

# Safety Data Sheet

fluorochem.

## 1. Identification of the substance/mixture

### 1.1 Product identification

|                           |                                                 |
|---------------------------|-------------------------------------------------|
| Product name              | tert-Butyl 3-phenyl-1,4-diazepane-1-carboxylate |
| Other names               |                                                 |
| Product code              | F640730                                         |
| CAS                       | 1211596-44-9                                    |
| MDL                       | MFCD06660435                                    |
| EINECS                    | N/A                                             |
| REACH Registration number |                                                 |

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

|                      |                                        |
|----------------------|----------------------------------------|
| Relevant uses        | For research and development purposes. |
| Uses advised against | No uses advised.                       |

### 1.3 Safety Data Sheet supplier details

|           |                                                                                 |
|-----------|---------------------------------------------------------------------------------|
| Company   | Fluorochem Ltd                                                                  |
| Address   | Unit 14, Graphite Way<br>Hadfield<br>Glossop Derbys. SK13 1QH<br>United Kingdom |
| Telephone | +44 1457 860111                                                                 |
| Email     | sds@fluorochem.co.uk                                                            |

### 1.4 Emergency Telephone

|                     |                                       |
|---------------------|---------------------------------------|
| Emergency Telephone | +44 20 3807 3798 (Poison Information) |
|---------------------|---------------------------------------|

## 2. Hazard Identification

### 2.1 Classification of the substance or mixture

|                |                                                                                |
|----------------|--------------------------------------------------------------------------------|
| Classification | H315 Skin Irrit. 2<br>H319 Eye Irrit. 2<br>H335 STOT SE 3<br>H302 Acute Tox. 4 |
|----------------|--------------------------------------------------------------------------------|

### 2.2 Label Elements

**Signal Word**

**Warning**

**Pictograms**



**GHS07**

**Hazards**

**H315** Causes skin irritation.  
**H319** Causes serious eye irritation.  
**H335** May cause respiratory irritation.  
**H302** Harmful if swallowed.

**Precautions**

**P101** If medical advice is needed, have product container or label at hand.  
**P264** Wash hands thoroughly after handling.  
**P271** Use only outdoors or in a well-ventilated area.  
**P305+P351+P338** IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
**P362+P364** Take off contaminated clothing and wash it before reuse.  
**P303+P361+P353** IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.  
**P302+P352** IF ON SKIN: Wash with plenty of water and soap.  
**P405** Store locked up.  
**P301+P310** IF SWALLOWED: Immediately call a POISON CENTER/doctor.  
**P270** Do not eat, drink or smoke when using this product.  
**P280** Wear protective gloves/protective clothing and eye/face protection.  
**P403+P233** Store in a well-ventilated place. Keep container tightly closed.  
**P308+P313** IF exposed or concerned: Get medical advice/attention.  
**P260** Do not breathe dust/fume/gas/mist/vapours/spray.  
**P301+P330+P331** IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.  
**P304+P340** IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
**P321** Specific treatment (see Section 4 on this SDS).  
**P501** Dispose of contents/container to hazardous waste disposal.

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**2.3 Other Hazards**

**Other Classification Hazards**

## 3. Composition

**3.1 SUBSTANCE**

| Name | CAS | Einecs | Composition | Hazards |
|------|-----|--------|-------------|---------|
|------|-----|--------|-------------|---------|

tert-Butyl 3-phenyl- 1211596-44-9 N/A  
1,4-diazepane-1-  
carboxylate

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### **3.2 MIXTURE**

Not applicable. Product is a substance.

