SAFETY DATA SHEET
tert-Butyl isocyanate

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

1.1. Product identifier

Product name tert-Butyl isocyanate
Product number FB01362
CAS number 1609-86-5
EC number 216-544-9

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

Identified uses Laboratory reagent. Manufacture of substances. Research and development.

1.3. Details of the supplier of the safety data sheet

Supplier Carbosynth Ltd
8&9 Old Station Business Park
Compton
Berkshire
RG20 6NE
UK
+44 1635 578444
+44 1635 579444
info@carbosynth.com

1.4. Emergency telephone number

Emergency telephone +44 7887 998634

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (EC 1272/2008)

Physical hazards Flam. Liq. 2 - H225

Environmental hazards Not Classified

2.2. Label elements

EC number 216-544-9

Pictogram

Signal word Danger
tert-Butyl isocyanate

Hazard statements
H225 Highly flammable liquid and vapour.
H302+H312 Harmful if swallowed or in contact with skin.
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.
H335 May cause respiratory irritation.

Precautionary statements
P264 Wash contaminated skin thoroughly after handling.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing.
Rinse skin with water or shower.
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.

Supplemental label information
EUH014 Reacts violently with water.

2.3. Other hazards
No data available.

SECTION 3: Composition/information on ingredients

3.1. Substances
Product name tert-Butyl isocyanate
CAS number 1609-86-5
EC number 216-544-9
Chemical formula C₅H₉NO

SECTION 4: First aid measures

4.1. Description of first aid measures
General information Get medical advice/attention if you feel unwell.
Inhalation Remove person to fresh air and keep comfortable for breathing. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. If breathing stops, provide artificial respiration. Get medical attention if symptoms are severe or persist.
Ingestion Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth thoroughly with water. Give plenty of water to drink. Get medical attention if symptoms are severe or persist.
Skin contact Remove contaminated clothing. Rinse with water. Continue to rinse for at least 15 minutes. Wash contaminated clothing before reuse. Get medical attention if symptoms are severe or persist.
Eye contact Rinse immediately with plenty of water. Continue to rinse for at least 15 minutes. Get medical attention if symptoms are severe or persist.

4.2. Most important symptoms and effects, both acute and delayed
General information See Section 11 for additional information on health hazards.

4.3. Indication of any immediate medical attention and special treatment needed
Notes for the doctor Treat symptomatically.

SECTION 5: Firefighting measures
tert-Butyl isocyanate

5.1. Extinguishing media

Suitable extinguishing media
Extinguish with alcohol-resistant foam, carbon dioxide or dry powder. Use fire-extinguishing media suitable for the surrounding fire.

5.2. Special hazards arising from the substance or mixture

Specific hazards
The product is flammable. Vapours are heavier than air and may spread near ground and travel a considerable distance to a source of ignition and flash back. Reacts violently with water.

Hazardous combustion products
Thermal decomposition or combustion products may include the following substances: Oxides of carbon. Oxides of nitrogen.

5.3. Advice for firefighters

Special protective equipment for firefighters
Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter’s clothing conforming to European standard EN469 (including helmets, protective boots and gloves) will provide a basic level of protection for chemical incidents. Use protective equipment appropriate for surrounding materials.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions
Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Avoid inhalation of vapours. Provide adequate ventilation. Keep unnecessary and unprotected personnel away from the spillage. Vapours may accumulate on the floor and in low-lying areas. Eliminate all sources of ignition.

6.2. Environmental precautions

Environmental precautions
Avoid discharge into drains or watercourses or onto the ground.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up
Wear protective clothing as described in Section 8 of this safety data sheet. Absorb spillage with sand or other inert absorbent. Clear up spills immediately and dispose of waste safely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Provide adequate ventilation. For waste disposal, see Section 13.

6.4. Reference to other sections

Reference to other sections
For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Usage precautions
Wear protective clothing as described in Section 8 of this safety data sheet. Wash hands thoroughly after handling. Provide adequate ventilation. Avoid contact with skin and eyes. Do not breathe vapours. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Take precautionary measures against static discharges.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions
Keep container tightly closed. Keep containers upright. Store away from incompatible materials (see Section 10). Never allow product to get in contact with water. Store contents under inert gas. Store at room temperature.

7.3. Specific end use(s)

Specific end use(s)
The identified uses for this product are detailed in Section 1.2.
tert-Butyl isocyanate

SECTION 8: Exposure Controls/personal protection

8.1. Control parameters

Occupational exposure limits
No exposure limits known for ingredient(s).

8.2. Exposure controls

Appropriate engineering controls
Provide adequate ventilation.

Eye/face protection
Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses. Personal protective equipment for eye and face protection should comply with European Standard EN166.

Hand protection
Wear protective gloves. To protect hands from chemicals, gloves should comply with European Standard EN374.

Other skin and body protection
Wear appropriate clothing to prevent repeated or prolonged skin contact.

