

Printing date 14.09.2011 Version number 1 Revision: 14.09.2011

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

· Product identifier

· Trade name: Alliin ROTICHROM®, HPLC, (S)-3-(Allylsulphinyl)-L-alanine

· Article number: K031

• CAS Number: 556-27-4 • EC number:

209-118-9

 $\cdot \ Relevant \ identified \ uses \ of \ the \ substance \ or \ mixture \ and \ uses \ advised \ against$

· Application of the substance / the preparation Laboratory chemical

· Details of the supplier of the safety data sheet

· Manufacturer/Supplier:

Carl Roth GmbH + Co.KG Schoemperlenstraße 3-5

76185 Karlsruhe

Telefon: +49/(0)721 5606-0

Telefax: +49/(0)721 5606-149 e-mail: info@carlroth.de

· Further information obtainable from: Department Health, Safety and Environment

• Emergency telephone number: Poison Centre Munich Telefon +49/(0)89 19240

2 Hazards identification

- · Classification of the substance or mixture
- · Classification according to Regulation (EC) No 1272/2008 Void
- · Classification according to Directive 67/548/EEC or Directive 1999/45/EC Void
- · Label elements
- · Labelling according to Regulation (EC) No 1272/2008 Void
- · Hazard pictograms Void
- · Signal word Void
- · Hazard statements Void
- · Other hazards All chemicals are potentially dangerous. They should only be handled by specially trained personnel.
- · Results of PBT and vPvB assessment
- · **PBT:** Not applicable.
- · vPvB: Not applicable.

3 Composition/information on ingredients

· Chemical characterization: Substances

· CAS No. Description

556-27-4 (S)-3-(Allylsulphinyl)-L-alanine

· Identification number(s)

• **EC number:** 209-118-9

4 First aid measures

- · Description of first aid measures
- · After inhalation: Supply fresh air; consult doctor in case of complaints.
- · After skin contact:

Immediately rinse with water.

If skin irritation continues, consult a doctor.

- · After eye contact: Rinse opened eye for 10 minutes under running water. If symptoms persist, consult a doctor.
- · After swallowing:

Rinse out mouth and drink a glass of water. Do not induce vomiting.

If symptoms persist consult doctor.

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- · Information for doctor:
- · Most important symptoms and effects, both acute and delayed No further relevant information available.
- · Indication of any immediate medical attention and special treatment needed

No further relevant information available.

5 Firefighting measures

- · Extinguishing media
- · Suitable extinguishing agents: CO2, powder, foam or water spray.
- · Special hazards arising from the substance or mixture No further relevant information available.
- · Advice for firefighters
- · Protective equipment: No special measures required.

6 Accidental release measures

- · Personal precautions, protective equipment and emergency procedures Avoid formation of dust.
- Environmental precautions: Do not allow to enter sewers/ surface or ground water.
- · Methods and material for containment and cleaning up:

Pick up mechanically.

Dispose of the material collected according to regulations.

· Reference to other sections

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

7 Handling and storage

- · Handling:
- · Precautions for safe handling Handling corresponding to laboratory safety guidelines.
- · Information about fire and explosion protection: No special measures required.
- · Conditions for safe storage, including any incompatibilities
- · Storage:
- · Requirements to be met by storerooms and receptacles: No special requirements.
- · Information about storage in one common storage facility: Store away from foodstuffs.
- Further information about storage conditions: Store in cool, dry conditions in well sealed receptacles.
- · Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

- · Additional information about design of technical facilities: No further data; see item 7.
- · Control parameters
- · Ingredients with limit values that require monitoring at the workplace: Not required.
- · Additional information: The lists valid during the making were used as basis.
- $\cdot \ Exposure \ controls$
- · Personal protective equipment:
- · General protective and hygienic measures:

Do not eat, drink or smoke while working.

Wash hands before breaks and at the end of work.

Avoid contact with the eyes and skin.

· Respiratory protection: Not required.

