

Chemical Safety Data Sheet MSDS / SDS

N-Allylthiourea

Revision Date:2025-05-17 Revision Number:1

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

Product identifier

Product name : N-Allylthiourea
CBnumber : CB3145441
CAS : 109-57-9
EINECS Number : 203-683-5
Synonyms : Allylthiourea,N-allylthiourea

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 : 400-158-6606

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

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

P270 Do not eat, drink or smoke when using this product.

P264 Wash skin thoroughly after handling.

P264 Wash hands thoroughly after handling.

P262 Do not get in eyes, on skin, or on clothing.

P501 Dispose of contents/container to....

P405 Store locked up.

P310 Immediately call a POISON CENTER or doctor/physician.

P309 IF exposed or if you feel unwell:

Hazard statements

H319 Causes serious eye irritation

H317 May cause an allergic skin reaction

H315 Causes skin irritation

H301 Toxic if swallowed

SECTION 3: Composition/information on ingredients

Substance

Product name	: N-Allylthiourea
Synonyms	: Allylthiourea, N-allylthiourea
CAS	: 109-57-9
EC number	: 203-683-5
MF	: C ₄ H ₈ N ₂ S
MW	: 116.18

SECTION 4: First aid measures

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Special hazards arising from the substance or mixture

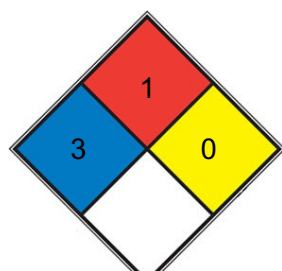
Carbon oxides Nitrogen oxides (NO_x) Sulfur oxides Combustible.

Advice for firefighters

No data available

Further information

No data available

NFPA 704



■ HEALTH	3	Short exposure could cause serious temporary or moderate residual injury (e.g. liquid hydrogen , sulfuric acid , calcium hypochlorite , hexafluorosilicic acid)
		Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. mineral oil , ammonia)
■ 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

For personal protection see section 8.

Environmental precautions

No data available

Methods and materials for containment and cleaning up

No data available

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

No data available

Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Personal protective equipment

Skin protection

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested:KCL 741 Dermatrill? L

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested:KCL 741 Dermatrill? L

Control of environmental exposure

Prevent product from entering drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	beige crystalline
Odour	unpleasant
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 70 - 72 °C - lit.
Initial boiling point and boiling range	191.3±33.0 °C(Predicted)
Flash point	Not applicable
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	1,11 g/mL at 25 °C
Water solubility	H2O: soluble30 parts
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available

Explosive properties	No data available
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Oxidizing properties	No data available
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Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

No data available

Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

Conditions to avoid

No data available

Incompatible materials

no information available

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 200 mg/kg Remarks:

(RTECS)

Inhalation: No data available Dermal: No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Toxicity

LD50 orally in rats: 200 mg/kg (Dieke)

SECTION 12: Ecological information

Toxicity**Toxicity to fish**

LC50 - *Leuciscus idus melanotus* - 3.200 mg/l - 48 h

Toxicity to daphnia and other aquatic invertebrates

LC50 - *Daphnia magna* (Water flea) - 39 mg/l - 24 h

Persistence and degradability

No data available

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods**Product**

No data available

SECTION 14: Transport information

UN number

ADR/RID: 2811 IMDG: 2811 IATA: 2811

UN proper shipping name

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (N-Allylthiourea) IMDG: TOXIC SOLID, ORGANIC, N.O.S. (N-Allylthiourea)

IATA: Toxic solid, organic, n.o.s. (N-Allylthiourea)

14.3	Transport hazard class(es) ADR/RID: 6.1 IMDG: 6.1	IATA: 6.1
14.4	Packaging group ADR/RID: III IMDG: III	IATA: III
14.5	Environmental hazards ADR/RID: no IMDG Marine pollutant: no	IATA: no
14.6	Special precautions for user No data available	

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

EC Inventory:Listed.

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

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

【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

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

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

【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

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

【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

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.