

SAFETY DATA SHEET

Version: v1

Revision Date: 2025-09-14

Print Date: 2025-09-21

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

1.1 Product identifiers

Product name	: Hexyl isothiocyanate
Product Number	: H140517
Brand	: aladdin
CAS-No.	: 4404-45-9

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

Identified uses	: Laboratory chemicals, Manufacture of substances.
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1.3 Company

Company	: ALADDIN SCIENTIFIC CORPORATION
Address	: 14078 Meridian Parkway, Riverside, CA. 92518
Telephone	: +1 (833) 552-7181
Fax	: no data available

1.4 Emergency telephone number

CHEMTREC®, Inside the USA	: 1-800-424-9300
CHEMTREC®, Outside the USA	:

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Danger

Hazard statement(s)

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

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Precautionary statement(s)

P261	Avoid breathing dust/fume/gas/mist/vapors/spray.
P264	Wash hands [and ...] 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.
P321	Specific treatment (see ... on this label).
P330	Rinse mouth.
P302+P352	IF ON SKIN: wash with plenty of 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.
P361+P364	Take off immediately all contaminated clothing and wash it before reuse.
P362+P364	Take off contaminated clothing and wash it before reuse.
P405	Store locked up.
P403+P233	Store in a well-ventilated place. Keep container tightly closed.
P501	Dispose of contents/container to an approved waste disposal plant.
P264+P265	Wash hands [and ...] thoroughly after handling. Do not touch eyes.
P301+P316	IF SWALLOWED: Get emergency medical help immediately.
P337+P317	If eye irritation persists: Get medical help.
P332+P317	If skin irritation occurs: Get medical help.
P316	Get emergency medical help immediately.
P319	Get medical help if you feel unwell.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS**SECTION 3: Composition/information on ingredients****3.1 Substances**

Synonyms	: 1-Isothiocyanatohexane;n-Hexyl mustard oil;1-Hexyl isothiocyanate
Formula	: C7H13NS
Molecular weight	: 143.25
CAS No.	: 4404-45-9
EC-NO.	: 224-549-2

Component	Classification	Concentration
Hexyl isothiocyanate	no data available	≥97%

SECTION 4: First aid measures

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

no data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Foam, Carbon dioxide (CO₂), Dry powder

Unsuitable extinguishing media

no data available

5.2 Special hazards arising from the substance or mixture

Carbon oxides, nitrogen oxides (NO_x), Sulphur oxides

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas. For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

7.3 Specific end use(s)

no data available

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching gloves outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multipurpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators

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and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

no data available

SECTION 9: Physical and chemical properties
9.1 Information on basic physical and chemical properties

a) Appearance	no data available
b) Odour	no data available
c) Odour Threshold	no data available
d) pH	no data available
e) Melting point/freezing point	no data available
f) Initial boiling point and boiling range	no data available
g) Flash point	no data available
h) Evaporation rate	no data available
i) Flammability (solid, gas)	no data available
j) Upper/lower flammability or explosive limits	no data available
k) Vapour pressure	no data available
l) Vapour density	no data available
m) Relative density	no data available
n) Water solubility	no data available
o) Partition coefficient: n-octanol/water	no data available
p) Auto-ignition temperature	no data available
q) Decomposition temperature	no data available
r) Viscosity	no data available
s) Explosive properties N	no data available
t) Oxidizing properties N	no data available

9.2 Other safety information

no data available

SECTION 10: Stability and reactivity
10.1 Reactivity

no data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

no data available

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10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Strong oxidizing agents Strong bases

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

no data available

Skin corrosion/irritation

no data available

Serious eye damage/eye irritation

no data available

Respiratory or skin sensitisation

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

no data available

Specific target organ toxicity - single exposure

no data available

Specific target organ toxicity - repeated exposure

no data available

Aspiration hazard

Inhalation - May cause respiratory irritation.

Additional Information

no data available

SECTION 12: Ecological information

12.1 Toxicity

no data available

12.2 Persistence and degradability

no data available

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12.3 Bioaccumulative potential

no data available

12.4 Mobility in soil

no data available

12.5 Results of PBT and vPvB assessment

no data available

12.6 Other adverse effects

no data available

SECTION 13:**13.1 Disposal considerations****Product**

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information**DOT (US)**

UN number: 3334

Packing group: no data available

Class: 9

Proper shipping name: A Aviation regulated liquid, n.o.s.(1-Hexyl isothiocyanate)

Reportable Quantity(RQ): no data available

Poison Inhalation Hazard: no data available

Environmental Hazards: No

IMDG

UN number: 3334

Packing group: no data available

EMS-No: no data available

Proper shipping name: A Aviation regulated liquid, n.o.s.(1-Hexyl isothiocyanate)

IATA

UN number: 3334

Packing group: no data available

Class: 9

Proper shipping name: A Aviation regulated liquid, n.o.s.(1-Hexyl isothiocyanate)

SECTION 15: Regulatory information

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

SECTION 16: Other information

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Creation Date

10-Sep-2020

Revision Date

14-Sep-2025

Print Date

21-Sep-2025

Revision Summary

SDS sections updated v1

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