

## SAFETY DATA SHEET

Version 8.5  
Revision Date 03/02/2024  
Print Date 03/23/2024

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

Product name : Butyl isocyanate

Product Number : B95736  
Brand : Aldrich  
CAS-No. : 111-36-4

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

**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)**

Flammable liquids (Category 2), H225  
Acute toxicity, Oral (Category 4), H302  
Acute toxicity, Inhalation (Category 1), H330  
Skin corrosion (Category 1B), H314

Serious eye damage (Category 1), H318  
 Respiratory sensitization (Category 1), H334  
 Skin sensitization (Category 1), H317  
 Short-term (acute) aquatic hazard (Category 3), H402  
 Long-term (chronic) aquatic hazard (Category 3), H412

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 Statements

H225	Highly flammable liquid and vapor.
H302	Harmful if swallowed.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H330	Fatal if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H412	Harmful to aquatic life with long lasting effects.

Precautionary Statements

P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
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.
P272	Contaminated work clothing must not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P284	Wear respiratory protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately 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.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.

P342 + P311	If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
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

Lachrymator.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Molecular weight	: 99.13 g/mol
CAS-No.	: 111-36-4
EC-No.	: 203-862-8

Component	Classification	Concentration
<b>butyl isocyanate</b>		
	Flam. Liq. 2; Acute Tox. 4; Acute Tox. 1; Skin Corr. 1B; Eye Dam. 1; Resp. Sens. 1; Skin Sens. 1; Aquatic Acute 3; Aquatic Chronic 3; H225, H302, H330, H314, H318, H334, H317, H402, H412	<= 100 %

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 aiders need to protect themselves. 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. Call a physician immediately.

**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: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

**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**

Carbon dioxide (CO<sub>2</sub>) Dry powder

**Unsuitable extinguishing media**

Foam Water

**5.2 Special hazards arising from the substance or mixture**

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

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

Forms explosive mixtures with air at ambient temperatures.

**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**

Remove container from danger zone and cool with water. 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: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

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. Risk of explosion.

### **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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

### **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. Avoid generation of vapours/aerosols.

#### **Advice on protection against fire and explosion**

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

#### **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**

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Store under inert gas.

#### **Storage class**

Storage class (TRGS 510): 3: Flammable liquids

### **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

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's 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.

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.2 mm

Break through time: 30 min

Material tested: Dermatrill® P (KCL 743 / Aldrich Z677388, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### Body Protection

Flame retardant antistatic protective clothing.

### Respiratory protection

Recommended Filter type: Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

required when vapours/aerosols 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. Risk of explosion.

---

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |                   |  |
|-------------------|--|
| a) Appearance     | Form: clear, liquid<br>Color: light yellow |
| b) Odor           | No data available                          |
| c) Odor Threshold | No data available                          |

d) pH	No data available
e) Melting point/freezing point	Melting point/freezing point: -75 °C (-103 °F) - (ECHA)
f) Initial boiling point and boiling range	115 °C 239 °F - lit.
g) Flash point	11 °C (52 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 10 %(V) Lower explosion limit: 1.3 %(V)
k) Vapor pressure	24.8 hPa at 21 °C (70 °F)
l) Vapor density	3.42 - (Air = 1.0)
m) Density	0.88 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	425 °C (797 °F) at 1,013 hPa
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

Relative vapor density	3.42 - (Air = 1.0)
------------------------	--------------------

---

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Vapors may form explosive mixture with air.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

Exothermic reaction with:  
Alcohols

Amines  
Bases  
Oxidizing agents  
Acids  
Water  
Release of:  
Carbon dioxide (CO<sub>2</sub>)

#### **10.4 Conditions to avoid**

Heat. Avoid moisture. Do not allow water to enter container because of violent reaction. Warming.

#### **10.5 Incompatible materials**

No data available

#### **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**

Acute toxicity estimate Oral - 360 mg/kg

(Calculation method)

LD<sub>50</sub> Oral - Rat - male - 360 mg/kg

Remarks: (ECHA)

Acute toxicity estimate Inhalation - 0.06 mg/l (Calculation method)

LC<sub>50</sub> Inhalation - Rat - male and female - 4 h - 0.059 mg/l - vapor

(OECD Test Guideline 403)

Acute toxicity estimate Dermal - 700 mg/kg

(Calculation method)

Dermal: No data available

No data available

##### **Skin corrosion/irritation**

Skin - Rabbit

Result: Causes burns.

Remarks: (ECHA)

##### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Causes burns.

Remarks: (ECHA)

##### **Respiratory or skin sensitization**

Sensitisation test: - Guinea pig

Result: positive

Remarks: (ECHA)

##### **Germ cell mutagenicity**

Aldrich - B95736

Page 8 of 12



Test Type: Ames test  
Test system: *S. typhimurium*  
Metabolic activation: with and without metabolic activation  
Result: negative  
Remarks: (ECHA)

### **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**

No data available

### **Aspiration hazard**

No data available

## **11.2 Additional Information**

Repeated dose toxicity - Rat - male - inhalation (vapor)  
Remarks: (ECHA)

RTECS: NQ8250000

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Cough, Shortness of breath, Headache, Nausea, 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	static test LC50 - <i>Lepomis macrochirus</i> - 32 mg/l - 96 h Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - <i>Daphnia magna</i> (Water flea) - > 100 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test EC50 - <i>Desmodesmus subspicatus</i> (green algae) - 51.1 mg/l - 72 h (Regulation (EC) No. 440/2008, Annex, C.3)

### **12.2 Persistence and degradability**

Aldrich - B95736

Page 9 of 12

Biodegradability      aerobic - Exposure time 20 d  
Result: 62 % - Readily biodegradable.  
Remarks: (ECHA)

### **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 Endocrine disrupting properties**

No data available

### **12.7 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](http://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: 2485    Class: 6.1I (3)    Packing group: I  
Proper shipping name: n-Butyl isocyanate  
Reportable Quantity (RQ):

Poison Inhalation Hazard: Hazard Zone B

#### **IMDG**

UN number: 2485    Class: 6.1 (3)    Packing group: I    EMS-No: F-E, S-D  
Proper shipping name: n-BUTYL ISOCYANATE

#### **IATA**

UN number: 2485    Class: 6.1 (3)  
Proper shipping name: n-Butyl isocyanate  
IATA Passenger: Not permitted for transport  
IATA Cargo: Not permitted for transport

Aldrich - B95736

Page 10 of 12

---

## SECTION 15: Regulatory information

### SARA 302 Components

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

### SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

### Massachusetts Right To Know Components

butyl isocyanate	CAS-No. 111-36-4	Revision Date 2007-03-01
------------------	---------------------	-----------------------------

butyl isocyanate	CAS-No. 111-36-4	Revision Date 2007-03-01
------------------	---------------------	-----------------------------

### Pennsylvania Right To Know Components

butyl isocyanate	CAS-No. 111-36-4	Revision Date 2007-03-01
------------------	---------------------	-----------------------------

butyl isocyanate	CAS-No. 111-36-4	Revision Date 2007-03-01
------------------	---------------------	-----------------------------

### New Jersey Right To Know Components

butyl isocyanate	CAS-No. 111-36-4	Revision Date 2007-03-01
------------------	---------------------	-----------------------------

---

## SECTION 16: Other information

### Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 8.5

Revision Date: 03/02/2024

Print Date: 03/23/2024