

para-Toluenesulfonyl Chloride

Document History

Published: 1997

Revised: 2001

Revised: 2008

Published: 2009

Rebranded: 2025

I. IDENTIFICATION

Chemical Name: para-Toluenesulfonyl chloride

Synonyms: Benzene sulfonyl chloride, 4-methyl; PTSC; Tosyl chloride; p-methylbenzylsulfonyl chloride; p-Toluenesulfonic acid chloride

CAS Number: 98-59-9

Molecular Formula: $C_7H_7ClO_2S$

Structural Formula:

$CH_3 SO_2Cl$



II. CHEMICAL AND PHYSICAL PROPERTIES⁽¹⁻³⁾

Physical State and Appearance: Colorless, off-white or gray crystalline powder (at room temperature)

Odor Description: Pungent

Molecular Weight: 190.64

Conversion Factors: 1 ppm = 7.8 mg/m³;
1 mg/m³ = 0.64 ppm

Melting Point: 67.4°C (153°F)

Boiling Point: 134.5°C (274°F) at 10 mmHg; 151.6°C (305°F) at 20 mmHg

Specific Gravity: 1.24 at 100°C (212°F)

Vapor Pressure: 1 mmHg at 88°C (190°F)

Flash Point: 128°C (262°F) (closed cup)

Solubility: Slightly soluble in water; soluble in ethanol, acetone, ether, benzene, chloroform, and toluene.

Reactivities and Incompatibilities: Highly reactive, hygroscopic crystals. Slowly hydrolyzes in hot water to HCl and p-toluene sulfonic acid.

Decomposition takes place at 220°C (428°F).

III. USES

PTSC is used mainly in the preparation of chemical derivatives for the pharmaceutical, specialty chemical, and plastics industries. Current production volumes are unknown; however, the material is produced in Asia and Europe, not in the U.S.

IV. ANIMAL TOXICITY DATA

A. Acute Toxicity and Irritancy

1. Oral Toxicity

Rats: LD₅₀ = 4680 mg/kg⁽⁴⁾

Rats: LD₅₀ = 5300 mg/kg⁽⁵⁾

2. Eye Irritation

PTSC was severely irritating to the eyes in a study with rabbits. Corneal opacity was noted and did not clear after a 7-day observation.⁽⁴⁾

In another irritation study, irreversible damage resulted after PTSC was introduced into the conjunctival sac of the rabbit for 24 hr; the material was considered corrosive to the rabbit eye.⁽⁵⁾

3. Skin Absorption

No data available.

4. Skin Irritation

In studies with rabbits, PTSC caused severe skin irritation.⁽⁴⁾

The dermal LD₅₀ for rabbits was estimated to be greater than 5.01 g/kg when held in continuous contact with rabbit skin for 24 hr.⁽⁵⁾

5. Skin Sensitization

No data available.

6. Inhalation Toxicity

No data available.

B. Subacute Toxicity

No data available.

C. Subchronic Toxicity

No data available.

D. Chronic Toxicity/Carcinogenicity

No data available.

E. Reproductive/Developmental Toxicity

No data available.

F. Genotoxicity

A mutagenicity test in *Salmonella typhimurium* and *Saccharomyces cerevisiae* indicated that PTSC was not mutagenic in the presence or absence of metabolic activation.^(4,6)

G. Metabolism/Pharmacokinetics

No data available.

V. HUMAN USE AND EXPERIENCE

Organic acid halides as a group are strong irritants of the eyes, skin, and respiratory tract. With PTSC, this is probably due to slow hydrolysis resulting in formation of HCL and p-toluenesulfonic acid.⁽¹⁾ Actual human use and experience data are limited.

Although airborne concentrations of PTSC are likely to be low because of its low vapor pressure, aerosols may be generated in sufficient concentrations to cause irritation.

VI. RATIONALE

Skin and eye irritation are the prevalent hazards associated with the handling of solid p-toluenesulfonyl chloride. The material was classified as severely irritating to the eyes and skin in animal testing.

Human use and experience with PTSC has not been well-documented; however, the material slowly hydrolyses in the presence of water to form HCl and p-toluenesulfonic acid — both strong acids — which probably accounts for the irritant properties. The deep vesicles produced by some organic acid halides, including PTSC, suggest that the molecule may penetrate intact surfaces, followed by slow hydrolysis.

PTSC vapors, dusts, and mists are the vehicles by which the material would contact respiratory surfaces and the eyes. This OEL is set to prevent irritation to the skin and respiratory tract, and irritation and damage to the eyes.

VII. RECOMMENDED OEL

Ceiling: 5 mg/m³

VIII. REFERENCES

1. **Monsanto Company:** “Para-Toluenesulfonyl Chloride” (Technical Bulletin No. IN-7). Monsanto Company, Organic Chemicals Division. St. Louis, MO: Monsanto, 1959.
2. **AKZO Nobel Chemicals, Inc.:** *Para-Toluenesulfonyl Chloride* (Material Safety Data Sheet). AKZO Nobel Chemicals, Inc. Dobbs Ferry, NY: AKZO Nobel Chemicals, Inc., 1994.
3. **Sigma Chemical Company:** *Para-Toluenesulfonyl Chloride* (Material Safety Data Sheet). St. Louis, MO: Sigma Chemical Company, 1996.
4. **AKZO Nobel Chemicals, Inc.:** “Results of Toxicological Data from Unpublished Reports of Studies Conducted in 1978.” [Personal Communication from AKZO Nobel Chemicals, Inc., to the AIHA WEEL Committee.] Dobbs Ferry, NY: AKZO Nobel Chemicals, Inc., 1996.
5. **Monsanto Company:** “Para-Toluenesulfonyl Chloride—Toxicity Information.” Monsanto Company, Department of Medicine & Environmental Health. St. Louis, MO: Monsanto, 1976.
6. **Monsanto Company:** [Unpublished data.] St. Louis, MO: Monsanto, 1979.

NOTE: The following databases were searched in developing this OEL:

CANCERLIT and Chemical Safety Newsbase
Hazardous Substances Data Bank
MEDLINE (1966–1995)
Merck Index
NIOSH
RTECS
TOXLINE (1965–1995)
TOXLIT (1965–1995)