Chemical Safety Data Sheet MSDS / SDS

3-(allylsulphinyl)-L-alanine

Revision Date:2025-05-03 Revision Number:1

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

Product identifier

Product name	: 3-(allylsulphinyl)-L-alanine
CBnumber	: CB8892362
CAS	: 17795-26-5
EINECS Number	: 241-773-6
Synonyms	: L-(±)-Alliin,(±)-L-Alliin
Relevant identified uses of the s	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

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SECTION 2: Hazards identification

Classification of the substance or mixture

no data available

Telephone

Label elements

Pictogram(s)

Signal word

Warning

: 010-86108875

Hazard statement(s)

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

Precautionary statement(s)

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

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

Continuerinsing.

no data available

Response

no data available

Storage

no data available

Disposal

no data available

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: 3-(allylsulphinyl)-L-alanine
Synonyms	: L-(±)-Alliin,(±)-L-Alliin
CAS	: 17795-26-5
EC number	: 241-773-6
MF	: C6H11NO3S
MW	: 177.22

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms and effects, both acute and delayed

no data available

Indication of any immediate medical attention and special treatment needed

no data available

SECTION 5: Firefighting measures

Extinguishing media

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

Specific Hazards Arising from the Chemical

no data available

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

NFPA 704



HEALTH	2	Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. <u>diethyl</u> <u>ether</u> , ammonium phosphate, iodine)
FIRE	0	Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, 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. HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use sparkproof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the riskelimination area.

Individual protection measures

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The

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

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	no data available
Colour	no data available
Odour	no data available
Melting point/freezing point	163 °C

Boiling point or initial boiling point and 416.132°C at 760 mmHg

boiling range

Flammability	no data available
Lower and upper explosion	no data available
limit/flammability limit	
Flash point	205.469°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	no data available
Partition coefficient n-octanol/water	no data available
Vapour pressure	0mmHg at 25°C
Density and/or relative density	1.354g/cm3
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available Toxicity to daphnia and other aquatic invertebrates: no data available Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

Other adverse effects

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: no data available IMDG: no data available IATA: no data available

UN Proper Shipping Name

ADR/RID: no data available IMDG: no data available IATA: no data available

Transport hazard class(es)

ADR/RID: no data available

IMDG: no data available

IATA: no data available

Packing group, if applicable

ADR/RID: no data available

IMDG: no data available

IATA: no data available

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed. **EC Inventory** Listed. United States Toxic Substances Control Act (TSCA) Inventory Not Listed. China Catalog of Hazardous chemicals 2015 Not Listed. New Zealand Inventory of Chemicals (NZIoC) Not Listed. PICCS Not Listed. **Vietnam National Chemical Inventory** Listed. IECSC Not Listed. Korea Existing Chemicals List (KECL) Not Listed.

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

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

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

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

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index? pageID=0&request_locale=en

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

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

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

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

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

Disclaimer:

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