

SAFETY DATA SHEET

Version 6.11 Revision Date 12/18/2024 Print Date 12/19/2024

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : p-Toluenesulfonyl chloride

Product Number : T35955

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

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Corrosive to Metals : Category 1

Skin irritation : Category 2

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Merck

Serious eye damage : Category 1

Skin sensitization : Category 1

GHS label elements

Hazard pictograms





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 : **Prevention:**

P234 Keep only in original container.

P261 Avoid breathing dust.

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 pro-

tection.

Response:

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 medi-

cal advice/ attention.

P362 Take off contaminated clothing and wash before

reuse.

P390 Absorb spillage to prevent material damage.

Storage:

P406 Store in corrosive resistant container with a re-

sistant inner liner.

Disposal:

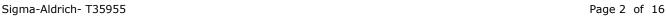
P501 Dispose of contents/ container to an approved

waste disposal plant.

Other hazards

Vesicant.

Lachrymator.



SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Chemical name	CAS-No.	Concentration (% w/w)
p-toluenesulphonyl chloride	98-59-9	>= 90 - <= 100

Actual concentration is withheld as a trade secret

SECTION 4. 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 con-

taminated 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 wa-

ter (two glasses at most).

Consult a physician.

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

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

SECTION 5. FIRE-FIGHTING MEASURES

Suitable extinguishing

media

: Carbon dioxide (CO2)

Dry powder

Unsuitable extinguishing

media

Foam Water

Specific hazards during

fire fighting

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: Combustible.

Vapors are heavier than air and may spread along

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floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products

: Carbon oxides

Sulfur oxides

Hydrogen chloride gas

Hazardous combustion products

Carbon oxides

Sulfur oxides

Hydrogen chloride gas

Specific extinguishing methods

: No data available

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.

Special protective equipment for fire-fighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation.

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Evacuate the danger area, observe emergency proce-

dures, consult an expert.

Advice for emergency responders: For personal protection see section 8.

Environmental precau-

tions

: Do not let product enter drains.

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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Conditions for safe stor- : Store under inert gas.

age

No metal containers.

Further information on

storage conditions

: Tightly closed.

Dry.

: 8A, Combustible, corrosive hazardous materials Storage class

Recommended storage

temperature

: Recommended storage temperature see product label.

Further information on

storage stability

: Store under inert gas. Moisture sensitive.

Packaging material : Suitable material: Poly Drum, Amber Glass Bottle/Jar

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

g and a grant of the contract					
Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis	
p-toluenesulphonyl chlo- ride	98-59-9	CEIL	5 mg/m3	US WEEL	

Engineering measures : No data available

Personal protective equipment

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Respiratory protection : 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.

Recommended Filter

type:

: filter E-(P2)

The entrepeneur 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.

Hand protection

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Full contact

Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Splash contact

Manufacturer : KCL 741 Dermatril® L

Remarks : 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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-

36124 Eichenzell, Internet: www.kcl.de).

Eye protection : Use equipment for eye protection tested and ap-

proved under appropriate government standards such

as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply

preventive skin protection. Wash hands and face af-

ter working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

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Appearance : crystalline

Color : white, to, gray

Odor : characteristic

Odor Threshold : No data available

: strongly acid

Melting point/ range : 149 - 156 °F / 65 - 69 °C

Boiling point/boiling range : 273 °F / 134 °C

(13 hPa)

Flash point : 262 °F / 128 °C

Method: c.c., closed cup

Evaporation rate : No data available

Burning rate : No data available

Upper explosion limit / Upper flammability limit : No data available

Lower explosion limit /

Lower flammability limit

: No data available

Vapor pressure : 0.13 Pa (68 °F / 20 °C)

Relative vapor density : No data available

Relative density : No data available

Density : 1.492 g/cm3 (68 °F / 20 °C)

Method: OECD Test Guideline 109

Solubility(ies)

: Hydrolysis (68 °F / 20 °C) Water solubility

Partition coefficient: n-

octanol/water

: No data available

Autoignition temperature : No data available

Decomposition tempera- : No data available

ture

Viscosity, dynamic : No data available

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Viscosity, kinematic : No data available

Flow time : No data available

Explosive properties : Not classified as explosive.

