

## SAFETY DATA SHEET

Version 6.3  
Revision Date 09/11/2021  
Print Date 10/30/2021**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 3-(Trifluoromethyl)phenol

Product Number : 156035  
Brand : Aldrich  
CAS-No. : 98-17-9**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 STATESTelephone : +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  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335  
Short-term (acute) aquatic hazard (Category 3), H402  
Long-term (chronic) aquatic hazard (Category 3), H412

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

Warning

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Hazard statement(s)	
H227	Combustible liquid.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H412	Harmful to aquatic life with long lasting effects.
Precautionary statement(s)	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P271	Use only outdoors or in a well-ventilated area.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: 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.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
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	: 3-Hydroxybenzotrifluoride a,a,a-Trifluoro-m-cresol
Formula	: C <sub>7</sub> H <sub>5</sub> F <sub>3</sub> O
Molecular weight	: 162.11 g/mol
CAS-No.	: 98-17-9
EC-No.	: 202-645-5

Component	Classification	Concentration
<b>a,a,a-Trifluoro-m-cresol</b>	Flam. Liq. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; Aquatic Acute 3; Aquatic Chronic 3; H227, H315, H319, H335, H402, H412	<= 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**

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

#### **If inhaled**

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### **In case of skin contact**

Wash off with soap and plenty of water. Consult a physician.

#### **In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### **If swallowed**

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

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## **SECTION 5: Firefighting measures**

### **5.1 Extinguishing media**

#### **Suitable extinguishing media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

#### **Unsuitable extinguishing media**

Do NOT use water jet.

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

Carbon oxides  
Hydrogen fluoride

### **5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

### **5.4 Further information**

Use water spray to cool unopened containers.

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## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of

vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

## **6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

## **6.3 Methods and materials for containment and cleaning up**

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Keep in suitable, closed containers for disposal.

## **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**

#### **Advice on safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

#### **Advice on protection against fire and explosion**

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

#### **Hygiene measures**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

For precautions see section 2.2.

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

#### **Storage conditions**

Keep container tightly closed in a dry and well-ventilated place.

#### **Storage class**

Storage class (TRGS 510): 10: Combustible liquids

### **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**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

## Personal protective equipment

### Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

#### Full contact

Material: Fluorinated rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

#### Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### Body Protection

Impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |               |                                      |
|---------------|--------------------------------------|
| a) Appearance | Form: clear, liquid<br>Color: yellow |
| b) Odor       | No data available                    |

c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: -2 - -1.8 °C (28 - 28.8 °F) - lit.
f) Initial boiling point and boiling range	178 - 179 °C 352 - 354 °F - lit.
g) Flash point	73 °C (163 °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	7.51 hPa at 70 °C (158 °F) 0.75 hPa at 40 °C(104 °F)
l) Vapor density	No data available
m) Density	1.333 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	insoluble
o) Partition coefficient: n-octanol/water	No data available
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	No data available

## 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

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Heat, flames and sparks.

## 10.5 Incompatible materials

Acid chlorides, Acid anhydrides, 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

Oral: No data available

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

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

Inhalation - May cause respiratory irritation.

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

No data available

### 11.2 Additional Information

RTECS: GP3510000

Depending on the intensity and duration of exposure, effects may vary from mild irritation to severe destruction of tissue., prolonged or repeated exposure can cause:, Damage to the eyes.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates EC50 - Daphnia magna (Water flea) - 11 mg/l - 48 h

### 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 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Harmful to aquatic life.

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Offer surplus and non-recyclable solutions to a licensed disposal company. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Contact a licensed professional waste disposal service to dispose of this material.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### DOT (US)

NA-Number: 1993 Class: NONE Packing group: III  
Proper shipping name: Combustible liquid, n.o.s. (a,a,a-Trifluoro-m-cresol)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

Not dangerous goods

### IATA

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Not dangerous goods

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## SECTION 15: Regulatory information

### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### 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, Chronic Health Hazard

### Massachusetts Right To Know Components

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

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

### Pennsylvania Right To Know Components

$\alpha,\alpha,\alpha$ -Trifluoro-m-cresol	CAS-No. 98-17-9	Revision Date
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$\alpha,\alpha,\alpha$ -Trifluoro-m-cresol	CAS-No. 98-17-9	Revision Date
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### New Jersey Right To Know Components

$\alpha,\alpha,\alpha$ -Trifluoro-m-cresol	CAS-No. 98-17-9	Revision Date
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## SECTION 16: Other information

### Further information

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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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