

Hexyl isothiocyanate

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830
Date of issue: 4/15/2019 Version: 1.0

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

1.1. Product identifier

Product form	: Substance
Substance name	: Hexyl isothiocyanate
IUPAC name	: 1-Isothiocyanatohexane
EC-No.	: 224-549-2
CAS-No.	: 4404-45-9
Product code	: 12971778
Formula	: C7H13NS
Product group	: Raw material

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

1.2.1. Relevant identified uses

Main use category	: Laboratory use, Industrial use, Professional use
Industrial/Professional use spec	: For professional use only

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Supplier

Scafell Organics
Molekula Ltd
Lingfield Way
Darlington - England
T +44 (0) 1949 823777 / +44 (0) 7590 545705
info@molekula.com / kbowen@molekula.com - www.molekula.com

1.4. Emergency telephone number

Emergency number : +44 (0) 7590 545705

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Acute toxicity (oral), Category 3	H301
Acute toxicity (dermal), Category 3	H311
Acute toxicity (inhal.), Category 3	H331
Skin corrosion/irritation, Category 2	H315
Serious eye damage/eye irritation, Category 2	H319
Specific target organ toxicity — Single exposure, Category 3, Respiratory tract irritation	H335
Full text of H statements : see section 16	

Adverse physicochemical, human health and environmental effects

No additional information available

2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS06

Signal word (CLP) :

Danger

Hazard statements (CLP) :

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

Precautionary statements (CLP) :

P260 - Do not breathe mist, spray, vapours.
P280 - Wear protective clothing, eye protection, face protection, protective gloves.
P301+P310 - IF SWALLOWED: Immediately call a POISON CENTER.
P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308+P311 - IF exposed or concerned: Call a POISON CENTER.

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2.3. Other hazards

This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII

This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

SECTION 3: Composition/information on ingredients

3.1. Substances

Name	Product identifier	%
Hexyl isothiocyanate	(CAS-No.) 4404-45-9 (EC-No.) 224-549-2	100

Full text of H-statements: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general	: If possible show this sheet, if not available show packaging or label. Never give anything by mouth to an unconscious person. Do not leave affected person unattended.
First-aid measures after inhalation	: If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing. Give oxygen or artificial respiration if necessary. If breathing difficulties persist : Get medical advice/attention.
First-aid measures after skin contact	: After contact with skin, take off immediately all contaminated clothing, and wash immediately with plenty of water. Do not remove clothing if it sticks to the skin. If irritation persists, consult a doctor.
First-aid measures after eye contact	: Rinse immediately with plenty of water. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.
First-aid measures after ingestion	: Rinse mouth out with water. Do not induce vomiting. Get medical advice/attention.

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

Symptoms/effects after inhalation	: May cause irritation to the respiratory tract, sneezing, coughing, burning sensation of throat with constricting sensation of the larynx and difficulty in breathing. Headache. Toxic if inhaled. More severe symptoms are also possible.
Symptoms/effects after skin contact	: Could cause toxic effects if inhaled or absorbed through skin. May cause skin irritation. Redness, pain. More severe symptoms are also possible.
Symptoms/effects after eye contact	: May cause severe irritation. Blurred vision. redness, itching, tears. stinging. More severe symptoms are also possible.
Symptoms/effects after ingestion	: Swallowing a small quantity of this material will result in serious health hazard. Symptoms of ingestion include drowsiness, weakness, headache, dizziness, nausea, vomiting. More severe symptoms are also possible.

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

Immediately call a POISON CENTER/doctor.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	: Foam. Dry powder. Carbon dioxide. Water spray. Sand.
Unsuitable extinguishing media	: Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

Hazardous decomposition products in case of fire	: Carbon oxides (CO, CO ₂). Nitrogen oxides. Sulphur oxides.
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5.3. Advice for firefighters

Precautionary measures fire	: Keep container tightly closed and away from heat, sparks and flame. Keep away from combustible materials.
Firefighting instructions	: Use water spray or fog for cooling exposed containers. Exercise caution when fighting any chemical fire. Prevent fire fighting water from entering the environment.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection.
Other information	: Warn all persons of toxic hazard.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures	: Isolate from fire, if possible, without unnecessary risk. Do not breathe gas, fumes, vapour or spray. No flames, no sparks. Eliminate all sources of ignition.
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6.1.1. For non-emergency personnel

Protective equipment	: Wear recommended personal protective equipment.
Emergency procedures	: Evacuate unnecessary personnel. Mark out the contaminated area with signs and prevent access to unauthorized personnel. Do not touch or walk on the spilled product. Avoid contact with skin, eyes and clothing.

