

## SAFETY DATA SHEET

### 1. CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product Name: tert-Butyl 3-cyano-4-fluorobenzoate  
 CAS Number: 171050-07-0  
 Catalog Numbers: BD587342

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

Identified uses: For laboratory research purposes. Not for drug or household use.

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

488 Taoqiao Road, Building 6, 1F, HuiNan Town,  
 Pudong New Area, Shanghai 201399, China  
 Telephone: 86-21-61629022 | Fax: 86-21-61629029

#### 1.4 Emergency telephone

Emergency Phone: 1-352-323-3500  
 400 120 0761

### 2. HAZARDS IDENTIFICATION

#### 2.1 Classification of the substance or mixture

##### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, oral(Category 4)	H302
Skin corrosion/irritation (Category 2)	H315
Serious eye damage/eye irritation(Category 2A)	H319
Specific target organ toxicity, single exposure;Respiratory system(Category 3)	H335
No Resource File	

#### 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Warning

Hazard statement(s)

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

Precautionary statement(s)

P261	Avoid breathing dust/fume/gas/mist/vapours/spray.
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.

Additional precautionary phrases are located throughout the safety data sheet.

### 3. COMPOSITION, INFORMATION ON INGREDIENTS

Molecular Formula: C<sub>12</sub>H<sub>12</sub>FNO<sub>2</sub>  
 Molecular Weight: 221.23

Component	Concentration
tert-Butyl 3-cyano-4-fluorobenzoate	
CAS Number	171050-07-0

### 4. FIRST AID MEASURES

#### 4.1 Description of first aid measures

General advice

---

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

**If inhaled**

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**In case of skin contact**

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

**If swallowed**

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

**4.2 Most important symptoms and effects, both acute and delayed**

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

**4.3 Indication of any immediate medical attention and special treatment needed**

No data available

---

**5. FIRE FIGHTING MEASURES**

**5.1 Extinguishing media**

Suitable extinguishing media: alcohol-resistant foam, dry chemical or carbon dioxide

Unsuitable extinguishing media: no data

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

In combustion toxic fumes may form.

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus.

Wear protective clothing to prevent contact with skin and eyes.

---

**6. ACCIDENTAL RELEASE MEASURES**

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

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas.

Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

Do not attempt to take action without suitable protective clothing.

For personal protection see section 8.

**6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains or river.

Alert the neighbourhood to the presence of fumes or gas.

**6.3 Methods and materials for containment and cleaning up**

Mix with sand or vermiculite. Sweep up and shovel. Transfer to a closable, labelled salvage container for disposal by an appropriate method.

**6.4 Reference to other sections**

For disposal see section 13.

---

**7. HANDLING AND STORAGE**

**7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Wash hands thoroughly after handling. Ensure there is sufficient ventilation of the area.

Normal measures for preventive fire protection. For precautions see section 2.2.

**7.2 Conditions for safe storage, including any incompatibilities**

Keep container tightly closed in a dry and well-ventilated area. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Sealed in dry, 2-8°C

**7.3 Specific end use(s)**

The end use(s) have not been fully determined. The substance is supplied for Research and Development purposes by professionals only.

## 8. EXPOSURE CONTROLS, PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

##### Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. 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.

##### Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

Do not let product enter drains.

## 9 PHYSICAL AND CHEMICAL PROPERTIES

Appearance	Solid or liquid
Boiling Point	No data available
Melting Point	No data available
Odour	No data available
Odour Threshold	No data available
pH	No data available
Flash point	No data available
Evaporation rate	No data available
Vapour pressure	No data available
Vapor Density	No data available
Relative density	No data available
Solubility in water	No data available
Auto-ignition temperature	No data available
Decomposition temperature	No data available
Viscosity No Data	No data available
Explosive properties	No data available
Oxidizing properties	No data available

## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

#### 10.4 Conditions to avoid

Not data available

#### 10.5 Incompatible materials

Not data available

#### 10.6 Hazardous decomposition products

Carbon monoxide , carbon dioxide , hydrogen fluoride , nitrogen oxides

---

### 11. TOXICOLOGICAL INFORMATION

#### 11.1 Information on toxicological effects

Acute Toxicity	No data available
Skin corrosion/irritation	No data available
Serious eye Damage/irritation	No data available
Respiratory or skin sensitisation	No data available
Germ Cell mutagenicity	No data available
Carcinogenicity	No data available
Reproductive toxicity	No data available
STOT-single exposure	No data available
STOT-repeated exposure	No data available
Aspiration hazard	No data available

#### 11.2 Additional

To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH

---

### 12. ECOLOGICAL INFORMATION

#### 12.1 Toxicity

No data available

#### 12.2 Persistence and degradability

No data available

#### 12.3 Bioaccumulative potential

No data available

#### 12.4 Mobility in soil

No data available

#### 12.5 Results of PBT and vPvB assessment

No data available

#### 12.6 Other adverse effects

No data available

---

### 13. DISPOSAL CONSIDERATIONS

#### 13.1 Waste treatment methods

##### Disposal Operations

Consult state, local or national regulations for proper disposal. Hand over to authorised disposal company as hazardous waste.

##### Disposal of Packaging

Disposal must be made according to official regulations.

