

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 8.4
Revision Date 05.06.2021
Print Date 27.09.2021

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

1.1 Product identifiers

Product name : Toluene-4-sulfonic acid monohydrate for analysis EMSURE® ACS

Product Number : 1.09613
Catalogue No. : 109613
Brand : Millipore
Index-No. : 016-030-00-2
REACH No. : 01-2119538811-39-XXXX
CAS-No. : 6192-52-5

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

Identified uses : Reagent for analysis

1.3 Details of the supplier of the safety data sheet

Company : Merck Life Science UK Limited
New Road
The Old Brickyard
GILLINGHAM
Dorset
SP8 4XT
UNITED KINGDOM

Telephone : +44 (0)1747 833-000
Fax : +44 (0)1747 833-313

1.4 Emergency telephone

Emergency Phone # : +44 (0)870 8200418 (CHEMTREC)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture


Classification according to Regulation (EC) No 1272/2008

Corrosive to Metals (Category 1), H290
Skin corrosion (Sub-category 1B), H314
Serious eye damage (Category 1), H318
Long-term (chronic) aquatic hazard (Category 3), H412


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

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram	
Signal word	Danger
Hazard statement(s)	
H290	May be corrosive to metals.
H314	Causes severe skin burns and eye damage.
H412	Harmful to aquatic life with long lasting effects.
Precautionary statement(s)	
P234	Keep only in original packaging.
P260	Do not breathe dusts or mists.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection/ hearing protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with 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.
Supplemental Hazard Statements	none

Reduced Labeling (<= 125 ml)

Pictogram	
Signal word	Danger
Hazard statement(s)	
H314	Causes severe skin burns and eye damage.
H412	Harmful to aquatic life with long lasting effects.
Precautionary statement(s)	
P260	Do not breathe dusts or mists.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection/ hearing protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with 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.
Supplemental Hazard Statements	none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula	: C7H8O3S.H2O
Molecular weight	: 190.22 g/mol
CAS-No.	: 6192-52-5

Index-No. : 016-030-00-2

Component	Classification	Concentration
p-Toluensulphonic acid monohydrate		
CAS-No. 6192-52-5 Index-No. 016-030-00-2	Met. Corr. 1; Skin Corr. 1B; Eye Dam. 1; Aquatic Chronic 3; H290, H314, H318, H412	<= 100 %

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

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

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

In case of eye contact

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

If swallowed

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Sulfur oxides

Combustible.

Fire may cause evolution of:

Sulfur oxides

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

5.3 Advice 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.

5.4 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

6.1 Personal precautions, protective equipment and emergency procedures

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.

For personal protection 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

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

No metal containers.

Tightly closed. Dry.

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

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

Skin protection

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).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 Dermatril® L

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).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 Dermatril® L

Body Protection

protective clothing

Respiratory protection

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type 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.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|--|-------------------------------------|
| a) Appearance | Form: crystals
Color: light pink |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: 56 °C |
| f) Initial boiling point and boiling range | 92 - 119 °C |
| g) Flash point | No data available |

h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapor pressure	No data available
l)	Vapor density	No data available
m)	Relative density	No data available
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Autoignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information

Bulk density ca.510 kg/m³

SECTION 10: Stability and reactivity

10.1 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.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Exothermic reaction with:

Generates dangerous gases or fumes in contact with:

Acids

Bases

strong oxidising agents

Acetic anhydride

with

Water

10.4 Conditions to avoid

no information available

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 toxicity

LD50 Oral - Rat - male and female - 1,410 mg/kg

(OECD Test Guideline 401)

Symptoms: Irritation symptoms in the respiratory tract., mucosal irritations, Cough, Shortness of breath, Possible damages:., damage of respiratory tract

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Corrosive - 4 h

(OECD Test Guideline 404)

Remarks: (anhydrous substance)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Corrosive - 30 s

Remarks: (anhydrous substance)

Causes serious eye damage.

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(Regulation (EC) No. 440/2008, Annex, B.6)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster lung cells

Metabolic activation: without metabolic activation

Method: OECD Test Guideline 473

Result: positive

Test Type: Chromosome aberration test in vitro

Test system: Other cell types

Metabolic activation: without metabolic activation

Method: OECD Test Guideline 473

Result: positive

Test Type: Micronucleus test

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

Remarks: (in analogy to similar products)

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 28 Days - NOAEL (No observed adverse effect level) - \geq 500 mg/kg

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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 - <i>Leuciscus idus melanotus</i> - $>$ 500 mg/l - 96 h (OECD Test Guideline 203) Remarks: (anhydrous substance)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - $>$ 103 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> - 73 mg/l - 72 h (OECD Test Guideline 201) Remarks: (anhydrous substance) The value is given in analogy to the following substances: toluene-4-sulphonic acid The value is given in analogy to the following substances: benzenesulphonic acid
Toxicity to bacteria	static test NOEC - activated sludge - 580 mg/l - 3 h (OECD Test Guideline 209)

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

15.2 Chemical Safety Assessment

A Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

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

H290	May be corrosive to metals.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H412	Harmful to aquatic life with long lasting effects.

