

1 Identification

Product identifier

Product name: tert-Butyl isothiocyanate

Stock number: L02668

CAS Number:

590-42-1

EC number:

209-682-6

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. 3 H226 Flammable liquid and vapour.



GHS06 Skull and crossbones

Acute Tox. 2 H300 Fatal if swallowed.

Acute Tox. 2 H310 Fatal in contact with skin.

Acute Tox. 2 H330 Fatal if inhaled.



GHS05 Corrosion

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

Eye Dam. 1 H318 Causes serious eye damage.

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

Signal word Danger

Hazard statements

H226 Flammable liquid and vapour.

H300+H310+H330 Fatal if swallowed, in contact with skin or if inhaled.

H314 Causes severe skin burns and eye damage.

Precautionary statements

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

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor/...

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).

P361 Take off immediately all contaminated clothing.

P405 Store locked up.

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

WHMIS classification

B3 - Combustible liquid

D1A - Very toxic material causing immediate and serious toxic effects

D2B - Toxic material causing other toxic effects

E - Corrosive material



Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH 3 Health (acute effects) = 3

FIRE 2 Flammability = 2

REACTIVITY 1 Physical Hazard = 1

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

Product name: **tert-Butyl isothiocyanate**

vPvB: Not applicable. (Contd. of page 1)

3 Composition/information on ingredients
Chemical characterization: Substances
CAS# Description:
590-42-1 tert-Butyl isothiocyanate
Identification number(s):
EC number: 209-682-6

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 Do not induce vomiting; immediately call for medical help.
Information for doctor
Most important symptoms and effects, both acute and delayed
Causes severe skin burns.
Causes serious eye damage.
Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures
Extinguishing media
Suitable extinguishing agents CO2, sand, extinguishing powder. Do not use water.
Special hazards arising from the substance or mixture
If this product is involved in a fire, the following can be released:
Carbon monoxide and carbon dioxide
Nitrogen oxides (NOx)
Hydrogen cyanide (HCN)
Sulfur oxides (SOx)
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 material to be released to the environment without proper governmental permits.
Methods and material for containment and cleaning up:
Keep away from ignition sources.
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.
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.

7 Handling and storage
Handling
Precautions for safe handling
Handle under dry protective gas.
Keep container tightly sealed.
Store in cool, dry place in tightly closed containers.
Ensure good ventilation at the workplace.
Open and handle container with care.
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: No special requirements.
Information about storage in one common storage facility:
Store away from oxidizing agents.
Store away from water/moisture.
Further information about storage conditions:
Store under dry inert gas.
This product is moisture sensitive.
Keep container tightly sealed.
Store in cool, dry conditions in well sealed containers.
Protect from humidity and water.
Specific end use(s) No further relevant information available.

Product name: **tert-Butyl isothiocyanate**

(Contd. of page 2)

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: Not required.
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.
Avoid contact with the eyes and skin.
Maintain an ergonomically appropriate working environment.

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

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.

Penetration time of glove material (in minutes) Not determined

Eye protection:
Tightly sealed goggles
Full face protection

Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties	
General Information	
Appearance:	
Form:	Liquid
Color:	Pale yellow
Odor:	Pungent
Odor threshold:	Not determined.
pH-value: Not determined.	
Change in condition	
Melting point/Melting range:	10-12 °C (50-54 °F)
Boiling point/Boiling range:	141-145 °C (286-293 °F)
Sublimation temperature / start:	Not determined
Flash point:	38 °C (100 °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):	0.908 g/cm³ (7.577 lbs/gal)
Relative density	Not determined.
Vapor density	Not determined.
Evaporation rate	Not determined.
Solubility in / Miscibility with	
Water:	Reacts
Partition coefficient (n-octanol/water):	Not determined.
Viscosity:	
dynamic:	Not determined.
kinematic:	Not determined.
Other information	No further relevant information available.

10 Stability and reactivity

Reactivity No information known.

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 No dangerous reactions known

Conditions to avoid No further relevant information available.








