

1 Identification of substance**Product details**

Trade name

Allyl isothiocyanate

Stock number:

L02901

Manufacturer/Supplier:

Alfa Aesar GmbH & Co.KG
Benzstrasse 3
D-76185 Karlsruhe / GermanyE-mail: gcat@matthey.com
www.alfa-chemcat.com

Informing department:

Product safety department.

Emergency information:

Giftnotruf Universität Mainz / Poison Information Center Mainz
www.giftinfo.uni-mainz.de Telefon:+49(0)6131/19240**2 Hazards identification**

Hazard designation:

T Toxic
N Dangerous for the environment

Information pertaining to particular dangers for man and environment

R 10 Flammable.
R 23/24/25 Toxic by inhalation, in contact with skin and if swallowed.
R 37/38 Irritating to respiratory system and skin.
R 41 Risk of serious damage to eyes.
R 50/53 Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

GHS label elements

**Danger**

H301 - Toxic if swallowed.
H310 - Fatal in contact with skin.
H331 - Toxic if inhaled.

**Danger**

H318 - Causes serious eye damage.

**Warning**

H226 - Flammable liquid and vapour.

**Warning**

H400 - Very toxic to aquatic life.
H410 - Very toxic to aquatic life with long lasting effects.

Warning

H315 - Causes skin irritation.
H335 - May cause respiratory irritation.

Prevention:

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P273 Avoid release to the environment.

Response:

P280 Wear protective gloves/protective clothing/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.
P309 IF exposed or if you feel unwell:
P310 Immediately call a POISON CENTER or doctor/physician.

3 Composition/information on ingredients

Chemical characterization:

Allyl isothiocyanate (CAS# 57-06-7)

Designation: (CAS#)

Identification number(s):

200-309-2

EINECS Number:

Stabilized with:

Additional information:

BHT (butylated hydroxytoluene) (CAS# 128-37-0)

4 First aid measures

General information

Instantly remove any clothing soiled by the product.
Remove breathing apparatus only after soiled clothing has been completely removed.
In case of irregular breathing or respiratory arrest provide artificial respiration.

After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

After skin contact

Seek immediate medical advice.
Instantly wash with water and soap and rinse thoroughly.
Seek immediate medical advice.

After eye contact

Rinse opened eye for several minutes under running water. Then consult doctor.

After swallowing

Do not induce vomiting; instantly call for medical help.
Seek immediate medical advice.

5 Fire fighting measures

Suitable extinguishing agents

CO₂, sand, extinguishing powder. Do not use water.

For safety reasons unsuitable extinguishing agents

Water.

Special hazards caused by the material, its products of combustion or flue gases:

Can be released in case of fire:
Carbon monoxide and carbon dioxide
Nitrogen oxides (NO_x)
Possibly Hydrogen cyanide (HCN)
Sulphur oxides (SO_x)

Protective equipment:

Wear self-contained breathing apparatus.
Wear full protective suit.

6 Accidental release measures

Person-related safety precautions:

Wear protective equipment. Keep unprotected persons away.
Ensure adequate ventilation
Keep away from ignition sources

Measures for environmental protection:

Do not allow material to be released to the environment without proper governmental permits.
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Dispose of contaminated material as waste according to item 13.

Measures for cleaning/collecting:

Ensure adequate ventilation.
Keep away from ignition sources.

Additional information:

See Section 7 for information on safe handling

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See section 8 for information on personal protection equipment.
See Section 13 for information on disposal.

7 Handling and storage**Handling
Information for safe handling:**

Handle under dry protective gas.
Keep containers tightly sealed.
Ensure good ventilation/exhaustion at the workplace.
Open and handle container with care.

**Information about protection against
explosions and fires:**

Keep ignition sources away - Do not smoke.
Protect against electrostatic charges.
Fumes can combine with air to form an explosive mixture.

**Storage
Requirements to be met by storerooms and
containers:
Information about storage in one common
storage facility:**

Refrigerate

Store away from oxidizing agents.
Store in the dark.
Protect from heat.
Store away from water.

**Further information about storage
conditions:**

Store under dry inert gas.
This product is moisture sensitive.
Keep container tightly sealed.
Protect from humidity and keep away from water.
Protect from the effects of light.
Store in a locked cabinet or with access restricted to technical experts or their assistants.
Refrigerate

8 Exposure controls and personal protection**Additional information about design of
technical systems:**

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

**Components with critical values that require
monitoring at the workplace:**

Not required.

Additional information:

No data

Personal protective equipment**General protective and hygienic measures**

The usual precautionary measures should be adhered to in handling the chemicals.
Keep away from foodstuffs, beverages and food.
Instantly remove any soiled and impregnated garments.
Wash hands during breaks and at the end of the work.
Store protective clothing separately.
Avoid contact with the eyes and skin.

Breathing equipment:**Protection of hands:****Material of gloves**

Use breathing protection with high concentrations.
Check protective gloves prior to each use for their proper condition.
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**Eye protection:****Body protection:**

Impervious gloves
Not determined
Safety glasses
Face protection
Protective work clothing.

