

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

### 1.1. Product identifier

|                           |                                    |
|---------------------------|------------------------------------|
| Product Description:      | <b>3,5-Dinitrobenzotrifluoride</b> |
| Cat No. :                 | <b>B24248</b>                      |
| CAS No                    | 401-99-0                           |
| Molecular Formula         | C7 H3 F3 N2 O4                     |
| REACH registration number | -                                  |

### 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.<br>(Part of Thermo Fisher Scientific)<br>Shore Road, Heysham<br>Lancashire, LA3 2XY,<br>United Kingdom<br>Office Tel: +44 (0) 1524 850506<br>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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Acute dermal toxicity  
Acute Inhalation Toxicity - Dusts and Mists  
Skin Corrosion/Irritation  
Serious Eye Damage/Eye Irritation  
Specific target organ toxicity - (single exposure)

Category 4 (H312)  
Category 4 (H332)  
Category 2 (H315)  
Category 2 (H319)  
Category 3 (H335)

## **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**

H335 - May cause respiratory irritation  
H319 - Causes serious eye irritation  
H315 - Causes skin irritation  
H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

## **Precautionary Statements**

P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell  
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

## **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                                              |
|------------------------------------------------------|----------|-------------------|----------|--------------------------------------------------------------------------------------------------------------------------------------|
| .alpha.,.alpha.,.alpha.-Trifluoro-3,5-dinitrotoluene | 401-99-0 | EEC No. 206-935-2 | 99       | STOT SE 3 (H335)<br>Skin Irrit. 2 (H315)<br>Eye Irrit. 2 (H319)<br>Acute Tox. 4 (H302)<br>Acute Tox. 4 (H312)<br>Acute Tox. 4 (H332) |

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|                           |   |
|---------------------------|---|
| REACH registration number | - |
|---------------------------|---|

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

|                                           |                                                                                                                                                  |
|-------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Eye Contact</b>                        | Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.                                  |
| <b>Skin Contact</b>                       | Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.                     |
| <b>Ingestion</b>                          | Clean mouth with water. Get medical attention.                                                                                                   |
| <b>Inhalation</b>                         | Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.                       |
| <b>Self-Protection of the First Aider</b> | Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination. |

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

No information available.

### 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**

Water spray. Carbon dioxide (CO<sub>2</sub>). Dry chemical. Chemical foam.

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

No information available.

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

Thermal decomposition can lead to release of irritating gases and vapors.

#### **Hazardous Combustion Products**

Nitrogen oxides (NO<sub>x</sub>), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Gaseous hydrogen fluoride (HF).

### 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.

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## 6.2. Environmental precautions

See Section 12 for additional Ecological Information.

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

Sweep up and shovel into suitable containers for disposal. Do not let this chemical enter the environment.

## 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe handling

Avoid contact with skin and eyes. Do not breathe dust. Do not ingest. If swallowed then seek immediate medical assistance.

#### **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 in a dry, cool and well-ventilated place. Keep container tightly closed.

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 11  
**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.

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## 8.2. Exposure controls

### Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

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

Goggles (European standard - EN 166)

#### Hand Protection

Protective gloves

| Glove material | Breakthrough time | Glove thickness | EU standard | Glove comments        |
|----------------|-------------------|-----------------|-------------|-----------------------|
| Nitrile rubber | See manufacturers | -               | EN 374      | (minimum requirement) |
| Neoprene       | recommendations   |                 |             |                       |
| Natural rubber |                   |                 |             |                       |
| PVC            |                   |                 |             |                       |

#### Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

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

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

**Recommended Filter type:** Particulates filter conforming to EN 143

#### 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.

**Recommended half mask:-** Particle filtering: EN149:2001

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

#### Physical State

Powder Solid

#### Appearance

Light yellow

#### Odor

No information available

#### Odor Threshold

No data available

#### Melting Point/Range

47 - 50 °C / 116.6 - 122 °F

#### Softening Point

No data available

#### Boiling Point/Range

127 - 129 °C / 260.6 - 264.2 °F @ 9 mmHg

#### Flammability (liquid)

Not applicable

Solid

#### Flammability (solid,gas)

No information available

#### Explosion Limits

No data available

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|                                         |                          |                                   |
|-----------------------------------------|--------------------------|-----------------------------------|
| Flash Point                             | > 110 °C / > 230 °F      | Method - No information available |
| Autoignition Temperature                | Not applicable           |                                   |
| Decomposition Temperature               | No data available        |                                   |
| pH                                      | No information available |                                   |
| Viscosity                               | Not applicable           | Solid                             |
| Water Solubility                        | No information available |                                   |
| Solubility in other solvents            | No information available |                                   |
| Partition Coefficient (n-octanol/water) |                          |                                   |
| Vapor Pressure                          | No data available        |                                   |
| Density / Specific Gravity              | No data available        |                                   |
| Bulk Density                            | No data available        |                                   |
| Vapor Density                           | Not applicable           | Solid                             |
| Particle characteristics                | No data available        |                                   |

