

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

### 1.1. Product identifier

Product Description: tert-Butyl cyanoacetate  
Cat No. : **L00123**  
CAS No 1116-98-9  
Molecular Formula NCCH2CO2C(CH3)3

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

Recommended Use Laboratory chemicals.  
Uses advised against No Information available

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

Company  
Avocado Research Chemicals Ltd.  
(Part of Thermo Fisher Scientific)  
Shore Road, Heysham  
Lancashire, LA3 2XY,  
United Kingdom  
Office Tel: +44 (0) 1524 850506  
Office Fax: +44 (0) 1524 850608

E-mail address begel.sdsdesk@thermofisher.com

### 1.4. 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

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

##### Physical hazards

Based on available data, the classification criteria are not met

##### Health hazards

Acute oral toxicity

Category 4 (H302)

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## Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## 2.2. Label elements



Signal Word

Warning

## Hazard Statements

H302 - Harmful if swallowed  
Combustible liquid

## Precautionary Statements

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting  
P312 - Call a POISON CENTER or doctor if you feel unwell  
P264 - Wash face, hands and any exposed skin thoroughly after handling

## 2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

| Component                                    | CAS No    | EC No             | Weight % | CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567 |
|----------------------------------------------|-----------|-------------------|----------|-----------------------------------------------------------------------------------------|
| Acetic acid, cyano-, 1,1-dimethylethyl ester | 1116-98-9 | EEC No. 214-243-7 | <=100    | Acute Tox. 4 (H302)                                                                     |

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of 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.

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|                                    |                                                                                                              |
|------------------------------------|--------------------------------------------------------------------------------------------------------------|
| Ingestion                          | Clean mouth with water and drink afterwards plenty of water.                                                 |
| Inhalation                         | Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur. |
| Self-Protection of the First Aider | No special precautions required.                                                                             |

## 4.2. Most important symptoms and effects, both acute and delayed

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

## 4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician Treat symptomatically.

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### **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.

### 5.2. Special hazards arising from the substance or mixture

Combustible material. Containers may explode when heated.

#### **Hazardous Combustion Products**

None under normal use conditions.

### 5.3. Advice 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

### 6.1. Personal precautions, protective equipment and emergency procedures

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

### 6.2. Environmental precautions

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

### 6.3. Methods and material for containment and cleaning up

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

### 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: HANDLING AND STORAGE

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## 7.1. Precautions for safe 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.

### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

## 7.2. Conditions for safe storage, including any incompatibilities

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

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 10  
**Storage Class (LGK) (Germany)**

## 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

#### **Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)**

No information available

#### **Predicted No Effect Concentration (PNEC)**

No information available.

### 8.2. 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**

##### **Eye Protection**

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

##### **Hand Protection**

Protective gloves

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| Glove material                  | Breakthrough time | Glove thickness        | EU standard | Glove comments        |
|---------------------------------|-------------------|------------------------|-------------|-----------------------|
| Viton (R)                       | 480 minutes       | 0.7 mm                 | EN 374      | (minimum requirement) |
| <b>Skin and body protection</b> |                   | Long sleeved clothing. |             |                       |

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.

## Respiratory Protection

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

## Large scale/emergency use

In case of insufficient ventilation, wear suitable respiratory equipment

**Recommended Filter type:** Multi-purpose/ABEK conforming to EN14387

## Small scale/Laboratory use

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

## Environmental exposure controls

No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

|                                                |                               |  |                                          |
|------------------------------------------------|-------------------------------|--|------------------------------------------|
| <b>Physical State</b>                          | Liquid                        |  |                                          |
| <b>Appearance</b>                              |                               |  |                                          |
| <b>Odor</b>                                    | Odorless                      |  |                                          |
| <b>Odor Threshold</b>                          | No data 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>Flammability (liquid)</b>                   | Combustible liquid            |  | On basis of test data                    |
| <b>Flammability (solid,gas)</b>                | Not applicable                |  | Liquid                                   |
| <b>Explosion Limits</b>                        | No data available             |  |                                          |
| <b>Flash Point</b>                             | 91 °C / 195.8 °F              |  | <b>Method -</b> No information available |
| <b>Autoignition Temperature</b>                | No data available             |  |                                          |
| <b>Decomposition Temperature</b>               | No data available             |  |                                          |
| <b>pH</b>                                      | No information available      |  |                                          |
| <b>Viscosity</b>                               | No data available             |  |                                          |
| <b>Water Solubility</b>                        | Immiscible                    |  |                                          |
| <b>Solubility in other solvents</b>            | No information available      |  |                                          |
| <b>Partition Coefficient (n-octanol/water)</b> |                               |  |                                          |
| <b>Vapor Pressure</b>                          | No data available             |  |                                          |
| <b>Density / Specific Gravity</b>              | 0.987 g/cm3                   |  | @ 20 °C                                  |
| <b>Bulk Density</b>                            | Not applicable                |  | Liquid                                   |
| <b>Vapor Density</b>                           | No data available             |  | (Air = 1.0)                              |
| <b>Particle characteristics</b>                | Not applicable (liquid)       |  |                                          |

### 9.2. Other information

|                             |                                                                    |
|-----------------------------|--------------------------------------------------------------------|
| <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                                                             |
| <b>Explosive Properties</b> | explosive air/vapour mixtures possible                             |

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## SECTION 10: STABILITY AND REACTIVITY

### 10.1. Reactivity

None known, based on information available

### 10.2. Chemical stability

Stable under normal conditions.

