

## SAFETY DATA SHEET

Version 6.12  
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 : *p*-Toluenesulfonyl chloride

Product Number : 240877  
Brand : Sigma-Aldrich  
CAS-No. : 98-59-9

**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)**

Corrosive to Metals (Category 1), H290  
Skin irritation (Category 2), H315  
Serious eye damage (Category 1), H318  
Skin sensitization (Category 1), H317

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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

H290 May be corrosive to metals.  
H315 Causes skin irritation.  
H317 May cause an allergic skin reaction.  
H318 Causes serious eye damage.

Precautionary Statements

P234 Keep only in original container.  
P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.  
P264 Wash skin thoroughly after handling.  
P272 Contaminated work clothing must not be allowed out of the workplace.  
P280 Wear protective gloves/ eye protection/ face protection.  
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.  
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.  
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.  
P362 Take off contaminated clothing and wash before reuse.  
P390 Absorb spillage to prevent material damage.  
P406 Store in corrosive resistant container with a resistant inner liner.  
P501 Dispose of contents/ container to an approved waste disposal plant.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Vesicant., Lachrymator.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : Tosyl chloride  
Formula : C<sub>7</sub>H<sub>7</sub>ClO<sub>2</sub>S  
Molecular weight : 190.65 g/mol  
CAS-No. : 98-59-9  
EC-No. : 202-684-8

Component	Classification	Concentration
<b>p-toluenesulphonyl chloride</b>		
	Met. Corr. 1; Skin Irrit. 2; Eye Dam. 1; Skin Sens. 1; H290, H315, H318, H317	<= 100 %

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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. 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

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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

Sulfur oxides

Hydrogen chloride gas

Carbon oxides

Sulfur oxides

Hydrogen chloride gas

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**

Water hydrolyzes material liberating acidic gas which in contact with metal surfaces can generate flammable and/or explosive hydrogen gas. 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: Avoid inhalation of dusts. 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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### **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**

Store under inert gas. No metal containers.

Tightly closed. Dry.

Store under inert gas. Moisture sensitive.

#### **Storage class**

Storage class (TRGS 510): 8B: Non-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

Component	CAS-No.	Value	Control parameters	Basis
p-toluenesulphonyl chloride	98-59-9	CEIL	5 mg/m <sup>3</sup>	USA. Workplace Environmental Exposure Levels (WEEL)

### 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

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: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

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

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (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 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

protective clothing

##### Respiratory protection

Recommended Filter type: Filter type P2

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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 dusts 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: crystalline Color: white, to, gray
b) Odor	characteristic
c) Odor Threshold	No data available
d) pH	strongly acid
e) Melting point/freezing point	Melting point/ range: 65 - 69 °C (149 - 156 °F) - lit.
f) Initial boiling point and boiling range	134 °C 273 °F at 13 hPa - lit.
g) Flash point	128 °C (262 °F) - closed cup - c.c.
h) Evaporation rate	No data available
i) Flammability (solid, gas)	The product is not flammable.
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	0.00 hPa at 20 °C (68 °F)
l) Vapor density	No data available
m) Density	1.492 g/cm <sup>3</sup> at 20 °C (68 °F) - OECD Test Guideline 109
Relative density	No data available
n) Water solubility	Hydrolysis
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 Not classified as explosive.
- t) Oxidizing properties none

## **9.2 Other safety information**

No data available

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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.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### **10.2 Chemical stability**

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

### **10.3 Possibility of hazardous reactions**

Risk of explosion with:

Alkali metals

conc. sulfuric acid

Risk of ignition or formation of inflammable gases or vapours with:

carbides

lithium silicide

Fluorine

Generates dangerous gases or fumes in contact with:

Aluminum

hydrides

formaldehyde

Metals

strong alkalis

Sulfides

Exothermic reaction with:

Amines

potassium permanganate

salts of oxyhalogenic acids

semimetallic oxides

semimetallic hydrogen compounds

Aldehydes

vinylmethyl ether

### **10.4 Conditions to avoid**

Exposure to moisture.

Strong heating.

### **10.5 Incompatible materials**

Metals

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## 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 - 4,680 mg/kg

(OECD Test Guideline 401)

Inhalation: No data available

Dermal: No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h

(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage.

(OECD Test Guideline 405)

#### Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: positive

(OECD Test Guideline 429)

#### Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Metabolic activation: Metabolic activation

Method: OECD Test Guideline 476

Result: positive

Test Type: Micronucleus test

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Intraperitoneal injection

Method: OECD Test Guideline 474

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**

Repeated dose toxicity - Rat - male and female - Oral - LOAEL (Lowest observed adverse effect level) - 150 mg/kg

RTECS: DB8929000

spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, Blistering, Lachrymation, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin.

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	static test LC50 - <i>Oryzias latipes</i> (Orange-red killifish) - > 100 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - > 334 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> (green algae) - > 100 mg/l - 72 h (US-EPA)  static test NOEC - <i>Pseudokirchneriella subcapitata</i> (green algae) - 2.6 mg/l - 72 h (US-EPA)
Toxicity to bacteria	static test NOEC - activated sludge - 580 mg/l - 3 h (OECD Test Guideline 209)

**12.2 Persistence and degradability**

Biodegradability      aerobic - Exposure time 28 d  
Result: 60 % - Readily biodegradable.  
(OECD Test Guideline 301D)

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

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## 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.

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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: 3261    Class: 8    Packing group: III  
Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (p-toluenesulphonyl chloride)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 3261    Class: 8    Packing group: III    EMS-No: F-A, S-B  
Proper shipping name: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (p-toluenesulphonyl chloride)

### IATA

UN number: 3261    Class: 8    Packing group: III  
Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (p-toluenesulphonyl chloride)

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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

Components	CAS-No.	Component TPQ (lbs)
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**SARA 311/312 Hazards** : Acute Health Hazard

**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.

#### **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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