Safety Data Sheet
acc. to OSHA HCS

Date of issue: 03/13/2025 Revision date 03/13/2025

*
1 Identification

· **Product identifier**

· **Trade name: Allicin**
· **Synonym** 2-propene-1-sulfinothioic acid, S-2-propen-1-yl ester
· **Other means of identification**

· **Article number:** 15570
· **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**


GHS02 Flame

Flammable liquids 2	H225 Highly flammable liquid and vapor.


GHS06 Skull and crossbones

Acute toxicity - oral 3	H301 Toxic if swallowed.
Acute toxicity - dermal 3	H311 Toxic in contact with skin.
Acute toxicity - inhalation 3	H331 Toxic if inhaled.


GHS08 Health hazard

Specific target organ toxicity (single exposure) 1	H370 Causes damage to the central nervous system and the visual organs.

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

GHS02 GHS06 GHS08

· **Signal word** Danger

· **Hazard-determining components of labeling:**
Methanol
· **Hazard statements**

H225	Highly flammable liquid and vapor.
H301+H311+H331	Toxic if swallowed, in contact with skin or if inhaled.
H370	Causes damage to the central nervous system and the visual organs.

· **Precautionary statements**

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P240	Ground / bond container and receiving equipment.
P241	Use explosion-proof [electrical/ventilating/lighting] equipment.
P242	Use non-sparking tools.
P243	Take action to prevent static discharge.
P260	Do not breathe dust/fume/gas/mist/vapors/spray.
P264	Wash thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
P301+P310	If swallowed: Immediately call a poison center/doctor.
P321	Specific treatment (see on this label).
P330	Rinse mouth.
P303+P361+P353	If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower].
P304+P340	If inhaled: Remove person to fresh air and keep comfortable for breathing.
P308+P311	IF exposed or concerned: Call a poison center/doctor.
P312	Call a poison center/doctor if you feel unwell.
P361+P364	Take off immediately all contaminated clothing and wash it before reuse.
P370+P378	In case of fire: Use CO2, powder or water spray to extinguish.
P403+P233	Store in a well-ventilated place. Keep container tightly closed.
P403+P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
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 = 3
Reactivity = 0

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· **HMIS-ratings (scale 0 - 4)**

HEALTH *2	Health = *2
FIRE 3	Fire = 3
REACTIVITY 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.

3 Composition/information on ingredients

· **Chemical characterization: Mixtures**
· **Description:** Mixture of the substances listed below with nonhazardous additions.

· **Dangerous components:**		
CAS: 67-56-1 RTECS: PC1400000	Methanol	59.45%
CAS: 539-86-6 RTECS: UD1900000	S-Allyl acrylo-1-sulphinothioate	1.0%

· **Other ingredients**		
CAS: 7732-18-5 RTECS: ZC0110000	Water	39.45%
CAS: 64-18-6 RTECS: LQ4900000	Formic acid	0.1%

4 First-aid measures

· **Description of first aid measures**
· **General information:**
Immediately remove any clothing soiled by the product.
Remove breathing apparatus only after contaminated clothing have been completely removed.
In case of irregular breathing or respiratory arrest provide artificial respiration.
· **After inhalation:**
Supply fresh air or oxygen; call for doctor.
In case of unconsciousness place patient stably in side position for transportation.
· **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
· **After eye contact:** Rinse opened eye for several minutes under running water. Then consult a doctor.
· **After swallowing:** Do not induce vomiting; immediately call for medical help.
· **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.

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5 Fire-fighting measures

· **Extinguishing media**
· **Suitable extinguishing agents:**
CO2, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
· **Special hazards arising from the substance or mixture**
67-56-1During heating or in case of fire poisonous gases are produced.
· **Advice for firefighters**
· **Protective equipment:** Mouth respiratory protective device.

6 Accidental release measures

· **Personal precautions, protective equipment and emergency procedures**
Mount respiratory protective device.
Wear protective equipment. Keep unprotected persons away.
· **Environmental precautions:**
Dilute with plenty of water.
Do not allow to enter sewers/ surface or ground water.
· **Methods and material for containment and cleaning up:**
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Dispose contaminated material as waste according to section 13.
Ensure adequate ventilation.
· **Protective Action Criteria for Chemicals**

· **PAC-1:**		
67-56-1	Methanol	530 ppm
64-18-6	Formic acid	3 ppm

· **PAC-2:**		
67-56-1	Methanol	2,100 ppm
64-18-6	Formic acid	25 ppm

· **PAC-3:**		
67-56-1	Methanol	7200* ppm
64-18-6	Formic acid	250 ppm

· **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**
Ensure good ventilation/exhaustion at the workplace.
Open and handle receptacle with care.
Prevent formation of aerosols.
· **Information about protection against explosions and fires:**
Keep ignition sources away - Do not smoke.
Protect against electrostatic charges.
Keep respiratory protective device available.

