

Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



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

article number: **4796**
Version: **3.0 en**
Replaces version of: 2019-12-03
Version: (2)

date of compilation: 2016-07-04
Revision: 2022-06-28

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 \geq 98%, for synthesis
Article number	4796
EC number	203-180-0
CAS number	6192-52-5
Alternative name(s)	Paratoluolsulphonic acid

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household).

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 Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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Classification acc. to GHS

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.2	Skin corrosion/irritation	2	Skin Irrit. 2	H315
3.3	Serious eye damage/eye irritation	2	Eye Irrit. 2	H319
3.8R	Specific target organ toxicity - single exposure (respiratory tract irritation)	3	STOT SE 3	H335

For full text of abbreviations: see SECTION 16

2.2 Label elements

Labelling

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

2.3 Other hazards

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Toluene-4-sulfonic acid monohydrate
Molecular formula	$C_7H_8O_3S \cdot H_2O$
Molar mass	190,2 g/mol
CAS No	6192-52-5
EC No	203-180-0

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Substance, Specific Conc. Limits, M-factors, ATE			
Specific Conc. Limits	M-Factors	ATE	Exposure route
STOT SE 3; H335: C \geq 20 %	-	-	

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 immediately and drink plenty of water. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

Corrosion, Risk of blindness, Gastric perforation, Irritation, Cough, Dyspnoea

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 firefighting measures to the fire surroundings
water, foam, alcohol resistant foam, dry extinguishing powder, ABC-powder

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

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

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5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus. Wear full chemical protective clothing.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

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

6.2 Environmental precautions

Keep away from drains, surface and ground water. The product is an acid. Before discharge into sewage plants the product normally needs to be neutralised.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains. Take up mechanically.

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

Provision of sufficient 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. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

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

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7.3 Specific end use(s)

No information available.

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	Identifier	TWA [mg/m ³]	STEL [mg/m ³]	Ceiling-C [mg/m ³]	Notation	Source
GB	dust		WEL	10			i	EH40/2005
GB	dust		WEL	4			r	EH40/2005

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)

Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	53,6 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	7,6 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

Environmental values

Relevant PNECs and other threshold levels				
Endpoint	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0,073 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0,007 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	58 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,058 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0,006 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0,016 mg/kg	terrestrial organisms	soil	short-term (single instance)

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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

• 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.

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SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	solid
Form	crystalline
Colour	light pink
Odour	faintly perceptible
Melting point/freezing point	99 – 103 °C
Boiling point or initial boiling point and boiling range	140 °C at 26 hPa
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	180 °C
Auto-ignition temperature	600 °C
Decomposition temperature	>150 °C
pH (value)	~ 0,2 (in aqueous solution: 200 g/l, 20 °C)
Kinematic viscosity	not relevant
<u>Solubility(ies)</u>	
Water solubility	~ 700 g/l at 20 °C
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	-0,96 (pH value: 6, 50 °C) (ECHA)
Vapour pressure	not determined
<u>Density and/or relative density</u>	
Density	~ 1,345 g/cm ³ at 20 °C (ECHA)
Relative vapour density	information on this property is not available
Bulk density	500 – 600 kg/m ³
Particle characteristics	No data available.
<u>Other safety parameters</u>	
Oxidising properties	none

9.2 Other information

Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
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Other safety characteristics:

Surface tension 48,77 mN/m (20 °C) (ECHA)

SECTION 10: Stability and reactivity

10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

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, Strong alkali

10.4 Conditions to avoid

Keep away from heat. Decomposition takes place from temperatures above: >150 °C.

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

Classification acc. to GHS

Acute toxicity

Shall not be classified as acutely toxic.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	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.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

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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

Causes serious eye irritation

• If inhaled

Irritation to respiratory tract, cough, Dyspnoea

• If on skin

causes skin irritation

• Other information

none

11.2 Endocrine disrupting properties

Not listed.

11.3 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LC50	$>500 \text{ mg/l}$	fish	ECHA	96 h
EC50	$>103 \text{ mg/l}$	aquatic invertebrates	ECHA	48 h
ErC50	73 mg/l	algae	ECHA	72 h

Biodegradation

Data are not available.

