

## SAFETY DATA SHEET

Version 5.3  
Revision Date 03/18/2016  
Print Date 11/18/2018

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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : 3,4,5-Trifluorophenol

Product Number : 51092  
Brand : Aldrich

CAS-No. : 99627-05-1

## 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  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

## 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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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  
Skin corrosion (Category 1B), H314  
Serious eye damage (Category 1), H318  
Acute aquatic toxicity (Category 2), H401  
Chronic aquatic toxicity (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

Pictogram



Signal word : Danger

Hazard statement(s)

H301 : Toxic if swallowed.  
H314 : Causes severe skin burns and eye damage.  
H318 : Causes serious eye damage.  
H411 : Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P260 : Do not breathe dust or mist.  
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/ protective clothing/ eye protection/ face protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/doctor. Rinse mouth.
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.
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

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Formula	: C <sub>6</sub> H <sub>3</sub> F <sub>3</sub> O
Molecular weight	: 148.08 g/mol
CAS-No.	: 99627-05-1
EC-No.	: 436-120-9

#### Hazardous components

Component	Classification	Concentration
<b>3,4,5-Trifluorophenol</b>		
	Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Aquatic Acute 2; Aquatic Chronic 2; H301, H314, H318, H411	<= 100 %

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

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this 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

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

#### 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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## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### **Suitable extinguishing media**

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

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

No data available

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

No data available

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## 6. ACCIDENTAL RELEASE MEASURES

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

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

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

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

### 6.4 Reference to other sections

For disposal see section 13.

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## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

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

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

Storage class (TRGS 510): Non-combustible, acute toxic Cat.3 / toxic hazardous materials or hazardous materials 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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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### **Components with workplace control parameters**

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### **Appropriate engineering controls**

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

#### **Personal protective equipment**

##### **Eye/face protection**

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

### Skin protection

Handle with impervious gloves. Wash and dry hands. 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.

#### Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

#### Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, 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 CE 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

Complete suit protecting against chemicals, 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 by a qualified industrial hygienist 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 EN 14387 (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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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |                                                 |                                                |
|-------------------------------------------------|------------------------------------------------|
| a) Appearance                                   | Form: crystalline<br>Colour: colourless        |
| b) Odour                                        | No data available                              |
| c) Odour Threshold                              | No data available                              |
| d) pH                                           | No data available                              |
| e) Melting point/freezing point                 | Melting point/range: 52 - 55 °C (126 - 131 °F) |
| f) Initial boiling point and boiling range      | 188 °C (370 °F) at 1,013 hPa (760 mmHg)        |
| 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) Vapour pressure                              | 1.7 hPa (1.3 mmHg) at 25 °C (77 °F)            |
| l) Vapour density                               | No data available                              |

m) Relative density	No data available
n) Water solubility	soluble
o) Partition coefficient: n-octanol/water	log Pow: 1.9 at 25 °C (77 °F)
p) Auto-ignition 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

Surface tension	68.1 mN/m at 20 °C (68 °F)
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## 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

No data available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen fluoride

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - 200 - 2,000 mg/kg

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: Causes burns. - 4 h

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Risk of serious damage to eyes.

#### Respiratory or skin sensitisation

Maximisation Test - Guinea pig

Result: Does not cause skin sensitisation.

**Germ cell mutagenicity**

Ames test

Result: Not mutagenic in Ames Test

**Carcinogenicity**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

**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

**Additional Information**

Repeated dose toxicity Rat - Oral - NOAEL : 450 mg/kg - OECD Test Guideline 407

RTECS: Not available

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**12. ECOLOGICAL INFORMATION****12.1 Toxicity**

Toxicity to fish semi-static test LC50 - Danio rerio (zebra fish) - 7.5 mg/l - 96.0 h (OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates EC50 - Daphnia magna (Water flea) - 5.1 mg/l - 48 h

Toxicity to algae EC50 - Desmodesmus subspicatus (green algae) - 16.5 mg/l - 72 h

**12.2 Persistence and degradability**

Biodegradability Result: 1 % - Not readily biodegradable.

**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**

Toxic to aquatic life with long lasting effects.

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

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

#### Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

#### Contaminated packaging

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

### DOT (US)

UN number: 2923      Class: 8 (6.1)      Packing group: II  
Proper shipping name: Corrosive solids, toxic, n.o.s. (3,4,5-Trifluorophenol)  
Reportable Quantity (RQ):

Poison Inhalation Hazard: No

### IMDG

UN number: 2923      Class: 8 (6.1)      Packing group: II      EMS-No: F-A, S-B  
Proper shipping name: CORROSIVE SOLID, TOXIC, N.O.S. (3,4,5-Trifluorophenol)  
Marine pollutant:yes

### IATA

UN number: 2923      Class: 8 (6.1)      Packing group: II  
Proper shipping name: Corrosive solid, toxic, n.o.s. (3,4,5-Trifluorophenol)

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## 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

Acute Health Hazard

### Massachusetts Right To Know Components

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

### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
3,4,5-Trifluorophenol	99627-05-1	

### New Jersey Right To Know Components

	CAS-No.	Revision Date
3,4,5-Trifluorophenol	99627-05-1	

### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## 16. OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity

Eye Dam.	Serious eye damage
H301	Toxic if swallowed.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H401	Toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.

**HMIS Rating**

Health hazard:	2
Chronic Health Hazard:	
Flammability:	0
Physical Hazard	0

**NFPA Rating**

Health hazard:	2
Fire Hazard:	0
Reactivity Hazard:	0

**Further information**

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**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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