· **Conditions for safe storage, including any incompatibilities**
· **Storage:** Store in accordance with information listed on the product insert.

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· **Requirements to be met by storerooms and receptacles:** Store in a cool location.
· **Information about storage in one common storage facility:** Not required.
· **Further information about storage conditions:**
Keep receptacle tightly sealed.
Store in cool, dry conditions in well sealed receptacles.
· **Specific end use(s)** No further relevant information available.

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8 Exposure controls/personal protection

· **Control parameters**
· **Components with limit values that require monitoring at the workplace:**
The following constituent is the only constituent of the product which has a PEL, TLV or other recommended exposure limit.
At this time, the remaining constituent has no known exposure limits.

67-56-1 Methanol	
PEL	Long-term value: 260 mg/m³, 200 ppm
REL	Short-term value: 325 mg/m³, 250 ppm Long-term value: 260 mg/m³, 200 ppm Skin
TLV	Short-term value: 328 mg/m³, 250 ppm Long-term value: 262 mg/m³, 200 ppm Skin; BEI

· **Ingredients with biological limit values:**

67-56-1 Methanol	
BEI	15 mg/L Medium: urine Time: end of shift Parameter: Methanol (background, nonspecific)

· **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.
Store protective clothing separately.
Avoid contact with the eyes and skin.
· **Breathing equipment:**
In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.
· **Protection of hands:**

Protective gloves

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

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· **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. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.
· **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**	Liquid
· **Color:**	According to product specification
· **Odor:**	Characteristic
· **Structural Formula**	C6H10OS2
· **Molecular Weight**	162.3 g/mol
· **Storage Buffer**	
· **Odor threshold:**	Not determined.
· **Formulation**	A solution in methanol:water:formic acid
· **Melting point/Melting range:**	Undetermined.
· **Boiling point/Boiling range:**	64.7 °C (148.5 °F)
· **Flammability:**	Highly flammable.
· **Explosion limits:**	
· **Lower:**	5.5 Vol %
· **Upper:**	44 Vol %
· **Flash point:**	11 °C (51.8 °F)
· **Decomposition temperature:**	Not determined.
· **pH-value:**	Not determined.
· **Viscosity:**	
· **Kinematic:**	Not determined.
· **SOLUBILITY**	DMF: 10 mg/ml; DMF:PBS (pH 7.2) (1:4): 0.2 mg/ml; DMSO: 5 mg/ml; Ethanol: 3 mg/ml
· **Dynamic:**	Not determined.
· **Solubility in / Miscibility with**	
· **Water:**	Fully miscible.
· **Partition coefficient (n-octanol/water):**	Not determined.
· **Vapor pressure at 20 °C (68 °F):**	128 hPa (96 mm Hg)
· **Vapor pressure:**	
· **Density at 20 °C (68 °F):**	0.87409 g/cm³ (7.29428 lbs/gal)
· **Relative density**	Not determined.
· **Bulk density:**	874 kg/m³
· **Vapor density**	Not determined.
· **Particle characteristics**	Not applicable.

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· **Other information**	
· **Appearance:**	
· **Form:**	Liquid
· **Important information on protection of health and environment, and on safety.**	
· **Ignition temperature:**	Product is not selfigniting.
· **Danger of explosion:**	Product is not explosive. However, formation of explosive air/vapor mixtures are possible.
· **Solvent content:**	
· **Organic solvents:**	59.5 %
· **Water:**	39.5 %
· **VOC content:**	59.45 % 519.6 g/l / 4.34 lb/gal
· **Solids content:**	0.0 %
· **Change in condition**	
· **Evaporation rate**	Not determined.

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:** reducing agents, oxidizing agents, acid chlorides, acid anhydrides, acids
· **Hazardous decomposition products:** hydrogen sulfide, carbon monoxide, carbon dioxide

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11 Toxicological information

· **Information on toxicological effects**
· **Acute toxicity:**

· **LD/LC50 values that are relevant for classification:**		
ATE (Acute Toxicity Estimate)		
Oral	LD50	168 mg/kg (rat)
Dermal	LD50	505 mg/kg (rabbit)
Inhalative	LC50/4 h	5.21 mg/l (rat)

67-56-1 Methanol		
Oral	LD50	100.1 mg/kg (rat) (Expert judgment) Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2) Symptoms: Nausea, Vomiting

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Dermal	LD50	300.1 mg/kg (rabbit) (Expert judgment) Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Inhalative	LC50/4 h	3.1 mg/l (rat) (Expert judgment) Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2) Symptoms: Irritation symptoms in the respiratory tract.