12.2 Process of degradability

Theoretical Oxygen Demand: $1,514 \text{ mg/mg}$

Theoretical Carbon Dioxide: $1,62 \text{ mg/mg}$

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Process of degradability		
Process	Degradation rate	Time
biotic/abiotic	79 %	25 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	-0,96 (pH value: 6, 50 °C) (ECHA)
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12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Not listed.

12.7 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. Waste catalogue ordinance (Germany).

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.

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SECTION 14: Transport information

14.1 UN number or ID number

ADRRID	UN 2585
IMDG-Code	UN 2585
ICAO-TI	UN 2585

14.2 UN proper shipping name

ADRRID	ALKYLSULPHONIC ACIDS, SOLID
IMDG-Code	ALKYLSULPHONIC ACIDS, SOLID
ICAO-TI	Alkylsulphonic acids, solid

14.3 Transport hazard class(es)

ADRRID	8
IMDG-Code	8
ICAO-TI	8

14.4 Packing group

ADRRID	III
IMDG-Code	III
ICAO-TI	III

14.5 Environmental hazards

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 Maritime transport in bulk according to IMO instruments

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) - Additional information

Proper shipping name	ALKYLSULPHONIC ACIDS, SOLID
Particulars in the transport document	UN2585, ALKYLSULPHONIC ACIDS, SOLID, 8, III, (E)
Classification code	C4
Danger label(s)	8
	
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 kg
Transport category (TC)	3
Tunnel restriction code (TRC)	E

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Hazard identification No 80

Emergency Action Code 2X

Regulations concerning the International Carriage of Dangerous Goods by Rail (RID) Additional information

Classification code C4

Danger label(s) 8



Excepted quantities (EQ) E1

Limited quantities (LQ) 5 kg

Transport category (TC) 3

Hazard identification No 80

International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name ALKYL SULPHONIC ACIDS, SOLID

Particulars in the shipper's declaration UN2585, ALKYL SULPHONIC ACIDS, SOLID, 8, III

Marine pollutant -

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) - Additional information

Proper shipping name Alkylsulphonic acids, solid

Particulars in the shipper's declaration UN2585, Alkylsulphonic acids, solid, 8, III

Danger label(s) 8



Excepted quantities (EQ) E1

Limited quantities (LQ) 5 kg

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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)

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		

Deco-Paint Directive

VOC content	100 % 1.345 g/l
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Industrial Emissions Directive (IED)

VOC content	100 %
VOC content	1.345 g/l

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

not listed

Regulation on the marketing and use of explosives precursors

not listed

Regulation on drug precursors

not listed

Regulation on substances that deplete the ozone layer (ODS)

not listed

Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

Regulation on persistent organic pollutants (POP)

not listed

National regulations(GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

Restrictions according to GB REACH, Annex 17

not listed

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Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

Country	Inventory	Status
AU	AIIC	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

AIIC	Australian Inventory of Industrial Chemicals
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 (PICCS)
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)

Alignment to regulation:

Restructuring: section 9, section 14

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.1		Classification acc. to GHS: change in the listing (table)	yes
2.2	Labelling of packages where the contents do not exceed 125 ml: Signal word: Warning		yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.3	Other hazards: There is no additional information.	Other hazards	yes
2.3		Results of PBT and vPvB assessment: According to the results of its assessment, this substance is not a PBT or a vPvB.	yes

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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 relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
ATE	Acute Toxicity Estimate
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	Ceiling value
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
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
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
EH40/2005	EH40/2005 Workplace exposure limits (http://www.nationalarchives.gov.uk/doc/open-government-licence/)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
ErC50	\equiv EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
GB REACH	The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended)
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
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
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
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
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)

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Abbr.	Descriptions of used abbreviations
STEL	Short-term exposure limit
TWA	Time-weighted average
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative
WEL	Workplace exposure limit

Key literature references and sources for data

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

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

Code	Text
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.