

ALFAAA14657

3-(Trifluoromethyl)benzenesulfonyl chloride

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明:
Product Description: 3-(三氟甲基)苯磺酰氯, 98%
3-(Trifluoromethyl)benzenesulfonyl chloride

Cat No. : A14657
CAS No 777-44-6
Molecular Formula C7 H4 Cl F3 O2 S

Supplier Avocado Research Chemicals Ltd.
(Part of Thermo Fisher Scientific)
Shore Road, Heysham
Lancashire, LA3 2XY,
United Kingdom
Office Tel: +44 (0) 1524 850506
Office Fax: +44 (0) 1524 850608

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

E-mail address begel.sdsdesk@thermofisher.com

Recommended Use Laboratory chemicals.
Uses advised against No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State
Liquid

Appearance
Light yellow

Odor
No information available

Emergency Overview
Causes severe skin burns and eye damage. Moisture sensitive.

Classification of the substance or mixture

Skin Corrosion/Irritation	Category 1 B
Serious Eye Damage/Eye Irritation	Category 1

Label Elements



Signal Word

Danger

Hazard Statements

H314 - Causes severe skin burns and eye damage

SAFETY DATA SHEET

3-(Trifluoromethyl)benzenesulfonyl chloride

Precautionary Statements

Prevention

P264 - Wash face, hands and any exposed skin thoroughly after handling

P280 - Wear protective gloves/protective clothing/eye protection/face protection

Response

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting

P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P310 - Immediately call a POISON CENTER or doctor

P362 + P364 - Take off contaminated clothing and wash it before reuse

Storage

P403 - Store in a well-ventilated place

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Physical and Chemical Hazards

None identified.

Health Hazards

Corrosive. Causes skin and eye burns.

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Will likely be mobile in the environment due to its volatility. The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces.

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

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
3-(Trifluoromethyl)benzenesulfonyl chloride	777-44-6	95

SECTION 4. FIRST AID MEASURES

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.

Inhalation

Remove to fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.

Ingestion

Do NOT induce vomiting. Call a physician or poison control center immediately.

Most important symptoms and effects

Causes burns by all exposure routes. . Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation: Inhalation of corrosive fumes/gases may cause coughing, choking, headache, dizziness, and weakness for several hours. Pulmonary edema may occur with tightness in the chest, shortness of breath, bluish skin, decreased blood pressure and increased heart rate

Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of

contamination.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES**Suitable Extinguishing Media**

Carbon dioxide (CO₂). Dry chemical. Chemical foam.

Extinguishing media which must not be used for safety reasons

Water.

Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors.

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.

SECTION 6. ACCIDENTAL RELEASE MEASURES**Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required. Evacuate personnel to safe areas.

Environmental Precautions

Prevent further leakage or spillage if safe to do so.

Methods for Containment and Clean Up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Do not expose spill to water.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE**Handling**

Use only under a chemical fume hood. Wear personal protective equipment/face protection. Do not breathe mist/vapors/spray. Do not get in eyes, on skin, or on clothing. Do not ingest. If swallowed then seek immediate medical assistance. Wash hands before breaks and immediately after handling the product.

Storage

Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep under nitrogen.

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**Control Parameters****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. MDHS70 General methods for sampling airborne gases and vapours MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS

SAFETY DATA SHEET

3-(Trifluoromethyl)benzenesulfonyl chloride

96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Exposure Controls

Engineering Measures

Ensure adequate ventilation, especially in confined areas. 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
Nitrile rubber	See manufacturers	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
PVC				

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 compatibility, 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.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure

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: Organic gases and vapours filter Type A Brown conforming to EN14387

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:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141
 When RPE is used a face piece Fit Test should be conducted

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance Light yellow
Physical State Liquid

Odor No information available
Odor Threshold No data available
pH No information available
Melting Point/Range No data available
Softening Point No data available

3-(Trifluoromethyl)benzenesulfonyl chloride

Boiling Point/Range	77 - 79 °C / 170.6 - 174.2 °F	@ 0.8 mmHg
Flash Point	> 110 °C / > 230 °F	Method - No information available
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Vapor Pressure	No data available	
Vapor Density	8.44	(Air = 1.0)
Specific Gravity / Density	1.520	
Bulk Density	Not applicable	Liquid
Water Solubility	Reacts with water	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	No data available	
Explosive Properties	No information available	
Oxidizing Properties	No information available	
Molecular Formula	C7 H4 Cl F3 O2 S	
Molecular Weight	244.62	

SECTION 10. STABILITY AND REACTIVITY

Stability	Water reactive. Contact with water liberates toxic gas.
Hazardous Reactions	Contact with water liberates toxic gas.
Hazardous Polymerization	Hazardous polymerization does not occur.
Conditions to Avoid	Incompatible products. Exposure to moist air or water.
Materials to avoid	Strong oxidizing agents. Amines. Strong acids. Bases.
Hazardous Decomposition Products	Carbon monoxide (CO). Carbon dioxide (CO ₂). Sulfur oxides. Gaseous hydrogen fluoride (HF). Hydrogen chloride gas.

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information	No acute toxicity information is available for this product
(a) acute toxicity;	
(b) skin corrosion/irritation;	Category 1 B
(c) serious eye damage/irritation;	Category 1
(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

SAFETY DATA SHEET

3-(Trifluoromethyl)benzenesulfonyl chloride

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

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

Symptoms / effects, both acute and delayed Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation: Inhalation of corrosive fumes/gases may cause coughing, choking, headache, dizziness, and weakness for several hours. Pulmonary edema may occur with tightness in the chest, shortness of breath, bluish skin, decreased blood pressure and increased heart rate

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

Persistence and Degradability
Persistence No information available
Persistence is unlikely, based on information available.

Bioaccumulative Potential Bioaccumulation is unlikely

Mobility in soil The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Will likely be mobile in the environment due to its volatility. Disperses rapidly in air.

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant This product does not contain any known or suspected substance
Ozone Depletion Potential This product does not contain any known or suspected substance

SECTION 13. DISPOSAL CONSIDERATIONS

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.

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. Do not flush to sewer. Large amounts will affect pH and harm aquatic organisms.

SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport

SAFETY DATA SHEET

3-(Trifluoromethyl)benzenesulfonyl chloride

UN-No UN3265
Proper Shipping Name Corrosive liquid, acidic, organic, n.o.s.
Technical Shipping Name 3-(TRIFLUOROMETHYL)BENZENESULFONYL CHLORIDE
Hazard Class 8
Packing Group II

IMDG/IMO

UN-No UN3265
Proper Shipping Name Corrosive liquid, acidic, organic, n.o.s.
Technical Shipping Name 3-(TRIFLUOROMETHYL)BENZENESULFONYL CHLORIDE
Hazard Class 8
Packing Group II

IATA

UN-No UN3265
Proper Shipping Name Corrosive liquid, acidic, organic, n.o.s.
Technical Shipping Name 3-(TRIFLUOROMETHYL)BENZENESULFONYL CHLORIDE
Hazard Class 8
Packing Group II

Special Precautions for User No special precautions required

SECTION 15. REGULATORY INFORMATION

International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
3-(Trifluoromethyl)benzenesulfonyl chloride	-	-	X	-	-	-	-	-	-	-	-	-

National Regulations

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Creation Date 26-Sep-2009
Revision Date 27-Apr-2024
Revision Summary New emergency telephone response service provider.

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.

Legend

SAFETY DATA SHEET

3-(Trifluoromethyl)benzenesulfonyl chloride

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

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

DSL/NDSL - 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

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

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 Safety Data Sheet