

## SAFETY DATA SHEET

Version 4.2  
Revision Date 07/03/2014  
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1. PRODUCT AND COMPANY IDENTIFICATION

## 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, Manufacture of substances

## 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

## 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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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  
Acute toxicity, Dermal (Category 3), H311  
Skin corrosion (Category 1B), H314  
Serious eye damage (Category 1), H318  
Respiratory sensitisation (Category 1), H334

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)

H225 : Highly flammable liquid and vapour.  
H302 : Harmful if swallowed.  
H311 : Toxic in contact with skin.  
H314 : Causes severe skin burns and eye damage.  
H330 : Fatal if inhaled.  
H334 : May cause allergy or asthma symptoms or breathing difficulties if inhaled.

Precautionary statement(s)

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/ vapours/ 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.                                                                                  |
| P280               | Wear protective gloves/ protective clothing/ eye protection/ face protection.                                                    |
| P284               | Wear respiratory protection.                                                                                                     |
| P301 + P312        | IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell.                                                      |
| P301 + P330 + P331 | IF SWALLOWED: rinse mouth. Do NOT induce vomiting.                                                                               |
| P303 + P361 + P353 | IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.                     |
| P304 + P340        | IF INHALED: Remove victim to fresh air and keep at rest in a position 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. |
| P310               | Immediately call a POISON CENTER or doctor/ physician.                                                                           |
| P320               | Specific treatment is urgent (see supplemental first aid instructions on this label).                                            |
| P361               | Remove/Take off immediately all contaminated clothing.                                                                           |
| P363               | Wash contaminated clothing before reuse.                                                                                         |
| P370 + P378        | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.                                            |
| 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.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

|                  |                                    |
|------------------|------------------------------------|
| Formula          | : C <sub>5</sub> H <sub>9</sub> NO |
| Molecular Weight | : 99.13 g/mol                      |
| CAS-No.          | : 111-36-4                         |
| EC-No.           | : 203-862-8                        |

#### Hazardous components

| Component               | Classification                                                                                                                       | Concentration |
|-------------------------|--------------------------------------------------------------------------------------------------------------------------------------|---------------|
| <b>Butyl isocyanate</b> |                                                                                                                                      |               |
|                         | Flam. Liq. 2; Acute Tox. 4; Acute Tox. 1; Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Resp. Sens. 1; H225, H302, H311, H314, H330, H334 | -             |

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

## 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**

Take off contaminated clothing and shoes immediately. 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. Continue rinsing eyes during transport to hospital.

**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

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**5. FIREFIGHTING MEASURES****5.1 Extinguishing media****Suitable extinguishing media**

For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

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

Carbon oxides, nitrogen oxides (NO<sub>x</sub>)

**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.

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**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).

**6.4 Reference to other sections**

For disposal see section 13.

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**7. HANDLING AND STORAGE****7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Use explosion-proof equipment. 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**

Store in cool place. 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.

Store under inert gas.

### 7.3 Specific end use(s)

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

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 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

Tightly fitting safety goggles. Faceshield (8-inch minimum). 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 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: Dermatril® 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 CE 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

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing, 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 multi-purpose 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 and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

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

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |                                 |                                             |
|---------------------------------|---------------------------------------------|
| a) Appearance                   | Form: clear, liquid<br>Colour: light yellow |
| 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      | 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 | no data available                       |
| k) Vapour pressure                              | no data available                       |
| l) Vapour density                               | 3.42 - (Air = 1.0)                      |
| m) Relative density                             | 0.88 g/cm <sup>3</sup> at 25 °C (77 °F) |
| 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                         | no data available                       |
| t) Oxidizing properties                         | no data available                       |

## 9.2 Other safety information

Relative vapour density 3.42 - (Air = 1.0)

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## 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

Vapours may form explosive mixture with air.

### 10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

### 10.5 Incompatible materials

Alcohols, Strong bases, Amines, acids, Strong oxidizing agents

### 10.6 Hazardous decomposition products

Other decomposition products - no data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - rat - 360 mg/kg

LC50 Inhalation - rat - 4 h - 0.06 mg/l

LD50 Dermal - rabbit - 700 mg/kg

no data available

**Skin corrosion/irritation**

no data available

**Serious eye damage/eye irritation**

no data available

**Respiratory or skin sensitisation****Germ cell mutagenicity**

no data available

**Carcinogenicity**

IARC: 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.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**

no data available

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

**Additional Information**

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

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**12. ECOLOGICAL INFORMATION****12.1 Toxicity**

Toxicity to fish LC0 - Leuciscus idus (Golden orfe) - 100 mg/l - 96 h

**12.2 Persistence and degradability**

no data available

**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

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

#### Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

#### Contaminated packaging

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

### DOT (US)

UN number: 2485      Class: 6.1 (3)      Packing group: I  
Proper shipping name: n-Butyl isocyanate  
Marine pollutant: No  
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: BUTYL ISOCYANATE  
Marine pollutant: No

### 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

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## 15. REGULATORY INFORMATION

### SARA 302 Components

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### SARA 313 Components

SARA 313: 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

|                  | CAS-No.  | Revision Date |
|------------------|----------|---------------|
| Butyl isocyanate | 111-36-4 | 1993-04-24    |

### Pennsylvania Right To Know Components

|                  | CAS-No.  | Revision Date |
|------------------|----------|---------------|
| Butyl isocyanate | 111-36-4 | 1993-04-24    |

### New Jersey Right To Know Components

|                  | CAS-No.  | Revision Date |
|------------------|----------|---------------|
| Butyl isocyanate | 111-36-4 | 1993-04-24    |

### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## 16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

|             |                                                                            |
|-------------|----------------------------------------------------------------------------|
| Acute Tox.  | Acute toxicity                                                             |
| Eye Dam.    | Serious eye damage                                                         |
| Flam. Liq.  | Flammable liquids                                                          |
| H225        | Highly flammable liquid and vapour.                                        |
| H302        | Harmful if swallowed.                                                      |
| H311        | Toxic in contact with skin.                                                |
| H314        | Causes severe skin burns and eye damage.                                   |
| H318        | Causes serious eye damage.                                                 |
| H330        | Fatal if inhaled.                                                          |
| H334        | May cause allergy or asthma symptoms or breathing difficulties if inhaled. |
| Resp. Sens. | Respiratory sensitisation                                                  |
| Skin Corr.  | Skin corrosion                                                             |

#### HMIS Rating

|                        |   |
|------------------------|---|
| Health hazard:         | 3 |
| Chronic Health Hazard: | * |
| Flammability:          | 3 |
| Physical Hazard        | 0 |

#### NFPA Rating

|                    |   |
|--------------------|---|
| Health hazard:     | 4 |
| Fire Hazard:       | 3 |
| Reactivity Hazard: | 0 |

#### Further information

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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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

#### Preparation Information

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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