## **4. First Aid Measures**

### **4.1 Description of First Aid Measures**

|                       |                                                                                                                                                                                                                                      |
|-----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Eye Contact</b>    | Where Diphoterine is not available, rinse eyes with copious amounts of water for at least 20 minutes. Protect uninjured eye. Remove contact lenses if present and easy to do. Continue rinsing and seek immediate medical attention. |
| <b>Ingestion</b>      | If swallowed rinse the mouth with plenty of water (only if the person is conscious) and contact a poison centre or physician if you feel unwell.                                                                                     |
| <b>Inhalation</b>     | Remove person to fresh air and keep comfortable for breathing. Call a poison centre or physician if you feel unwell. If breathing is irregular or stopped, administer artificial respiration.                                        |
| <b>Skin Contact</b>   | Where Diphoterine is not available, wash immediately with plenty of water and soap. Remove contaminated clothing immediately. Immediately seek medical attention.                                                                    |
| <b>General Advice</b> | No additional advice.                                                                                                                                                                                                                |

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### **4.2 Most Important Symptoms and Effects**

**Most Important Symptoms and Effects** No known symptoms or effects.

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### **4.3 Indication of any urgent medical attention and special treatments needed**

**Immediate First Aid Measures** No special immediate treatment required.

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## **5. Fire Fighting Measures**

### **5.1 Extinguishing Media**

|                                            |                                                                                               |
|--------------------------------------------|-----------------------------------------------------------------------------------------------|
| <b>Suitable Fire Extinguishing Media</b>   | Carbon dioxide, alcohol resistant foam or dry chemical powder., Use water to extinguish fire. |
| <b>Unsuitable Fire Extinguishing Media</b> | No known unsuitable media.                                                                    |

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

**Special Hazards** Thermal decomposition can lead to release of irritating gases and vapours.

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### **5.3 Recommendations for firefighting personnel**

## Advice for Fire Fighters

As in any fire, wear self-contained breathing apparatus and full protective gear.

## 6. Accidental Release Measures

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

#### Personal precautions

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Keep personnel away from spill/leak.

### 6.2 Environmental Precautions

#### Environmental Precautions

Prevent further leakage if safe to do so. Prevent product from entering drains. Do not let product enter waterways or sewer systems. Discharge into the environment must be avoided.

### 6.3 Containment and cleaning methods and materials

#### Containment - Methods and Materials

Absorb the spilled material with an inert absorbent (e.g. sand, silica gel, rag, vermiculite) before transferring into an airtight container. Remove all sources of ignition. Dispose of appropriately according to local regulations.

### 6.4 References to other sections

#### Referenced SDS Sections

For personal protection see section 8. For disposal see section 13.

## 7. Handling and Storage

### 7.1 Precautions for safe handling

#### Safe Handling

Wear appropriate personal protective equipment. Use only under a chemical fume hood. Keep away from heat/sparks/open flame/hot surfaces. Take measures to prevent the build-up of electrostatic charge. Ensure adequate exhaust ventilation, especially if dust, aerosol or fumes will be generated. Avoid contact with skin, eyes and clothing. For precautions see section 2.2.

#### Protection Against Explosion and Fire

Where possible, use anti static and spark proof equipment when handling.

#### General Occupational Hygiene

Handle in accordance with good industrial hygiene and safety practice. Wash hands before and after use. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing before re-use.

### 7.2 Conditions for Safe Storage and Incompatibilities

#### Managing Storage Risks

Keep container tightly closed and upright. Store in a cool, dry and well-ventilated place.

#### Storage Controls

No special requirements.

#### Maintaining Integrity

Keep container tightly closed in a cool area away from sunlight or heat sources.

**Other Advice**

No other specific advice available.

### **7.3 Specific End Use(s)**

**Specific End Use(s)**

No specific end uses are advised. The products supplied are for research purposes only.

## **8. Exposure Controls / Personal Protection**

### **8.1 Control Parameters**

**Control Parameters**

No data available.

### **8.2 Exposure Controls**

**Engineering Measures**

Use only under a chemical fume hood ensuring adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting/equipment. Ensure that eyewash stations and safety showers are close to the workstation location.

**Face Protection**

Wear tightly fitting safety goggles which adhere to European standard EN 166. Ensure eye bath is to hand.

