SAFETY DATA SHEET
Allyl isothiocyanate

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

1.1. Product identifier
Product name: Allyl isothiocyanate
Product number: FA02432
Synonyms; trade names: Mustard Oil, AITC
CAS number: 57-06-7
EC number: 200-309-2

1.2. Relevant identified uses of the substance or mixture and uses advised against
Identified uses: Laboratory reagent. Manufacture of substances. Research and development.

1.3. Details of the supplier of the safety data sheet
Supplier: Carbosynth Ltd
8&9 Old Station Business Park
Compton
Berkshire
RG20 6NE
UK
+44 1635 578444
+44 1635 579444
info@carbosynth.com

1.4. Emergency telephone number
Emergency telephone: +44 7887 998634

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture
Classification (EC 1272/2008)
Physical hazards: Flam. Liq. 3 - H226
Health hazards: Acute Tox. 3 - H301 Acute Tox. 2 - H310 Acute Tox. 3 - H331 Skin Irrit. 2 - H315 Eye Irrit. 2 - H319 Resp. Sens. 1 - H334 Skin Sens. 1 - H317 STOT SE 3 - H335
Environmental hazards: Aquatic Acute 1 - H400 Aquatic Chronic 1 - H410

2.2. Label elements
EC number: 200-309-2
Pictogram:

Signal word: Danger
Allyl isothiocyanate

Hazard statements
H226 Flammable liquid and vapour.
H301+H331 Toxic if swallowed or if inhaled.
H310 Fatal in contact with skin.
H315 Causes skin irritation.
H317 May cause an allergic skin reaction.
H319 Causes serious eye irritation.
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H335 May cause respiratory irritation.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.
P501 Dispose of contents/ container in accordance with national regulations.

2.3. Other hazards
No data available.

SECTION 3: Composition/information on ingredients

3.1. Substances
Product name Allyl isothiocyanate
CAS number 57-06-7
EC number 200-309-2
Chemical formula C₄H₅NS

SECTION 4: First aid measures

4.1. Description of first aid measures
General information Get medical advice/attention if you feel unwell.
Inhalation Remove person to fresh air and keep comfortable for breathing. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. If breathing stops, provide artificial respiration. Get medical attention if symptoms are severe or persist.
Ingestion Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth thoroughly with water. Give plenty of water to drink. Get medical attention if symptoms are severe or persist.
Skin contact Remove contaminated clothing. Rinse with water. Continue to rinse for at least 15 minutes. Wash contaminated clothing before reuse. Get medical attention if symptoms are severe or persist.
Eye contact Rinse immediately with plenty of water. Continue to rinse for at least 15 minutes. Get medical attention if symptoms are severe or persist.

4.2. Most important symptoms and effects, both acute and delayed
General information See Section 11 for additional information on health hazards.

4.3. Indication of any immediate medical attention and special treatment needed
Notes for the doctor Treat symptomatically.
Allyl isothiocyanate

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media: Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fireextinguishing media suitable for the surrounding fire.

5.2. Special hazards arising from the substance or mixture

Specific hazards: None known.

Hazardous combustion products: Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours. Oxides of carbon. Oxides of nitrogen. Oxides of sulphur.

5.3. Advice for firefighters

Special protective equipment for firefighters: Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing conforming to European standard EN469 (including helmets, protective boots and gloves) will provide a basic level of protection for chemical incidents. Use protective equipment appropriate for surrounding materials.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions: Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Avoid inhalation of vapours. Provide adequate ventilation. Eliminate all sources of ignition. Vapours may form explosive mixtures with air. Vapours may accumulate on the floor and in low-lying areas. Keep unnecessary and unprotected personnel away from the spillage.

6.2. Environmental precautions

Environmental precautions: Avoid discharge into drains or watercourses or onto the ground.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up: Wear protective clothing as described in Section 8 of this safety data sheet. Absorb spillage with sand or other inert absorbent. Clear up spills immediately and dispose of waste safely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Provide adequate ventilation. For waste disposal, see Section 13.

6.4. Reference to other sections

Reference to other sections: For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Usage precautions: Wear protective clothing as described in Section 8 of this safety data sheet. Wash hands thoroughly after handling. Provide adequate ventilation. Avoid contact with skin and eyes. Avoid inhalation of vapours. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Take precautionary measures against static discharge.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions: Keep container tightly closed. Store in a cool and well-ventilated place. Protect from moisture. Keep away from heat. Store at temperatures between 2°C and 8°C.

