

ALFAAL10866

## 1-Heptyl isothiocyanate

### SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

**产品说明:**  
**Product Description:** 1-异硫代氰酸庚酯  
1-Heptyl isothiocyanate

**Cat No. :** L10866  
**CAS No** 4426-83-9  
**Molecular Formula** C8 H15 N S

**Supplier** Avocado Research Chemicals Ltd.  
(Part of Thermo Fisher Scientific)  
Shore Road, Heysham  
Lancashire, LA3 2XY,  
United Kingdom  
Office Tel: +44 (0) 1524 850506  
Office Fax: +44 (0) 1524 850608

**Emergency Telephone Number** For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

**E-mail address** begel.sdsdesk@thermofisher.com

**Recommended Use** Laboratory chemicals.  
**Uses advised against** No Information available

### SECTION 2. HAZARD IDENTIFICATION

**Physical State**  
Liquid

**Appearance**  
Yellow

**Odor**  
No information available

#### Emergency Overview

Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation. Moisture sensitive. Lachrymator (substance which increases the flow of tears).

#### Classification of the substance or mixture

|  |            |
|--|------------|
| Acute Oral Toxicity                                | Category 4 |
| Acute Dermal Toxicity                              | Category 4 |
| Acute Inhalation Toxicity - Vapors                 | Category 4 |
| Skin Corrosion/Irritation                          | Category 2 |
| Serious Eye Damage/Eye Irritation                  | Category 2 |
| Specific target organ toxicity - (single exposure) | Category 3 |

#### Label Elements



**Signal Word****Warning****Hazard Statements**

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray

P264 - Wash face, hands and any exposed skin 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

**Response**

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

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

P312 - Call a POISON CENTER or doctor if you feel unwell

P330 - Rinse mouth

P362 + P364 - Take off contaminated clothing and wash it before reuse

**Storage**

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

**Disposal**

P501 - Dispose of contents/ container to an approved waste disposal plant

**Physical and Chemical Hazards**

None identified.

**Health Hazards**

Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation. Lachrymator (substance which increases the flow of tears).

**Environmental hazards**

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Will likely be mobile in the environment due to its water solubility. The product is water soluble, and may spread in water systems.

**Other Hazards**

Lachrymator (substance which increases the flow of tears)

This product does not contain any known or suspected endocrine disruptors.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

| Component                  | CAS No    | Weight % |
|----------------------------|-----------|----------|
| Heptane, 1-isothiocyanato- | 4426-83-9 | 97       |

**SECTION 4. FIRST AID MEASURES****Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

**Skin Contact**

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.

**Inhalation**

Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.

**Ingestion**

Clean mouth with water. Get medical attention.

**Most important symptoms and effects**

No information available.

**Self-Protection of the First Aider**

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

**Notes to Physician**

Treat symptomatically.

**SECTION 5. FIRE-FIGHTING MEASURES****Suitable Extinguishing Media**

Carbon dioxide (CO<sub>2</sub>). Dry chemical. Chemical foam.

**Extinguishing media which must not be used for safety reasons**

No information available.

**Specific Hazards Arising from the Chemical**

Thermal decomposition can lead to release of irritating gases and vapors.

**Protective Equipment and Precautions for Firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

**SECTION 6. ACCIDENTAL RELEASE MEASURES****Personal Precautions**

Ensure adequate ventilation.

**Environmental Precautions**

See Section 12 for additional Ecological Information.

**Methods for Containment and Clean Up**

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE****Handling**

Avoid contact with skin and eyes. Do not breathe mist/vapors/spray.

**Storage**

Keep in a dry, cool and well-ventilated place. Keep container tightly closed.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters**

**Exposure Controls****Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

**Personal protective equipment**

**Eye Protection** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

| Glove material | Breakthrough time | Glove thickness | EU standard | Glove comments        |
|----------------|-------------------|-----------------|-------------|-----------------------|
| Nitrile rubber | See manufacturers | -               | EN 374      | (minimum requirement) |
| Neoprene       | recommendations   |                 |             |                       |
| Natural rubber |                   |                 |             |                       |
| PVC            |                   |                 |             |                       |

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

**Skin and body protection** Wear appropriate protective gloves and clothing to prevent skin exposure

**Respiratory Protection** When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

**Large scale/emergency use** Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced  
**Recommended Filter type:** Organic gases and vapours filter Type A Brown conforming to EN14387

**Small scale/Laboratory use** Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.  
**Recommended half mask:-** Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141  
When RPE is used a face piece Fit Test should be conducted

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice.

**Environmental exposure controls** No information available.

**SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

**Appearance** Yellow  
**Physical State** Liquid

**Odor** No information available  
**Odor Threshold** No data available  
**pH** No information available  
**Melting Point/Range** No data available  
**Softening Point** No data available  
**Boiling Point/Range** 235 °C / 455 °F  
**Flash Point** 106 °C / 222.8 °F

@ 760 mmHg  
**Method** - No information available

## 1-Heptyl isothiocyanate

|   |                          |             |
|---|--------------------------|-------------|
| Evaporation Rate                        | No data available        |             |
| Flammability (solid,gas)                | Not applicable           | Liquid      |
| Explosion Limits                        | No data available        |             |
| Vapor Pressure                          | 0.05 mmHg @ 20 °C        |             |
| Vapor Density                           | 5.42                     | (Air = 1.0) |
| Specific Gravity / Density              | 0.910                    |             |
| Bulk Density                            | Not applicable           | Liquid      |
| Water Solubility                        | Negligible               |             |
| Solubility in other solvents            | No information available |             |
| Partition Coefficient (n-octanol/water) |                          |             |
| Autoignition Temperature                | No data available        |             |
| Decomposition Temperature               | No data available        |             |
| Viscosity                               | No data available        |             |
| Explosive Properties                    | No information available |             |
| Oxidizing Properties                    | No information available |             |
| Molecular Formula                       | C8 H15 N S               |             |
| Molecular Weight                        | 157.28                   |             |

