

SAFETY DATA SHEET

Creation Date 22-May-2014

Revision Date 20-Dec-2025

Revision Number 7

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

1. Identification

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

Cat No. : AC456900000, AC456902500, AC456900010, AC456900050

CAS No 887144-97-0
Synonyms Togni's Reagent

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

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

2. Hazard(s) identification

Classification

This chemical is considered hazardous according to [US] OSHA (29 CFR 1910.1200, 2024)

Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

Label Elements

Signal Word

Warning

Hazard Statements

Causes skin irritation

Causes serious eye irritation
May cause respiratory irritation

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Wear protective gloves/protective clothing/eye protection/face protection
Avoid breathing dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing
Call a POISON CENTER or doctor if you feel unwell

Skin

IF ON SKIN: Wash with plenty of soap and water
If skin irritation occurs: Get medical advice/attention
Take off contaminated clothing

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
If eye irritation persists: Get medical advice/attention

Storage

Store in a well-ventilated place. Keep container tightly closed
Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

3. Composition/information on Ingredients

Component	CAS No	Weight %
3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole	887144-97-0	>90

4. First-aid measures

General Advice	If symptoms persist, call a physician.
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Skin Contact	If skin irritation persists, call a physician. Wash off immediately with plenty of water for at least 15 minutes.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Ingestion	Clean mouth with water and drink afterwards plenty of water. Get medical attention if

symptoms occur.

Most important symptoms and effects

None reasonably foreseeable.

Notes to Physician

Treat symptomatically

5. Fire-fighting measures

Unsuitable Extinguishing Media

No information available

Flash Point

No information available

Method -

No information available

Autoignition Temperature

Not applicable

Explosion Limits

Upper

No data available

Lower

No data available

Sensitivity to Mechanical Impact

No information available

Sensitivity to Static Discharge

No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen iodide. Hydrogen fluoride.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health
2

Flammability
1

Instability
1

Physical hazards
N/A

6. Accidental release measures

Personal Precautions

Use personal protective equipment as required. Ensure adequate ventilation. Avoid dust formation.

Environmental Precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

7. Handling and Storage

Handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

Storage.

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

8. Exposure controls / personal protection

Exposure Guidelines

This product does not contain any hazardous materials with occupational exposure limit established by the region specific regulatory bodies.

Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment

Eye/face Protection	Tight sealing safety goggles.
Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure.
Respiratory Protection	Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Recommended Filter type:	Particulates filter conforming to EN 143.
Hygiene Measures	When using do not eat, drink or smoke. Provide regular cleaning of equipment, work area and clothing.

9. Physical and chemical properties

Appearance

Physical State	Powder Solid
Color	Beige
Odor	No information available
Odor Threshold	No information available
Property	Values
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
Flammability (liquid)	Not applicable
Flammability (solid,gas)	No information available
Explosion Limits	No data available

Remarks**• Method**

Method - No information available
Solid

Autoignition Temperature	Not applicable
Decomposition Temperature	130°C
pH	No information available
Viscosity	Not applicable
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
Particle characteristics	No data available

Solid

Solid

Other Information

Molecular Formula	C10 H10 F3 I O
Molecular Weight	330.09
Evaporation Rate	Not applicable - Solid

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	heat sensitive. Moisture sensitive.
Conditions to Avoid	Heat. Exposure to moisture.

Incompatible Materials Strong oxidizing agents

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO₂), Hydrogen iodide, Hydrogen fluoride

Hazardous Polymerization No information available.

Hazardous Reactions None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation May cause irritation of respiratory tract.
Ingestion Ingestion may cause irritation to mucous membranes.
Eyes Irritating to eyes.
Skin Irritating to skin.

Toxicology data for the components

Toxicologically Synergistic Products No information 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;

The table below indicates whether each agency has listed any ingredient as a carcinogen

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole	887144-97-0	Not listed	Not listed	Not listed	Not listed	Not listed

(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

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

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

Endocrine Disrupting Properties This product does not contain any known or suspected endocrine disruptors.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability No information available

Bioaccumulation/ Accumulation No information available.

Mobility No information available.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT Not regulated

TDG Not regulated

IATA Not regulated

IMDG/IMO Not regulated

15. Regulatory Information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole	887144-97-0	-	-	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole	887144-97-0	-	-	-	-	-		-	-	-

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations

SARA 313

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ): N

DOT Marine Pollutant N

DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

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)
3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole	887144-97-0	-	-	-

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole	887144-97-0	Not applicable	Not applicable	Not applicable	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)
3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole (CAS #: 887144-97-0)	-	-	Listed	Listed	-

PFAS Legend

Listed = Meets the PFAS definition of the named authority

Other International Regulations

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	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
3,3-Dimethyl-1-(trifluoromethyl)-1,2-benziodoxole	887144-97-0	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information**Prepared By**

Product stewardship (Regulatory Affairs)
Thermo Fisher Scientific
email - begel.sdsdesk@thermofisher.com

Creation Date

22-May-2014

Revision Date

20-Dec-2025

Print Date

20-Dec-2025

Revision Summary

Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

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 SDS