

1. Chemical Product and company Identification

Product Name: 异绿原酸A

English Name: 3,5-Dicaffeoylquinic acid

Catalogue No: 2450-53-5

Supplier: Chengdu Biopurify Phytochemicals Ltd.

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2. Composition, Information on Ingredients

Alias: Isochlorogenic acid A

CAS Number: 2450-53-5

Mol. Formula: C₂₅H₂₄O₁₂

Mol. Weight: 516.455

Identified uses: Laboratory chemicals, for R&D

Storage: Room temperature for transportation, for long term storage, protected from strong light, keep package airproofed when not in use.

3. Hazards identification

Classification of the substance or mixture

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

This substance is not classified as dangerous according to Directive 67/548/EEC.

Label elements

Not a hazardous substance or mixture according to EC-directives 67/548/EEC or 1999/45/EC.

Other hazards -

The chemical, Physical and toxicological properties of this product have not been thoroughly investigated. Use appropriate procedures to prevent opportunities for direct contact with the skin or eyes and to prevent inhalation.

4. First-aid measures

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration.

Consult a doctor.

In case of skin contact

Wash off with soap and plenty of water. Consult a doctor.

In case of eye contact

Flush eyes with water as a precaution. Consult a doctor.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a doctor.

Indication of any immediate medical attention and special treatment needed

No data available

Show this safety data sheet to the doctor in attendance.

Immediate medical attention is required.

5. Fire-fighting measures

Conditions of flammability

Not flammable or combustible.

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special protective equipment for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.
Hazardous combustion products
Hazardous decomposition products formed under fire conditions. – Carbon oxides

6、Accidental release measures

Personal precautions

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

7、Handling and storage

Handling:

Wash thoroughly after handling. Remove contaminated clothing and wash before reuse. Avoid contact with eyes, skin, and clothing. Avoid ingestion and inhalation. Keep away from sources of ignition. Avoid prolonged or repeated exposure.

Storage:

Store in a well closed container. Protected from air and light, put into refrigerator or freeze for long term storage.

Specific end uses

Use in a laboratory fume hood where possible. Refer to employer is COSHH risk assessment.

8、Exposure controls, personal protection

Contains no substances with occupational exposure limit values.

Personal protective equipment

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Hand protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Eye protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin and body protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

9、Physical and chemical properties

Physical Description : Off-white Powder

Property	Values
pH	No information available
Melting point/freezing point	170–172°C
Boiling point	826.2°C at 760 mmHg
Flash point	280.4°C
Density	1.645 g/cm ³
Evaporation rate	No information available
Upper flammability limits	No information available
Lower flammability limit	No information available
Vapor pressure	No information available

Vapor density	No information available
Specific gravity	No information available
Water solubility	No information available
Solubility in other solvents	No information available
Partition coefficient	No information available
Autoignition temperature	No information available
Kinematic viscosity	No information available
Decomposition temperature	No information available
Explosive properties	No information available
Oxidizing properties	No information available

10、Stability and reactivity

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Materials to avoid

Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - no data available

11、Toxicological information

Acute toxicity

Oral LD50: no data available

Inhalation LC50: no data available

Dermal LD50: no data available

Other information on acute toxicity: no data available

no data available

Serious eye damage/eye irritation

no data available

Respiratory or skin sensitisation

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

no data available

Teratogenicity

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)

no data available

Specific target organ toxicity - repeated exposure (Globally Harmonized System)

no data available

Aspiration hazard

no data available

Potential health effects

Inhalation May be harmful if inhaled. Causes respiratory tract irritation.

Ingestion May be harmful if swallowed.

Skin May be harmful if absorbed through skin. Causes skin irritation.

Eyes May be caused eye irritation.

Synergistic effects

no data available

Additional Information
RTECS: Not available

12、Ecological information

Toxicity

no data available

Persistence and degradability

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

PBT and vPvB assessment

no data available

Other adverse effects

no data available

13、Disposal considerations

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14、Transport information

Classified according to the criteria of the UN Model Regulations as reflected in the IMDG Code, ADR, RID and IATA.

UN number

Does not meet the criteria for classification as hazardous for transport.

UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

Transport hazard class(es)

Does not meet the criteria for classification as hazardous for transport.

Packaging group

Does not meet the criteria for classification as hazardous for transport.

Environmental hazards

This product is not classified as environmentally hazardous according to the UN Model Regulations, nor a marine pollutant according to the IMDG Code.

Special precautions for user

no data available

15、Regulatory information

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

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

no data available

Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

16、Other information

DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Biopurify and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.phytopurify.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

