

Material Safety Data Sheet

Printed : 09/08/2024

Revised : LSI_2023-1-CLP from 09/08/2024

ALLYL ISOTHIOCYANATE

1. PRODUCT AND COMPANY IDENTIFICATION

1.1. Product identifier

ALLYL ISOTHIOCYANATE

Product identification : ALLYL ISOTHIOCYANATE code AIT
C.A.S number : 57-06-7 ; ;
CAS EINECS number :
EINECS number : 200-309-2
EC (REACH) number :
REACH registration number : Exempted (Used Flavours only)

1.2. Relevant identified uses of the substance or mixture and uses advised against

Concentrated aromatic raw material.
Not intended for personal use in this form or concentration.
For industrial use only, not for retail sale.

USE : **Flavouring substance**

1.3. Details of the supplier of the safety data sheet

Company : SASU DIFFUSIONS AROMATIQUES
558 allée des Parfums
Parc d'activités "Les Hauts de Grasse"
06530 SAINT-CEZAIRE-SUR-SIAGNE
Tel:+33 (0)4 93 60 82 82
Fax :+33 (0)4 93 60 82 79
Web :www.diffusions-aromatiques.fr
Email :contact@diffusions-aromatiques.fr

1.4. Emergency telephone number

Emergency telephone number 24h/24 - 7d/7: ORFILA (INRS) : +33.(0)1.45.42.59.59

2. HAZARD IDENTIFICATION

2.1. Classification of the substance or mixture

GHS Classification :

(RegulationCLP)

ATD3 Acute toxicity dermal 3
ATI2 Acute toxicity inhalation 2
ATO4 Acute toxicity oral 4
EDI1 Serious eye damage / eye irritation 1
EHA1 Hazardous to the aquatic environment, acute hazard 1
EHC1 Hazardous to the aquatic environment, long-term hazard 1
FL3 Flammable Liquids 3
RS1A Sensitisation, respiratory 1A
SCI1C Skin corrosion / irritation 1C
SS1 Sensitisation skin 1

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H226 - Flammable liquid and vapour.
H302 - Harmful if swallowed.
H311 - Toxic in contact with skin.
H314 - Causes severe skin burns and eye damage.
H317 - May cause an allergic skin reaction.
H318 - Causes serious eye damage.
H330 - Fatal if inhaled.
H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H400 - Very toxic to aquatic life.
H410 - Very toxic to aquatic life with long lasting effects.

2.2. Label elements

GHS Classification :

(RegulationCLP)



Warning mention : Danger

ATD3 Acute toxicity dermal 3
ATI2 Acute toxicity inhalation 2
ATO4 Acute toxicity oral 4
EDI1 Serious eye damage / eye irritation 1
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P260 - Do not breathe dust/fume/gas/mist/vapours/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.
P273 - Avoid release to the environment.
P284 - Wear respiratory protection.

2.3. Other hazards

- Endocrine disruptors : No components concerned

- **Contains substances that may cause allergies : Allyl isothiocyanate PROHIBE IFRA**

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3. COMPOSITION / INFORMATION ON INGREDIENT

3.1. Substances

Identification number	Substance	Hazard classes & H-phrases	LCS / M-factors / ATE	Percentage %
CAS# 57-06-7 EINECS# 200-309-2 REACH# 01-2120771363-54-*** *	Allyl isothiocyanate PROHIBE IFRA	ATD3, AT12, ATO4, EDI1, EHA1, EHC1, FL3, RS1A, SC11C, SS1 H311, H330, H302, H318, H400, H410, H226, H334, H314, H317	EHA1 (M=10) ATE (Dermale) : 300mg/kg ATE (Orale) : 425mg/kg ATE (Inhalation) : 0.051mg/L	[90-100]

- Endocrine disruptors : No components concerned

3.2. Mixtures

NO CONCERNED

4. FIRST AID MEASURES

4.1. Description of first aid measures

General notes: Take Risk and Safety phrases (section 15) into account.

Following inhalation:

Remove from exposure site to fresh air and keep at rest. Obtain medical advice.

Following skin contact:

Remove contaminated clothes. Wash thoroughly with water (and soap). Contact physician if symptoms persist.

Following eye contact:

Flush immediately with water for at least 15 minutes. Contact physician if symptoms persist.

Following ingestion:

Rinse mouth with water and obtain medical advice.

Notes for the doctor:

Treat symptomatically and supportively.

Treatment may vary with condition of victim and specifics of incident.

4.2. Most important symptoms and effects, both acute and delayed

No data available

Please note the risk and safety phrases

4.3. Indication of any immediate medical attention and special treatment needed

No data available

Please note the risk and safety phrases

5. FIRE FIGHTING

5.1. Extinguishing media

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Suitable extinguishing media

Depending on the type of product:

- CO₂, dry powder or foam extinguishers
- Water spray or fog to cool the package (if necessary)

Unsuitable extinguishing media :

Direct water jet

5.2. Special hazards arising from the substance or mixture

Flammability : The product is not easily flammable.

