

SAFETY DATA SHEET

Version 6.8
Revision Date 03/07/2024
Print Date 05/12/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : 3-(Trifluoromethyl)aniline

Product Number : A41801
Brand : Aldrich
CAS-No. : 98-16-8

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

Identified uses : Laboratory chemicals, Synthesis of substances

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)**

Flammable liquids (Category 4), H227
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Dermal (Category 4), H312
Skin irritation (Category 2), H315
Serious eye damage (Category 1), H318
Short-term (acute) aquatic hazard (Category 2), H401
Long-term (chronic) aquatic hazard (Category 2), H411

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

2.2 GHS Label elements, including precautionary statements

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Pictogram



Signal Word

Danger

Hazard Statements

H227

Combustible liquid.

H302 + H312

Harmful if swallowed or in contact with skin.

H315

Causes skin irritation.

H318

Causes serious eye damage.

H411

Toxic to aquatic life with long lasting effects.

Precautionary Statements

P210

Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.

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 protective gloves/ eye protection/ face protection.

P301 + P312 + P330

IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.

P302 + P352 + P312

IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.

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.

P332 + P313

If skin irritation occurs: Get medical advice/ attention.

P362

Take off contaminated clothing and wash before reuse.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P391

Collect spillage.

P403 + P235

Store in a well-ventilated place. Keep cool.

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 : 3-Aminobenzotrifluoride
α,α,α-Trifluoro-m-toluidine

Formula : C₇H₆F₃N
Molecular weight : 161.12 g/mol
CAS-No. : 98-16-8
EC-No. : 202-643-4

Component	Classification	Concentration
3-aminobenzotrifluoride		
	Flam. Liq. 4; Acute Tox. 4;	<= 100 %

	Skin Irrit. 2; Eye Dam. 1; Aquatic Acute 2; Aquatic Chronic 2; H227, H302, H312, H315, H318, H401, H411	
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For the full text of the H-Statements mentioned in this Section, see Section 16.

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. Consult a physician.

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: immediately make victim drink water (two glasses at most). Consult a physician.

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) 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_x)

Hydrogen fluoride

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.

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

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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. Keep away from heat and sources of ignition. 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 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.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

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

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face 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.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|-------------------|---|
| a) Appearance | Form: clear, liquid
Color: light brown |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |

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e) Melting point/freezing point	Melting point/range: 5 - 6 °C (41 - 43 °F) - lit.
f) Initial boiling point and boiling range	187 °C 369 °F - lit.
g) Flash point	87 °C (189 °F) - closed cup
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	1.29 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	1.2920 °C - Regulation (EC) No. 440/2008, Annex, A.3
n) Water solubility	4.68 g/l at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.6 - soluble
o) Partition coefficient: n-octanol/water	log Pow: 2.09 at 30 °C (86 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	< 400 °C (< 752 °F) at 0.009 - 0.01 hPanot auto-flammable
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

Surface tension	64.5 mN/m at 22.2 °C (72.0 °F) - Surface tension
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SECTION 10: Stability and reactivity

10.1 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.

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

Strong heating.

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 477 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity).
(RTECS)

Inhalation: No data available

Acute toxicity estimate Dermal - 1,100.1 mg/kg
(Expert judgment)

LD50 Dermal - Rabbit - 1,330 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity).

Lungs, Thorax, or Respiration:Dyspnea.

Prolonged skin contact may cause skin irritation and/or dermatitis.
(RTECS)

No data available

Skin corrosion/irritation

Skin - In vitro study

Result: irritating

Remarks: (ECHA)

Skin - In vitro study

Result: non-corrosive

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irreversible effects on the eye

Remarks: (ECHA)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: Not a skin sensitizer.

(OECD Test Guideline 429)

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

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: XU9180000

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.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 2.7 mg/l - 48 h Remarks: (ECOTOX Database)
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12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 4 % - Not readily biodegradable. (OECD Test Guideline 301B)
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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

Discharge into the environment must be avoided.

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.

SECTION 14: Transport information

DOT (US)

UN number: 2948 Class: 6.1 Packing group: II
Proper shipping name: 3-Trifluoromethylaniline
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2948 Class: 6.1 Packing group: II EMS-No: F-A, S-A
Proper shipping name: 3-TRIFLUOROMETHYLANILINE

IATA

UN number: 2948 Class: 6.1 Packing group: II
Proper shipping name: 3-Trifluoromethylaniline

SECTION 15: Regulatory information

SARA 302 Components

3-aminobenzotrifluoride	CAS-No. 98-16-8	Revision Date 2007-03-01
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SARA 313 Components

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.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

3-aminobenzotrifluoride	CAS-No. 98-16-8	Revision Date 2007-03-01
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Pennsylvania Right To Know Components

3-aminobenzotrifluoride	CAS-No. 98-16-8	Revision Date 2007-03-01
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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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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