**Hand Protection**

Handle with impermeable gloves. Inspect gloves before use. Gloves must satisfy the specifications of EU Directive 89/686/EEC and the standard EN374 derived from it. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

**Skin Protection**

Wear appropriate protective clothing ensuring all skin is covered. Wear safety shoes that meet at least S1 standards. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

**Respiratory Protection**

Product should be handled in a fume cupboard with adequate extraction. No respiratory equipment is needed under normal use conditions.

**Hygiene Measures**

Ensure hair or skin particles cannot enter the chemical container.

**Environment Exposure Controls**

Avoid discharge into the environment, see section 6.2.

## **9. Physical and Chemical Properties**

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

**a) State**

No data available.

**b) Colour**

No data available.

**c) Odour**

No data available.

**d) Melting Point / Freezing Point**

No data available.

**e) Initial Boiling point or Boiling range**

No data available.

**f) Flammability**

No data available.

|                                     |                    |
|-------------------------------------|--------------------|
| <b>Explosion Limits</b>             | No data available. |
| <b>h) Flash Point</b>               | No data available. |
| <b>i) Auto Ignition Temperature</b> | No data available. |
| <b>j) Decomposition Temperature</b> | No data available. |
| <b>k) pH</b>                        | No data available. |
| <b>l) Viscosity</b>                 | No data available. |
| <b>m) Solubility</b>                | No data available. |
| <b>n) Partition Coefficient</b>     | No data available. |
| <b>o) Vapour Pressure</b>           | No data available. |
| <b>p) Relative Density</b>          | No data available. |
| <b>q) Vapour Density</b>            | No data available. |
| <b>r) Appearance</b>                | No data available. |

## **9.2 Other Safety Information**

|                          |                    |
|--------------------------|--------------------|
| <b>Other Information</b> | No data available. |
|--------------------------|--------------------|

# **10. Stability and Reactivity**

## **10.1 Reactivity**

|                   |                    |
|-------------------|--------------------|
| <b>Reactivity</b> | No data available. |
|-------------------|--------------------|

## **10.2 Stability**

|                  |                                              |
|------------------|----------------------------------------------|
| <b>Stability</b> | Stable under recommended storage conditions. |
|------------------|----------------------------------------------|

## **10.3 Possibility of Hazardous Reactions**

|                                           |                                       |
|-------------------------------------------|---------------------------------------|
| <b>Possibility of Hazardous Reactions</b> | None under normal storage conditions. |
|-------------------------------------------|---------------------------------------|

## **10.4 Conditions to Avoid**

|                            |                                                                       |
|----------------------------|-----------------------------------------------------------------------|
| <b>Conditions to Avoid</b> | Heat, sparks, open flames, sources of ignition. Exposure to moisture. |
|----------------------------|-----------------------------------------------------------------------|

## **10.5 Incompatible Materials**

|                               |                          |
|-------------------------------|--------------------------|
| <b>Incompatible Materials</b> | Strong oxidizing agents. |
|-------------------------------|--------------------------|

## **10.6 Hazardous Decomposition Products**

|                                         |                    |
|-----------------------------------------|--------------------|
| <b>Hazardous Decomposition Products</b> | No data available. |
|-----------------------------------------|--------------------|

# **11. Toxicology Information**

## **11.1 Information on Hazard Classes, as defined in Regulation (EC) No. 1271/2008**

|                                        |                                                   |
|----------------------------------------|---------------------------------------------------|
| <b>Acute Toxicity</b>                  | No toxicological data available for this product. |
| <b>Skin Corrosion / Irritation</b>     | No Toxicology data available for this product.    |
| <b>Serious Eye Damage / Irritation</b> | No Toxicology data available for this product.    |

|                                          |                                                |
|------------------------------------------|------------------------------------------------|
| <b>Respiratory or Skin Sensitisation</b> | No Toxicology data available for this product. |
| <b>Germ Cell Mutagenicity</b>            | No Toxicology data available for this product. |
| <b>Carcinogenicity</b>                   | No Toxicology data available for this product. |
| <b>Reproductive Toxicity</b>             | No Toxicology data available for this product. |
| <b>STOT-single Exposure</b>              | No Toxicology data available for this product. |
| <b>STOT-repeated Exposure</b>            | No Toxicology data available for this product. |
| <b>Aspiration Hazard</b>                 | No Toxicology data available for this product. |

