

## SAFETY DATA SHEET

Version 6.9  
Revision Date 09/07/2024  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 4-(Trifluoromethyl)aniline

Product Number : 224936  
Brand : Aldrich  
CAS-No. : 455-14-1

**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****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Acute toxicity, Oral (Category 3), H301  
Serious eye damage (Category 1), H318  
Short-term (acute) aquatic hazard (Category 1), H400  
Long-term (chronic) aquatic hazard (Category 1), H410

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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

Danger

Hazard Statements

H301

Toxic if swallowed.

H318

Causes serious eye damage.

H410

Very toxic to aquatic life with long lasting effects.

Precautionary Statements

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P273

Avoid release to the environment.

P280

Wear eye protection/ face protection.

P301 + P310 + P330

IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.

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.

P391

Collect spillage.

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

Synonyms : 4-Aminobenzotrifluoride  
α,α,α-Trifluoro-p-toluidine

Formula : C<sub>7</sub>H<sub>6</sub>F<sub>3</sub>N  
Molecular weight : 161.12 g/mol  
CAS-No. : 455-14-1  
EC-No. : 207-236-5

| Component                          | Classification  | Concentration |
|------------------------------------|---|---------------|
| <b>α,α,α-Trifluoro-p-toluidine</b> |   |               |
|                                    | Acute Tox. 3; Eye Dam. 1;<br>Aquatic Acute 1; Aquatic<br>Chronic 1; H301, H318,<br>H400, H410<br>M-Factor - Aquatic Acute:<br>1 | <= 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

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

#### If swallowed

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

### 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

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

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

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Hydrogen fluoride

Combustible.

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

### 5.3 Advice for firefighters

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

## 5.4 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.

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## SECTION 6: Accidental release measures

### 6.1 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.

For personal protection see section 8.

### 6.2 Environmental precautions

Do not let product enter drains.

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

### 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

For precautions see section 2.2.

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

#### Storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

**Storage stability** Recommended storage temperature

2 - 8 °C

Handle and store under inert gas. Moisture sensitive.

#### Storage class

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

### 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

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

### Personal protective equipment

#### Eye/face 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 protection

required

#### Body Protection

protective clothing

#### Respiratory protection

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.

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.

### Control of environmental exposure

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: liquid<br>Color: colorless                      |
| b) Odor                                    | No data available                                     |
| c) Odor Threshold                          | No data available                                     |
| d) pH                                      | No data available                                     |
| e) Melting point/freezing point            | Melting point/freezing point: 38 °C (100 °F) - (ECHA) |
| f) Initial boiling point and boiling range | 83 °C 181 °F at 16 hPa - lit.                         |
| g) Flash point                             | No data available                                     |
| h) Evaporation rate                        | No data available                                     |
| i) Flammability (solid, gas)               | No data available                                     |

|   |  |
|---|--|
| j) Upper/lower flammability or explosive limits | No data available  |
| k) Vapor pressure                               | No data available  |
| l) Vapor density                                | No data available  |
| m) Density                                      | 1.283 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.          |
| Relative density                                | 1.2925 °C  |
| n) Water solubility                             | 0.229 g/l at 20 °C (68 °F) - partly soluble              |
| o) Partition coefficient: n-octanol/water       | log Pow: 1.95 - (ECHA), Bioaccumulation is not expected. |
| p) Autoignition temperature                     | No data available  |
| q) Decomposition temperature                    | No data available  |
| r) Viscosity                                    | No data available  |
| s) Explosive properties                         | No data available  |
| t) Oxidizing properties                         | none   |

## 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

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

no information available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 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

LD50 Oral - Rat - male and female - 128 mg/kg

Remarks: (ECHA)

Inhalation: No data available

LD50 Dermal - Rat - male and female - > 2,002 mg/kg  
(OECD Test Guideline 402)

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage. - 72 h

(OECD Test Guideline 405)

#### Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

#### Germ cell mutagenicity

Test Type: reverse mutation assay

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

#### 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

#### 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

RTECS: XU9260000

Cough, Shortness of breath, Headache, Nausea, Vomiting, May cause cyanosis., prolonged or repeated exposure can cause:, Dizziness

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

|   |   |
|---|---|
| Toxicity to fish  | semi-static test EC50 - Oncorhynchus mykiss (rainbow trout) - > 0.93 mg/l - 96 h<br>(OECD Test Guideline 203)   |
| Toxicity to daphnia and other aquatic invertebrates                   | static test EC50 - Daphnia magna (Water flea) - 0.85 mg/l - 48 h<br>(Directive 67/548/EEC, Annex V, C.2.)   |
| Toxicity to algae   | static test EbC50 - Pseudokirchneriella subcapitata (green algae) - 3.67 mg/l - 72 h<br>(OECD Test Guideline 201)<br><br>static test NOEC - Pseudokirchneriella subcapitata (green algae) - 0.61 mg/l - 72 h<br>(OECD Test Guideline 201) |
| Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) | flow-through test EC10 - Daphnia magna (Water flea) - 0.25 mg/l - 20 d<br>(OECD Test Guideline 211)<br><br>flow-through test NOEC - Daphnia magna (Water flea) - 0.4 mg/l - 20 d<br>(OECD Test Guideline 211)                             |

### 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 Endocrine disrupting properties

No data available

### 12.7 Other adverse effects

No data available



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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14: Transport information

#### DOT (US)

UN number: 2810    Class: 6.1    Packing group: III  
Proper shipping name: Toxic, liquids, organic, n.o.s. (a,a,a-Trifluoro-p-toluidine)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### IMDG

UN number: 2810    Class: 6.1    Packing group: III    EMS-No: F-A, S-A  
Proper shipping name: TOXIC LIQUID, ORGANIC, N.O.S. (a,a,a-Trifluoro-p-toluidine)  
Marine pollutant : yes

#### IATA

UN number: 2810    Class: 6.1    Packing group: III  
Proper shipping name: Toxic liquid, organic, n.o.s. (a,a,a-Trifluoro-p-toluidine)

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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 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.

#### US State Regulations

##### Massachusetts Right To Know

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

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**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 : All substances listed as active on the 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****Further information**

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 applicable to appropriate safety precautions for the product. 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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