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Measures in case of dust release : Shelter from vapours by keeping upwind. Ventilate the area thoroughly, especially low lying areas (basements, workpits etc).

6.1.2. For emergency responders

Protective equipment : Equip cleanup crew with proper protection. Use self-contained breathing apparatus and chemically protective clothing.

Emergency procedures : Ventilate area.

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

For containment : Collect spillage. Contain the spilled material by bunding.

Methods for cleaning up : Soak up spills with inert solids, such as clay or diatomaceous earth as soon as possible. Try to stop release if without risk.

6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Avoid formation of vapours. Provide local exhaust or general room ventilation.

Hygiene measures : Take off immediately all contaminated clothing and wash it before reuse. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Do not eat, drink or smoke when using this product.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Ensure adequate ventilation, especially in confined areas.

Storage conditions : Keep only in the original container in a cool, well ventilated place away from : Heat sources, Direct sunlight. Keep container closed when not in use. Moisture sensitive. Store contents under inert gas.

Incompatible products : Strong oxidisers. Strong bases.

Incompatible materials : Sources of ignition. Direct sunlight. Heat sources. Moisture. Water, humidity.

Heat and ignition sources : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Storage area : Store below 20 °C. Store in dry protected location to prevent any moisture contact.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Appropriate engineering controls:

Handle in accordance with good industrial hygiene and safety procedures. Floors should be impervious, resistant to liquids and easy to clean.

Personal protective equipment:

Avoid all unnecessary exposure.

Hand protection:					
The protective gloves to be used must comply with the specifications of the regulation 2016/425 and the resultant standard EN 374					
Type	Material	Permeation	Thickness (mm)	Penetration	Standard
Disposable gloves	Butyl rubber	6 (> 480 minutes)	0.11		EN 374
Eye protection:					
Emergency eye wash fountains should be available in the immediate vicinity of any potential exposure. Use eye protection according to EN 166, designed to protect against liquid splashes.					
Type	Use	Characteristics	Standard		
Safety goggles, Face shield	Droplet, vapours	tightly fitting safety goggles, With side shields	EN 166		
Skin and body protection:					
Emergency safety showers should be available in the immediate vicinity of any potential exposure. Keep suitable chemically resistant protective clothing readily available for emergency use					

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Type	Standard		
Total impervious protective suits, gloves, and boots must be worn to prevent any contact with the product	EN 14605		
Respiratory protection:			
Keep self contained breathing apparatus readily available for emergency use. Where exposure through inhalation may occur from use, respiratory protection equipment is recommended			
Device	Filter type	Condition	Standard
Air-Purifying Respirator (APR), reusable	ABEK	Moist condition, Mist formation, Protection for Liquid particles, Vapour protection	EN 14387

Other information:

Do not eat, drink or smoke during use.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Appearance	: Clear.
Molecular mass	: 143.25 g/mol
Colour	: Colourless to pale yellow.
Odour	: No data available.
Odour threshold	: No data available
pH	: No data available
Relative evaporation rate (butylacetate=1)	: No data available
Melting point	: No data available
Freezing point	: No data available
Boiling point	: 136 - 138 °C lit.
Flash point	: 91 °C closed cup.
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: Non flammable.
Vapour pressure	: No data available
Relative vapour density at 20 °C	: No data available
Relative density	: 0.929 g/cm ³
Solubility	: No data available
Log Pow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidising properties	: No data available
Explosive limits	: No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

10.2. Chemical stability

Stable under recommended handling and storage conditions (see section 7).

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

Protect from sunlight. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Moisture. Water, humidity.

10.5. Incompatible materials

Strong oxidizers. Strong bases.

10.6. Hazardous decomposition products

No hazardous decomposition products known at room temperature. Thermal decomposition generates : Carbon oxides (CO, CO₂). Nitrogen oxides. Sulphur oxides.

