

1 Identification

Product identifier

Product name: tert-Butyl isocyanate

Stock number: 96680

CAS Number:

1609-86-5

EC number:

216-544-9

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

Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar

Thermo Fisher Scientific Chemicals, Inc.

30 Bond Street

Ward Hill, MA 01835-8099

Tel: 800-343-0660

Fax: 800-322-4757

Email: tech@alfa.com

www.alfa.com

Information Department: Health, Safety and Environmental Department

Emergency telephone number:

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)



GHS02 Flame

Flam. Liq. 2 H225 Highly flammable liquid and vapor.



GHS06 Skull and crossbones

Acute Tox. 1 H330 Fatal if inhaled.



GHS08 Health hazard

Resp. Sens. 1 H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.



GHS05 Corrosion

Skin Corr. 1B H314 Causes severe skin burns and eye damage.

Eye Dam. 1 H318 Causes serious eye damage.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Skin Sens. 1 H317 May cause an allergic skin reaction.

Hazards not otherwise classified Lachrymator

Label elements

GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms



GHS02 GHS05 GHS06 GHS08

Signal word

Danger

Hazard statements

H225 Highly flammable liquid and vapor.

H302 Harmful if swallowed.

H330 Fatal if inhaled.

H314 Causes severe skin burns and eye damage.

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.

H317 May cause an allergic skin reaction.

Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P303+P361+P353 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

P305+P351+P338 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P320 Specific treatment is urgent (see on this label).

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

WHMIS classification

B2 - Flammable liquid

D1A - Very toxic material causing immediate and serious toxic effects

D2A - Very toxic material causing other toxic effects

E - Corrosive material



Product name: *tert-Butyl isocyanate*

Classification system
HMIS ratings (scale 0-4)
(Hazardous Materials Identification System)

HEALTH	3	Health (acute effects) = 3
FIRE	3	Flammability = 3
REACTIVITY	2	Physical Hazard = 2

Other hazards
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.

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3 Composition/information on ingredients

Chemical characterization: Substances
CAS# Description:
1609-86-5 *tert-Butyl isocyanate*
Concentration: ≤100%
Identification number(s):
EC number: 216-544-9

4 First-aid measures

Description of first aid measures
General information
Immediately remove any clothing soiled by the product.
Remove breathing apparatus only after contaminated clothing has been completely removed.
In case of irregular breathing or respiratory arrest provide artificial respiration.
After inhalation
Supply fresh air. If required, provide artificial respiration. Keep patient warm.
Seek immediate medical advice.
After skin contact
Immediately wash with water and soap and rinse thoroughly.
Seek immediate medical advice.
After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.
After swallowing Seek medical treatment.
Information for doctor
Most important symptoms and effects, both acute and delayed
Causes severe skin burns.
Harmful if swallowed.
Fatal if inhaled.
Causes serious eye damage.
May cause allergy or asthma symptoms or breathing difficulties if inhaled.
May cause an allergic skin reaction.
This product is a lachrymator.
Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures

Extinguishing media
Suitable extinguishing agents In case of fire, use sand, carbon dioxide or powdered extinguishing agent. Never use water.
For safety reasons unsuitable extinguishing agents Water
Special hazards arising from the substance or mixture
Reacts violently with water
If this product is involved in a fire, the following can be released:
Carbon monoxide and carbon dioxide
Nitrogen oxides (NOx)
Advice for firefighters
Protective equipment:
Wear self-contained respirator.
Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures
Wear protective equipment. Keep unprotected persons away.
Ensure adequate ventilation
Keep away from ignition sources
Environmental precautions: Do not allow product to reach sewage system or any water course.
Methods and material for containment and cleaning up:
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Use neutralizing agent.
Dispose of contaminated material as waste according to section 13.
Ensure adequate ventilation.
Do not flush with water or aqueous cleansing agents
Prevention of secondary hazards: Keep away from ignition sources.
Reference to other sections
See Section 7 for information on safe handling
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.
Protective Action Criteria for Chemicals
PAC-1: 0.0099 ppm
PAC-2: 0.11 ppm
PAC-3: 0.65 ppm

7 Handling and storage

Handling
Precautions for safe handling
Handle under dry protective gas.
Keep container tightly sealed.
Ensure good ventilation at the workplace.
Open and handle container with care.

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Product name: *tert-Butyl isocyanate*

Information about protection against explosions and fires:
Protect against electrostatic charges.
Fumes can combine with air to form an explosive mixture.
Keep ignition sources away.