Respiratory protection
Respiratory protection complying with an approved standard should be worn if a risk assessment indicates inhalation of contaminants is possible. Ensure all respiratory protective equipment is suitable for its intended use and is ‘CE’-marked. Gas and combination filter cartridges should comply with European Standard EN14387. Full face mask respirators with replaceable filter cartridges should comply with European Standard EN136. Half mask and quarter mask respirators with replaceable filter cartridges should comply with European Standard EN140.

Environmental exposure controls
Keep container tightly sealed when not in use.

SECTION 9: Physical and Chemical Properties

9.1. Information on basic physical and chemical properties

Appearance
Liquid.

Colour
Colourless.

Odour
No data available.

Odour threshold
No data available.

pH
No data available.

Melting point
No data available.

Initial boiling point and range
No data available.

Flash point
- 4°C Closed cup.

Evaporation rate
No data available.

Flammability (solid, gas)
No data available.

Upper/lower flammability or explosive limits
No data available.

Vapour pressure
No data available.

Vapour density
No data available.

Relative density
0.868 g/cm³
tert-Butyl isocyanate

Solubility(ies) No data available.
Partition coefficient No data available.
Auto-ignition temperature No data available.
Decomposition Temperature No data available.
Viscosity No data available.
Explosive properties No data available.
Oxidising properties No data available.

9.2. Other information
Molecular weight 99.13

SECTION 10: Stability and reactivity

10.1. Reactivity
Reactivity No data available.

10.2. Chemical stability
Stability Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions
Possibility of hazardous reactions No data available.

10.4. Conditions to avoid
Conditions to avoid Avoid heat, flames and other sources of ignition. Avoid exposure to high temperatures or direct sunlight.

10.5. Incompatible materials

10.6. Hazardous decomposition products

SECTION 11: Toxicological information

11.1. Information on toxicological effects
Acute toxicity - oral
Acute toxicity oral (LD₅₀ mg/kg) 360.0
Species Rat
Notes (oral LD₅₀) Acute Tox. 4 - H302 Harmful if swallowed.
ATE oral (mg/kg) 500.0

Acute toxicity - dermal
Notes (dermal LD₅₀) Acute Tox. 4 - H312 Harmful in contact with skin.
ATE dermal (mg/kg) 1,100.0

Acute toxicity - inhalation
# tert-Butyl isocyanate

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Description</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Acute toxicity inhalation (LC₅₀ vapours mg/l)</strong></td>
<td>0.06</td>
<td>Rat</td>
<td>Acute Tox. 1 - H330 Fatal if inhaled.</td>
</tr>
<tr>
<td><strong>ATE inhalation (vapours mg/l)</strong></td>
<td>0.05</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Skin corrosion/irritation</strong></td>
<td></td>
<td></td>
<td>Animal data</td>
</tr>
<tr>
<td><strong>serious eye damage/irritation</strong></td>
<td></td>
<td></td>
<td>Eye Dam. 1 - H318 Corrosive to skin. Corrosivity to eyes is assumed.</td>
</tr>
<tr>
<td><strong>Respiratory sensitisation</strong></td>
<td></td>
<td></td>
<td>There is evidence that the product can cause respiratory hypersensitivity.</td>
</tr>
<tr>
<td><strong>Skin sensitisation</strong></td>
<td></td>
<td></td>
<td>May cause skin sensitisation or allergic reactions in sensitive individuals.</td>
</tr>
<tr>
<td><strong>Germ cell mutagenicity</strong></td>
<td></td>
<td></td>
<td>Genotoxicity - in vitro Based on available data the classification criteria are not met.</td>
</tr>
<tr>
<td><strong>Carcinogenicity</strong></td>
<td></td>
<td></td>
<td>Carcinogenicity</td>
</tr>
<tr>
<td><strong>IARC carcinogenicity</strong></td>
<td></td>
<td></td>
<td>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.</td>
</tr>
<tr>
<td><strong>Reproductive toxicity</strong></td>
<td></td>
<td></td>
<td>Reproductive toxicity</td>
</tr>
<tr>
<td><strong>Specific target organ toxicity - single exposure</strong></td>
<td></td>
<td></td>
<td>STOT - single exposure STOT SE 3 - H335 May cause respiratory irritation.</td>
</tr>
<tr>
<td><strong>Target organs</strong></td>
<td></td>
<td></td>
<td>Respiratory system, lungs</td>
</tr>
<tr>
<td><strong>Specific target organ toxicity - repeated exposure</strong></td>
<td></td>
<td></td>
<td>STOT - repeated exposure Not classified as a specific target organ toxicant after repeated exposure.</td>
</tr>
<tr>
<td><strong>Aspiration hazard</strong></td>
<td></td>
<td></td>
<td>Aspiration hazard</td>
</tr>
<tr>
<td><strong>General information</strong></td>
<td></td>
<td></td>
<td>The severity of the symptoms described will vary dependent on the concentration and the length of exposure.</td>
</tr>
<tr>
<td><strong>Inhalation</strong></td>
<td></td>
<td></td>
<td>May cause sensitisation or allergic reactions in sensitive individuals. A single exposure may cause the following adverse effects: Difficulty in breathing. Unconsciousness, possibly death.</td>
</tr>
<tr>
<td><strong>Ingestion</strong></td>
<td></td>
<td></td>
<td>May cause sensitisation or allergic reactions in sensitive individuals. May cause chemical burns in mouth, oesophagus and stomach. Symptoms following overexposure may include the following: Severe stomach pain. Nausea, vomiting.</td>
</tr>
<tr>
<td><strong>Skin contact</strong></td>
<td></td>
<td></td>
<td>May cause skin sensitisation or allergic reactions in sensitive individuals. Causes severe burns. Symptoms following overexposure may include the following: Pain or irritation. Redness. Blistering may occur.</td>
</tr>
</tbody>
</table>
tert-Butyl isocyanate

