

ALFAAL00123

## tert-Butyl cyanoacetate

### SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明:  
Product Description: 氰乙酸叔丁酯  
tert-Butyl cyanoacetate

Cat No. : L00123  
CAS No 1116-98-9  
Molecular Formula NCCH<sub>2</sub> CO<sub>2</sub> C(CH<sub>3</sub>)<sub>3</sub>

Supplier Avocado Research Chemicals Ltd.  
(Part of Thermo Fisher Scientific)  
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United Kingdom  
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Emergency Telephone Number For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

E-mail address begel.sdsdesk@thermofisher.com

Recommended Use Laboratory chemicals.  
Uses advised against No Information available

### SECTION 2. HAZARD IDENTIFICATION

Physical State  
Liquid

Appearance  
No information available

Odor  
Odorless

Emergency Overview  
Combustible liquid. Harmful if swallowed.

#### Classification of the substance or mixture

Flammable liquids.	Category 4
Acute Oral Toxicity	Category 4

#### Label Elements



Signal Word

Warning

Hazard Statements  
H227 - Combustible liquid

H302 - Harmful if swallowed

**Precautionary Statements****Prevention**

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

P264 - Wash face, hands and any exposed skin thoroughly after handling

P270 - Do not eat, drink or smoke when using this product

P280 - Wear protective gloves/protective clothing/eye protection/face protection

**Response**

P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor if you feel unwell

P330 - Rinse mouth

P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish

**Storage**

P403 + P235 - Store in a well-ventilated place. Keep cool

**Disposal**

P501 - Dispose of contents/ container to an approved waste disposal plant

**Physical and Chemical Hazards**

Combustible material.

**Health Hazards**

Harmful if swallowed.

**Environmental hazards**

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil. The product is insoluble and floats on water. The product evaporates slowly.

This product does not contain any known or suspected endocrine disruptors.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Component	CAS No	Weight %
Acetic acid, cyano-, 1,1-dimethylethyl ester	1116-98-9	<=100

**SECTION 4. FIRST AID MEASURES****General Advice**

If symptoms persist, call a physician.

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

**Inhalation**

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

**Ingestion**

Clean mouth with water and drink afterwards plenty of water.

**Most important symptoms and effects**

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

**Self-Protection of the First Aider**

No special precautions required.

**Notes to Physician**

Treat symptomatically.

**SECTION 5. FIRE-FIGHTING MEASURES****Suitable Extinguishing Media**

Carbon dioxide (CO<sub>2</sub>). Powder. Water spray. In case of major fire and large quantities: Evacuate area. Fight fire remotely due to the risk of explosion. Water mist may be used to cool closed containers.

**Extinguishing media which must not be used for safety reasons**

No information available.

**Specific Hazards Arising from the Chemical**

Combustible material. Containers may explode when heated.

**Protective Equipment and Precautions for Firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

**SECTION 6. ACCIDENTAL RELEASE MEASURES****Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.

**Environmental Precautions**

Should not be released into the environment. See Section 12 for additional Ecological Information.

**Methods for Containment and Clean Up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE****Handling**

Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid ingestion and inhalation. Do not get in eyes, on skin, or on clothing. Keep away from open flames, hot surfaces and sources of ignition.

**Storage**

Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters****Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours

**Exposure Controls****Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of

properly designed ventilation systems, should be adopted to control hazardous materials at source.

### Personal protective equipment

<b>Eye Protection</b>	Wear safety glasses with side shields (or goggles) (European standard - EN 166)
<b>Hand Protection</b>	Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Viton (R)	480 minutes	0.7 mm	EN 374	(minimum requirement)

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.  
(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

<b>Skin and body protection</b>	Long sleeved clothing
<b>Respiratory Protection</b>	When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly
<b>Large scale/emergency use</b>	In case of insufficient ventilation, wear suitable respiratory equipment <b>Recommended Filter type:</b> Multi-purpose/ABEK conforming to EN14387
<b>Small scale/Laboratory use</b>	Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. When RPE is used a face piece Fit Test should be conducted

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice.

**Environmental exposure controls** No information available.

## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

<b>Appearance</b>	
<b>Physical State</b>	Liquid
<b>Odor</b>	Odorless
<b>Odor Threshold</b>	No data available
<b>pH</b>	No information available
<b>Melting Point/Range</b>	No data available
<b>Softening Point</b>	No data available
<b>Boiling Point/Range</b>	67 - 68 °C / 152.6 - 154.4 °F @ 1.5mmHg
<b>Flash Point</b>	91 °C / 195.8 °F <b>Method -</b> No information available
<b>Evaporation Rate</b>	No data available
<b>Flammability (solid,gas)</b>	Not applicable Liquid
<b>Explosion Limits</b>	No data available
<b>Vapor Pressure</b>	No data available
<b>Vapor Density</b>	No data available (Air = 1.0)
<b>Specific Gravity / Density</b>	0.987 g/cm3 @ 20 °C
<b>Bulk Density</b>	Not applicable Liquid
<b>Water Solubility</b>	Immiscible
<b>Solubility in other solvents</b>	No information available
<b>Partition Coefficient (n-octanol/water)</b>	
<b>Autoignition Temperature</b>	No data available
<b>Decomposition Temperature</b>	No data available
<b>Viscosity</b>	No data available