### **11.2 Information about Other Hazards**

|                                        |                                                |
|----------------------------------------|------------------------------------------------|
| <b>Endocrine Disrupting Properties</b> | Avoid release to the environment.              |
| <b>Addition Toxicology Information</b> | No Toxicology data available for this product. |

## **12. Ecological Information**

### **12.1 Toxicity**

|                 |                                                |
|-----------------|------------------------------------------------|
| <b>Toxicity</b> | No Ecological data available for this product. |
|-----------------|------------------------------------------------|

### **12.2 Persistence and Degradability**

|                                      |                                                |
|--------------------------------------|------------------------------------------------|
| <b>Persistence and Degradability</b> | No Ecological data available for this product. |
|--------------------------------------|------------------------------------------------|

### **12.3 Bio-Accumulative Potential**

|                                   |                                                |
|-----------------------------------|------------------------------------------------|
| <b>Bio-Accumulative Potential</b> | No Ecological data available for this product. |
|-----------------------------------|------------------------------------------------|

### **12.4 Mobility in Soil**

|                         |                                                |
|-------------------------|------------------------------------------------|
| <b>Mobility in Soil</b> | No Ecological data available for this product. |
|-------------------------|------------------------------------------------|

### **12.5 Results of PBT and vPvB assessment**

|                                           |                                                |
|-------------------------------------------|------------------------------------------------|
| <b>Results of PBT and vPvB assessment</b> | No Ecological data available for this product. |
|-------------------------------------------|------------------------------------------------|

### **12.6 Endocrine Disrupting Properties**

|                                        |                                   |
|----------------------------------------|-----------------------------------|
| <b>Endocrine Disrupting Properties</b> | Avoid release to the environment. |
|----------------------------------------|-----------------------------------|

### **12.7 Other Adverse Effects**

|                              |                                   |
|------------------------------|-----------------------------------|
| <b>Other Adverse Effects</b> | Avoid release to the environment. |
|------------------------------|-----------------------------------|

## **13. Disposal Considerations**

### **13.1 Waste Treatment Methods**

|                              |                                                                                                                               |
|------------------------------|-------------------------------------------------------------------------------------------------------------------------------|
| <b>Disposal Operations</b>   | Ensure product is disposed of by licensed waste carriers.                                                                     |
| <b>Disposal of Packaging</b> | Ensure INNER PACKAGING is disposed of by licensed waste carriers. Some OUTER PACKAGING MAY be recyclable if not contaminated. |

## **14. Transport Information**

### 14.1 UN Number

|                       |                    |                      |                    |                       |                    |
|-----------------------|--------------------|----------------------|--------------------|-----------------------|--------------------|
| <b>IATA UN Number</b> | No data available. | <b>ADR UN Number</b> | No data available. | <b>IMDG UN Number</b> | No data available. |
|-----------------------|--------------------|----------------------|--------------------|-----------------------|--------------------|

### 14.2 Official UN Shipping Name

|                                  |                                                                               |                                 |                                                                               |                                  |                                                                               |
|----------------------------------|-------------------------------------------------------------------------------|---------------------------------|-------------------------------------------------------------------------------|----------------------------------|-------------------------------------------------------------------------------|
| <b>IATA Proper Shipping Name</b> | Non Hazardous For Transport (tert-Butyl 3-phenyl-1,4-diazepane-1-carboxylate) | <b>ADR Proper Shipping Name</b> | Non Hazardous For Transport (tert-Butyl 3-phenyl-1,4-diazepane-1-carboxylate) | <b>IMDG Proper Shipping Name</b> | Non Hazardous For Transport (tert-Butyl 3-phenyl-1,4-diazepane-1-carboxylate) |
|----------------------------------|-------------------------------------------------------------------------------|---------------------------------|-------------------------------------------------------------------------------|----------------------------------|-------------------------------------------------------------------------------|