**Eye contact**
Causes serious eye damage. Symptoms following overexposure may include the following:
Pain. Profuse watering of the eyes. Redness.

**Route of exposure**
Ingestion Inhalation Skin and/or eye contact

**Target organs**
Respiratory system, lungs

**Medical considerations**
Skin disorders and allergies.

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**SECTION 12: Ecological Information**

**Ecotoxicity**
Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.

**12.1. Toxicity**

**Acute aquatic toxicity**

**Acute toxicity - fish**
LC₅₀, : 100 mg/l, Leuciscus idus (Golden orfe)

**12.2. Persistence and degradability**

**Persistence and degradability**
The degradability of the product is not known.

**12.3. Bioaccumulative potential**

**Bioaccumulative potential**
No data available on bioaccumulation.

**Partition coefficient**
No data available.

**12.4. Mobility in soil**

**Mobility**
No data available.

**12.5. Results of PBT and vPvB assessment**

**Results of PBT and vPvB assessment**
No data available.

**12.6. Other adverse effects**

**Other adverse effects**
None known.

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**SECTION 13: Disposal considerations**

**13.1. Waste treatment methods**

**General information**
Dispose of waste to licensed waste disposal site in accordance with the requirements of the local Waste Disposal Authority. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered.

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**SECTION 14: Transport information**

**14.1. UN number**

**UN No. (ADR/RID)**
2484

**UN No. (IMDG)**
2484

**UN No. (ICAO)**
2484

**UN No. (ADN)**
2484

**14.2. UN proper shipping name**

**Proper shipping name (ADR/RID)**
tert-BUTYL ISOCYANATE
tert-Butyl isocyanate

Proper shipping name (IMDG) tert-BUTYL ISOCYANATE
Proper shipping name (ICAO) tert-BUTYL ISOCYANATE
Proper shipping name (ADN) tert-BUTYL ISOCYANATE

14.3. Transport hazard class(es)
ADR/RID class 6.1
ADR/RID subsidiary risk 3
ADR/RID classification code TF1
ADR/RID label 6.1
IMDG class 6.1
IMDG subsidiary risk 3
ICAO class/division 6.1
ICAO subsidiary risk 3
ADN class 6.1
ADN subsidiary risk 3

Transport labels

14.4. Packing group
ADR/RID packing group I
IMDG packing group I
ADN packing group I
ICAO packing group I

14.5. Environmental hazards
Environmentally hazardous substance/marine pollutant
No.

14.6. Special precautions for user
EmS F-E, S-D
ADR transport category 1
Emergency Action Code •3WE
Hazard Identification Number (ADR/RID) 663
Tunnel restriction code (C/D)

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

SECTION 15: Regulatory information

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

National regulations

Health and Safety at Work etc. Act 1974 (as amended).  
The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"].  
EH40/2005 Workplace exposure limits.

EU legislation


15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

Inventories

US - TSCA  
Present.

SECTION 16: Other information

Abbreviations and acronyms used in the safety data sheet

ADR:  European Agreement concerning the International Carriage of Dangerous Goods by Road.  
ADN:  European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.  
RID:  European Agreement concerning the International Carriage of Dangerous Goods by Rail.  
IATA:  International Air Transport Association.  
IMDG:  International Maritime Dangerous Goods.  
CAS:  Chemical Abstracts Service.  
ATE:  Acute Toxicity Estimate.  
LC₅₀:  Lethal Concentration to 50 % of a test population.  
LD₅₀:  Lethal Dose to 50% of a test population (Median Lethal Dose).  
EC₅₀:  50% of maximal Effective Concentration.  
PBT:  Persistent, Bioaccumulative and Toxic substance.  
vPvB:  Very Persistent and Very Bioaccumulative.

Training advice

Only trained personnel should use this material.

Revision date

28/11/2017

Revision

1

SDS number

144929

Hazard statements in full

H225 Highly flammable liquid and vapour.  
H302 Harmful if swallowed.  
H312 Harmful in contact with skin.  
H314 Causes severe skin burns and eye damage.  
H317 May cause an allergic skin reaction.  
H318 Causes serious eye damage.  
H330 Fatal if inhaled.  
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.  
H335 May cause respiratory irritation.
tert-Butyl isocyanate