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· Protection of hands:



Protective gloves

· Material of gloves

Nitrile, thickness: 0,4 mm

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

· Penetration time of glove material

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

· Eye protection:



Tightly sealed goggles

· **Body protection:** Protective work clothing

9 Physical and chemical properties

· Information on basic physical and chemical properties

· General Information

· Appearance:

Form: Solid
Colour: White

Odour: Odourless

Odour threshold: Not determined.

pH-value: Not applicable.

· Change in condition

Melting point/Melting range: 164-166°C (Lit.)
Boiling point/Boiling range: Undetermined.

• Flash point: Not applicable.

• Flammability (solid, gaseous): Product is not flammable.

 \cdot Ignition temperature:

Decomposition temperature: Not determined.
· **Self-igniting:** Not determined.

• **Danger of explosion:** Product does not present an explosion hazard.

· Explosion limits:

Lower: Not determined.
Upper: Not determined.

· Vapour pressure: Not applicable.

· Density: Not determined.

· Relative density Not determined.

· Vapour density Not applicable.

· Evaporation rate Not applicable.

 \cdot Solubility in / Miscibility with

water: Not determined.

· Segregation coefficient (n-octanol/water): Not determined.

· Viscosity:

Dynamic: Not applicable.

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Kinematic: Not applicable.

Other information No further relevant information available.

10 Stability and reactivity

- · Reactivity
- · Chemical stability
- · Thermal decomposition / conditions to be avoided: No decomposition if used and stored according to specifications.
- · Possibility of hazardous reactions No information available.
- · Conditions to avoid No further relevant information available.
- · **Incompatible materials:** Strong oxidizing agents.
- · Hazardous decomposition products: No information available.

11 Toxicological information

- · Information on toxicological effects
- · Acute toxicity:
- LD/LC50 values relevant for classification:

Oral LD50 4200 mg/kg (rat)

- · Primary irritant effect:
- · on the skin: Slight irritations.
- · on the eye: Slight irritations
- · after inhalation: Slight irritations.
- · Sensitization: No sensitizing effects known.
- · Additional toxicological information:

When used and handled according to specifications, the product does not have any harmful effects to our experience and the information provided to us.

The substance is not subject to classification according to the latest version of the EU lists.

• Further information: The product should be handled with the care usual when dealing with chemicals.

12 Ecological information

- · Toxicity
- · Acquatic toxicity: Quantitative data on the ecological effect of this product are not available.
- · Persistence and degradability No further relevant information available.
- · Behaviour in environmental systems:
- · Bioaccumulative potential No further relevant information available.
- · Mobility in soil No further relevant information available.
- · Ecotoxical effects:
- · **Remark:** Do not allow to enter waters, waste water, or soil!
- · Results of PBT and vPvB assessment
- · **PBT:** Not applicable.
- · vPvB: Not applicable.
- · Other adverse effects No further relevant information available.

13 Disposal considerations

- · Waste treatment methods
- · Recommendation

The disposal is regionally differently regulated, therefore the kind of disposal is to be inquired at the responsible authorities.

- · Uncleaned packaging:
- · Recommendation: Disposal according to official regulations.

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14 Transport information

· UN-Number

· ADR, ADN, IMDG, IATA Void

· UN proper shipping name

· ADR, ADN, IMDG, IATA Void

· Transport hazard class(es)

· ADR, ADN, IMDG, IATA

· Class Void

· Packing group

· ADR, IMDG, IATA Void

· Environmental hazards:

· Marine pollutant: No

· Special precautions for user Not applicable.

· Transport in bulk according to Annex II of

MARPOL73/78 and the IBC Code Not applicable.

· Transport/Additional information:

 $\cdot \, ADR$

• **Remarks:** Not subject to transport regulations.

· UN "Model Regulation":

15 Regulatory information

- · Safety, health and environmental regulations/legislation specific for the substance or mixture
- · National regulations:
- · Waterhazard class: Not subject to classification.
- · Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

- · Department issuing MSDS: Department: Health, Safety and Environment
- · Contact: Herr Dr. Hagel
- · Abbreviations and acronyms:

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

ICAO: International Civil Aviation Organization

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

* * Data compared to the previous version altered.

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