7.3. Specific end use(s)

Specific end use(s): The identified uses for this product are detailed in Section 1.2.
Allyl isothiocyanate

SECTION 8: Exposure Controls/personal protection

8.1. Control parameters

Occupational exposure limits
No exposure limits known for ingredient(s).

8.2. Exposure controls

Appropriate engineering controls
Provide adequate ventilation.

Eye/face protection
Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses. Personal protective equipment for eye and face protection should comply with European Standard EN166.

Hand protection
Wear protective gloves. To protect hands from chemicals, gloves should comply with European Standard EN374.

Other skin and body protection
Wear appropriate clothing to prevent repeated or prolonged skin contact.

Respiratory protection
Respiratory protection complying with an approved standard should be worn if a risk assessment indicates inhalation of contaminants is possible. Ensure all respiratory protective equipment is suitable for its intended use and is ‘CE’-marked. Gas and combination filter cartridges should comply with European Standard EN14387. Full face mask respirators with replaceable filter cartridges should comply with European Standard EN136. Half mask and quarter mask respirators with replaceable filter cartridges should comply with European Standard EN140.

Environmental exposure controls
Keep container tightly sealed when not in use.

SECTION 9: Physical and Chemical Properties

9.1. Information on basic physical and chemical properties

Appearance
Liquid.

Colour
Colourless. or Yellow.

Odour
Pungent.

Odour threshold
No data available.

pH
No data available.

Melting point
-80°C

Initial boiling point and range
150°C

Flash point
46°C Closed cup.

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
3.4

Relative density
1.013 g/cm³ @ 25°C

Solubility(ies)
2 g/l water @ 20°C
Allyl isothiocyanate

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SECTION 10: Stability and reactivity

10.1. Reactivity
Reactivity
No data available.

10.2. Chemical stability
Stability
Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions
Possibility of hazardous reactions
No data available.

10.4. Conditions to avoid
Conditions to avoid

10.5. Incompatible materials
Materials to avoid

10.6. Hazardous decomposition products
Hazardous decomposition products

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral
Acute toxicity oral (LD₅₀ mg/kg) 112.0
Species Rat
Notes (oral LD₅₀) Acute Tox. 3 - H301 Toxic if swallowed.
ATE oral (mg/kg) 112.0

Acute toxicity - dermal
Acute toxicity dermal (LD₅₀ mg/kg) 88.0
Species Rabbit
Notes (dermal LD₅₀) Acute Tox. 2 - H310 Fatal in contact with skin.
ATE dermal (mg/kg) 88.0

Acute toxicity - inhalation
Allyl isothiocyanate

Notes (inhalation LC₅₀) Acute Tox. 3 - H331 Toxic if inhaled.

ATE Inhalation (vapours mg/l) 3.0

Skin corrosion/irritation
Animal data Irritating.

Serious eye damage/irritation
Serious eye damage/irritation Causes serious eye irritation.

Respiratory sensitisation
Respiratory sensitisation There is evidence that the product can cause respiratory hypersensitivity.

Skin sensitisation
Skin sensitisation May cause skin sensitisation or allergic reactions in sensitive individuals.

Germ cell mutagenicity
Genotoxicity - in vitro Based on available data the classification criteria are not met.

Carcinogenicity
Carcinogenicity Based on available data the classification criteria are not met.

IARC carcinogenicity IARC Group 3 Not classifiable as to its carcinogenicity to humans.

Reproductive toxicity
Reproductive toxicity - fertility Based on available data the classification criteria are not met.

Reproductive toxicity - development Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure
STOT - single exposure STOT SE 3 - H335 May cause respiratory irritation.

Target organs Respiratory system, lungs

Specific target organ toxicity - repeated exposure
STOT - repeated exposure Not classified as a specific target organ toxicant after repeated exposure.

Aspiration hazard
Aspiration hazard Based on available data the classification criteria are not met.

General information The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation May cause sensitisation or allergic reactions in sensitive individuals. A single exposure may cause the following adverse effects: Drowsiness, dizziness, disorientation, vertigo. Unconsciousness. High concentrations may be fatal.