Conditions for safe storage, including any incompatibilities
Storage
Requirements to be met by storerooms and receptacles: Refrigerate
Information about storage in one common storage facility:
Protect from heat.
Store away from water/moisture.
Do not store together with acids.
Store away from strong bases.
Store away from oxidizing agents.
Store away from reducing agents.
Store away from alcohols.
Store away from amines.

Further information about storage conditions:
Store under dry inert gas.
This product is moisture sensitive.
Protect from humidity and water.
Keep container tightly sealed.
Refrigerate

Specific end use(s) No further relevant information available.

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8 Exposure controls/personal protection

Additional information about design of technical systems:
Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Control parameters
Components with limit values that require monitoring at the workplace:
The product does not contain any relevant quantities of materials with critical values that have to be monitored at the workplace.

Additional information: No data

Exposure controls
Personal protective equipment
General protective and hygienic measures
The usual precautionary measures for handling chemicals should be followed.
Keep away from foodstuffs, beverages and feed.
Remove all soiled and contaminated clothing immediately.
Wash hands before breaks and at the end of work.
Store protective clothing separately.
Do not inhale dust / smoke / mist.
Avoid contact with the eyes and skin.
Maintain an ergonomically appropriate working environment.

Breathing equipment: Use self-contained respiratory protective device in emergency situations.

Recommended filter device for short term use:
Use a respirator with multi-purpose combination (US) or type ABEK (EN 14387) as a backup to engineering controls. Risk assessment should be performed to determine if air-purifying respirators are appropriate. Only use equipment tested and approved under appropriate government standards such as NIOSH (USA) or CEN (EU).

Protection of hands:
Impervious gloves
Check protective gloves prior to each use for their proper condition.
The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.

Eye protection:
Tightly sealed goggles
Full face protection
Safety glasses with side shields / NIOSH (US) or EN 166(EU)

Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties
General Information
Appearance:
Form: Liquid
Odor: Acid
Odor threshold: Not determined.

pH-value: Not determined.

Change in condition
Melting point/Melting range: Not determined
Boiling point/Boiling range: 85-86 °C (185-187 °F)
Sublimation temperature / start: Not determined

Flash point: -4 °C (25 °F)
Flammability (solid, gaseous): Not determined.
Ignition temperature: Not determined
Decomposition temperature: Not determined
Auto igniting: Not determined.

Danger of explosion: Product is not explosive. However, formation of explosive air/vapor mixtures is possible.
Explosion limits:
Lower: Not determined
Upper: Not determined
Vapor pressure: Not determined
Density at 20 °C (68 °F): 0.868 g/cm³ (7.243 lbs/gal)
Relative density: Not determined.
Vapor density: Not determined.
Evaporation rate: Not determined.
Solubility in / Miscibility with
Water: Reacts
Reacts violently

Partition coefficient (n-octanol/water): Not determined.

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Product name: *tert-Butyl isocyanate*

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Viscosity:
dynamic: Not determined.
kinematic: Not determined.
Other information No further relevant information available.

10 Stability and reactivity

Reactivity Reacts violently with water.
Chemical stability Stable under recommended storage conditions.
Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.
Possibility of hazardous reactions
Reacts with strong oxidizing agents
Reacts violently with water
Conditions to avoid No further relevant information available.
Incompatible materials:
Acids
Bases
Oxidizing agents
Reducing agents
Alcohols
Amines
Water/moisture
Heat
Hazardous decomposition products:
Carbon monoxide and carbon dioxide
Nitrogen oxides

11 Toxicological information

Information on toxicological effects
Acute toxicity:
Harmful if swallowed.
Fatal if inhaled.
Swallowing will lead to a strong corrosive effect on mouth and throat and to the danger of perforation of esophagus and stomach.
LD/LC50 values that are relevant for classification:

Oral	LD50	360 mg/kg (rat)
Inhalative	LC50/4H	0.06 mg/l/4H (rat)

Skin irritation or corrosion: Causes severe skin burns.
Eye irritation or corrosion:
This product is a lachrymator.
Causes serious eye damage.
Sensitization:
May cause allergy or asthma symptoms or breathing difficulties if inhaled.
May cause an allergic skin reaction.
Germ cell mutagenicity: No effects known.
Carcinogenicity: No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.
Reproductive toxicity: No effects known.
Specific target organ system toxicity - repeated exposure: No effects known.
Specific target organ system toxicity - single exposure: No effects known.
Aspiration hazard: No effects known.
Subacute to chronic toxicity: No effects known.
Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

Toxicity
Aquatic toxicity: No further relevant information available.
Persistence and degradability No further relevant information available.
Bioaccumulative potential No further relevant information available.
Mobility in soil No further relevant information available.
Additional ecological information:
General notes:
Do not allow product to reach ground water, water course or sewage system.
Danger to drinking water if even small quantities leak into the ground.
Avoid transfer into the environment.
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.
Other adverse effects No further relevant information available.