### 10.3. Possibility of hazardous reactions

**Hazardous Polymerization**  
**Hazardous Reactions**

No information available.  
None under normal processing.

### 10.4. Conditions to avoid

Keep away from open flames, hot surfaces and sources of ignition.

### 10.5. Incompatible materials

Reducing Agent. Oxidizing agent.

### 10.6. Hazardous decomposition products

None under normal use conditions.

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Product Information

#### (a) acute toxicity;

|            |                   |
|------------|-------------------|
| Oral       | Category 4        |
| Dermal     | No data available |
| Inhalation | No data available |

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

#### (d) respiratory or skin sensitization;

|             |                   |
|-------------|-------------------|
| Respiratory | No data available |
| Skin        | No data available |

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

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**Target Organs** No information available.

**(j) aspiration hazard;** No data available

**Symptoms / effects, both acute and delayed** Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

## 11.2. Information on other hazards

**Endocrine Disrupting Properties** Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## SECTION 12: ECOLOGICAL INFORMATION

**12.1. Toxicity**  
**Ecotoxicity effects** Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

**12.2. Persistence and degradability**  
**Persistence** Immiscible with water, May persist, based on information available.

**12.3. Bioaccumulative potential** May have some potential to bioaccumulate

**12.4. Mobility in soil** 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

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

**12.6. Endocrine disrupting properties**  
**Endocrine Disruptor Information** This product does not contain any known or suspected endocrine disruptors

**12.7. Other adverse effects**  
**Persistent Organic Pollutant** This product does not contain any known or suspected substance  
**Ozone Depletion Potential** This product does not contain any known or suspected substance

## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

**Waste from Residues/Unused Products** 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.

**Contaminated Packaging** Dispose of this container to hazardous or special waste collection point.

**European Waste Catalogue (EWC)** According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

**Other Information** Waste codes should be assigned by the user based on the application for which the product

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was used. Do not empty into drains.

## SECTION 14: TRANSPORT INFORMATION

**IMDG/IMO** Not regulated

**14.1. UN number**  
**14.2. UN proper shipping name**  
**14.3. Transport hazard class(es)**  
**14.4. Packing group**

**ADR** Not regulated

**14.1. UN number**  
**14.2. UN proper shipping name**  
**14.3. Transport hazard class(es)**  
**14.4. Packing group**

**IATA** Not regulated

**14.1. UN number**  
**14.2. UN proper shipping name**  
**14.3. Transport hazard class(es)**  
**14.4. Packing group**

**14.5. Environmental hazards** No hazards identified

**14.6. Special precautions for user** No special precautions required.

**14.7. Maritime transport in bulk according to IMO instruments** Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

#### International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

| Component                                    | CAS No    | EINECS    | ELINCS | NLP | IECSC | TCSI | KECL | ENCS | ISHL |
|----------------------------------------------|-----------|-----------|--------|-----|-------|------|------|------|------|
| Acetic acid, cyano-, 1,1-dimethylethyl ester | 1116-98-9 | 214-243-7 | -      | -   | -     | X    | -    | X    | X    |

| Component                                    | CAS No    | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|----------------------------------------------|-----------|------|-----------------------------------------------|-----|------|------|-------|-------|
| Acetic acid, cyano-, 1,1-dimethylethyl ester | 1116-98-9 | X    | INACTIVE                                      | -   | X    | X    | -     | -     |

**Legend:** X - Listed '-' - Not Listed

**KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

**Authorisation/Restrictions according to EU REACH** Not applicable

| Component | CAS No | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous | REACH Regulation (EC 1907/2006) article 59 - Candidate List of |
|-----------|--------|---------------------------------------------------------------------|--------------------------------------------------------------------|----------------------------------------------------------------|
|-----------|--------|---------------------------------------------------------------------|--------------------------------------------------------------------|----------------------------------------------------------------|

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|                                              |           |   | Substances | Substances of Very High Concern (SVHC) |
|----------------------------------------------|-----------|---|------------|----------------------------------------|
| Acetic acid, cyano-, 1,1-dimethylethyl ester | 1116-98-9 | - | -          | -                                      |

## Seveso III Directive (2012/18/EC)

| Component                                    | CAS No    | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements |
|----------------------------------------------|-----------|-------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Acetic acid, cyano-, 1,1-dimethylethyl ester | 1116-98-9 | Not applicable                                                                            | Not applicable                                                                           |

## Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

## Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

## National Regulations

**UK** - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

**WGK Classification** Water endangering class = 3 (self classification)

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

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

H302 - Harmful if swallowed

### 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/NDSL** - 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%

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

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**NOEC** - No Observed Effect Concentration  
**PBT** - Persistent, Bioaccumulative, Toxic

**POW** - Partition coefficient Octanol:Water  
**vPvB** - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**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

## Training Advice

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

## Prepared By

Health, Safety and Environmental Department

## Revision Date

14-Feb-2024

## Revision Summary

New emergency telephone response service provider.

**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.**

## 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**