Incompatible materials:
Alcohols
Amines
Oxidizing agents
Water/moisture

Hazardous decomposition products:
Carbon monoxide and carbon dioxide
Nitrogen oxides
Hydrogen cyanide
Sulfur oxides (SOx)

11 Toxicological information

Information on toxicological effects
Acute toxicity:
Fatal if inhaled.
Fatal in contact with skin.
Fatal if swallowed.
Danger through skin absorption.
Swallowing will lead to a strong corrosive effect on mouth and throat and to the danger of perforation of esophagus and stomach.

(Contd. on page 4)
USA

Product name: tert-Butyl isothiocyanate	
<div>LD/LC50 values that are relevant for classification: No data</div> <div>Skin irritation or corrosion: Causes severe skin burns.</div> <div>Eye irritation or corrosion: Causes serious eye damage. This product is a lachrymator.</div> <div>Sensitization: No sensitizing effects known.</div> <div>Germ cell mutagenicity: No effects known.</div> <div>Carcinogenicity: No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.</div> <div>Reproductive toxicity: No effects known.</div> <div>Specific target organ system toxicity - repeated exposure: No effects known.</div> <div>Specific target organ system toxicity - single exposure: No effects known.</div> <div>Aspiration hazard: No effects known.</div> <div>Subacute to chronic toxicity: No effects known.</div> <div>Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.</div>	(Contd. of page 3)
12 Ecological information <div>Toxicity</div> <div>Aquatic toxicity: No further relevant information available.</div> <div>Persistence and degradability: No further relevant information available.</div> <div>Bioaccumulative potential: No further relevant information available.</div> <div>Mobility in soil: No further relevant information available.</div> <div>Additional ecological information:</div> <div>General notes: Do not allow material to be released to the environment without proper governmental permits. Do not allow undiluted product or large quantities to reach ground water, water course or sewage system. Avoid transfer into the environment.</div> <div>Results of PBT and vPvB assessment</div> <div>PBT: Not applicable.</div> <div>vPvB: Not applicable.</div> <div>Other adverse effects: No further relevant information available.</div>	
13 Disposal considerations <div>Waste treatment methods</div> <div>Recommendation: Consult state, local or national regulations to ensure proper disposal.</div> <div>Uncleaned packagings:</div> <div>Recommendation: Disposal must be made according to official regulations.</div>	
14 Transport information	
UN-Number DOT, IMDG, IATA	UN2929
UN proper shipping name DOT IMDG, IATA	Toxic liquids, flammable, organic, n.o.s. (tert-Butyl isothiocyanate) TOXIC LIQUID, FLAMMABLE, ORGANIC, N.O.S. (tert-Butyl isothiocyanate)
Transport hazard class(es) DOT	<div></div>
Class Label Class Label IMDG, IATA	6.1 Toxic substances. 6.1+3 6.1 (TF1) Toxic substances 6.1+3
<div></div> Class Label	6.1 Toxic substances. 6.1+3
Packing group DOT, IMDG, IATA	II
Environmental hazards:	Not applicable.
Special precautions for user EMS Number:	Warning: Toxic substances F-E,S-D
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information: DOT Marine Pollutant (DOT):	No
UN "Model Regulation":	UN2929, Toxic liquids, flammable, organic, n.o.s. (tert-Butyl isothiocyanate), 6.1 (3), II
15 Regulatory information <div>Safety, health and environmental regulations/legislation specific for the substance or mixture</div> <div>GHS label elements: The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)</div> <div>Hazard pictograms</div> <div></div> <div>GHS02 GHS05 GHS06</div> <div>Signal word: Danger</div> <div>Hazard statements H226: Flammable liquid and vapour.</div>	
(Contd. on page 5) USA	

Product name: **tert-Butyl isothiocyanate**

(Contd. of page 4)

H300+H310+H330 *Fatal if swallowed, in contact with skin or if inhaled.*
H314 *Causes severe skin burns and eye damage.*
Precautionary statements
P210 *Keep away from heat/sparks/open flames/hot surfaces. No smoking.*
P301+P310 *IF SWALLOWED: Immediately call a POISON CENTER/ doctor/...*
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).*
P361 *Take off immediately all contaminated clothing.*
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.*
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 Material 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 / last revision *11/23/2015 / -*
Abbreviations and acronyms:
RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)
IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)
ICAO: International Civil Aviation Organization
ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)
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
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)

USA