13 Disposal considerations

Waste treatment methods
Recommendation Consult state, local or national regulations to ensure proper disposal.
Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.





14 Transport information

UN-Number DOT, IMDG, IATA	UN2484
UN proper shipping name DOT ADR IMDG, IATA	<i>tert-Butyl isocyanate</i> 2484 <i>tert-Butyl isocyanate</i> <i>tert-BUTYL ISOCYANATE</i>





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Transport hazard class(es)	
DOT	
	
Class Label ADR	6.1 Toxic substances 6.1, 3
	
Class Label IMDG	6.1 (TF1) Toxic substances 6.1+3
	
Class Label IATA	6.1 Toxic substances 6.1/3
	
Class Label	6.1 Toxic substances 6.1 (3)
Packing group DOT, ADR, IMDG, IATA	I
Environmental hazards:	Not applicable.
Special precautions for user	Warning: Toxic substances
EMS Number:	F-E,S-D
Stowage Category	D
Stowage Code	SW2 Clear of living quarters.
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information:	
DOT	
Quantity limitations	On passenger aircraft/rail: Forbidden On cargo aircraft only: Forbidden
Marine Pollutant (DOT):	No
Remarks:	This material is poisonous by inhalation in Hazard Zone A.
IMDG	
Limited quantities (LQ)	0
Excepted quantities (EQ)	Code: E0 Not permitted as Excepted Quantity
UN "Model Regulation":	UN 2484 TERT-BUTYL ISOCYANATE, 6.1 (3), I

15 Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture	
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)	
Hazard pictograms	
   	
GHS02 GHS05 GHS06 GHS08	
Signal word Danger	
Hazard statements	
H225 Highly flammable liquid and vapor.	
H302 Harmful if swallowed.	
H330 Fatal if inhaled.	
H314 Causes severe skin burns and eye damage.	
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.	
H317 May cause an allergic skin reaction.	
Precautionary statements	
P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.	
P303+P361+P353 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.	
P305+P351+P338 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.	
P320 Specific treatment is urgent (see on this label).	
P405 Store locked up.	
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.	
National regulations	
All components of this product are listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical substance Inventory.	
All components of this product are listed on the Canadian Non-Domestic Substances List (NDSL).	
SARA Section 313 (specific toxic chemical listings) Substance is not listed.	
California Proposition 65	
Prop 65 - Chemicals known to cause cancer Substance is not listed.	
Prop 65 - Developmental toxicity Substance is not listed.	
Prop 65 - Developmental toxicity, female Substance is not listed.	
Prop 65 - Developmental toxicity, male Substance is not listed.	
Information about limitation of use: For use only by technically qualified individuals.	

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Other regulations, limitations and prohibitive regulations
Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.
The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.
Substance is not listed.
Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.
Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department

Date of preparation/Revision: Print date, revision date and version number are in the header of each page.

Abbreviations and acronyms:
ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
EINECS: European Inventory of Existing Commercial Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
HMIS: Hazardous Materials Identification System (USA)
WHMIS: Workplace Hazardous Materials Information System (Canada)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
PBT: Persistent, Bioaccumulative and Toxic
SVHC: Substances of Very High Concern
vPvB: very Persistent and very Bioaccumulative
ACGIH: American Conference of Governmental Industrial Hygienists (USA)
OSHA: Occupational Safety and Health Administration (USA)
NTP: National Toxicology Program (USA)
IARC: International Agency for Research on Cancer
EPA: Environmental Protection Agency (USA)
Flam. Liq. 2: Flammable liquids – Category 2
Acute Tox. 4: Acute toxicity – Category 4
Acute Tox. 1: Acute toxicity – Category 1
Skin Corr. 1B: Skin corrosion/irritation – Category 1B
Eye Dam. 1: Serious eye damage/eye irritation – Category 1
Resp. Sens. 1: Respiratory sensitisation – Category 1
Skin Sens. 1: Skin sensitisation – Category 1

USA