



MATERIAL SAFETY DATA SHEET

according to the Hazard Communication Standard (29 CFR 1910.1200)

Date of issue: 10/21/2012

Version 1.0

SECTION 1. Identification

Product identifier

Product number	814725
Product name	Toluene-4-sulfonic acid monohydrate for synthesis

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

Identified uses	Chemical for synthesis
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Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation 290 Concord Road, Billerica, MA 01821, United States of America SDS Phone Support: +1-978-715-1335 General Inquiries: +1-978-751-4321 Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5) e-mail: mm_sds@merckgroup.com
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Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week
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SECTION 2. Hazards identification

GHS Classification

Skin irritation, Category 2, H315
Eye irritation, Category 2, H319
Specific target organ systemic toxicity - single exposure, Category 3, H335
For the full text of the H-Statements mentioned in this Section, see Section 16.

GHS-Labeling

Hazard pictograms



Signal Word
Warning

Hazard Statements

H315 Causes skin irritation.
H319 Causes serious eye irritation.

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H335 May cause respiratory irritation.

Precautionary Statements

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

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

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

OSHA Hazards

This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	$\text{CH}_3\text{C}_6\text{H}_4\text{SO}_3\text{H} \cdot \text{H}_2\text{O}$	$\text{C}_7\text{H}_8\text{O}_3\text{S} \cdot \text{H}_2\text{O}$ (Hill)
CAS-No.	6192-52-5	
Molar mass	190.22 g/mol	

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

toluene-4-sulphonic acid ($\geq 90\%$ - $\leq 100\%$)

104-15-4

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air. Get medical attention.

Skin contact

After skin contact: wash off with plenty of water. Remove contaminated clothing. Get medical attention.

Eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist.

Ingestion

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

irritant effects, Cough, Shortness of breath, gastric pain

Indication of any immediate medical attention and special treatment needed

No information available.

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SECTION 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

Water, Carbon dioxide (CO₂), Foam, Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Special hazards arising from the substance or mixture

Combustible material

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

Fire may cause evolution of:

Sulfur oxides

Advice for firefighters

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.

Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Avoid inhalation of dusts.

Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

Environmental precautions

Do not empty into 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

Precautions for safe handling

Observe label precautions.

Conditions for safe storage, including any incompatibilities

Tightly closed. Dry.

Requirements for storage areas and containers

No metal containers.

Store at +15°C to +25°C (+59°F to +77°F).

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SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Contains no substances with occupational exposure limit values.

Engineering measures

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

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

Eye/face protection

Safety glasses

Hand protection

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Recommended:

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

Other protective equipment:

protective clothing

Respiratory protection

required when dusts are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

SECTION 9. Physical and chemical properties

Physical state	crystals
Color	light pink
Odor	weak

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Odor Threshold	No information available.
pH	1 at 650 g/l 68 °F (20 °C) (anhydrous substance)
Melting point	133 °F (56 °C) Elimination of water of crystallization ca. 221 °F (105 °C) (anhydrous substance)
Boiling point/boiling range	284 °F (140 °C) at 27 hPa
Flash point	ca. 356 °F (180 °C)
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapor pressure	No information available.
Relative vapor density	No information available.
Relative density	No information available.
Water solubility	ca. 750 g/l at 68 °F (20 °C)
Partition coefficient: n-octanol/water	log Pow: -0.62 (calculated) (Lit.) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	338 °F (170 °C)
Viscosity, dynamic	No information available.
Ignition temperature	1112 °F (600 °C)
Bulk density	ca. 510 kg/m ³

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SECTION 10. Stability and reactivity

Reactivity

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

releases water of crystallization when heated.

Possibility of hazardous reactions

Generates dangerous gases or fumes in contact with:

Acids, metals, bases, strong oxidizing agents, Acetic anhydride, Water

Exothermic reaction with:

Conditions to avoid

Strong heating.

Incompatible materials

Metals

Hazardous decomposition products

in the event of fire: See section 5.

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Eye contact, Skin contact, Ingestion

Acute oral toxicity

LD50 rat: 2,570 mg/kg (RTECS)

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

Acute inhalation toxicity

Symptoms: Irritation symptoms in the respiratory tract., Cough, Shortness of breath

Skin irritation

Irritations

Causes skin irritation.

Eye irritation

rabbit

Result: Severe irritations
(anhydrous substance) (IUCLID)

Causes serious eye irritation.

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Sensitization

Sensitization test: guinea pig
Result: negative
Method: OECD Test Guideline 406

Genotoxicity in vitro

Ames test
Result: negative
Method: OECD Test Guideline 471

Specific target organ systemic toxicity - single exposure

May cause respiratory irritation.

Specific target organ systemic toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

Regarding the available data the classification criteria are not fulfilled.

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.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
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.
ACGIH	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish

LC50 Lepomis macrochirus (Bluegill sunfish): > 500 mg/l; 96 h (anhydrous substance) (IUCLID)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): > 500 mg/l; 96 h (anhydrous substance) (IUCLID)

Toxicity to algae

IC50 Chlorella vulgaris (Fresh water algae): 245 mg/l; 96 h (anhydrous substance) (IUCLID)

Toxicity to bacteria

EC0 Bacteria: > 2,500 mg/l; 24 h (anhydrous substance) (IUCLID)

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Persistence and degradability

Biodegradability

Easily eliminable.

79 %; 25 d

OECD Test Guideline 302B
(anhydrous substance)

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: -0.62

(calculated)

(Lit.) Bioaccumulation is not expected (log Pow <1).

Mobility in soil

No information available.

Other adverse effects

Additional ecological information

Harmful effect due to pH shift.

Further information on ecology

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)

UN number	UN 2585
Proper shipping name	ARYLSULPHONIC ACIDS, SOLID
Class	8
Packing group	III
Environmentally hazardous	--

Air transport (IATA)

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Product number 814725
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UN number UN 2585
Proper shipping name ARYLSULPHONIC ACIDS, SOLID
Class 8
Packing group III
Environmentally hazardous --
Special precautions for user no

Sea transport (IMDG)

UN number UN 2585
Proper shipping name ARYLSULPHONIC ACIDS, SOLID
Class 8
Packing group III
Environmentally hazardous --
Special precautions for user yes
EmS F-A S-B

SECTION 15. Regulatory information

United States of America

OSHA Hazards

Skin irritant
Eye irritant
Moderate respiratory irritant

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

TSCA list

Not relevant

SARA 311/312 Hazards

Acute Health Hazard

Clean Water Act

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

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

US State Regulations

Massachusetts Right To Know

Ingredients
toluene-4-sulphonic acid

Pennsylvania Right To Know

Ingredients
toluene-4-sulphonic acid
water of crystallization

New Jersey Right To Know

Ingredients
toluene-4-sulphonic acid
water of crystallization

California Prop 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

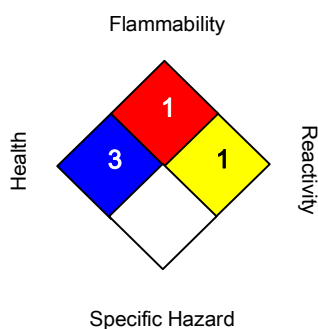
Notification status

TSCA: On TSCA Inventory

DSL: All components of this product are on the Canadian DSL.

SECTION 16. Other information

National Fire Protection Association (U.S.A)



Training advice

Provide adequate information, instruction and training for operators.

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

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

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.

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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