## SECTION 10. STABILITY AND REACTIVITY

|                          |  |
|--------------------------|--|
| Stability                | Stable. Moisture sensitive.                            |
| Hazardous Reactions      | No information available.                              |
| Hazardous Polymerization | Hazardous polymerization does not occur.               |
| Conditions to Avoid      | Incompatible products. Exposure to moist air or water. |
| Materials to avoid       | Acids. Water. Strong oxidizing agents. Alcohols.       |

**Hazardous Decomposition Products** Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Sulfur oxides.

## SECTION 11. TOXICOLOGICAL INFORMATION

## Product Information

|  |   |
|--|---|
| (a) acute toxicity;                    |   |
| (b) skin corrosion/irritation;         | Category 2  |
| (c) serious eye damage/irritation;     | Category 2  |
| (d) respiratory or skin sensitization; |   |
| Respiratory                            | No data available   |
| Skin                                   | No data available   |
| (e) germ cell mutagenicity;            | No data available   |
| (f) carcinogenicity;                   | No data available   |
|  | There are no known carcinogenic chemicals in this product |
| (g) reproductive toxicity;             | No data available   |

|  |  |
|--|--|
| (h) STOT-single exposure;                  | Category 3   |
| Results / Target organs                    | Respiratory system   |
| (i) STOT-repeated exposure;                | No data available  |
| Target Organs                              | No information available.                                      |
| (j) aspiration hazard;                     | No data available  |
| Other Adverse Effects                      | The toxicological properties have not been fully investigated. |
| Symptoms / effects, both acute and delayed | No information available                                       |

**SECTION 12. ECOLOGICAL INFORMATION**

|  |   |
|--|---|
| Ecotoxicity effects  | Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.   |
| Persistence and Degradability<br>Persistence   | Soluble in water, Persistence is unlikely, based on information available.  |
| Bioaccumulative Potential  | Bioaccumulation is unlikely   |
| Mobility in soil   | The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility Highly mobile in soils   |
| Endocrine Disruptor Information<br>Persistent Organic Pollutant<br>Ozone Depletion Potential | This product does not contain any known or suspected endocrine disruptors<br>This product does not contain any known or suspected substance<br>This product does not contain any known or suspected substance |

**SECTION 13. DISPOSAL CONSIDERATIONS**

|                                     |  |
|-------------------------------------|--|
| Waste from Residues/Unused Products | Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations. |
| Contaminated Packaging              | Dispose of this container to hazardous or special waste collection point.  |
| Other Information                   | Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.  |

**SECTION 14. TRANSPORT INFORMATION****Road and Rail Transport**

|                      |                               |
|----------------------|-------------------------------|
| UN-No                | UN2810                        |
| Proper Shipping Name | Toxic liquid, organic, n.o.s. |
| Hazard Class         | 6.1                           |
| Packing Group        | III                           |

**IMDG/IMO**

**UN-No** UN2810  
**Proper Shipping Name** Toxic liquid, organic, n.o.s.  
**Hazard Class** 6.1  
**Packing Group** III

**IATA**

**UN-No** UN2810  
**Proper Shipping Name** TOXIC LIQUID, ORGANIC, N.O.S.\*  
**Hazard Class** 6.1  
**Packing Group** III

**Special Precautions for User** No special precautions required

**SECTION 15. REGULATORY INFORMATION****International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

| Component                  | The Inventory of Hazardous Chemicals (2015 Edition) | List of dangerous goods GB 12268 - 2012 | TCSI | IECSC | EINECS    | TSCA | DSL | PICCS | ENCS | ISHL | AICS | KECL |
|----------------------------|---|---|------|-------|-----------|------|-----|-------|------|------|------|------|
| Heptane, 1-isothiocyanato- | -   | -                                       |      | -     | 224-610-3 | X    | X   | -     | -    |      | -    | -    |

**National Regulations****SECTION 16. OTHER INFORMATION**

**Prepared By** Health, Safety and Environmental Department  
**Revision Date** 16-May-2024  
**Revision Summary** New emergency telephone response service provider.

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

**Legend**

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer

## 1-Heptyl isothiocyanate

**DNEL** - Derived No Effect Level  
**RPE** - Respiratory Protective Equipment  
**LC50** - Lethal Concentration 50%  
**NOEC** - No Observed Effect Concentration  
**PBT** - Persistent, Bioaccumulative, Toxic

**PNEC** - Predicted No Effect Concentration  
**LD50** - Lethal Dose 50%  
**EC50** - Effective Concentration 50%  
**POW** - Partition coefficient Octanol:Water  
**vPvB** - very Persistent, very Bioaccumulative

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association  
**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road  
**OECD** - Organisation for Economic Co-operation and Development  
**BCF** - Bioconcentration factor

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code  
**MARPOL** - International Convention for the Prevention of Pollution from Ships  
**ATE** - Acute Toxicity Estimate  
**VOC** - (Volatile Organic Compound)

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**Disclaimer**

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**End of Safety Data Sheet**