

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 26.03.2018

Version 10.2

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

1.1 Product identifier

Catalogue No. 808326

Product name 4-Toluenesulfonyl chloride for synthesis

REACH Registration Number A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. 98-59-9

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses Chemical for synthesis
For additional information on uses please refer to the Merck Chemicals portal (www.merckgroup.com).

1.3 Details of the supplier of the safety data sheet

Company Merck KGaA * 64271 Darmstadt * Germany * Phone: +49 6151 72-0

Responsible Department LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number Please contact the regional company representation in your country.

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

Classification (REGULATION (EC) No 1272/2008)

Corrosive to metals, Category 1, H290

Skin irritation, Category 2, H315

Serious eye damage, Category 1, H318

Skin sensitisation, Category 1, H317

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

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

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

P280 Wear protective gloves.

P280 Wear eye protection.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P313 Get medical advice/ attention.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 808326
Product name 4-Toluenesulfonyl chloride for synthesis

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H317 May cause an allergic skin reaction.

H318 Causes serious eye damage.

Precautionary statements

P280 Wear protective gloves.

P280 Wear eye protection.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P313 Get medical advice/ attention.

Contains: p-toluenesulphonyl chloride

CAS-No. 98-59-9

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	4-(CH ₃)C ₆ H ₄ SO ₂ Cl	C ₇ H ₇ ClO ₂ S (Hill)
EC-No.	202-684-8	
Molar mass	190,65 g/mol	

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 808326
Product name 4-Toluenesulfonyl chloride for synthesis

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical name (Concentration)

CAS-No. Registration number Classification

p-toluenesulphonyl chloride ($\geq 80\%$ - $\leq 100\%$)

98-59-9 *)

Corrosive to metals, Category 1, H290

Skin irritation, Category 2, H315

Serious eye damage, Category 1, H318

Skin sensitisation, Category 1, H317

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

3.2 Mixture

Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Consult a physician.

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

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

Irritation and corrosion, Allergic reactions

Risk of serious damage to eyes.

4.3 Indication of any immediate medical attention and special treatment needed

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂), Dry powder

Unsuitable extinguishing media

Water, Foam

5.2 Special hazards arising from the substance or mixture

Combustible.

May not get in touch with:

Water

Caution! in contact with water product releases:

Hydrogen chloride gas

Has a fire-promoting effect due to release of oxygen.

Forms explosive mixtures with air on intense heating.

Vapours are heavier than air and may spread along floors.

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

Fire may cause evolution of:

Sulphur oxides, Hydrogen chloride gas

5.3 Advice for firefighters

Special protective equipment 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.

Further information

Suppress (knock down) gases/vapours/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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

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.

Advice for emergency responders:

Protective equipment 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

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Requirements for storage areas and containers

No metal containers.

Storage conditions

Protected from light.

Away from combustible materials and sources of ignition and heat.

Tightly closed. Dry.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 808326
Product name 4-Toluenesulfonyl chloride for synthesis

Recommended storage temperature see product label.

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

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Tightly fitting safety goggles

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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).

Other protective equipment

protective clothing

Respiratory protection

required when dusts are generated.

Recommended Filter type: filter E-(P2)

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.

Environmental exposure controls

Do not let product enter drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	crystalline solid
Colour	white to grey
Odour	characteristic

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

Odour Threshold	No information available.
pH	strongly acid
Melting point	ca. 67 °C
Boiling point/boiling range	> 160 °C at 1.013 hPa Method: OECD Test Guideline 103
Flash point	128 °C Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	The product is not flammable.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	No information available.
Relative vapour density	No information available.
Density	1,49 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	at 20 °C Hydrolysis
Partition coefficient: n-octanol/water	No information available.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

Auto-ignition temperature	No information available.
Decomposition temperature	> 220 °C
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	The substance or mixture is not classified as oxidizing.

9.2 Other data

Bulk density	800 kg/m ³
Particle size	Particle size > 0,1 mm
Corrosion	> 6,25 mm/a Method: (Aluminium, 55 °C) > 6,25 mm/a Method: (Steel, 55 °C) May be corrosive to metals.

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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

sensitive to moisture

Sensitivity to light

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:

Aluminium, hydrides, formaldehyde, Metals, strong alkalis, Sulphides

Exothermic reaction with:

Amines, potassium permanganate, salts of oxyhalogenic acids, semimetallic oxides, semimetallic hydrogen compounds, Aldehydes, vinylmethyl ether

10.4 Conditions to avoid

Moisture.

Strong heating.

10.5 Incompatible materials

Metals

10.6 Hazardous decomposition products

in the event of fire: See section 5.

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: 4.680 mg/kg

OECD Test Guideline 401

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

Acute inhalation toxicity

Symptoms: Possible damages:, mucosal irritations

Acute dermal toxicity

This information is not available.

Skin irritation

Rabbit

Result: Irritations

OECD Test Guideline 404

Causes skin irritation.

Eye irritation

Rabbit

Result: Causes serious eye damage.

OECD Test Guideline 405

Causes serious eye damage.

Sensitisation

Sensitisation test: Mouse

Result: positive

Method: OECD Test Guideline 429

May cause an allergic skin reaction.

Germ cell mutagenicity

Genotoxicity in vivo

Micronucleus test

Mouse

male

Intraperitoneal injection

Red blood cells (erythrocytes)

Result: negative

Method: OECD Test Guideline 474

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

Decomposition of the substance with tissue moisture.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

static test LC50 *Oryzias latipes* (Orange-red killifish): > 100 mg/l; 96 h

Analytical monitoring: yes

OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

static test EC50 *Daphnia magna* (Water flea): > 334 mg/l; 48 h

Analytical monitoring: yes

OECD Test Guideline 202

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

Toxicity to algae

static test EC50 *Pseudokirchneriella subcapitata* (green algae): > 100 mg/l; 72 h

Analytical monitoring: yes

US-EPA

static test NOEC *Pseudokirchneriella subcapitata* (green algae): 2,6 mg/l; 72 h

Analytical monitoring: yes

US-EPA

Toxicity to bacteria

EC10 Bacteria: 114 mg/l; 30 min

(External MSDS)

12.2 Persistence and degradability

Biodegradability

60 %; 28 d; aerobic

OECD Test Guideline 301D

Readily biodegradable

12.3 Bioaccumulative potential

No information available.

12.4 Mobility in soil

No information 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

Additional ecological information

Discharge into the environment must be avoided.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number	UN 3261
14.2 Proper shipping name	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (4-TOLUENESULFONYL CHLORIDE)
14.3 Class	8
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 3261
14.2 Proper shipping name	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (4-TOLUENESULFONYL CHLORIDE)
14.3 Class	8
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

Sea transport (IMDG)

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

14.1 UN number	UN 3261
14.2 Proper shipping name	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (4-TOLUENESULFONYL CHLORIDE)
14.3 Class	8
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
EmS	F-A S-B
14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	Not relevant

SECTION 15. Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulations

Major Accident Hazard	SEVESO III
Legislation	Not applicable
Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work.

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 808326
Product name 4-Toluenesulfonyl chloride for synthesis

Substances of very high concern (SVHC)

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w).

National legislation

Storage class 8A

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

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

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

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Danger

Hazard statements

H290 May be corrosive to metals.
H315 Causes skin irritation.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	808326
Product name	4-Toluenesulfonyl chloride for synthesis

H317 May cause an allergic skin reaction.

H318 Causes serious eye damage.

Precautionary statements

Prevention

P280 Wear eye protection.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P313 Get medical advice/ attention.

Contains: p-toluenesulphonyl chloride

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.