9 Physical and chemical properties:**General Information**

Form: Liquid
Colour: Yellow
Smell: Pungent

Change in condition

Melting point/Melting range: -80°C
Boiling point/Boiling range: 149-151°C
Sublimation temperature / start: Not determined

Flash point: 46°C

Ignition temperature: Not determined

Decomposition temperature: Not determined

Critical values for explosion:

Lower: Not determined
Upper: Not determined

Steam pressure at 20°C: 5.3 hPa

Density at 20°C 1.013 g/cm³

**Solubility in / Miscibility with
Water at 20°C:** 2 g/l

10 Stability and reactivity**Thermal decomposition / conditions to be
avoided:**

No decomposition if used and stored according to specifications.
Danger of containers bursting upon heating.

Stable until:**Materials to be avoided:**

Depletion of inhibitor.
Oxidizing agents
Amines
Heat
Ultraviolet radiation
Free radical initiators
Water/moisture
Light

Dangerous reactions:

Danger of polymerisation
Spontaneous polymerisation can be caused in unstabilised product e.g. by ambient heat

Dangerous products of decomposition:

Carbon monoxide and carbon dioxide

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Additional information:

Nitrogen oxides (NO_x)
Sulphur oxides (SO_x)
Possibly Hydrogen cyanide (HCN)
Unless inhibited, the product can polymerize resulting in a temperature and pressure increase that may rupture the container.

11 Toxicological information**Acute toxicity:****LD/LC50 values that are relevant for classification:**

Oral	LD50	308 mg/kg (mouse) 112 mg/kg (rat)
Dermal	LD50	88 mg/kg (rabbit)
Irritation of eyes	severe	unknown mg (rabbit)

Primary irritant effect:**on the skin:****on the eye:**

Irritant for skin and mucous membranes.
Strong irritant with the danger of severe eye injury.
Lachrymatory effect.
No sensitizing effect known.

Sensitization:**Other information (about experimental toxicology):****Additional toxicological information:**

Tumorigenic effects have been observed on tests with laboratory animals.
To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.
Danger by skin resorption.
IARC-3: Not classifiable as to carcinogenicity to humans.

12 Ecological information:**Ecotoxicological effects:****Remark:****Additional ecological information:****General notes:**

Very toxic for fish

Water danger class 3 (Self-assessment): extremely hazardous for water.
Do not allow product to reach ground water, water bodies or sewage system, even in small quantities.
Danger to drinking water if even extremely small quantities leak into soil.
Also poisonous for fish and plankton in water bodies.
Do not allow material to be released to the environment without proper governmental permits.
Very toxic for aquatic organisms

13 Disposal considerations**Product:****Recommendation**

Hand over to disposers of hazardous waste.
Must be specially treated under adherence to official regulations.
Consult state, local or national regulations for proper disposal.

Uncleaned packagings:**Recommendation:**

Disposal must be made according to official regulations.

14 Transport information**Land transport ADR/RID and GGVS/GGVE (cross-border/domestic)****ADR/RID-GGVS/E Class:**

6.1 (TF1) Toxic substances.

Kemler Number:

639

UN-Number:

1545

Packaging group:

II

Label

6.1+3

Special marking:

Symbol (fish and tree)

Designation of goods:

1545 ALLYL ISOTHIOCYANATE, STABILIZED

Limited quantities (LQ)

LQ17

Tunnel restriction code

D/E

Maritime transport IMDG/GGVSea:**IMDG/GGVSea Class:**

6.1

UN Number:

1545

Label

6.1+3

Packaging group:

II

Marine pollutant:

No

Correct technical name:

ALLYL ISOTHIOCYANATE, STABILIZED

Air transport ICAO-TI and IATA-DGR:**ICAO/IATA Class:**

6.1

UN/ID Number:

1545

Label

6.1+3

Packaging group:

II

Correct technical name:

ALLYL ISOTHIOCYANATE, STABILIZED

UN "Model Regulation":

UN1545, ALLYL ISOTHIOCYANATE, STABILIZED, 6.1 (3), II

Environmental hazards:

Environmentally hazardous substance, liquid; Marine Pollutant

15 Regulatory information**Designation according to EC guidelines:****Code letter and hazard designation of product:**

T Toxic

N Dangerous for the environment

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Risk phrases:	10 Flammable. 23/24/25 Toxic by inhalation, in contact with skin and if swallowed. 37/38 Irritating to respiratory system and skin. 41 Risk of serious damage to eyes. 50/53 Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
Safety phrases:	26 In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. 36/37 Wear suitable protective clothing and gloves. 45 In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). 60 This material and its container must be disposed of as hazardous waste. 61 Avoid release to the environment. Refer to special instructions/safety data sheets.
National regulations	
Information about limitation of use:	Employment restrictions concerning young persons must be observed. For use only by technically qualified individuals.
Water hazard class:	Water danger class 3 (Self-assessment): extremely hazardous for water.

16 Other information:

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing data specification sheet: Health, Safety and Environmental Department.

Contact: Zachariah Holt

Abbreviations and acronyms:

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)
IMDG: International Maritime Code for Dangerous Goods
IATA: International Air Transport Association
IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)
ICAO: International Civil Aviation Organization
ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)
GHS: Globally Harmonized System of Classification and Labelling of Chemicals
EINECS: European Inventory of Existing Commercial Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent

GB