

ALFAAA12223

## 1-Hexyl isothiocyanate

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

**产品说明:** 1-己基异硫代氰酸酯  
**Product Description:** 1-Hexyl isothiocyanate

**Cat No. :** A12223  
**CAS No** 4404-45-9  
**Molecular Formula** C7 H13 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**  
Colorless to yellow

**Odor**  
No information available

#### Emergency Overview

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

#### Classification of the substance or mixture

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

#### Label Elements

**Signal Word****Danger****Hazard Statements**

H227 - Combustible liquid  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation  
H301 + H311 + H331 - Toxic if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking  
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**

P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor  
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  
P311 - Call a POISON CENTER or doctor  
P330 - Rinse mouth  
P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish  
P361 + P364 - Take off immediately all contaminated clothing and wash it before reuse

**Storage**

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed  
P405 - Store locked up

**Disposal**

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

**Physical and Chemical Hazards**

Combustible material.

**Health Hazards**

Toxic if swallowed. Toxic in contact with skin. Causes skin irritation. Causes serious eye irritation. Toxic if inhaled. May cause respiratory irritation.

**Environmental hazards**

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants.

**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 %
1-Hexyl isothiocyanate	4404-45-9	97

**SECTION 4. FIRST AID MEASURES**

**General Advice**

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.

**Inhalation**

Remove to fresh air. If breathing is difficult, give oxygen. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.

**Ingestion**

Do NOT induce vomiting. Call a physician or poison control center immediately.

**Most important symptoms and effects**

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

**Self-Protection of the First Aider**

Use personal protective equipment as required.

**Notes to Physician**

Treat symptomatically.

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

Water mist may be used to cool closed containers. Carbon dioxide (CO<sub>2</sub>). Powder. Alcohol resistant foam.

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

No information available.

**Specific Hazards Arising from the Chemical**

Keep product and empty container away from heat and sources of ignition. Risk of ignition. Combustible material. Containers may explode when heated.

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

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

Use personal protective equipment as required. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.

**Environmental Precautions**

Should not be released into the environment. See Section 12 for additional Ecological Information.

**Methods for Containment and Clean Up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition.

Refer to protective measures listed in Sections 8 and 13.

## 1-Hexyl isothiocyanate

## SECTION 7. HANDLING AND STORAGE

**Handling**

Use only under a chemical fume hood. Wear personal protective equipment/face protection. Do not breathe mist/vapors/spray. Do not get in eyes, on skin, or on clothing. Do not ingest. If swallowed then seek immediate medical assistance. Keep away from open flames, hot surfaces and sources of ignition. Wash hands before breaks and immediately after handling the product.

**Storage**

Keep away from heat, sparks and flame. Keep container tightly closed in a dry and well-ventilated place. Store under an inert atmosphere. Keep refrigerated.

**Specific Use(s)**

Use in laboratories

## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

**Control Parameters****Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours

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

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. 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
Natural rubber	See manufacturers	-	EN 374	(minimum requirement)
Nitrile rubber	recommendations			
Neoprene				
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**

Long sleeved clothing

**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**

Colorless to 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**

108 - 110 °C / 226.4 - 230 °F

@ 15 mmHg

**Flash Point**

91 °C / 195.8 °F

**Method -** CC (closed cup)

**Evaporation Rate**

No data available

**Flammability (solid,gas)**

Not applicable

Liquid

**Explosion Limits**

No data available

**Vapor Pressure**

No data available

**Vapor Density**

No data available

(Air = 1.0)

**Specific Gravity / Density**

0.933

**Bulk Density**

Not applicable

Liquid

**Water Solubility**

No information available

**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**

explosive air/vapour mixtures possible

**Oxidizing Properties**

No information available

**Molecular Formula**

C7 H13 N S

**Molecular Weight**

143.25

**SECTION 10. STABILITY AND REACTIVITY****Stability**

Stable under recommended storage conditions.

**Hazardous Reactions**

None under normal processing.

**Hazardous Polymerization**

Hazardous polymerization does not occur.

**Conditions to Avoid**

Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition. Exposure to moist air or water.

**Materials to avoid**

Strong oxidizing agents. Bases. Amines. Strong reducing agents.

**Hazardous Decomposition Products** Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Nitrogen oxides (NO<sub>x</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
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(i) STOT-repeated exposure; No data available

Target Organs	No information available.
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(j) aspiration hazard; No data available

Symptoms / effects, both acute and delayed	Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
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**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.
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Persistence and Degradability	No information available
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Bioaccumulative Potential	No information available
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Mobility in soil	No information available
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Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant	This product does not contain any known or suspected substance
Ozone Depletion Potential	This product does not contain any known or suspected substance

**SECTION 13. DISPOSAL CONSIDERATIONS**

## 1-Hexyl isothiocyanate

**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.  
**Technical Shipping Name** (Hexyl isothiocyanate)  
**Hazard Class** 6.1  
**Packing Group** III

**IMDG/IMO**

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

**IATA**

**UN-No** UN2810  
**Proper Shipping Name** Toxic liquid, organic, n.o.s.  
**Technical Shipping Name** (Hexyl isothiocyanate)  
**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
1-Hexyl isothiocyanate	-	-	X	-	224-549-2	-	-	-	-		-	-

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

## 1-Hexyl isothiocyanate

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<b>Prepared By</b>	Health, Safety and Environmental Department
<b>Revision Date</b>	27-Apr-2024
<b>Revision Summary</b>	New emergency telephone response service provider.

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**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/NDL** - 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

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

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

**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**

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The 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, unless specified in the text

**End of Safety Data Sheet**