

## SAFETY DATA SHEET

Version 6.10  
Revision Date 04/28/2025  
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## SECTION 1. IDENTIFICATION

## 1.1 Product identifiers

Product name : 2-(Trifluoromethyl)benzenesulfonyl chloride

Product Number : 491624

Brand : Aldrich

CAS-No. : 776-04-5

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

## 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

**GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)**

Skin corrosion : Category 1B

Serious eye damage : Category 1

**Other hazards**

None known.

**GHS label elements**

Hazard pictograms

:



Signal Word

: Danger

Hazard Statements

: H314 Causes severe skin burns and eye damage.

Precautionary Statements :

**Prevention:**

P264 Wash 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/ shower.

P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

Immediately call a POISON CENTER/ doctor.

P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.

P363 Wash contaminated clothing before reuse.

**Storage:**

P405 Store locked up.

**Disposal:**

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

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**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Substance / Mixture

: Substance

**Components**

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
2-(Trifluoromethyl)benzenesulfonyl chloride	776-04-5*	>= 90 - <= 100	-

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\* Indicates that the identifier is a CAS No.  
Actual concentration is withheld as a trade secret

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## SECTION 4. FIRST AID MEASURES

General advice	: First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.
If inhaled	: After inhalation: fresh air. Call in physician.
In case of skin contact	: In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.
In case of eye contact	: After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.
If swallowed	: After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.
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
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

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## SECTION 5. FIRE-FIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO <sub>2</sub> ) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products : Carbon oxides

Sulfur oxides

Hydrogen chloride gas

Hydrogen fluoride

Specific extinguishing methods : No data available

Further information : Suppress (knock down) gases/vapors/mists with a water spray jet.  
Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:  
Do not breathe vapors, aerosols.  
Avoid substance contact.  
Ensure adequate ventilation.  
Evacuate the danger area, observe emergency procedures, consult an expert.  
Advice for emergency responders:  
For personal protection see section 8.

Environmental precautions : Do not let product enter drains.

Methods and materials for containment and cleaning up : Cover drains. Collect, bind, and pump off spills.  
Observe possible material restrictions (see sections 7 and 10).

Take up with liquid-absorbent material (e.g. Chemizorb® ). Dispose of properly. Clean up affected area.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Further information on storage conditions	: Tightly closed. Keep locked up or in an area accessible only to qualified or authorized persons.
Storage class	: 8A, Combustible, corrosive hazardous materials
Recommended storage temperature	: Recommended storage temperature see product label.

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

### Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Remarks : required

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Tightly fitting safety goggles

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid

Color : colorless

Odor : No data available

Odor Threshold : No data available

pH : No data available

Melting point : No data available

Boiling point/boiling range : 271 - 275 °F / 133 - 135 °C (19 hPa)  
Method: lit.

Flash point : 278.6 °F / 137.0 °C  
Method: closed cup

Evaporation rate : No data available

Flammability (solid, gas) : No data available

Flammability (liquids) : No data available

Burning rate : No data available

Upper explosion limit /  
Upper flammability limit : No data available

Lower explosion limit /  
Lower flammability limit : No data available

Vapor pressure : No data available

Relative vapor density : No data available

Relative density : No data available

Density : 1.585 g/cm<sup>3</sup> (77 °F / 25 °C)

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Method: lit.

Water solubility	: No data available
Partition coefficient: n-octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 244.62 g/mol
Particle characteristics Particle size	: No data available

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## SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Forms explosive mixtures with air on intense heating.  A range from approx. 15 Kelvin below the flash point is to be rated as critical.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: No data available
Conditions to avoid	: Avoid moisture.  Strong heating.
Incompatible materials	: Strong oxidizing agents
Hazardous decomposition products	: In the event of fire: see section 5

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## SECTION 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

Remarks: No data available

#### Serious eye damage/eye irritation

Remarks: 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

No data available

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

No data available

### 11.2 Additional Information

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea



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## SECTION 12. ECOLOGICAL INFORMATION

### Ecotoxicity

#### Components:

##### **2-(Trifluoromethyl)benzenesulfonyl chloride:**

Toxicity to fish : Remarks: No data available

### Persistence and degradability

#### Components:

##### **2-(Trifluoromethyl)benzenesulfonyl chloride:**

Biodegradability : Remarks: No data available

### Bioaccumulative potential

#### Components:

##### **2-(Trifluoromethyl)benzenesulfonyl chloride:**

Bioaccumulation : Remarks: No data available

### Mobility in soil

#### Components:

##### **2-(Trifluoromethyl)benzenesulfonyl chloride:**

Stability in soil : Remarks: No data available

### Other adverse effects

#### Product:

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances  
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

#### Components:

##### **2-(Trifluoromethyl)benzenesulfonyl chloride:**

Additional ecological information : No data available

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## SECTION 13. DISPOSAL CONSIDERATIONS

### Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave

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chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14. TRANSPORT INFORMATION

### International Regulations

#### IATA-DGR

UN/ID No. : UN 3265  
Proper shipping name : Corrosive liquid, acidic, organic, n.o.s.  
(2-(Trifluoromethyl)benzenesulfonyl chloride)  
Class : 8  
Packing group : II  
Labels : Class 8 - Corrosive substances  
Packing instruction (cargo : 855  
aircraft)  
Packing instruction : 851  
(passenger aircraft)

#### IMDG-Code

UN number : UN 3265  
Proper shipping name : CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.  
(2-(Trifluoromethyl)benzenesulfonyl chloride)  
Class : 8  
Packing group : II  
Labels : 8  
EmS Code : F-A, S-B  
Marine pollutant : no

#### Transport in bulk according to IMO instruments

Not applicable for product as supplied.

### National regulation

#### 49 CFR Road

UN/ID/NA number : UN 3265  
Proper shipping name : Corrosive liquid, acidic, organic, n.o.s.  
(2-(Trifluoromethyl)benzenesulfonyl chloride)  
Class : 8  
Packing group : II  
Labels : Class 8 - Corrosive substances  
ERG Code : 153  
Marine pollutant : no

Poison Inhalation Hazard : No

### Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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## SECTION 15. REGULATORY INFORMATION

### **CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

### **SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

### **SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : No SARA Hazards

**SARA 313** : 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.

### **Clean Air Act**

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489).

### **Clean Water Act**

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

### **US State Regulations**

#### **Massachusetts Right To Know**

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

#### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

**The ingredients of this product are reported in the following inventories:**

TSCA : Product contains substance(s) not listed on TSCA inventory.

### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## **SECTION 16. OTHER INFORMATION**

### **Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is

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