

## SAFETY DATA SHEET

Version 8.2  
Revision Date 09/16/2020  
Print Date 06/01/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole

Product Number : 754218  
Brand : Aldrich  
CAS-No. : 887144-97-0

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

Identified uses : Laboratory chemicals, Synthesis of substances

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

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable solids (Category 2), H228  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

For the full text of the H-Statements mentioned in this Section, see Section 16.

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

Pictogram



Signal word

Warning

|                            |                                                                                                                                  |
|----------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| Hazard statement(s)        |                                                                                                                                  |
| H228                       | Flammable solid.                                                                                                                 |
| H315                       | Causes skin irritation.                                                                                                          |
| H319                       | Causes serious eye irritation.                                                                                                   |
| H335                       | May cause respiratory irritation.                                                                                                |
| Precautionary statement(s) |                                                                                                                                  |
| P210                       | Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.                                                              |
| P240                       | Ground/bond container and receiving equipment.                                                                                   |
| P241                       | Use explosion-proof electrical/ ventilating/ lighting/ equipment.                                                                |
| P261                       | Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.                                                                            |
| P264                       | Wash skin thoroughly after handling.                                                                                             |
| P271                       | Use only outdoors or in a well-ventilated area.                                                                                  |
| P280                       | Wear protective gloves/ eye protection/ face protection.                                                                         |
| P302 + P352                | IF ON SKIN: Wash with plenty of soap and water.                                                                                  |
| P304 + P340 + P312         | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.      |
| P305 + P351 + P338         | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P332 + P313                | If skin irritation occurs: Get medical advice/ attention.                                                                        |
| P337 + P313                | If eye irritation persists: Get medical advice/ attention.                                                                       |
| P362                       | Take off contaminated clothing and wash before reuse.                                                                            |
| P370 + P378                | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.                                             |
| P403 + P233                | Store in a well-ventilated place. Keep container tightly closed.                                                                 |
| P405                       | Store locked up.                                                                                                                 |
| P501                       | Dispose of contents/ container to an approved waste disposal plant.                                                              |

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                                     |
|------------------|-----------------------------------------------------|
| Formula          | : C <sub>10</sub> H <sub>10</sub> F <sub>3</sub> IO |
| Molecular weight | : 330.09 g/mol                                      |
| CAS-No.          | : 887144-97-0                                       |

| Component                                                | Classification                                                                | Concentration |
|----------------------------------------------------------|-------------------------------------------------------------------------------|---------------|
| <b>3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole</b> |                                                                               |               |
|                                                          | Flam. Sol. 2; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H228, H315, H319, H335 | <= 100 %      |

For the full text of the H-Statements mentioned in this Section, see Section 16.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Consult a physician. Show this material 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

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

Carbon oxides, Hydrogen fluoride, Hydrogen iodide

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers.

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## SECTION 6: Accidental release measures

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

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Avoid breathing dust.  
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.

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

Sweep up and shovel. Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal. Contain spillage, pick up with an electrically protected vacuum cleaner or by wet-brushing and transfer to a container for disposal according to local regulations (see section 13).

### **6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

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 place.

Recommended storage temperature 2 - 8 °C

Moisture sensitive. Heat sensitive. Handle under nitrogen, protect from moisture. Store under nitrogen. Keep in a dry place.

Storage class (TRGS 510): 4.1B: Flammable solid hazardous materials

### **7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients 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**

Safety glasses with side-shields conforming to EN166 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**

Impervious clothing, Flame retardant antistatic protective clothing., 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**

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

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## **SECTION 9: Physical and chemical properties**

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

|                                                 |                                                                    |
|-------------------------------------------------|--------------------------------------------------------------------|
| a) Appearance                                   | Form: powder<br>Color: beige                                       |
| b) Odor                                         | No data available                                                  |
| c) Odor Threshold                               | No data available                                                  |
| d) pH                                           | No data available                                                  |
| e) Melting point/freezing point                 | Melting point/range: 75 - 79 °C (167 - 174 °F)                     |
| f) Initial boiling point and boiling range      | No data available                                                  |
| g) Flash point                                  | ( )No data available                                               |
| h) Evaporation rate                             | No data available                                                  |
| i) Flammability (solid, gas)                    | The substance or mixture is a flammable solid with the category 2. |
| j) Upper/lower flammability or explosive limits | No data available                                                  |
| k) Vapor pressure                               | No data available                                                  |
| l) Vapor density                                | No data available                                                  |
| m) Relative density                             | No data available                                                  |
| n) Water solubility                             | No data available                                                  |
| o) Partition coefficient: n-octanol/water       | No data available                                                  |
| p) Autoignition temperature                     | No data available                                                  |
| q) Decomposition temperature                    | 130 °C (266 °F) -<br>, 611.95 kJ/kg                                |

- r) Viscosity No data available
- s) Explosive properties No data available
- t) Oxidizing properties No data available

## **9.2 Other safety information**

No data available

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## **SECTION 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**

Heat, flames and sparks.

### **10.5 Incompatible materials**

Strong oxidizing agents

### **10.6 Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen fluoride, Hydrogen iodide

Other decomposition products - No data available

In the event of fire: see section 5

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## **SECTION 11: Toxicological information**

### **11.1 Information on toxicological effects**

#### **Acute toxicity**

No data available

Inhalation: No data available

Dermal: No data available

No data available

#### **Skin corrosion/irritation**

No data available

#### **Serious eye damage/eye irritation**

No data available

#### **Respiratory or skin sensitization**

No data available

#### **Germ cell mutagenicity**

No data available

#### **Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is

identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

**Reproductive toxicity**

No data available

No data available

**Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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**SECTION 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**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**12.6 Other adverse effects**

No data available

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**SECTION 13: Disposal considerations**

**13.1 Waste treatment methods**

**Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**

Dispose of as unused product.

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## SECTION 14: Transport information

### DOT (US)

UN number: 1325    Class: 4.1    Packing group: III  
Proper shipping name: Flammable solids, organic, n.o.s. (3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 1325    Class: 4.1    Packing group: III    EMS-No: F-A, S-G  
Proper shipping name: FLAMMABLE SOLID, ORGANIC, N.O.S. (3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole)

### IATA

UN number: 1325    Class: 4.1    Packing group: III  
Proper shipping name: Flammable solid, organic, n.o.s. (3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole)

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## SECTION 15: Regulatory information

### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

### Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

No components are subject to the Massachusetts Right to Know Act.

### Pennsylvania Right To Know Components

|                                                   |                        |               |
|---------------------------------------------------|------------------------|---------------|
| 3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole | CAS-No.<br>887144-97-0 | Revision Date |
|---------------------------------------------------|------------------------|---------------|

|                                                   |                        |               |
|---------------------------------------------------|------------------------|---------------|
| 3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole | CAS-No.<br>887144-97-0 | Revision Date |
|---------------------------------------------------|------------------------|---------------|

### New Jersey Right To Know Components

|                                                   |                        |               |
|---------------------------------------------------|------------------------|---------------|
| 3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole | CAS-No.<br>887144-97-0 | Revision Date |
|---------------------------------------------------|------------------------|---------------|

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## SECTION 16: Other information

### Further information

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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