## tert-Butyl cyanoacetate

<b>Explosive Properties</b>		explosive air/vapour mixtures possible
<b>Oxidizing Properties</b>	No information available	

<b>Molecular Formula</b>	NCCH <sub>2</sub> CO <sub>2</sub> C(CH <sub>3</sub> ) <sub>3</sub>
<b>Molecular Weight</b>	141.17

## SECTION 10. STABILITY AND REACTIVITY

<b>Stability</b>	Stable under normal conditions.
<b>Hazardous Reactions</b>	None under normal processing.
<b>Hazardous Polymerization</b>	No information available.
<b>Conditions to Avoid</b>	Keep away from open flames, hot surfaces and sources of ignition.
<b>Materials to avoid</b>	Reducing Agent. Oxidizing agent.

**Hazardous Decomposition Products** None under normal use conditions.

## SECTION 11. TOXICOLOGICAL INFORMATION

## Product Information

<b>(a) acute toxicity;</b>	
<b>(b) skin corrosion/irritation;</b>	No data available
<b>(c) serious eye damage/irritation;</b>	No data available
<b>(d) respiratory or skin sensitization;</b>	
Respiratory	No data available
Skin	No data available
<b>(e) germ cell mutagenicity;</b>	No data available
<b>(f) carcinogenicity;</b>	No data available
	There are no known carcinogenic chemicals in this product
<b>(g) reproductive toxicity;</b>	No data available
<b>(h) STOT-single exposure;</b>	No data available
<b>(i) STOT-repeated exposure;</b>	No data available
Target Organs	No information available.
<b>(j) aspiration hazard;</b>	No data available
<b>Symptoms / effects, both acute and delayed</b>	Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

## SECTION 12. ECOLOGICAL INFORMATION

<b>Ecotoxicity effects</b>	Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.
<b>Persistence and Degradability</b> <b>Persistence</b>	Immiscible with water, May persist, based on information available.
<b>Bioaccumulative Potential</b>	May have some potential to bioaccumulate
<b>Mobility in soil</b>	Spillage unlikely to penetrate soil The product is insoluble and floats on water The product evaporates slowly Is not likely mobile in the environment due its low water solubility Spillage unlikely to penetrate soil
<b>Endocrine Disruptor Information</b> <b>Persistent Organic Pollutant</b> <b>Ozone Depletion Potential</b>	This product does not contain any known or suspected endocrine disruptors This product does not contain any known or suspected substance This product does not contain any known or suspected substance

## SECTION 13. DISPOSAL CONSIDERATIONS

<b>Waste from Residues/Unused Products</b>	Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.
<b>Contaminated Packaging</b>	Dispose of this container to hazardous or special waste collection point.
<b>Other Information</b>	Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

## SECTION 14. TRANSPORT INFORMATION

<b>Road and Rail Transport</b>	Not Regulated
<b>IMDG/IMO</b>	Not regulated
<b>IATA</b>	Not regulated

<b>Special Precautions for User</b>	No special precautions required
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## SECTION 15. REGULATORY INFORMATION

## International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL

**SAFETY DATA SHEET****tert-Butyl cyanoacetate**

Acetic acid, cyano-, 1,1-dimethylethyl ester	-	-	X	-	214-243-7	X	-	-	X	X	X	-
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**National Regulations****SECTION 16. OTHER INFORMATION**

**Prepared By** Health, Safety and Environmental Department  
**Revision Date** 01-May-2024  
**Revision Summary** New emergency telephone response service provider.

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

**Legend****CAS** - Chemical Abstracts Service**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances**PICCS** - Philippines Inventory of Chemicals and Chemical Substances**IECSC** - Chinese Inventory of Existing Chemical Substances**KECL** - Korean Existing and Evaluated Chemical Substances**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory**DSL/NDL** - Canadian Domestic Substances List/Non-Domestic Substances List**ENCS** - Japanese Existing and New Chemical Substances**AICS** - Australian Inventory of Chemical Substances**NZIoC** - New Zealand Inventory of Chemicals**WEL** - Workplace Exposure Limit**ACGIH** - American Conference of Governmental Industrial Hygienists**DNEL** - Derived No Effect Level**RPE** - Respiratory Protective Equipment**LC50** - Lethal Concentration 50%**NOEC** - No Observed Effect Concentration**PBT** - Persistent, Bioaccumulative, Toxic**TWA** - Time Weighted Average**IARC** - International Agency for Research on Cancer**PNEC** - Predicted No Effect Concentration**LD50** - Lethal Dose 50%**EC50** - Effective Concentration 50%**POW** - Partition coefficient Octanol:Water**vPvB** - very Persistent, very Bioaccumulative**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road**OECD** - Organisation for Economic Co-operation and Development**BCF** - Bioconcentration factor**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code**MARPOL** - International Convention for the Prevention of Pollution from Ships**ATE** - Acute Toxicity Estimate**VOC** - (Volatile Organic Compound)**Key literature references and sources for data**<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadviser - LOLI, Merck index, RTECS

**Disclaimer**

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**