

Safety data sheet Safety data sheet

acc. to Safe Work Australia - Code of Practice



Alliin ROTICHROM® HPLC

article number: **K031**
Version: **GHS 3.0 en**
Replaces version of: 2022-02-07
Version: (GHS 2)

date of compilation: 2020-09-01
Revision: 2024-03-01

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

1.1 Product identifier

Identification of the substance **Alliin ROTICHROM® HPLC**
Article number **K031**
CAS number **556-27-4**
Alternative name(s) **(S)-3-(Allylsulphinyl)-L-alanine**

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

Relevant identified uses: **Laboratory chemical
Laboratory and analytical use**
Uses advised against: **Do not use for private purposes (household).
Food, drink and animal feedingstuffs.**

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

Telephone:+49 (0) 721 - 56 06 0
Telefax: +49 (0) 721 - 56 06 149
e-mail: sicherheit@carlroth.de
Website: www.carlroth.de

Competent person responsible for the safety data sheet: **Department Health, Safety and Environment**

e-mail (competent person): **sicherheit@carlroth.de**

1.4 Emergency telephone number

| Name | Street | Postal code/city | Telephone | Website |
|--|-----------------|--------------------|-----------|---------|
| NSW Poisons Information Centre Childrens Hospital | Hawkesbury Road | 2145 Westmead, NSW | 131126 | |

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

| Section | Hazard class | Cat-egory | Hazard class and category | Hazard statement |
|---------|---|-----------|---------------------------|------------------|
| 3.2 | Skin corrosion/irritation | 2 | Skin Irrit. 2 | H315 |
| 3.3 | Serious eye damage/eye irritation | 2A | Eye Irrit. 2A | H319 |
| 3.8R | Specific target organ toxicity - single exposure (respiratory tract irritation) | 3 | STOT SE 3 | H335 |

For full text of abbreviations: see SECTION 16

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2.2 Label elements

Labelling

Signal word

Warning

Pictograms

GHS07



Hazard statements

| | |
|------|----------------------------------|
| H315 | Causes skin irritation |
| H319 | Causes serious eye irritation |
| H335 | May cause respiratory irritation |

Precautionary statements

Precautionary statements - prevention

| | |
|------|--|
| P261 | Avoid breathing dust/fume/gas/mist/vapours/spray |
| P280 | Wear protective gloves |

Precautionary statements - response

| | |
|----------------|---|
| P302+P352 | IF ON SKIN: Wash with plenty of soap and water |
| P305+P351+P338 | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing |
| P312 | Call a POISON CENTER or doctor/physician if you feel unwell |

Precautionary statements - storage

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

Precautionary statements - disposal

| | |
|------|--|
| P501 | Dispose of contents/container to industrial combustion plant |
|------|--|

2.3 Other hazards

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

SECTION 3: Composition/information on ingredients

3.1 Substances

| | |
|-------------------|-----------------------|
| Name of substance | Alliin |
| Molecular formula | $C_6H_{11}NO_3S$ |
| Molar mass | 177.2 g/mol |
| CAS No | 556-27-4 |

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SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In case of skin irritation, consult a physician.

Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Irritation, Cough, Dyspnoea

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!
water, foam, dry extinguishing powder, ABC-powder

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

In case of fire may be liberated: Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂), Sulphur oxides (SO_x)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Avoid contact with skin, eyes and clothes. Do not breathe dust.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically. Control of dust.

Other information relating to spills and releases

Place in appropriate containers for disposal.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation. Avoid dust formation.

Measures to prevent fire as well as aerosol and dust generation

Removal of dust deposits.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place. Keep in a cool place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Ventilation requirements

Use local and general ventilation.

Specific designs for storage rooms or vessels

Recommended storage temperature: 2 – 8 °C

7.3 Specific end use(s)

No information available.

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SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

| Country | Name of agent | CAS No | Identifier | TWA [mg/m ³] | STEL [mg/m ³] | Ceiling-C [mg/m ³] | Notation | Source |
|---------|----------------|--------|------------|--------------------------|---------------------------|--------------------------------|----------|--------|
| AU | nuisance dusts | | WES | 10 | | | i | WES |

Notation

Ceiling-C Ceiling value is a limit value above which exposure should not occur

i Inhalable fraction

STEL Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified)

TWA Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average (unless otherwise specified)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggles with side protection.

