

SAFETY DATA SHEET

Revision Date 21-Feb-2020

Revision Number 2

1. Identification

Product Name 3-Allyl-2-mercapto-3,5,6,7-tetrahydro-4H-cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one

Cat No. : H33943

CAS-No 113520-01-7
Synonyms No information available

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Emergency Telephone Number

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660.
After normal business hours, call Carechem 24 at (866) 928-0789.

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

Label Elements

Signal Word

Warning

Hazard Statements

Causes skin irritation
Causes serious eye irritation
May cause respiratory irritation



Precautionary Statements

Prevention

Wash face, hands and any exposed skin thoroughly after handling
Wear protective gloves/protective clothing/eye protection/face protection
Avoid breathing dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Call a POISON CENTER or doctor/physician if you feel unwell

Skin

IF ON SKIN: Wash with plenty of soap and water
If skin irritation occurs: Get medical advice/attention
Take off contaminated clothing and wash before reuse

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
If eye irritation persists: Get medical advice/attention

Storage

Store in a well-ventilated place. Keep container tightly closed
Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

3. Composition/Information on Ingredients

Component	CAS-No	Weight %
3-Allyl-2-mercapto-3,5,6,7-tetrahydro-4H-cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one	113520-01-7	<=100

4. First-aid measures

General Advice	If symptoms persist, call a physician.
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Ingestion	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
Most important symptoms and effects	None reasonably foreseeable.

Notes to Physician Treat symptomatically

5. Fire-fighting measures

Unsuitable Extinguishing Media No information available

Flash Point No information available
Method - No information available

Autoignition Temperature No information available

Explosion Limits

Upper No data available

Lower No data available

Sensitivity to Mechanical Impact No information available

Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

None known.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health
2

Flammability
1

Instability
0

Physical hazards
-

6. Accidental release measures

Personal Precautions Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

Environmental Precautions Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

7. Handling and storage

Handling Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

Storage Keep containers tightly closed in a dry, cool and well-ventilated place.

8. Exposure controls / personal protection

Exposure Guidelines This product does not contain any hazardous materials with occupational exposure limit established by the region specific regulatory bodies.

Engineering Measures Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard

EN166.

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Solid Crystalline
Appearance	Light grey
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	210 - 211 °C / 410 - 411.8 °F
Boiling Point/Range	No information available
Flash Point	No information available
Evaporation Rate	Not applicable
Flammability (solid,gas)	No information available
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	Not applicable
Specific Gravity	No information available
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	Not applicable
Molecular Formula	C12 H12 N2 OS2
Molecular Weight	264.37

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Incompatible products.
Incompatible Materials	Strong oxidizing agents
Hazardous Decomposition Products	None under normal use conditions
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity**Product Information****Component Information****Toxicologically Synergistic Products**

No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
3-Allyl-2-mercapto-3,5,6,7-tetrahydro-4H-cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one	113520-01-7	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Respiratory system

STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects, both acute and delayed No information available

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability No information available

Bioaccumulation/ Accumulation No information available.

Mobility No information available.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT Not regulated

TDG Not regulated

IATA Not regulated

IMDG/IMO Not regulated

15. Regulatory information

United States of America Inventory

Component	CAS-No	TSCA	TSCA Inventory notification - Active/Inactive	TSCA - EPA Regulatory Flags
3-Allyl-2-mercapto-3,5,6,7-tetrahydro-4H-cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one	113520-01-7	-	-	-

Legend:

TSCA - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Australia (AICS), China (IECSC), Korea (ECL).

Component	CAS-No	DSL	NDSL	EINECS	PICCS	ENCS	AICS	IECSC	KECL
3-Allyl-2-mercapto-3,5,6,7-tetrahydro-4H-cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one	113520-01-7	-	-	-	-	-	-	-	-

U.S. Federal Regulations

SARA 313 Not applicable

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA Not applicable

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ): N

DOT Marine Pollutant N

DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

16. Other information

Prepared By Health, Safety and Environmental Department
Email: tech@alfa.com
www.alfa.com

Revision Date	21-Feb-2020
Print Date	21-Feb-2020
Revision Summary	SDS authoring systems update, replaces ChemGes SDS No. 113520-01-7.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS