

SAFETY DATA SHEET

Version 6.4
Revision Date 02/25/2021
Print Date 05/28/2022

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : 3-Iodo-2-propynyl *N*-butylcarbamate

Product Number : 521949
Brand : Aldrich
CAS-No. : 55406-53-6

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 3), H331
Serious eye damage (Category 1), H318
Respiratory sensitization (Category 1), H334
Specific target organ toxicity - repeated exposure (Category 1), larynx, H372
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word	Danger
Hazard statement(s)	
H302	Harmful if swallowed.
H318	Causes serious eye damage.
H331	Toxic if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H372	Causes damage to organs (larynx) through prolonged or repeated exposure.
H410	Very toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
P260	Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash 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.
P273	Avoid release to the environment.
P280	Wear eye protection/ face protection.
P285	In case of inadequate ventilation wear respiratory protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P342 + P311	If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.
P391	Collect spillage.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Molecular weight	: 281.09 g/mol
CAS-No.	: 55406-53-6
EC-No.	: 259-627-5

Component	Classification	Concentration
3-Iodo-2-propynyl butylcarbamate		
	Acute Tox. 4; Acute Tox. 3; Eye Dam. 1; Resp. Sens. 1; STOT RE 1; Aquatic Acute 1; Aquatic Chronic 1; H302, H331, H318, H334, H372, H400, H410 M-Factor - Aquatic Acute:	<= 100 %

	10 M-Factor - Aquatic Chronic: 10	
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For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

First aider needs to protect himself. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Hydrogen iodide

Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.
For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.
Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

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

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

Body Protection

protective clothing

Respiratory protection

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---------------------------------|---|
| a) Appearance | Form: crystalline
Color: light yellow |
| b) Odor | weak |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: 64 - 68 °C (147 - 154 °F) - lit. |
| f) Initial boiling point | No data available |

and boiling range

- | | |
|---|---|
| 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) Vapor pressure | < 0.1 hPa at 25 °C (77 °F) - OECD Test Guideline 104 |
| l) Vapor density | No data available |
| m) Relative density | 1.76 |
| n) Water solubility | 0.168 g/l at 20 °C (68 °F) - OECD Test Guideline 105 |
| o) Partition coefficient: n-octanol/water | log Pow: 2.81 at 25 °C (77 °F) - OECD Test Guideline 107 - Bioaccumulation is not expected. |
| p) Autoignition temperature | does not ignite |
| q) Decomposition temperature | No data available |
| r) Viscosity | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | No data available |

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) . Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

Strong oxidizing agents

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

LD50 Oral - Rat - male and female - 1,470 mg/kg
(OECD Test Guideline 401)

Remarks:

(Regulation (EC) No 1272/2008, Annex VI)

LC50 Inhalation - Rat - male and female - 4 h - 0.68 mg/l
(OECD Test Guideline 403)

Remarks:

(Regulation (EC) No 1272/2008, Annex VI)

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg
(US-EPA)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(US-EPA)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage. - 30 s

(US-EPA)

Remarks:

(Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: positive

(OECD Test Guideline 406)

Remarks:

(Regulation (EC) No 1272/2008, Annex VI)

Germ cell mutagenicity

In vitro mammalian cell gene mutation test

Chinese hamster lung cells

Result: negative

Ames test

Escherichia coli/Salmonella typhimurium

Result: negative

OECD Test Guideline 474

Mouse - male and female - Red blood cells (erythrocytes)

Result: negative

Carcinogenicity

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

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Causes damage to organs through prolonged or repeated exposure. - larynx

Remarks:

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Aspiration hazard

No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - 91 Days - NOAEL (No observed adverse effect level) - 200 mg/kg - LOAEL (Lowest observed adverse effect level) - 500 mg/kg
RTECS: EZ0950000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish	LC50 - Oncorhynchus mykiss (rainbow trout) - 0.067 mg/l - 96 h Remarks: (ECOTOX Database)
Toxicity to daphnia and other aquatic invertebrates	LC50 - Daphnia magna (Water flea) - 0.04 mg/l - 48 h Remarks: (ECOTOX Database)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - 0.053 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - activated sludge - 44 mg/l - 3 h (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 5 % - Not readily biodegradable.
(OECD Test Guideline 301B)

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 2811 Class: 6.1 Packing group: III
Proper shipping name: Toxic solids, organic, n.o.s. (3-Iodo-2-propynyl butylcarbamate)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2811 Class: 6.1 Packing group: III EMS-No: F-A, S-A
Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (3-Iodo-2-propynyl butylcarbamate)
Marine pollutant : yes

IATA

UN number: 2811 Class: 6.1 Packing group: III
Proper shipping name: Toxic solid, organic, n.o.s. (3-Iodo-2-propynyl butylcarbamate)

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

3-Iodo-2-propynyl butylcarbamate	CAS-No. 55406-53-6	Revision Date 2007-07-01
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SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

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3-Iodo-2-propynyl butylcarbamate

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New Jersey Right To Know Components

3-Iodo-2-propynyl butylcarbamate

CAS-No.
55406-53-6

Revision Date
2007-07-01

SECTION 16: Other information

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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