Ingestion May cause sensitisation or allergic reactions in sensitive individuals. May cause stomach pain or vomiting. May cause severe internal injury.

Skin contact May cause skin sensitisation or allergic reactions in sensitive individuals. A single exposure may cause the following adverse effects: Pain. Unconsciousness, possibly death.

Eye contact Irritating to eyes.

Route of exposure Ingestion Inhalation Skin and/or eye contact

Target organs Respiratory system, lungs

Medical considerations Skin disorders and allergies.
Allyl isothiocyanate

SECTION 12: Ecological Information

Ecotoxicity
Very toxic to aquatic life with long lasting effects.

12.1. Toxicity

Acute aquatic toxicity
\[ \text{LE(C)}_{50} < 0.1 \leq \text{L(E)C50} < 1 \]
M factor (Acute) 1

Acute toxicity - fish
\[ \text{LC}_{50}, 96 \text{ hour}: 0.0856 \text{ mg/l}, \text{Pimephales promelas (Fat-head Minnow)} \]
\[ \text{LC}_{50}, 96 \text{ hour}: 0.054 - 0.109 \text{ mg/l}, \text{Freshwater fish} \]

Chronic aquatic toxicity
\[ \text{NOEC} < 0.01 \leq \text{NOEC} < 0.1 \]

Degradability
Non-rapidly degradable

M factor (Chronic) 1

12.2. Persistence and degradability

Persistence and degradability
The degradability of the product is not known.

12.3. Bioaccumulative potential

Bioaccumulative potential
No data available on bioaccumulation.

Partition coefficient
No data available.

12.4. Mobility in soil

Mobility
No data available.

12.5. Results of PBT and vPvB assessment

Results of PBT and vPvB assessment
No data available.

12.6. Other adverse effects

Other adverse effects
None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

General information
Dispose of waste to licensed waste disposal site in accordance with the requirements of the local Waste Disposal Authority. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered.

SECTION 14: Transport information

14.1. UN number

UN No. (ADR/RID) 1545
UN No. (IMDG) 1545
UN No. (ICAO) 1545
UN No. (ADN) 1545

14.2. UN proper shipping name

14.3. Transport hazard class(es)
Allyl isothiocyanate

ADR/RID class 6.1
ADR/RID subsidiary risk 3)
ADR/RID classification code TF1
ADR/RID label 6.1
IMDG class 6.1
IMDG subsidiary risk 3)
ICAO class/division 6.1
ICAO subsidiary risk 3)
ADN class 6.1
ADN subsidiary risk 3

Transport labels

14.4. Packing group
ADR/RID packing group II
IMDG packing group II
ADN packing group II
ICAO packing group II

14.5. Environmental hazards
Environmentally hazardous substance/marine pollutant
No.

14.6. Special precautions for user
EmS F-E, S-D
ADR transport category 2
Emergency Action Code 3WE
Hazard Identification Number 639
(ADR/RID)

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture
National regulations
Health and Safety at Work etc. Act 1974 (as amended).
The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"].
EH40/2005 Workplace exposure limits.
Allyl isothiocyanate

EU legislation

15.2. Chemical safety assessment
No chemical safety assessment has been carried out.

Inventories
US - TSCA
Present.

SECTION 16: Other information

Abbreviations and acronyms used in the safety data sheet
ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.
ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.
RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.
IATA: International Air Transport Association.
IMDG: International Maritime Dangerous Goods.
CAS: Chemical Abstracts Service.
ATE: Acute Toxicity Estimate.
LC₅₀: Lethal Concentration to 50 % of a test population.
LD₅₀: Lethal Dose to 50% of a test population (Median Lethal Dose).
EC₅₀: 50% of maximal Effective Concentration.
PBT: Persistent, Bioaccumulative and Toxic substance.
vPvB: Very Persistent and Very Bioaccumulative.

Training advice
Only trained personnel should use this material.

Revision date
19/07/2018

Revision
1

SDS number
144929

Hazard statements in full
H226 Flammable liquid and vapour.
H301 Toxic if swallowed.
H310 Fatal in contact with skin.
H315 Causes skin irritation.
H317 May cause an allergic skin reaction.
H319 Causes serious eye irritation.
H331 Toxic if inhaled.
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H335 May cause respiratory irritation.
H400 Very toxic to aquatic life.
H410 Very toxic to aquatic life with long lasting effects.

This 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. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.