Oxidizing properties : none

Molecular weight : 190.65 g/mol

Metal corrosion rate : 6.25 mm/a

6.25 mm/a

May be corrosive to metals.

Particle characteristics

Particle size : No data available

SECTION 10. STABILITY AND REACTIVITY

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.

Chemical stability : The product is chemically stable under standard ambi-

ent conditions (room temperature).

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

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Metals strong alkalis Sulfides

Exothermic reaction with:

Amines

potassium permanganate salts of oxyhalogenic acids

semimetallic oxides

semimetallic hydrogen compounds

Aldehydes

vinylmethyl ether

Conditions to avoid : Exposure to moisture.

Strong heating.

Incompatible materials : Metals

Hazardous decomposition : In the event of fire: see section 5

products

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

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Merc

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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.

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

p-toluenesulphonyl chloride:

Toxicity to fish : LC50 (Oryzias latipes (Orange-red killifish)): > 100

mg/l

End point: mortality Exposure time: 96 h Test Type: static test Analytical monitoring: yes

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Method: OECD Test Guideline 203

GLP: yes

Toxicity to daphnia and other aquatic inverte-

brates

: EC50 (Daphnia magna (Water flea)): > 334 mg/l

End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes

Method: OECD Test Guideline 202

GLP: yes

Toxicity to algae/aquatic

plants

ErC50 (Pseudokirchneriella subcapitata (green

algae)): > 100 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes

Method: US-EPA

GLP: yes

NOEC (Pseudokirchneriella subcapitata (green algae)):

2.6 mg/l

Exposure time: 72 h Test Type: static test Analytical monitoring: yes

Method: US-EPA

GLP: yes

Toxicity to microorgan-

isms

: NOEC (activated sludge): 580 mg/l

End point: Growth rate Exposure time: 3 h Test Type: static test

Method: OECD Test Guideline 209

Persistence and degradability

Components:

p-toluenesulphonyl chloride:

Biodegradability : aerobic

Inoculum: activated sludge Concentration: 2 mg/l

Result: Readily biodegradable.

Biodegradation: 60 % Exposure time: 28 d

Method: OECD Test Guideline 301D

GLP: yes

Bioaccumulative potential

No data available

Mobility in soil

No data available

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Other adverse effects

Product:

Ozone-Depletion Potential: Regulation: 40 CFR Protection of Environment; Part 82

Protection of Stratospheric Ozone - CAA Section 602

Class I Substances

Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR

82, Subpt. A, App.A + B).

Components:

p-toluenesulphonyl chloride:

Additional ecological in- : Discharge into the environment must be avoided.

formation

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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

International Regulations

IATA-DGR

UN/ID No. : UN 3261

Proper shipping name : Corrosive solid, acidic, organic, n.o.s.

(p-toluenesulphonyl chloride)

Class 8 Packing group III

Labels : Class 8 - Corrosive substances

Packing instruction (cargo: 864

aircraft)

Packing instruction (pas- : 860

senger aircraft)

IMDG-Code

UN number : UN 3261

: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. Proper shipping name

(p-toluenesulphonyl chloride)

: 8 Class : III Packing group Labels

EmS Code : F-A, S-B

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Marine pollutant : no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National regulation

49 CFR Road

UN/ID/NA number : UN 3261

Proper shipping name : Corrosive solid, acidic, organic, n.o.s.

(p-toluenesulphonyl chloride)

Class : 8 Packing group : III

Labels : Class 8 - Corrosive substances

ERG Code : 154 Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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

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

SARA 311/312 Haz- : Acute Health Hazard

ards

SARA 313 : This material does not contain any chemical compo-

nents with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by

SARA Title III, Section 313.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B). This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

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The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCMI Intermediate or Final VOC's (40 CFR 60.489):

p-toluenesulphonyl 98-59-9 >= 90 - <= 100 % chloride

cinoriae

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. Clean-Water Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

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.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

US WEEL : USA. Workplace Environmental Exposure Levels

(WEEL)

US WEEL / CEIL : Ceiling

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx

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- Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA -Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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. Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

Revision Date : 12/18/2024

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