

Chemical Safety Data Sheet MSDS / SDS

3-sulfanylidene-2,4,9-triazabicyclo[4.3.0]nona-7,10-dien-5-oneRevision Date:2026-05-31 Revision Number:1

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

Product name : 3-sulfanylidene-2,4,9-triazabicyclo[4.3.0]nona-7,10-dien-5-one
CBnumber : CB81257674
CAS : 67831-84-9
Synonyms : 2-thioxo-2,3-dihydro-1H-pyrrolo[2,3-d]pyrimidin-4(7H)-one,3-sulfanylidene-2,4,9-triazabicyclo[4.3.0]nona-7,10-dien-5-one

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**

Symbol(GHS)



Signal word

Warning

Precautionary statements

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

Continuerinsing.

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

Hazard statements

H302 Harmful if swallowed

SECTION 3: Composition/information on ingredients**Substance**

Product name	: 3-sulfanylidene-2,4,9-triazabicyclo[4.3.0]nona-7,10-dien-5-one
Synonyms	: 2-thioxo-2,3-dihydro-1H-pyrrolo[2,3-d]pyrimidin-4(7H)-one,3-sulfanylidene-2,4,9-triazabicyclo[4.3.0]nona-7,10-dien-5-one
CAS	: 67831-84-9
MF	: C6H5N3OS
MW	: 167.19

SECTION 4: First aid measures

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

If swallowed

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

Protection of first-aiders

For personal protection see section 8.

Notes to physician

No data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting

Combustible. Development of hazardous combustion gases or vapours possible in the event of fire.

Specific extinguishing methods

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters

In the event of fire, wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7: Handling and storage

Handling

Avoidance of contact

Strong oxidizing agents

Storage

Further information on storage conditions

Tightly closed. Dry.

Storage class

11, Combustible Solids

Recommended storage temperature

Recommended storage temperature see product label.

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures

No data available

Personal protective equipment

Respiratory protection

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type

Filter type P1

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Eye/face protection

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

Safety glasses

Hand protection

Material

Nitrile rubber

Break through time

480 min

Glove thickness

0.11 mm

Protective index

Full contact

Manufacturer

KCL 741 L

Material

Nitrile rubber

Break through time

480 min

Glove thickness

0.11 mm

Protective index

Splash contact

Manufacturer

KCL 741 L

Remarks

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D- 36124 Eichenzell, Internet: www.kcl.de).

Hygiene measures

Change contaminated clothing. Wash hands after working with substance.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

solid

Color

White to Off-White

Odor

No data available

Odor Threshold

No data available

pH

No data available

Melting point/ range

No data available

Boiling point/boiling range

No data available

Flash point

Not applicable

Evaporation rate

No data available

Flammability (solid, gas)

No data available

Flammability (liquids)

No data available

Burning rate

No data available

Upper explosion limit / Upper flammability limit

No data available

Lower explosion limit / Lower flammability limit

No data available

Vapor pressure

No data available

Relative vapor density

No data available

Relative density

1.65±0.1 g/cm³(Predicted)

Density

1.65±0.1 g/cm³(Predicted)

Water solubility

No data available

Partition coefficient: n-octanol/water

No data available

Autoignition temperature

No data available

Decomposition temperature

No data available

Viscosity, dynamic

No data available

Viscosity, kinematic

No data available

Flow time

No data available

Explosive properties

No data available

Oxidizing properties

none

Molecular weight

167.19 g/mol

Particle characteristics Particle size

No data available

Solubility

Aqueous Base (Slightly)i, DMSO (Slightly)

Physical state

Solid

SECTION 10: Stability and reactivity

Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

No data available

Conditions to avoid

no information available

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Classified based on available data. For more details, see section 2

Serious eye damage/eye irritation

Classified based on available data. For more details, see section 2

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

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

SECTION 12: Ecological information

Ecotoxicity

No data available

Persistence and degradability

No data available

Bioaccumulative potential

No data available

Mobility in soil

No data available

Other adverse effects

No data available

SECTION 13: Disposal considerations

Disposal methods

Waste from residues

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

SECTION 14: Transport information

International Regulations

IATA-DGR

UN/ID No. : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

Packing instruction (cargo aircraft) : Not applicable

Packing instruction (passenger aircraft) : Not applicable

IMDG-Code

UN number : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

EmS Code : Not applicable

Marine pollutant : no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National regulation GB 6944/12268

UN number : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

National regulatory information

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals

Hazardous Chemicals for Priority Management

under SAWS

Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals

China Severely Restricted Toxic Chemicals for Import and Export

SECTION 16: Other information

Full text of other abbreviations

AIIIC - Australian Inventory of Industrial Chemicals

ANTT - National Agency for Transport by Land of Brazil
 ASTM - American Society for the Testing of Materials
 bw - Body weight
 CMR - Carcinogen, Mutagen or Reproductive Toxicant
 DIN - Standard of the German Institute for Standardisation
 DSL - Domestic Substances List (Canada)
 EC_x - Concentration associated with x% response
 EL_x - Loading rate associated with x% response
 EmS - Emergency Schedule
 ENCS - Existing and New Chemical Substances (Japan)
 ErC_x - Concentration associated with x% growth rate response
 ERG - Emergency Response Guide
 GHS - Globally Harmonized System
 GLP - Good Laboratory Practice
 IARC - International Agency for Research on Cancer
 IATA - International Air Transport Association
 IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk
 IC₅₀ - Half maximal inhibitory concentration
 ICAO - International Civil Aviation Organization
 IECSC - Inventory of Existing Chemical Substances in China
 IMDG - International Maritime Dangerous Goods
 IMO - International Maritime Organization
 ISHL - Industrial Safety and Health Law (Japan)
 ISO - International Organisation for Standardization
 KECI - Korea Existing Chemicals Inventory
 LC₅₀ - Lethal Concentration to 50 % of a test population
 LD₅₀ - Lethal Dose to 50% of a test population (Median Lethal Dose)
 MARPOL - International Convention for the Prevention of Pollution from Ships
 n.o.s. - Not Otherwise Specified
 Nch - Chilean Norm
 NO(A)EC - No Observed (Adverse) Effect Concentration
 NO(A)EL - No Observed (Adverse) Effect Level
 NOELR - No Observable Effect Loading Rate
 NOM - Official Mexican Norm
 NTP - National Toxicology Program
 NZIoC - New Zealand Inventory of Chemicals
 OECD - Organization for Economic Co-operation and Development
 OPPTS - Office of Chemical Safety and Pollution Prevention
 PBT - Persistent, Bioaccumulative and Toxic substance
 PICCS - Philippines Inventory of Chemicals and Chemical Substances
 (Q)SAR - (Quantitative) Structure Activity Relationship
 REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals

SADT - Self-Accelerating Decomposition Temperature

SDS - Safety Data Sheet

TCSI - TaiwanChemical Substance Inventory

TDG - Transportation of Dangerous Goods

TECI -Thailand Existing Chemicals Inventory

TSCA - Toxic Substances Control Act (UnitedStates)

UN - United Nations

UNRTDG - United Nations Recommendations on theTransport of Dangerous Goods

vPvB - Very Persistent and Very Bioaccumulative

WHMIS - Workplace Hazardous Materials Information System

Disclaimer:

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.