

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Toluene-4-sulfonic acid monohydrate \geq 98%, for synthesis

article number: **4796**
Version: **2.0 en**
Replaces version of: 2016-07-04
Version: (1)

date of compilation: 2016-07-04
Revision: 2019-12-03

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

1.1 Product identifier

Identification of the substance	Toluene-4-sulfonic acid monohydrate
Article number	4796
Registration number (REACH)	01-2119538811-39-XXXX
Index No	016-030-00-2
EC number	203-180-0
CAS number	6192-52-5

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

Identified uses: laboratory chemical
laboratory and analytical use

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

Telephone: +49 (0) 721 - 56 06 0
Telefax: +49 (0) 721 - 56 06 149
e-mail: sicherheit@carlroth.de
Website: www.carlroth.de

Competent person responsible for the safety data sheet : Department Health, Safety and Environment

e-mail (competent person) : sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Centre Beaumont Hospital	Beaumont Road	Dublin 9	01 809 2166	https:// www.poisons.ie/

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
3.2	skin corrosion/irritation	(Skin Irrit. 2)	H315
3.3	serious eye damage/eye irritation	(Eye Irrit. 2)	H319

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Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
3.8R	specific target organ toxicity - single exposure (respiratory tract irritation)	(STOT SE 3)	H335

2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 (CLP)

Signal word

Warning

Pictograms

GHS07



Hazard statements

H315 Causes skin irritation
H319 Causes serious eye irritation
H335 May cause respiratory irritation

Precautionary statements

Precautionary statements - response

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

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Warning**

Symbol(s)



2.3 Other hazards

There is no additional information.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Toluene-4-sulfonic acid monohydrate
Index No	016-030-00-2
Registration number (REACH)	01-2119538811-39-XXXX
EC number	203-180-0
CAS number	6192-52-5
Molecular formula	C ₇ H ₈ O ₃ S*H ₂ O

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Molar mass

190,2 g/mol

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off immediately all contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In case of skin irritation, consult a physician.

Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. Consult an ophthalmologist.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Gastrointestinal complaints, Irritation, Cough, Breathing difficulties

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings
water spray, foam, dry extinguishing powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours may form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: carbon monoxide (CO), carbon dioxide (CO₂), sulphur oxides (SO_x)

5.3 Advice for firefighters

Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus. Wear full chemical protective clothing.

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SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Do not breathe dust. Avoid contact with skin and eyes.

6.2 Environmental precautions

Keep away from drains, surface and ground water.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains.

Advice on how to clean up a spill

Take up mechanically. Control of dust.

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provide adequate ventilation. Avoid dust formation.

• Measures to prevent fire as well as aerosol and dust generation

Removal of dust deposits.

Advice on general occupational hygiene

Wash hands before breaks and after work.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed. Store in a dry place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice

• Ventilation requirements

Use local and general ventilation.

• Specific designs for storage rooms or vessels

Recommended storage temperature: 15 – 25 °C.

7.3 Specific end use(s)

No information available.

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SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Country	Name of agent	CAS No	Notation	Identifier	TWA [mg/m ³]	STEL [mg/m ³]	Ceiling-C [ppm]	Ceiling-C [mg/m ³]	Source
IE	dusts non-specific		i	OELV	10				S.I. No. 619 of 2001
IE	dusts non-specific		r	OELV	4				S.I. No. 619 of 2001

Notation

Ceiling-C Ceiling value is a limit value above which exposure should not occur

i Inhalable fraction

r Respirable fraction

STEL Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified)

TWA Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average (unless otherwise specified)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



• hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 °C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

• type of material

NBR (Nitrile rubber)

• material thickness

>0,11 mm

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• breakthrough times of the glove material

>480 minutes (permeation: level 6)

• other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection



Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P2 (filters at least 94 % of airborne particles, colour code: White).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance

Physical state	solid (crystalline)
Colour	light pink
Odour	faintly perceptible
Odour threshold	No data available

