SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

<table>
<thead>
<tr>
<th>Product name</th>
<th>4-(Trifluoromethyl)benzoyl chloride</th>
</tr>
</thead>
<tbody>
<tr>
<td>Product Number</td>
<td>249475</td>
</tr>
<tr>
<td>Brand</td>
<td>Aldrich</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>329-15-7</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Company</th>
<th>Sigma-Aldrich Inc.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3050 SPRUCE ST</td>
</tr>
<tr>
<td></td>
<td>ST. LOUIS MO 63103</td>
</tr>
<tr>
<td></td>
<td>UNITED STATES</td>
</tr>
<tr>
<td>Telephone</td>
<td>+1 314 771-5765</td>
</tr>
<tr>
<td>Fax</td>
<td>+1 800 325-5052</td>
</tr>
</tbody>
</table>

1.4 Emergency telephone

<table>
<thead>
<tr>
<th>Emergency Phone #</th>
<th>800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>24 Hours/day; 7 Days/week</td>
</tr>
</tbody>
</table>

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 corrosion (Category 1B), H314
- Serious eye damage (Category 1), H318

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

2.2 GHS Label elements, including precautionary statements

<table>
<thead>
<tr>
<th>Pictogram</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Signal Word</td>
<td>Danger</td>
</tr>
</tbody>
</table>

Aldrich - 249475
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

### Hazard statement(s)
- H227: Combustible liquid.
- H314: Causes severe skin burns and eye damage.

### Precautionary statement(s)
- P210: Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
- P264: Wash skin thoroughly after handling.
- P280: Wear protective gloves/ protective clothing/ eye protection/ face protection.
- 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.
- P370 + P378: In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
- 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: α,α,α-Trifluoro-p-toluoyl chloride
- Formula: \( C_8H_4ClF_3O \)
- Molecular weight: 208.56 g/mol
- CAS-No.: 329-15-7
- EC-No.: 206-342-9

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-Trifluoromethylbenzoic acid chloride</td>
<td>Flam. Liq. 4; Skin Corr. 1B; Eye Dam. 1; H227, H314, H318</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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**
First aidsers 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.

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**
Carbon dioxide (CO2) Dry powder

**Unsuitable extinguishing media**
Foam Water

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Hydrogen chloride gas
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 locked up or in an area accessible only to qualified or authorized persons.

Moisture sensitive.

Storage class
Storage class (TRGS 510): 8A: Combustible, corrosive 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**
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

- Full contact
  - Material: Viton®
  - 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)

**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 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: 64 - 65 °C (147 - 149 °F)

f) **Initial boiling point and boiling range**
   - 78 - 79 °C 172 - 174 °F at 21 hPa - lit.
   - 188 - 190 °C (370 - 374 °F) - lit.

g) **Flash point**
   - 78 °C (172 °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**
   - 1.404 g/cm3 at 25 °C (77 °F) - lit.
   - Relative density
     - No data available

n) **Water solubility**
   - No data available

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**
   - none

9.2 Other safety information

- No data available

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
Violent reactions possible with:
- Water
- Alcohols
- Bases
- Oxidizing agents

10.4 Conditions to avoid
Strong heating.

10.5 Incompatible materials
No data available

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
Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.
Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract
Dermal: No data available

Skin corrosion/irritation
Remarks: Causes skin burns.

Serious eye damage/eye irritation
Remarks: Causes serious eye damage.

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
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. Cough, Shortness of breath, Headache, Nausea
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.
Other dangerous properties can not be excluded.
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity
No data available

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
Product reacts with water.
Hazardous decomposition products
hydrochloric acid
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: 3265  
  - Class: 8  
  - Packing group: II  
- Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (p-Trifluoromethylbenzoic acid chloride)  
- Reportable Quantity (RQ):  
  - Poison Inhalation Hazard: No

**IMDG**
- UN number: 3265  
  - Class: 8  
  - Packing group: II  
  - EMS-No: F-A, S-B  
- Proper shipping name: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (p-Trifluoromethylbenzoic acid chloride)

**IATA**
- UN number: 3265  
  - Class: 8  
  - Packing group: II  
- Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (p-Trifluoromethylbenzoic acid chloride)

SECTION 15: Regulatory information

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

**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.

**Massachusetts Right To Know Components**
No components are subject to the Massachusetts Right to Know Act.

SECTION 16: Other information

**Further information**
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...
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Version: 6.5 Revision Date: 08/11/2023 Print Date: 08/12/2023