## Chemical Safety Data Sheet MSDS / SDS

## Neochlorogenic acid

Revision Date: 2025-07-19 Revision Number: 1

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

#### **Product identifier**

Product name : Neochlorogenic acid

CBnumber : CB0914996

CAS : 906-33-2

EINECS Number : 212-997-1

Synonyms : Neochlorogenic Acid,5-Caffeoylquinic acid

#### 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

#### Pictogram(s)

Signal word

Warning

#### Hazard statement(s)

H335 May cause respiratory irritation

H319 Causes serious eye irritation

H315 Causes skin irritation

#### Prevention

P271 Use only outdoors or in a well-ventilated area.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P264 Wash ... thoroughly after handling.

#### Response

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue

rinsing.

P362+P364 Take off contaminated clothing and wash it before reuse.

P332+P317 If skin irritation occurs: Get medical help.

P321 Specific treatment (see ... on this label).

P302+P352 IF ON SKIN: Wash with plenty of water/...

P319 Get medical help if you feel unwell.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

#### Storage

P405 Store locked up.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

#### Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

## SECTION 3: Composition/information on ingredients

#### **Substance**

Product name : Neochlorogenic acid

Synonyms : Neochlorogenic Acid,5-Caffeoylquinic acid

CAS : 906-33-2 EC number : 212-997-1 MF : C16H18O9 MW : 354.31

## SECTION 4: First aid measures

#### Description of first aid measures

## If inhaled

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

#### In case of skin contact

Wash off with soap and plenty of water.

## In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

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

## 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

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

No data available

## SECTION 5: Firefighting measures

### **Extinguishing media**

#### Suitable extinguishing media

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

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

Carbon oxides

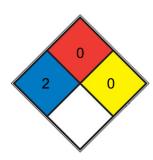
#### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### **Further information**

No data available

### **NFPA 704**



Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. <u>diethyl</u>

HEALTH 2

<u>ether</u>, ammonium phosphate, iodine)

Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete,

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

SPEC.

## SECTION 6: Accidental release measures

## Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing vapours, mist or gas. For personal protection see section 8.

### **Environmental precautions**

No special environmental precautions required.

## Methods and materials for containment and cleaning up

Sweep up and shovel. Keep in suitable, closed containers for disposal.

#### Reference to other sections

For disposal see section 13.

## SECTION 7: Handling and storage

#### Precautions for safe handling

Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

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

Keep container tightly closed in a dry and well-ventilated place. Store in cool place. Store with desiccant. Light sensitive. Store under inert gas.

#### Specific end use(s)

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

## SECTION 8: Exposure controls/personal protection

### control parameter

#### Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

#### **Exposure controls**

#### Appropriate engineering controls

General industrial hygiene practice.

#### Personal protective equipment

Eye/face protection

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

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it. Body Protection

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

No special environmental precautions required.

## SECTION 9: Physical and chemical properties

## Information on basic physicochemical properties

Appearance	white Powder with lumps
Odour	No data available
Odour Threshold	No data available
рН	No data available
Melting point/freezing point	204 - 206 °C
Initial boiling point and boiling range	665.0±55.0 °C(Predicted)
Flash point	No data available
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive	No data available
limits	
Vapour pressure	No data available
Vapour density	No data available
Relative density	No data available
Water solubility	soluble in hot water
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

## Other safety information

Solubility in other solvents

Ethanol - soluble

## SECTION 10: Stability and reactivity

## Reactivity

No data available

## **Chemical stability**

Stable under recommended storage conditions.

## Possibility of hazardous reactions

No data available

#### Conditions to avoid

No data available

### Incompatible materials

Strong oxidizing agents

### Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides Other decomposition products - No data available In the event of fire: see section 5

## **SECTION 11: Toxicological information**

## Information on toxicological effects

#### **Acute toxicity**

No data available

#### Skin corrosion/irritation

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.

#### 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

#### **Additional Information**

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

## SECTION 12: Ecological information

## **Toxicity**

No data available

## Persistence and degradability

No data available

## **Bioaccumulative potential**

No data available

### Mobility in soil

No data available

## Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

#### Other adverse effects

No data available

## **SECTION 13: Disposal considerations**

#### Waste treatment methods

#### **Product**

Offer surplus and non-recyclable solutions to a licensed disposal company.

### Contaminated packaging

Dispose of as unused product.

## **SECTION 14: Transport information**

## **UN** number

ADR/RID: - IMDG: - IATA: -

## **UN proper shipping name**

ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Not dangerous goods

## Transport hazard class(es)

ADR/RID: - IMDG: - IATA: -

### **Packaging group**

ADR/RID: - IMDG: - IATA: -

## **Environmental hazards**

ADR/RID: no IMDG Marine pollutant: no IATA: no

## Special precautions for user

No data available

## **SECTION 15: Regulatory information**

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

#### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: https://www.mem.gov.cn/

#### Measures for Environmental Management of New Chemical Substances

EC Inventory:Listed.

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: https://www.epa.govt.nz/

Korea Existing Chemicals List (KECL):Not Listed. website: http://ncis.nier.go.kr

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: https://echa.europa.eu/

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: https://www.mee.gov.cn/

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: https://emb.gov.ph/

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: https://www.epa.gov/

Vietnam National Chemical Inventory:Listed. website: https://chemicaldata.gov.vn/

## SECTION 16: Other information

### Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

#### References

[1] CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

[2] ChemlDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

[3] ECHA - European Chemicals Agency, website: https://echa.europa.eu/

[4] eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request\_locale=en

[5] ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

[6] Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

[7] HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

[8] IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

[9] IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

[10] Sigma-Aldrich, website: https://www.sigmaaldrich.com/

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.