Other physical and chemical parameters

pH (value)	~ 1 (water: 650 g/l, 20 °C)
Melting point/freezing point	56 °C
Initial boiling point and boiling range	140 °C
Flash point	>150 °C
Evaporation rate	no data available
Flammability (solid, gas)	These information are not available
<u>Explosive limits</u>	
• lower explosion limit (LEL)	this information is not available
• upper explosion limit (UEL)	this information is not available
Explosion limits of dust clouds	these information are not available
Vapour pressure	This information is not available.
Density	This information is not available.
Vapour density	This information is not available.
Bulk density	500 – 600 kg/m ³
Relative density	Information on this property is not available.
<u>Solubility(ies)</u>	
Water solubility	~ 700 g/l at 20 °C

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Partition coefficient

n-octanol/water (log KOW)	This information is not available.
Auto-ignition temperature	600 °C
Decomposition temperature	no data available
Viscosity	not relevant (solid matter)
Explosive properties	Shall not be classified as explosive
Oxidising properties	none

9.2 Other information

Temperature class (EU, acc. to ATEX)	T1 (Maximum permissible surface temperature on the equipment: 450°C)
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SECTION 10: Stability and reactivity

10.1 Reactivity

Dust explosibility. If heated. Vapours may form explosive mixtures with air.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Exothermic reaction with: Bases, Acetic anhydride, Acids

10.4 Conditions to avoid

Keep away from heat.

10.5 Incompatible materials

metals

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Shall not be classified as acutely toxic.

Exposure route	Endpoint	Value	Species	Source
oral	LD50	2.570 mg/kg	rat	TOXNET

Skin corrosion/irritation

Causes skin irritation.

Serious eye damage/eye irritation

Causes serious eye irritation.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

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Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor as a reproductive toxicant

• Specific target organ toxicity - single exposure

May cause respiratory irritation.

• Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

gastrointestinal complaints

• If in eyes

data are not available

• If inhaled

cough, Irritation to respiratory tract, breathing difficulties

• If on skin

causes skin irritation

Other information

None

SECTION 12: Ecological information

12.1 Toxicity

acc. to 1272/2008/EC: Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)

Endpoint	Value	Species	Method	Source	Exposure time
LC50	$>500 \text{ mg/l}$	bluegill (<i>Lepomis macrochirus</i>)	anhydrous	IUCLID	96 h
EC50	$>500 \text{ mg/l}$	daphnia magna	anhydrous	IUCLID	96 h

12.2 Process of degradability

The substance is readily biodegradable.
Theoretical Oxygen Demand: $1,514 \text{ mg/mg}$
Theoretical Carbon Dioxide: $1,62 \text{ mg/mg}$

Process	Degradation rate	Time
biotic/abiotic	79 %	25 d

12.3 Bioaccumulative potential

Data are not available.

12.4 Mobility in soil

Data are not available.

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12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.


13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions.

SECTION 14: Transport information

14.1	UN number	2585
14.2	UN proper shipping name	ARYLSULPHONIC ACIDS, SOLID
	Hazardous ingredients	Toluene-4-sulfonic acid monohydrate
14.3	Transport hazard class(es)	
	Class	8 (corrosive substances)
14.4	Packing group	III (substance presenting low danger)
14.5	Environmental hazards	none (non-environmentally hazardous acc. to the dangerous goods regulations)
14.6	Special precautions for user	Provisions for dangerous goods (ADR) should be complied within the premises.
14.7	Transport in bulk according to Annex II of MARPOL and the IBC Code	The cargo is not intended to be carried in bulk.
14.8	Information for each of the UN Model Regulations	
	• Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)	
	UN number	2585

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Proper shipping name	ARYLSULPHONIC ACIDS, SOLID
Particulars in the transport document	UN2585, ARYLSULPHONIC ACIDS, SOLID, 8, III, (E)
Class	8
Classification code	C4
Packing group	III
Danger label(s)	8



Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 kg
Transport category (TC)	3
Tunnel restriction code (TRC)	E
Hazard identification No	80

• International Maritime Dangerous Goods Code (IMDG)

UN number	2585
Proper shipping name	ARYLSULPHONIC ACIDS, SOLID
Particulars in the shipper's declaration	UN2585, ARYLSULPHONIC ACIDS, SOLID, 8, III
Class	8
Marine pollutant	-
Packing group	III
Danger label(s)	8



Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 kg
EmS	F-A, S-B
Stowage category	A
Segregation group	1 - Acids

• International Civil Aviation Organization (ICAO-IATA/DGR)

UN number	2585
Proper shipping name	Arylsulphonic acids, solid
Particulars in the shipper's declaration	UN2585, Arylsulphonic acids, solid, 8, III
Class	8
Packing group	III
Danger label(s)	8

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Excepted quantities (EQ)

E1

Limited quantities (LQ)

5 kg

SECTION 15: Regulatory information

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

Relevant provisions of the European Union (EU)

- **Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)**

Not listed.