Prévention: Do not smoke. Do not use flame near.

In case of fire, may produce toxic fumes of carbon monoxide (CO) or carbon dioxide (CO₂). Exposure to decomposition products may cause health hazards. Do not breathe fumes.

5.3. Advice for firefighters

Never use a direct water jet.

Workers should be equipped with suitable protective equipment (respiratory and protective suit).

High temperatures can cause high pressures inside closed packages.

6. ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

- Wear gloves (if possible made of natural rubber) when handling leaks to avoid contact with the skin, body cleansing should be observed in case of contact.
 - Avoid breathing vapours.
 - Follow normal hygiene rules in case of accidental spillage.
 - Ensure adequate ventilation of the workplace after spillage.
- Refer to protective measures listed under headings 7 and 8.

6.2. Environmental precautions

Prevent contamination of soil and water, runoff into sewers, gutters, rivers. Notify the authorities if the product enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

Methods of cleaning up:

- Large spills should be contained with sand or diatomaceous earth, pumped and rinsed with water after recovery of the waste in specific labelled plastic drums to be handed over to an approved recovery company.
- Clean the area carefully to eliminate any residual pollution
- Any sorbent used to mop up leaks must be destroyed quickly, according to local regulations, preferably by incineration; cases of spontaneous combustion of cloths soaked in perfumes or aromas are well known. Spills must be contained by appropriate means and the associated waste treated in accordance with the regulations in force.

6.4. Reference to other sections

See sections 8 and 13 of this safety data sheet where applicable.

7. HANDLING AND STORAGE

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7.1. Precautions for safe handling

- Wear suitable PPE: gloves (preferably natural rubber) and eye/face protection.
- Handle in well-ventilated areas, ventilated if necessary, at the lowest possible temperature, avoiding dust accumulation.
- Do not smoke. Do not expose to flames or other potential sources of ignition (electrical equipment)
- Observe safety and hygiene standards
- Close the packaging after use.
- Reproduce the labelling if transferring to another container.
- Prevent access by unauthorised persons

7.2. Conditions for safe storage, including any incompatibilities

- Store products in their original containers, preferably full and tightly capped, in a cool, dry place. Do not reuse empty containers.
- Keep away from air and light.
- Avoid unnecessary exposure.
- Keep away from food and drink.

7.3. Specific end use(s)

Wash hands and other exposed areas with mild soap and water before eating, drinking, smoking and before leaving work.

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

8.1. Control parameters

Components with Occupational Exposure Limits (OELs) :
No data available

8.2. Exposure controls

Technical measures: Avoid contact with eyes, skin or clothing. Do not ingest. Avoid contact with food, drink.

Personal protective equipment:

Do not eat, drink or smoke during use.



9. PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

FORMULA : **C4H5NS**
MOLECULAR WEIGHT : **99.15**
SHELF LIFE : **24 months in below conditions, after this time it can be used after control.**

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Storage conditions :	Keep in tightly closed container in a cool and dry place, protected from light.		
FREEZING POINT :	ND		
IGNITION POINT :	ND		
IGNITION TEMPERATURE (°C) :	ND		
EXPLOSIVE LIMITS :	ND		
ASSAY (%GC) :	>99%		
Appearance :	Liquid		
Color :	Colorless to light yellow		
ODOR :	Powerful ; mustard ; sulfurous		
Relative density (d20/20) :	[1.017 ; 1.024]		
Refractive index to 20°C :	[1.526 ; 1.533]		
Flash point :	46°C		
OPTICAL ROTATION (°) :	ND		
Solubility(ies) :	Insoluble in water, soluble in ethanol		
Vapor pressure :	7 kPa (50°C) ; 5.3 mbar (20°C)		
Partition coef (n-octanol/water) :	ND		
MELTING POINT (capillarity) °C :	ND		
BOILING POINT (°C) :	ND		
PH :	ND		
ACID VALUE (mg KOH/g) :	ND		
SPECIFIC GRAVITY (25°C g/cm3) :	ND		

9.2. Other information

No data available

10. STABILITY AND REACTIVITY

10.1. Reactivity

Dangerous reactions : No dangerous reactions known.

10.2. Chemical stability

Good stability if storage and handling standards/indications are taken into consideration.

10.3. Possibility of hazardous reactions

No dangerous reaction if storage and handling standards/indications are taken into account.

10.4. Conditions to avoid

Avoid excessive heat sources (open flame, sparks, etc.)
Do not heat closed containers.

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Avoid contact with oxidizing agents

10.5. Incompatible materials

Data not available

10.6. Hazardous decomposition products

Thermal decomposition / conditions to be avoided: Avoid contact with any flame or spark, flame, Overheat. Avoid Direct rays of the sun. No decomposition if used according to specifications.

Dangerous decomposition products: No dangerous decomposition products known.

11. TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

a) Skin corrosion/skin irritation :	Refer to heading 2, if applicable
b) Serious eye damage/eye irritation :	Refer to heading 2, if applicable
c) Respiratory or skin sensitisation :	Refer to heading 2, if applicable
d) Germ cell mutagenicity :	Refer to heading 2, if applicable
e) Carcinogenicity:	Refer to heading 2, if applicable
f) Reproductive toxicity :	Refer to heading 2, if applicable
g) Specific target organ toxicity (STOT) single exposure :	Refer to heading 2, if applicable
h) Specific target organ toxicity (STOT) repeated exposure :	Refer to heading 2, if applicable
i) Aspiration hazard :	Refer to heading 2, if applicable

j) Acute toxicity :

LD50 (dermal) mg/kg : **ND**

LD50 (ORAL) (mg/kg) : **ND**

LC50 (inhalatoire) : **TOXICITE AIGUË PAR INHALATION : Estimation de la toxicité aiguë : 0,5 mg/l - Temps d'exposition : 4 h - Atmosphère d'essai : vapeur - Méthode : Méthode de calcul TOXICITE AIGUË ORALE : Estimation de la toxicité aiguë : 500 mg/kg - Méthode : Méthode de calcul - TOXICITE AIGUË PAR VOIE CUTANEE : Estimation de la toxicité aiguë : 300 mg/kg - Méthode de calcul**

TOXICITE ORALE : **Estimation de la toxicité aiguë : 500 mg/kg - Méthode : Méthode de calcul**

11.2. Information on other hazards

Endocrine disrupting properties: The product does not contain substances identified as having endocrine disrupting properties for human health with a concentration equal to or greater than 0.1% (w/w).

11.2.2 Others informations

CMR SUBSTANCES : **Dont' contain CMR substances, category 1A, 1B et 2 of 1272/2008 EC regulation**

12. ECOLOGICAL INFORMATION

12.1. Toxicity

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Do not leave the product, even diluted or in great quantity, penetrate the ground water, water or the drains.

12.2. Persistence and degradability

BIODEGRADABILITY : **Not available**

12.3. Bioaccumulative potential

Data not available

12.4. Mobility in soil

Data not available

12.5. Results of PBT and vPvB assessment

Data not available

12.6. Endocrine disrupting properties

The product does not contain substances identified as having endocrine disrupting properties for the environment with a concentration equal to or greater than 0.1% (w/w).

12.7. Other adverse effects

Data not available

13. DISPOSAL RECOMMENDATIONS

13.1. Waste treatment methods

Product : Recommendation : Does not have to be evacuated with the refuse . Not to let penetrate in the sewers.

Not cleaned packing : Recommendation : Evacuation in accordance with the regulations.

14. TRANSPORT INFORMATION

ADR/ADN/RID:



IMDG:



14.1. UN number

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ADR/ADN/RID : 1545 ((D/E))
IMDG:1545
IATA :1545

14.2. UN proper shipping name

ADR/ADN/RID : ALLYL ISOTHIOCYANATE, STABILIZED
IMDG:ALLYL ISOTHIOCYANATE, STABILIZED
IATA :ALLYL ISOTHIOCYANATE, STABILIZED

14.3. Transport hazard class(es)

ADR/ADN/RID : 6.1 (3) (ENV)
IMDG:6.1 (3) (ENV)
IATA :NO CONCERNED

14.4. Packing group

ADR/ADN/RID : II
IMDG:II
IATA :NO CONCERNED

14.5. Environmental hazards

IMDG :

14.6. Special precautions for user

NO CONCERNED

14.7. Maritime transport in bulk according to IMO instruments

NO CONCERNED

15. REGULATORY INFORMATION

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

Valeur ICPE : **4120.2**

15.2. Chemical safety assessment

No chemical safety assessment has been carried out

16. OTHER INFORMATION

Full H sentences text in point 3 :

H226	Flammable liquid and vapour.
H302	Harmful if swallowed.
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H400 Very toxic to aquatic life.

H410 Very toxic to aquatic life with long lasting effects.

Acronyms used:

C.A.S: Chemical Abstract Service

TSCA: Toxic Substances Control Act

EINECS: European inventory of existing Commercial Chemical Substances

GHS Global Harmonized System

CLP: Classification and Labelling and Packaging of substances and mixtures

ADR: Agreement Dangerous goods by Road

IMDG: International Maritime Dangerous Goods

IATA: International Air Transport Association

The information contained in this sheet is based on our knowledge of the product concerned at the time of issue.

The information given in this safety data sheet is in accordance with Regulation 1907/2006/EC of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) establishing a European Chemicals Agency, (amended by Regulation 2015/830, 2020/878 (Annex II of REACH), amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94, as well as Council Directive 76/769/EEC, and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC, 200/21/EC and according to Regulation 453/2010/EC of 20 May 2010.

Users' attention is also drawn to the possible risks involved when a product is used for a purpose other than that for which it was designed.

The information provided is based on the current state of our knowledge, but does not constitute a guarantee of the product's properties and does not give rise to a contractual legal relationship.

REVISION DATE :

09/08/2024