

Creation Date 22-May-2014

Revision Date 22-May-2014

Revision Number 1

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

### 1.1. Product identifier

Product Description: **3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole**  
 Cat No. : **456900000, 456902500, 456900010, 456900050**  
 Synonyms Togni's Reagent  
 CAS-No 887144-97-0  
 Molecular Formula C<sub>10</sub> H<sub>10</sub> F<sub>3</sub> I O

### 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 Acros Organics BVBA  
 Janssen Pharmaceuticaaan 3a  
 2440 Geel, Belgium  
 E-mail address begel.sdsdesk@thermofisher.com

### 1.4. Emergency telephone number

For information **US** call: 001-800-ACROS-01 / **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 - Regulation (EC) No 1272/2008

##### Physical hazards

Based on available data, the classification criteria are not met

##### Health hazards

Skin Corrosion/irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3

##### Environmental hazards

Based on available data, the classification criteria are not met

#### Classification according to EU Directives 67/548/EEC or 1999/45/EC

Symbol(s) Xi - Irritant

R-phrases R36/37/38 - Irritating to eyes, respiratory system and skin

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

### 2.2. Label elements

# SAFETY DATA SHEET

3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole

Revision Date 22-May-2014



**Signal Word**

**Warning**

## Hazard Statements

- H315 - Causes skin irritation
- H319 - Causes serious eye irritation
- H335 - May cause respiratory irritation

## Precautionary Statements

- P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
- P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
- P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection

## 2.3. Other hazards

No information available

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

Component	CAS-No	EC-No.	Weight %	CLP Classification - Regulation (EC) No 1272/2008	DSD Classification - 67/548/EEC
3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole	887144-97-0		>90	Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) STOT SE 3 (H335)	Xi; R36/37/38

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

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

#### General Advice

If symptoms persist, call a physician. Show this safety data sheet to the doctor in attendance.

#### Eye Contact

Immediately flush with plenty of water. After initial flushing, remove any contact lenses and continue flushing for at least 15 minutes. Keep eye wide open while rinsing. If symptoms persist, call a physician.

#### Skin Contact

Call a physician immediately. SPEEDY ACTION IS CRITICAL, GET MEDICAL AID IMMEDIATELY. If symptoms persist, call a physician. If skin irritation persists, call a physician. Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.

#### Ingestion

Clean mouth with water and drink afterwards plenty of water. Do not induce vomiting without medical advice. Never give anything by mouth to an unconscious person. Consult a physician.

# SAFETY DATA SHEET

3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole

Revision Date 22-May-2014

**Inhalation** Move to fresh air. Artificial respiration and/or oxygen may be necessary. Consult a physician. Immediate medical attention is not required. Move to fresh air in case of accidental inhalation of vapors. If symptoms persist, call a physician.

**Protection of First-aiders** Use personal protective equipment.

## **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**

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

#### **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**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Hydrogen iodide, Hydrogen fluoride.

### **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**

Use personal protective equipment. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### **6.2. Environmental precautions**

Do not flush into surface water or sanitary sewer system. Prevent further leakage or spillage if safe to do so. Prevent product from entering drains. See Section 12 for additional ecological Information.

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

### **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**

Pay attention to flashback. No information available.

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

# SAFETY DATA SHEET

3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole

Revision Date 22-May-2014

Keep refrigerated. Store under an inert atmosphere. Keep in properly labeled containers. Keep container tightly closed in a dry and well-ventilated place.

## 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.

#### Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

**Derived No Effect Level (DNEL)** No information available

Route of exposure	Acute effects (local)	Acute effects (systemic)	Chronic effects (local)	Chronic effects (systemic)
Oral Dermal Inhalation				

**Predicted No Effect Concentration (PNEC)** No information available.

### 8.2. Exposure controls

#### Engineering Measures

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
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# SAFETY DATA SHEET

3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole

Revision Date 22-May-2014

Natural rubber Nitrile rubber Neoprene PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)
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## Skin and body protection

Long sleeved clothing Impervious gloves

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

## Hygiene Measures

When using, do not eat, drink or smoke. Provide regular cleaning of equipment, work area and clothing.

## Environmental exposure controls

No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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

Appearance	Beige	
Physical State	Powder Solid	
Odor	No information available	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	75 - 79 °C / 167 - 174.2 °F	
Softening Point	No data available	
Boiling Point/Range	No information available	
Flash Point	No information available	<b>Method -</b> No information available
Evaporation Rate	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Vapor Pressure	No data available	
Vapor Density	Not applicable	Solid
Specific Gravity / Density	No data available	
Bulk Density	No data available	
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	Not applicable	

# SAFETY DATA SHEET

3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole

Revision Date 22-May-2014

Decomposition temperature	130°C	
Viscosity	Not applicable	Solid
Explosive Properties	No information available	
Oxidizing Properties	No information available	

## 9.2. Other information

Molecular Formula	C10 H10 F3 I O
Molecular Weight	330.09

## SECTION 10: STABILITY AND REACTIVITY

### 10.1. Reactivity

None known, based on information available

### 10.2. Chemical stability

heat sensitive: Moisture sensitive

### 10.3. Possibility of hazardous reactions

Hazardous Polymerization	No information available.
Hazardous Reactions	No information available.

### 10.4. Conditions to avoid

Heat. Exposure to moisture.

### 10.5. Incompatible materials

Strong oxidizing agents.

### 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Hydrogen iodide. Hydrogen fluoride.

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on toxicological effects

#### Product Information

#### (a) acute toxicity;

Oral	No data available
Dermal	No data available
Inhalation	No data available

(b) skin corrosion/irritation; Category 2

(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

# SAFETY DATA SHEET

3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole

Revision Date 22-May-2014

(h) STOT-single exposure;	Category 3
(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	Not applicable Solid
Symptoms / effects, both acute and delayed	No information available

## 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** 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. Other adverse effects

Endocrine Disruptor Information  
Persistent Organic Pollutant  
Ozone Depletion Potential

This product does not contain any known or suspected endocrine disruptors  
This product does not contain any known or suspected substance  
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 Catalogue, 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

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

# SAFETY DATA SHEET

3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole

Revision Date 22-May-2014

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. Transport in bulk according to Not applicable, packaged goods

Annex II of MARPOL73/78 and the

IBC Code

## SECTION 15: REGULATORY INFORMATION

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

**International Inventories**

X = listed No information available

**National Regulations**

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

Take note of Dir 94/33/EC on the protection of young people at work

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

15.2. Chemical safety assessment

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

## SECTION 16: OTHER INFORMATION

Full text of R-phrases referred to under sections 2 and 3

R36/37/38 - Irritating to eyes, respiratory system and skin

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

H315 - Causes skin irritation

H319 - Causes serious eye 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

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDL** - 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

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer



# SAFETY DATA SHEET

3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole

Revision Date 22-May-2014

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**PNEC** - Predicted No Effect Concentration

**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

**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 Compounds

## Key literature references and sources for data

Suppliers safety data sheet,

Chemadvisor - LOLI,

Merck index,

RTECS

## 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.

**Creation Date**

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**Revision Summary**

Not applicable.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006**

## Disclaimer

The information provided on 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 guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as 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 material or in any process, unless specified in the text.

**End of Safety Data Sheet**