· **Primary irritant effect:**
· **on the skin:** No irritant effect.
· **on the eye:** No irritating effect.
· **Sensitization:** No sensitizing effects known.
· **Additional toxicological information:**
The product shows the following dangers according to internally approved calculation methods for preparations:
Toxic
· **Interactive effects** No interactive effects between components are known.

· **Carcinogenic categories**

· **IARC (International Agency for Research on Cancer)**
None of the ingredients is listed.

· **NTP (National Toxicology Program)**
None of the ingredients is listed.

· **OSHA-Ca (Occupational Safety & Health Administration)**
None of the ingredients is 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 2 (Self-assessment): hazardous for water
Do not allow product to reach ground water, water course or sewage system.
Danger to drinking water if even small quantities leak into the ground.

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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.
· **Recommended cleansing agent:** Water, if necessary with cleansing agents.

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14 Transport information

· **UN-Number**	
· **DOT, IMDG, IATA**	UN1992
· **UN proper shipping name**	
· **DOT**	Flammable liquids, toxic, n.o.s. (Methanol)
· **IMDG**	FLAMMABLE LIQUID, TOXIC, N.O.S. (Methanol)
· **IATA**	Flammable liquid, toxic, n.o.s. (Methanol)
· **Transport hazard class(es)**	
· **DOT**	

· **Class**	3 Flammable liquids
· **Label**	3, 6.1
· **IMDG**	

· **Class**	3 Flammable liquids
· **Label**	3/6.1
· **IATA**	

· **Class**	3 Flammable liquids
· **Label**	3 (6.1)
· **Packing group**	
· **DOT, IMDG, IATA**	II
· **Environmental hazards:**	Not applicable.
· **Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code**	Not applicable.

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· **Transport/Additional information:**

· **DOT**

· **Quantity limitations**	On passenger aircraft/rail: 1 L On cargo aircraft only: 60 L

· **IMDG**

· **Limited quantities (LQ)**	1L
· **Excepted quantities (EQ)**	Code: E2 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 500 ml

· **IATA**

· **Remarks:**	When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.

· **Special precautions for user**	Warning: Flammable liquids
· **Hazard identification number (Kemler code):**	336
· **EMS Number:**	F-E,S-D
· **Stowage Category**	B
· **Stowage Code**	SW2 Clear of living quarters.
· **UN "Model Regulation":**	UN 1992 FLAMMABLE LIQUID, TOXIC, N.O.S. (METHANOL), 3 (6.1), II

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):**

None of the ingredients is listed.

· **Section 313 (Specific toxic chemical listings):**

67-56-1	Methanol
64-18-6	Formic acid

· **TSCA (Toxic Substances Control Act):**

67-56-1	Methanol	ACTIVE
7732-18-5	Water	ACTIVE
64-18-6	Formic acid	ACTIVE

· **Hazardous Air Pollutants**

67-56-1	Methanol

· **Chemicals known to cause cancer:**

None of the ingredients is listed.

· **Chemicals known to cause reproductive toxicity for females:**

None of the ingredients is listed.

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· **Chemicals known to cause reproductive toxicity for males:**
None of the ingredients is listed.

· **Chemicals known to cause developmental toxicity:**

67-56-1	Methanol

· **Carcinogenic categories**

· **EPA (Environmental Protection Agency)**
None of the ingredients is listed.

· **TLV (Threshold Limit Value)**
None of the ingredients is listed.

· **NIOSH-Ca (National Institute for Occupational Safety and Health)**
None of the ingredients is 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** 09/19/2022
· **Date of preparation** 03/13/2025
· **Abbreviations and acronyms:**
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
EINECS: European Inventory of Existing Commercial Chemical Substances
ELINCS: European List of Notified Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
NFPA: National Fire Protection Association (USA)
HMIS: Hazardous Materials Identification System (USA)
VOC: Volatile Organic Compounds (USA, EU)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
PBT: Persistent, Bioaccumulative and Toxic
vPvB: very Persistent and very Bioaccumulative
NIOSH: National Institute for Occupational Safety
OSHA: Occupational Safety & Health
TLV: Threshold Limit Value
PEL: Permissible Exposure Limit
REL: Recommended Exposure Limit
BEI: Biological Exposure Limit
Flammable liquids 2: Flammable liquids – Category 2
Acute toxicity - oral 3: Acute toxicity – Category 3
Specific target organ toxicity (single exposure) 1: Specific target organ toxicity (single exposure) – Category 1
· *** Data compared to the previous version altered.**