Skin protection



• hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 °C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

• type of material

NBR (Nitrile rubber)

• material thickness

>0,11 mm

• breakthrough times of the glove material

>480 minutes (permeation: level 6)

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• other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection



Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P2 (filters at least 94 % of airborne particles, colour code: White).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

| | |
|--|---|
| Physical state | solid |
| Form | powder |
| Colour | white |
| Odour | odourless |
| Melting point/freezing point | 164 – 166 °C |
| Boiling point or initial boiling point and boiling range | not determined |
| Flammability | this material is combustible, but will not ignite readily |
| Lower and upper explosion limit | not determined |
| Flash point | not applicable |
| Auto-ignition temperature | not determined |
| Decomposition temperature | not relevant |
| pH (value) | not applicable |
| Kinematic viscosity | not relevant |
| <u>Solubility(ies)</u> | |
| Water solubility | not determined |
| <u>Partition coefficient</u> | |
| Partition coefficient n-octanol/water (log value): | -4.2 |
| Vapour pressure | not determined |
| <u>Density and/or relative density</u> | |
| Density | not determined |

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| | |
|--------------------------------|--|
| Relative vapour density | Information on this property is not available. |
| Particle characteristics | No data available. |
| <u>Other safety parameters</u> | |
| Oxidising properties | none |

9.2 Other information

| | |
|---|---|
| Information with regard to physical hazard classes: | hazard classes acc. to GHS (physical hazards): not relevant |
| Other safety characteristics: | There is no additional information. |

SECTION 10: Stability and reactivity

10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser

10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Shall not be classified as acutely toxic.

Skin corrosion/irritation

Causes skin irritation.

Serious eye damage/eye irritation

Causes serious eye irritation.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

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Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

Data are not available.

• If in eyes

Causes serious eye irritation

• If inhaled

Irritation to respiratory tract, cough, Dyspnoea

• If on skin

causes skin irritation

• Other information

none

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 1.444 mg/mg
Theoretical Oxygen Demand (with nitrification): 1.806 mg/mg
Theoretical Carbon Dioxide: 1.49 mg/mg

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

| | |
|---------------------------|------|
| n-octanol/water (log KOW) | -4.2 |
|---------------------------|------|

12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

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12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

Relevant provisions relating to waste(Basel Convention)

Properties of waste which render it hazardous

H11 Toxic (Delayed or chronic)

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

SECTION 14: Transport information

- | | | |
|------|--|---|
| 14.1 | UN number | not subject to transport regulations |
| 14.2 | UN proper shipping name | not assigned |
| 14.3 | Transport hazard class(es) | not assigned |
| 14.4 | Packing group | not assigned |
| 14.5 | Environmental hazards | non-environmentally hazardous acc. to the dangerous goods regulations |
| 14.6 | Special precautions for user | There is no additional information. |
| 14.7 | Transport in bulk according to IMO instruments | The cargo is not intended to be carried in bulk. |
| 14.8 | Information for each of the UN Model Regulations | |
| | Transport informationNational regulationsAdditional information(UN RTDG) | Not subject to transport regulations. UN RTDG |
| | International Maritime Dangerous Goods Code (IMDG) - Additional information | Not subject to IMDG. |

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International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Not subject to ICAO-IATA.

SECTION 15: Regulatory information

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

There is no additional information.

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

| Country | Inventory | Status |
|---------|-----------|---------------------|
| EU | ECSI | substance is listed |
| TW | TCSI | substance is listed |

Legend

ECSI EC Substance Inventory (EINECS, ELINCS, NLP)
TCSI Taiwan Chemical Substance Inventory

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Indication of changes (revised safety data sheet)

| Section | Former entry (text/value) | Actual entry (text/value) | Safety-relevant |
|---------|---------------------------|---|-----------------|
| 2.3 | | Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$. | yes |

Abbreviations and acronyms

| Abbr. | Descriptions of used abbreviations |
|-----------|---|
| CAS | Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances) |
| Ceiling-C | Ceiling value |
| DGR | Dangerous Goods Regulations (see IATA/DGR) |
| ED | Endocrine disruptor |
| EINECS | European Inventory of Existing Commercial Chemical Substances |
| ELINCS | European List of Notified Chemical Substances |
| GHS | "Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations |
| IATA | International Air Transport Association |
| IATA/DGR | Dangerous Goods Regulations (DGR) for the air transport (IATA) |
| ICAO | International Civil Aviation Organization |

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| Abbr. | Descriptions of used abbreviations |
|---------|---|
| IMDG | International Maritime Dangerous Goods Code |
| NLP | No-Longer Polymer |
| PBT | Persistent, Bioaccumulative and Toxic |
| STEL | Short-term exposure limit |
| TWA | Time-weighted average |
| UN RTDG | UN Recommendations on the Transport of Dangerous Good |
| vPvB | Very Persistent and very Bioaccumulative |
| WES | Safe Work Australia: Workplace exposure standards for airborne contaminants |

Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

| Code | Text |
|------|-----------------------------------|
| H315 | Causes skin irritation. |
| H319 | Causes serious eye irritation. |
| H335 | May cause respiratory irritation. |

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.