## 9.2. Other information

|                   |                        |
|-------------------|------------------------|
| Molecular Formula | C7 H3 F3 N2 O4         |
| Molecular Weight  | 236.11                 |
| Evaporation Rate  | Not applicable - Solid |

## 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 polymerization does not occur. |
| Hazardous Reactions      | No information available.                |

### 10.4. Conditions to avoid

Excess heat. Incompatible products.

### 10.5. Incompatible materials

Strong oxidizing agents. Strong bases.

### 10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Gaseous hydrogen fluoride (HF).

## 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     | Category 4 |
| Inhalation | Category 4 |

#### (b) skin corrosion/irritation;

Category 2

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(c) serious eye damage/irritation; Category 2

(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; Category 3

Results / Target organs Respiratory system.

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; Not applicable  
Solid

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed No information available.

## 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 Do not empty into drains.

12.2. Persistence and degradability No information available

12.3. Bioaccumulative potential No information available

12.4. Mobility in soil No information available

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

12.6. Endocrine disrupting properties

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**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 was used. Do not empty into drains.

## SECTION 14: TRANSPORT INFORMATION

**IMDG/IMO**

**14.1. UN number**

UN2811

**14.2. UN proper shipping name**

Toxic solid, organic, n.o.s.

**14.3. Transport hazard class(es)**

6.1

**14.4. Packing group**

III

**ADR**

**14.1. UN number**

UN2811

**14.2. UN proper shipping name**

Toxic solid, organic, n.o.s.

**14.3. Transport hazard class(es)**

6.1

**14.4. Packing group**

III

**IATA**

**14.1. UN number**

UN2811

**14.2. UN proper shipping name**

Toxic solid, organic, n.o.s.

**14.3. Transport hazard class(es)**

6.1

**14.4. Packing group**

III

**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**

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## 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 |
|------------------------------------------------------|----------|-----------|--------|-----|-------|------|------|------|------|
| .alpha.,.alpha.,.alpha.-Trifluoro-3,5-dinitrotoluene | 401-99-0 | 206-935-2 | -      | -   | X     | X    | -    | -    | -    |

| Component                                            | CAS No   | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|------------------------------------------------------|----------|------|-----------------------------------------------|-----|------|------|-------|-------|
| .alpha.,.alpha.,.alpha.-Trifluoro-3,5-dinitrotoluene | 401-99-0 | -    | -                                             | -   | -    | -    | -     | -     |

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 Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|------------------------------------------------------|----------|---------------------------------------------------------------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
| .alpha.,.alpha.,.alpha.-Trifluoro-3,5-dinitrotoluene | 401-99-0 | -                                                                   | -                                                                             | -                                                                                                     |

## 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 |
|------------------------------------------------------|----------|-------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| .alpha.,.alpha.,.alpha.-Trifluoro-3,5-dinitrotoluene | 401-99-0 | 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)?

See table for values

| Component                                                              | OECD PFAS | US (EPA) PFAS | EU (ECHA) PFAS | UK (HSE) PFAS | Chemsec PFAS (Sin List) |
|------------------------------------------------------------------------|-----------|---------------|----------------|---------------|-------------------------|
| .alpha.,.alpha.,.alpha.-Trifluoro-3,5-dinitrotoluene (CAS #: 401-99-0) | -         | -             | Listed         | Listed        | -                       |

## PFAS Legend

Listed = Meets the PFAS definition of the named authority

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)

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| Component                                                               | Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81) | Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC) | Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure |
|-------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| .alpha.,.alpha.,.alpha.-Trifluoro-3,5-dinitrobenzene<br>401-99-0 ( 99 ) | Prohibited and Restricted Substances                                                                           |                                                                                 |                                                                                             |

## 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  
H312 - Harmful in contact with skin  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H332 - Harmful if inhaled  
H335 - May cause respiratory irritation

### 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%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

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

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**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

### Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

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

**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)

### Training Advice

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

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Prepared By

Revision Date

Revision Summary

Health, Safety and Environmental Department

28-Jan-2024

New emergency telephone response service provider.

# **SAFETY DATA SHEET**

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**Revision Date 28-Jan-2024**

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**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**