- **Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)**

Not listed.

- **Regulation 850/2004/EC on persistent organic pollutants (POP)**

Not listed.

- **Restrictions according to REACH, Annex XVII**

not listed

- **Restrictions according to REACH, Title VIII**

None.

- **List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list**

not listed

- **Seveso Directive**

2012/18/EU (Seveso III)			
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements	Notes
	not assigned		

- **Directive 75/324/EEC relating to aerosol dispensers**

Filling batch

Deco-Paint Directive (2004/42/EC)

VOC content	100 %
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Directive on industrial emissions (VOCs, 2010/75/EU)

VOC content	0 %
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Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II

not listed

Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

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Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)

not listed

Regulation 98/2013/EU on the marketing and use of explosives precursors

not listed

Regulation 111/2005/EC laying down rules for the monitoring of trade between the Community and third countries in drug precursors

not listed

National inventories

Substance is listed in the following national inventories:

Country	National inventories	Status
AU	AICS	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
KR	KECI	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed

Legend

AICS	Australian Inventory of Chemical Substances
CICR	Chemical Inventory and Control Regulation
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
KECI	Korea Existing Chemicals Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances
TCSI	Taiwan Chemical Substance Inventory

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
1.1	Registration number (REACH): This information is not available.	Registration number (REACH): 01-2119538811-39-XXXX	yes
2.1	Remarks: For full text of Hazard- and EU Hazard-state-ments: see SECTION 16.		yes
2.2		Pictograms: change in the listing (table)	yes
14.2	Hazardous ingredients: p-Toluenesulphonic acid monohydrate	Hazardous ingredients: Toluene-4-sulfonic acid monohydrate	yes
14.3	Transport hazard class(es)	Transport hazard class(es): class 8 hazard - corrosive substances	yes

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Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
14.8	• International Maritime Dangerous Goods Code (IMDG): Not subject to IMDG.	• International Maritime Dangerous Goods Code (IMDG)	yes
14.8		Particulars in the shipper's declaration: UN2585, ARYLSULPHONIC ACIDS, SOLID, 8, III	yes
14.8		Marine pollutant: -	yes
14.8	Special provisions (SP): -		yes
14.8		• International Civil Aviation Organization (ICAO-IATA/DGR)	yes
14.8		UN number: 2585	yes
14.8		Proper shipping name: Arylsulphonic acids, solid	yes
14.8		Particulars in the shipper's declaration: UN2585, Arylsulphonic acids, solid, 8, III	yes
14.8		Class: 8	yes
14.8		Packing group: III	yes
14.8		Danger label(s): 8	yes
14.8		Danger label(s): change in the listing (table)	yes
14.8		Excepted quantities (EQ): E1	yes
14.8		Limited quantities (LQ): 5 kg	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	ceiling value
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DGR	Dangerous Goods Regulations (see IATA/DGR)
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule

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Abbr.	Descriptions of used abbreviations
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
index No	the Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
ppm	parts per million
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
S.I. No. 619 of 2001	Safety, Health and Welfare at Work (Chemical Agents) Regulations 2001
STEL	short-term exposure limit
SVHC	Substance of Very High Concern
TWA	time-weighted average
VOC	Volatile Organic Compounds
vPvB	very Persistent and very Bioaccumulative

Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)
- Dangerous Goods Regulations (DGR) for the air transport (IATA)
- International Maritime Dangerous Goods Code (IMDG)

List of relevant phrases (code and full text as stated in chapter 2 and 3)

Code	Text
H315	causes skin irritation
H319	causes serious eye irritation
H335	may cause respiratory irritation

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Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.