the supplier of the safety data sheet

Extrasynthese
 Z.I Lyon Nord
 Impasse Jacquard - C.S 30062
 69727 GENAY CEDEX - FRANCE
 Phone : (33)(0)478-98-20-34
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1.4 Emergency call number (I.N.R.S France) : Tel :

(33)(0)145-42-59-59

2 . HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

According to Regulation (EC) No 1272/2008

Not a hazardous substance or mixture according to Regulation (EC) No 1272/2008.

2.2 Label elements

Labelling according Regulation (CE) No 1272/2008

Not a hazardous substance or mixture according to Regulation (EC) No 1272/2008.

Pictogram

Not required

Hazard statement

Not required

Precautionary statements

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P262 Do not get in eyes, on skin, or on clothing.

Supplemental hazard statements

No additional information.

2.3 Other hazards

None

3 . COMPOSITION / INFORMATION ON INGREDIENTS

3.1 Substances

Product name : 3,5-Di-O-caffeoyl quinic acid
Empirical formula : C₂₅H₂₄O₁₂
CAS NUMBER : 2450-53-5
Synonyms : Isochlorogenic acid A
EC Number :

3,5-Di-O-caffeoyl quinic acid

CAS NUMBER	Concentration	Classification
2450-53-5	< 100%	

For the full text of the H-statements mentioned in this section, see section 16.

3.2 Mixtures

Not applicable

4 . FIRST AID MEASURES**4.1 Description of first aid measures****General advice**

Consult a physician. Show this safety data sheet to the doctor in attendance.

Inhalation

In case of inhalation, move the victim to fresh air. If breathing is difficult, put the victim on oxygen. If breathing stops, carry out artificial respiration.

In case of skin contact

Wash thoroughly with water and soap.

In case of eye contact

Rinse well with plenty of water for at least 15 minutes.

Ingestion

Do not make an unconscious person vomit or swallow anything. Rinse the mouth thoroughly with water.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

4.3 Indication of any immediate medical attention and special treatment needed

No data available.

5 . FIRE-FIGHTING MEASURES**5.1 Extinguishing media**

Carbon dioxide, dry powder.

5.2 Special hazards arising from the substance

Harmful/toxic vapours, carbon oxides may be released during the fire.

5.3 Advise for fire-fighters

Wear an autonomous breathing apparatus and suitable protection clothing against chemical agents.

6 . ACCIDENTAL RELEASE MEASURES**6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Evacuate the personnel from the contaminated zone. Ensure adequate ventilation.

6.2 Environmental precautions

Keeping away from drains, surface and ground waters.

6.3 Methods and materials for containment and cleaning up

Clean up without creating dust and place in adapted and sealed containers for elimination. Wash the contaminated area with water and soap. Confine washing water and dispose of it complying with the local regulations. After cleaning, quickly eliminate traces of water with a product absorbing liquids (for example : sand, sawdust, universal binder, Kieselguhr).

6.4 Reference to other sections

For disposal see section 13.

7 . HANDLING AND STORAGE**7.1 Precautions for safe handling**

Avoid formation of dust. Avoid contact with skin and eyes. During handling, wear suitable personal protective equipment (see section 8). Follow the normal measures for preventive fire protection.

7.2 Specific handling

No data available.

7.3 Conditions for safe storage, including any incompatibilities

Store in a cool well-ventilated place.
Keep container tightly closed in a dry place away from light.
Store at <-15°C

7.4 Specific end use(s)

No data available

8 . EXPOSURE CONTROL/PERSONAL PROTECTION**8.1 Control parameters****Occupational exposure limit values (Workplace Exposure Limits)**

This information is not available.

8.2 Exposure controls**Respiratory protection**

Wear imperatively an appropriated mask/respirator, tested and approved by standards such as NIOSH (US) or GEN (EU).

Hand protection

Handle with protective gloves. The selected gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Eye protection

Wear safety glasses.

Skin protection

Wear suitable protective clothing according to the quantity and the level of activity of the substance at the workplace.

9 . PHYSICAL AND CHEMICAL PROPERTIES**9.1 Information on basic physical and chemical properties**

a	Physical state	: Powder
b	Odour	: No data available
c	Odour threshold	: No data available
d	pH	: No data available
e	Melting point/freezing point	: No data available
f	Initial boiling point/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	Vapour pressure	: No data available
l	Vapour density	: No data available
m	Relative density	: No data available
n	Solubility	: No data available
o	Partition coefficient: n-octanol/water	: No data available
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

No data available

10 . STABILITY AND REACTIVITY**10.1 Reactivity**

No data available.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions during storage and handling complying with the instructions.

10.4 Conditions to avoid

No data available.

10.5 Incompatible materials

No data available.

10.6 Hazardous decomposition products

No hazardous decomposition products if the instructions for handling and storage are respected. During high overheating of the substance or during a fire, hazardous decomposition products may be produced.

11 . TOXICOLOGICAL INFORMATION

11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute oral toxicity

No data available.

Acute dermal toxicity

No data available.

Acute inhalation toxicity

No data available.

Skin Corrosion

No data available.

Skin Irritation

No data available.

Serious Eye Damage

No data available.

Eye Irritation

No data available.

Respiratory Sensitisation

No data available.

Skin Sensitisation

No data available.

Germ Cell Mutagenicity

No data available.

Carcinogenicity

No data available.

Reproductive Toxicity

No data available.

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 Information on other hazards

No data available.

12 . ECOLOGICAL INFORMATION

12.1 Toxicity

No data available.

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

No data available.

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

No data available.

12.6 Endocrine disrupting properties

No data available.

12.7 Other adverse effects

No data available.

13 . DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods**

Non-recyclable surplus and solutions must be sent to a licensed professional waste disposal service, while respecting the local statutory instructions. Contaminated packaging is to be eliminated in the same way as the product that is contained.

14 . TRANSPORT INFORMATION**14.1 UN number or ID number**

Not subject to transport regulations

14.2 UN proper shipping name

Not assigned.

14.3 Transport hazard classes

-

14.4 Packing group

-

14.5 Environmental hazards

No

14.6 Special precautions for user

There is no additional information.

14.7 Maritime transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

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

Directive 96/82/CE (SEVESO category/named substances) : not applicable.
Regulation CE 2037/2000 (substances that deplete the ozone layer) : not applicable.
Regulation 850/2004 (persistent organic pollutants) : not applicable.
Regulation REACH-Titre VII (authorisations) et Titre VIII (restrictions) : not applicable.

15.2 Chemical safety assessment

Not applicable.

16 . OTHER INFORMATION**Use**

The information contained in this safety data sheet are based on our experience and our current knowledge. The data may in no case be considered as product specifications. It is provided for information purposes only with no obligation on our part. In this respect, we shall not be held liable for the use which is made of our products and for the information given above.

Abbreviations and acronyms

ADR: Agreement on Dangerous Goods by Road
RID: Regulations concerning the International Transport of Dangerous Goods by Rail
IATA: International Air Transport Association
CAS: Chemical Abstract Service
PBT: Persistent, Bioaccumulative and Toxic
vPvB: Very Persistent and Very Bioaccumulative

Full text of R-phrase(s) and S-phrase(s) according to European Directive 67/548/EEC-Full text of hazard statement(s) mentioned in section 3

Not applicable.