Safety Data Sheet
acc. to OSHA HCS

Date of issue: 06/19/2025 Revision date 06/19/2025

*
1 Identification

· **Product identifier**

· **Trade name: Necrostatin-5**
· **Synonym**
2-[[3,4,5,6,7,8-hexahydro-3-(4-methoxyphenyl)-4-oxo[1]benzothieno[2,3-d]pyrimidin-2-yl]thio]-acetonitrile
Nec-5
· **CAS Number:**
337349-54-9
· **Other means of identification**

· **Article number:** 10527
· **Application of the substance / the mixture**
This product is for research use - Not for human or veterinary diagnostic or therapeutic use.

· **Details of the supplier of the safety data sheet**
· **Manufacturer/Supplier:**
Cayman Chemical Co.
1180 E. Ellsworth Rd.
Ann Arbor, MI 48108
USA

· **Information department:** Product safety department
· **Emergency telephone number:**
During normal opening times: +1 (734) 971-3335
US/CANADA: 800-424-9300
Outside US/CANADA: 703-741-5970

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2 Hazard(s) identification

· **Classification of the substance or mixture**

GHS07

Eye irritation 2A H319 Causes serious eye irritation.

Aquatic Chronic 4 H413 May cause long lasting harmful effects to aquatic life.

· **Label elements**
· **GHS label elements**
The substance is classified and labeled according to the Globally Harmonized System (GHS).

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· **Hazard pictograms**

GHS07

· **Signal word** Warning
· **Hazard statements**
H319 Causes serious eye irritation.
H413 May cause long lasting harmful effects to aquatic life.
· **Precautionary statements**

P264	Wash thoroughly after handling.
P273	Avoid release to the environment.
P280	Wear eye protection / face protection.
P305+P351+P338	If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337+P313	If eye irritation persists: Get medical advice/attention.
P501	Dispose of contents/container in accordance with local/regional/national/international regulations.

· **Information pertaining to particular dangers for man and environment:**
· **Classification system:**
· **NFPA ratings (scale 0 - 4)**

Health = 2
Fire = 0
Reactivity = 0

· **HMIS-ratings (scale 0 - 4)**

Health = 2
Fire = 0
Reactivity = 0

· **Other hazards**
· **Results of PBT and vPvB assessment**
· **PBT:** Not applicable.
· **vPvB:** Not applicable.
· **Classification according to (d)(1)(ii) of § 1910.1200**
The SDS issuer does not object to the classifications provided by importers or manufacturers of precursor products.
· **Hazards not otherwise classified**
There are no adverse physical or health effects known that are not covered by the hazard classes of the Hazard Communications Standard.

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3 Composition/information on ingredients

· **Chemical characterization: Substances**
· **CAS No. Description**
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4 First-aid measures

· **Description of first aid measures**
· **After inhalation:** Supply fresh air; consult doctor in case of complaints.
· **After skin contact:** Generally the product does not irritate the skin.
· **After eye contact:**
Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.
· **After swallowing:** If symptoms persist consult 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 Fire-fighting measures

· **Extinguishing media**
· **Suitable extinguishing agents:**
Use fire fighting measures that suit the environment.
A solid water stream may be inefficient.
· **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** Not required.
· **Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
· **Methods and material for containment and cleaning up:** Pick up mechanically.
· **Protective Action Criteria for Chemicals**
· **PAC-1:** Substance is not listed.
· **PAC-2:** Substance is not listed.
· **PAC-3:** Substance is not listed.
· **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

· **Precautions for safe handling**
No special precautions are necessary if used correctly.
Avoid breathing dust/fume/gas/mist/vapours/spray.
Avoid prolonged or repeated exposure.
Keep away from sources of ignition.
Take precautionary measures against static discharge.re.
· **Information about protection against explosions and fires:** No special measures required.

· **Conditions for safe storage, including any incompatibilities**
· **Storage:** Store in accordance with information listed on the product insert.
· **Requirements to be met by storerooms and receptacles:** No special requirements.
· **Information about storage in one common storage facility:** Not required.

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· **Further information about storage conditions:** Keep receptacle tightly sealed.
· **Specific end use(s)** No further relevant information available.

8 Exposure controls/personal protection

· **Control parameters**
· **Components with limit values that require monitoring at the workplace:** Not required.
· **Additional information:** The lists that were valid during the creation were used as basis.

· **Exposure controls**
· **Appropriate engineering controls** No further data; see section 7.
· **Personal protective equipment:**
· **General protective and hygienic measures:**
Keep away from foodstuffs, beverages and feed.
Immediately remove all soiled and contaminated clothing.
Wash hands before breaks and at the end of work.
Avoid contact with the eyes.
Avoid contact with the eyes and skin.
· **Breathing equipment:** Not required.
· **Protection of hands:**
The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.
Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.
Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation
· **Material of gloves**
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

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9 Physical and chemical properties

· **Information on basic physical and chemical properties**
· **General Information**

· **Physical state**	Solid
· **Color:**	Not determined.
· **Odor:**	Characteristic
· **Structural Formula**	C19H17N3O2S2
· **Molecular Weight**	383.5 g/mol
· **Storage Buffer**	
· **Odor threshold:**	Not determined.
· **Formulation**	
· **Melting point/Melting range:**	Undetermined.
· **Boiling point/Boiling range:**	Undetermined.