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SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity (oral)	: Oral: Toxic if swallowed.
Acute toxicity (dermal)	: Dermal: Toxic in contact with skin.
Acute toxicity (inhalation)	: Inhalation: Toxic if inhaled.
Skin corrosion/irritation	: Causes skin irritation.
Additional information	: Based on available data, the classification criteria are not met
Serious eye damage/irritation	: Causes serious eye irritation.
Additional information	: Based on available data, the classification criteria are not met
Respiratory or skin sensitisation	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Germ cell mutagenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Carcinogenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Reproductive toxicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-single exposure	: May cause respiratory irritation.
Additional information	: Based on available data, the classification criteria are not met
STOT-repeated exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Aspiration hazard	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Potential adverse human health effects and symptoms	: Based on available data, the classification criteria are not met.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity	: Not classified
Chronic aquatic toxicity	: Not classified

12.2. Persistence and degradability

Hexyl isothiocyanate (4404-45-9)

Persistence and degradability	No data available.
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12.3. Bioaccumulative potential

Hexyl isothiocyanate (4404-45-9)

Bioaccumulative potential	No data available.
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12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

Hexyl isothiocyanate (4404-45-9)

This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII

This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

12.6. Other adverse effects

Additional information	: Avoid release to the environment.
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SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product/Packaging disposal recommendations	: Dispose in a safe manner in accordance with local/national regulations.
Ecology - waste materials	: Avoid release to the environment. Hazardous waste due to toxicity.

SECTION 14: Transport information






In accordance with ADR / RID / IMDG / IATA / ADN

ADR	IMDG	IATA	ADN	RID
14.1. UN number				
2810	2810	2810	2810	2810


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14.2. UN proper shipping name				
TOXIC LIQUID, ORGANIC, N.O.S.	TOXIC LIQUID, ORGANIC, N.O.S.	Toxic liquid, organic, n.o.s.	TOXIC LIQUID, ORGANIC, N.O.S.	TOXIC LIQUID, ORGANIC, N.O.S.
Transport document description				
UN 2810 TOXIC LIQUID, ORGANIC, N.O.S. (Hexyl isothiocyanate), 6.1, III, (E)	UN 2810 TOXIC LIQUID, ORGANIC, N.O.S. (Hexyl isothiocyanate), 6.1, III	UN 2810 Toxic liquid, organic, n.o.s. (Hexyl isothiocyanate), 6.1, III	UN 2810 TOXIC LIQUID, ORGANIC, N.O.S. (Hexyl isothiocyanate), 6.1, III	UN 2810 TOXIC LIQUID, ORGANIC, N.O.S. (Hexyl isothiocyanate), 6.1, III
14.3. Transport hazard class(es)				
6.1	6.1	6.1	6.1	6.1
				
14.4. Packing group				
III	III	III	III	III
14.5. Environmental hazards				
Dangerous for the environment : No	Dangerous for the environment : No Marine pollutant : No	Dangerous for the environment : No	Dangerous for the environment : No	Dangerous for the environment : No
No supplementary information available				
14.6. Special precautions for user				

Overland transport

Classification code (ADR)	: T1
Special provisions (ADR)	: 274, 614
Limited quantities (ADR)	: 5I
Excepted quantities (ADR)	: E1
Packing instructions (ADR)	: P001, IBC03, LP01, R001
Mixed packing provisions (ADR)	: MP19
Portable tank and bulk container instructions (ADR)	: T7
Portable tank and bulk container special provisions (ADR)	: TP1, TP28
Tank code (ADR)	: L4BH
Tank special provisions (ADR)	: TU15, TE19
Vehicle for tank carriage	: AT
Transport category (ADR)	: 2
Special provisions for carriage - Packages (ADR)	: V12
Special provisions for carriage - Loading, unloading and handling (ADR)	: CV13, CV28
Special provisions for carriage - Operation (ADR)	: S9
Hazard identification number (Kemler No.)	: 60
Orange plates	: 

Tunnel restriction code (ADR)	: E
EAC code	: 2X
APP code	: B

Transport by sea

Special provisions (IMDG)	: 223, 274
Packing instructions (IMDG)	: P001, LP01
IBC packing instructions (IMDG)	: IBC03
Tank instructions (IMDG)	: T7
Tank special provisions (IMDG)	: TP1, TP28
EmS-No. (Fire)	: F-A
EmS-No. (Spillage)	: S-A

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Stowage category (IMDG) : A
Stowage and handling (IMDG) : SW2
Properties and observations (IMDG) : Toxic if swallowed, by skin contact or by inhalation.