### 14.3 Hazard classes for transport purposes

|                          |                    |                         |                    |                          |                    |
|--------------------------|--------------------|-------------------------|--------------------|--------------------------|--------------------|
| <b>IATA Hazard Class</b> | No data available. | <b>ADR Hazard Class</b> | No data available. | <b>IMDG Hazard Class</b> | No data available. |
|--------------------------|--------------------|-------------------------|--------------------|--------------------------|--------------------|

### 14.4 Packing Group

|                           |                    |                          |                    |                           |                    |
|---------------------------|--------------------|--------------------------|--------------------|---------------------------|--------------------|
| <b>IATA Packing Group</b> | No data available. | <b>ADR Packing Group</b> | No data available. | <b>IMDG Packing Group</b> | No data available. |
|---------------------------|--------------------|--------------------------|--------------------|---------------------------|--------------------|

### 14.5 Enviromental Hazards

|                                   |                    |                                  |                    |                                   |                    |
|-----------------------------------|--------------------|----------------------------------|--------------------|-----------------------------------|--------------------|
| <b>IATA Environmental Hazards</b> | No data available. | <b>ADR Environmental Hazards</b> | No data available. | <b>IMDG Environmental Hazards</b> | No data available. |
|-----------------------------------|--------------------|----------------------------------|--------------------|-----------------------------------|--------------------|

### 14.6 Special Precautions

No Information Available

### 14.7 Bulk Maritime Transport in accordance with IMO Instructions

|                       |                    |                      |                    |                       |                    |
|-----------------------|--------------------|----------------------|--------------------|-----------------------|--------------------|
| <b>IATA Sub Class</b> | No data available. | <b>ADR Sub Class</b> | No data available. | <b>IMDG Sub Class</b> | No data available. |
|-----------------------|--------------------|----------------------|--------------------|-----------------------|--------------------|

## 15. Regulatory Information

### 15.1 Health, safety and environmental regulations/legislation specific to the substance or mixture

|                               |                                                                                           |
|-------------------------------|-------------------------------------------------------------------------------------------|
| <b>Regulatory Information</b> | As far as Fluorochem is aware, there are no further regulations controlling this product. |
|-------------------------------|-------------------------------------------------------------------------------------------|

### 15.2 Chemical Safety Assessment

|                                   |                                                                    |
|-----------------------------------|--------------------------------------------------------------------|
| <b>Chemical Safety Assessment</b> | There is no chemical safety assessment available for this product. |
|-----------------------------------|--------------------------------------------------------------------|

## 16. Other Information

### Information Not Covered in Other Sections

ional transport of dangerous goods by road). RID: International Regulations concerning the Transport of Dangerous Goods by Rail (Regulations regarding the international transport of dangerous goods by rail). IMDG: International Maritime Code for Dangerous Goods. IATA: International Air Transport Association. IATA-DGR: Dangerous Goods Regulations fra International Air Transport Association. ICAO: International Civil Aviation Organisation. ICAO-TI: Technical instructions from ICAO. GHS: Globally Harmonized System for Classification and Labelling of Chemicals. CAS: Chemical Abstracts Service

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**Other Information**

|               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|---------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Revision      | 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| Date Modified | 19/12/2024 18:46:00                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| Disclaimer    | The product listed is for research and development purposes only and not for human or animal use. As such, in most cases, the toxicological, ecological and physico-chemical properties have not been fully determined and the product should be treated with respect and always handled under suitable conditions by appropriately qualified personnel. The responsible party shall use this datasheet only in conjunction with other sources of information gathered by them, and should make an independent judgement of suitability, 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. This SDS adheres to Regulation (EC) No 1907/2006, and as of 13th April 2023, also conforms to EU Regulation 2020/878. |