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· **Flammability:**	Product is not flammable.
· **Explosion limits:**	
· **Lower:**	Not determined.
· **Upper:**	Not determined.
· **Flash point:**	Not applicable.
· **Decomposition temperature:**	Not determined.
· **pH-value:**	Not applicable.
· **Viscosity:**	
· **Kinematic:**	Not applicable.
· **SOLUBILITY**	Chloroform: 10 mg/ml; DMF: Slightly Soluble; DMSO: Slightly Soluble
· **Dynamic:**	Not applicable.
· **Solubility in / Miscibility with**	
· **Water:**	Not determined.
· **Partition coefficient (n-octanol/water):**	Not determined.
· **Vapor pressure:**	Not applicable.
· **Vapor pressure:**	
· **Density:**	Not determined.
· **Relative density**	Not determined.
· **Vapor density**	Not applicable.
· **Particle characteristics**	Not determined.

· **Other information**	
· **Appearance:**	
· **Form:**	Solid
· **Important information on protection of health and environment, and on safety.**	
· **Ignition temperature:**	Not determined.
· **Danger of explosion:**	Product does not present an explosion hazard.
· **Change in condition**	
· **Evaporation rate**	Not applicable.

10 Stability and reactivity

· **Reactivity** No further relevant information available.
· **Chemical stability**
· **Thermal decomposition / conditions to be avoided:**
No decomposition if used according to specifications.
· **Possibility of hazardous reactions** No dangerous reactions known.
· **Conditions to avoid** No further relevant information available.
· **Incompatible materials:** strong oxidizing agents
· **Hazardous decomposition products:**
carbon dioxide, carbon monoxide, hydrogen cyanide,nitrogen oxides,sulfur oxides

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11 Toxicological information

· **Information on toxicological effects**
· **Acute toxicity:**
· **Primary irritant effect:**
· **on the skin:** No irritant effect.
· **on the eye:** Irritating effect.

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· **Sensitization:** No sensitizing effects known.
· **Additional toxicological information:**
· **Interactive effects** No interactive effects between components are known.

· **Carcinogenic categories**
· **IARC (International Agency for Research on Cancer)** Substance is not listed.
· **NTP (National Toxicology Program)** Substance is not listed.
· **OSHA-Ca (Occupational Safety & Health Administration)** Substance is not listed.
· **Alternative sources for toxicological information**
No non-standard sources for toxicological information where used.

12 Ecological information

· **Toxicity**
· **Aquatic toxicity:** No further relevant information available.
· **Persistence and degradability** No further relevant information available.
· **Bioaccumulative potential** No further relevant information available.
· **Mobility in soil** No further relevant information available.
· **Results of PBT and vPvB assessment**
· **PBT:** Not applicable.
· **vPvB:** Not applicable.
· **Other adverse effects**
· **Additional ecological information:**
· **General notes:**
Water hazard class 1 (Self-assessment): slightly hazardous for water
Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

13 Disposal considerations

· **Waste treatment methods**
· **Recommendation:**
Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

· **Uncleaned packagings:**
· **Recommendation:** Disposal must be made according to official regulations.

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14 Transport information

· **UN-Number**	
· **DOT, IMDG, IATA**	not regulated
· **UN proper shipping name**	
· **DOT, IMDG, IATA**	not regulated
· **Transport hazard class(es)**	
· **DOT, ADN, IMDG, IATA**	
· **Class**	not regulated

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· **Packing group** · **DOT, IMDG, IATA**	not regulated
· **Environmental hazards:**	Not applicable.
· **Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code**	Not applicable.
· **Special precautions for user**	Not applicable.
· **UN "Model Regulation":**	not regulated

15 Regulatory information

· **Safety, health and environmental regulations/legislation specific for the substance or mixture**
No further relevant information available.
· **Sara**
· **Section 355 (extremely hazardous substances):** Substance is not listed.
· **Section 313 (Specific toxic chemical listings):** Substance is not listed.
· **TSCA (Toxic Substances Control Act):** Substance is not listed.
· **Hazardous Air Pollutants** Substance is not listed.
· **Chemicals known to cause cancer:** Substance is not listed.
· **Chemicals known to cause reproductive toxicity for females:** Substance is not listed.
· **Chemicals known to cause reproductive toxicity for males:** Substance is not listed.
· **Chemicals known to cause developmental toxicity:** Substance is not listed.

· **Carcinogenic categories**
· **EPA (Environmental Protection Agency)** Substance is not listed.
· **TLV (Threshold Limit Value)** Substance is not listed.
· **NIOSH-Ca (National Institute for Occupational Safety and Health)** Substance is not listed.
· **Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

16 Other information

All chemicals may pose unknown hazards and should be used with caution. This SDS applies only to the material as packaged. If this product is combined with other materials, deteriorates, or becomes contaminated, it may pose hazards not mentioned in this SDS. Cayman Chemical Company assumes no responsibility for incidental or consequential damages, including lost profits, arising from the use of these data. It shall be the user's responsibility to develop proper methods of handling and personal protection based on the actual conditions of use. While this SDS is based on technical data judged to be reliable, Cayman Chemical Company assumes no responsibility for the completeness or accuracy of the information contained herein.

· **Department issuing SDS:** Environment protection department.
· **Contact:** -
· **Date of previous version** 08/16/2024
· **Date of preparation** 06/19/2025
· **Abbreviations and acronyms:**
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
CAS: Chemical Abstracts Service (division of the American Chemical Society)
NFPA: National Fire Protection Association (USA)
HMIS: Hazardous Materials Identification System (USA)
PBT: Persistent, Bioaccumulative and Toxic
vPvB: very Persistent and very Bioaccumulative

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NIOSH: National Institute for Occupational Safety
OSHA: Occupational Safety & Health
TLV: Threshold Limit Value
PEL: Permissible Exposure Limit
REL: Recommended Exposure Limit
Eye irritation 2A: Serious eye damage/eye irritation – Category 2A
Aquatic Chronic 4: Hazardous to the aquatic environment - long-term aquatic hazard – Category 4
· *** Data compared to the previous version altered.**