Air transport

PCA Excepted quantities (IATA) : E1
PCA Limited quantities (IATA) : Y642
PCA limited quantity max net quantity (IATA) : 2L
PCA packing instructions (IATA) : 655
PCA max net quantity (IATA) : 60L
CAO packing instructions (IATA) : 663
CAO max net quantity (IATA) : 220L
Special provisions (IATA) : A3, A4, A137
ERG code (IATA) : 6L

Inland waterway transport

Classification code (ADN) : T1
Special provisions (ADN) : 274, 614, 802
Limited quantities (ADN) : 5 L
Excepted quantities (ADN) : E1
Carriage permitted (ADN) : T
Equipment required (ADN) : PP, EP, TOX, A
Ventilation (ADN) : VE02
Number of blue cones/lights (ADN) : 0

Rail transport

Classification code (RID) : T1
Special provisions (RID) : 274, 614
Excepted quantities (RID) : E1
Packing instructions (RID) : P001, IBC03, LP01, R001
Mixed packing provisions (RID) : MP19
Portable tank and bulk container instructions (RID) : T7
Portable tank and bulk container special provisions (RID) : TP1, TP28
Tank codes for RID tanks (RID) : L4BH
Special provisions for RID tanks (RID) : TU15
Transport category (RID) : 2
Special provisions for carriage – Packages (RID) : W12
Special provisions for carriage - Loading, unloading and handling (RID) : CW13, CW28, CW31
Colis express (express parcels) (RID) : CE8
Hazard identification number (RID) : 60

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

Not applicable

SECTION 15: Regulatory information

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

15.1.1. EU-Regulations

No REACH Annex XVII restrictions
Hexyl isothiocyanate is not on the REACH Candidate List
Directive 2012/18/EU (SEVESO III)

15.1.2. National regulations

Germany

12th Ordinance Implementing the Federal Immission Control Act - 12.BImSchV : Is not subject of the 12. BImSchV (Hazardous Incident Ordinance)

Netherlands

SZW-lijst van kankerverwekkende stoffen : The substance is not listed
SZW-lijst van mutagene stoffen : The substance is not listed
NIET-limitatieve lijst van voor de voortplanting giftige stoffen – Borstvoeding : The substance is not listed

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NIET-limitatieve lijst van voor de voortplanting giftige stoffen – Vruchtbaarheid : The substance is not listed

NIET-limitatieve lijst van voor de voortplanting giftige stoffen – Ontwikkeling : The substance is not listed

Denmark

Class for fire hazard : Class III-1

Store unit : 50 liter

Classification remarks : Flammable according to the Danish Ministry of Justice; Emergency management guidelines for the storage of flammable liquids must be followed

Danish National Regulations : Young people below the age of 18 years are not allowed to use the product
Pregnant/breastfeeding women working with the product must not be in direct contact with the product

15.2. Chemical safety assessment

No chemical safety assessment has been carried out for the substance or the mixture by the supplier

SECTION 16: Other information

Data sources : REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

Other information : None.

Full text of H- and EUH-statements:	
Acute Tox. 3 (Dermal)	Acute toxicity (dermal), Category 3
Acute Tox. 3 (Inhalation)	Acute toxicity (inhal.), Category 3
Acute Tox. 3 (Oral)	Acute toxicity (oral), Category 3
Eye Irrit. 2	Serious eye damage/eye irritation, Category 2
Skin Irrit. 2	Skin corrosion/irritation, Category 2
STOT SE 3	Specific target organ toxicity — Single exposure, Category 3, Respiratory tract irritation
H301	Toxic if swallowed.
H311	Toxic in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H331	Toxic if inhaled.
H335	May cause respiratory irritation.

SDS EU (REACH Annex II)

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.