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Annex: Exposure scenario

Identified uses:

Use: Industrial use

SU 3: Industrial uses: Uses of substances as such or in preparations at industrial sites
SU 3, SU9, SU 10: Industrial uses: Uses of substances as such or in preparations at industrial sites, Manufacture of fine chemicals, Formulation [mixing] of preparations and/ or re-packaging (excluding alloys)
PC19: Intermediate PC21: Laboratory chemicals
PROC1: Use in closed process, no likelihood of exposure PROC3: Use in closed batch process (synthesis or formulation) PROC4: Use in batch and other process (synthesis) where opportunity for exposure arises PROC5: Mixing or blending in batch processes for formulation of preparations and articles (multistage and/ or significant contact) PROC8a: Transfer of substance or preparation (charging/ discharging) from/ to vessels/ large containers at non-dedicated facilities PROC8b: Transfer of substance or preparation (charging/ discharging) from/ to vessels/ large containers at dedicated facilities PROC9: Transfer of substance or preparation into small containers (dedicated filling line, including weighing) PROC10: Roller application or brushing PROC15: Use as laboratory reagent
ERC2, ERC4, ERC6a, ERC6b: Formulation of preparations, Industrial use of processing aids in processes and products, not becoming part of articles, Industrial use resulting in manufacture of another substance (use of intermediates), Industrial use of reactive processing aids

Use: Professional use

SU 22: Professional uses: Public domain (administration, education, entertainment, services, craftsmen)
SU 22: Professional uses: Public domain (administration, education, entertainment, services, craftsmen)
PC21: Laboratory chemicals PROC15: Use as laboratory reagent
ERC2, ERC6a, ERC6b: Formulation of preparations, Industrial use resulting in manufacture of another substance (use of intermediates), Industrial use of reactive processing aids

1. Short title of Exposure Scenario: Industrial use

Main User Groups	: SU 3
Sectors of end-use	: SU 3, SU9, SU 10
Chemical product category	: PC19, PC21
Process categories	: PROC1, PROC3, PROC4, PROC5, PROC8a, PROC8b, PROC9, PROC10, PROC15
Environmental Release Categories	: ERC2, ERC4, ERC6a, ERC6b:

2.2 Contributing scenario controlling worker exposure for: PROC1, PROC3, PROC4, PROC5, PROC8a, PROC8b, PROC9, PROC10, PROC15

Product characteristics

Concentration of the Substance in Mixture/Article : Covers the percentage of the substance in the product up to 100 % (unless stated differently).
 Physical Form (at time of use) : Solid, medium dustiness
 Process Temperature : < 116 °C

Frequency and duration of use

Frequency of use : 8 hours/day
 Frequency of use : 5 days/week

Other operational conditions affecting workers exposure

Outdoor / Indoor : Indoor without local exhaust ventilation (LEV)

Conditions and measures related to personal protection, hygiene and health evaluation

Wear suitable gloves tested to EN374., Tightly fitting safety goggles

Additional good practice advice beyond the REACH Chemical Safety Assessment

Wear suitable coveralls to prevent exposure to the skin.

3. Exposure estimation and reference to its source

Environment

A chemical safety assessment was performed according REACH Article 14(3), Annex I, sections 3 (Environmental Hazard assessment) and 4 (PBT/vPvB Assessment). As no hazard was identified, an exposure assessment and risk characterisation is not necessary (REACH Annex I section 5.0).

Workers

Contributing Scenario	Exposure Assessment Method	Specific conditions	Value	Level of Exposure	RCR*
PROC1	ECETOC TRA 3	longterm, inhalative, systemic			< 0.01
PROC1	ECETOC TRA 3	longterm, dermal, systemic			< 0.01
PROC1		longterm, combined, systemic			< 0.01
PROC3	ECETOC TRA 3	longterm, inhalative, systemic			0.018
PROC3	ECETOC TRA 3	longterm, dermal, systemic			0.018
PROC3		longterm, combined, systemic			0.036

PROC4	ECETOC TRA 3	longterm, inhalative, systemic			0.093
PROC4	ECETOC TRA 3	longterm, dermal, systemic			0.180
PROC4		longterm, combined, systemic			0.273
PROC5	ECETOC TRA 3	longterm, inhalative, systemic			0.093
PROC5	ECETOC TRA 3	longterm, dermal, systemic			0.361
PROC5		longterm, combined, systemic			0.454
PROC8a	ECETOC TRA 3	longterm, inhalative, systemic			0.093
PROC8a	ECETOC TRA 3	longterm, dermal, systemic			0.361
PROC8a		longterm, combined, systemic			0.454
PROC8b	ECETOC TRA 3	longterm, inhalative, systemic			0.019
PROC8b	ECETOC TRA 3	longterm, dermal, systemic			0.361
PROC8b		longterm, combined, systemic			0.379
PROC9	ECETOC TRA 3	longterm, inhalative, systemic			0.093
PROC9	ECETOC TRA 3	longterm, dermal, systemic			0.180
PROC9		longterm, combined, systemic			0.273
PROC10	ECETOC TRA 3	longterm, inhalative, systemic			0.093
PROC10	ECETOC TRA 3	longterm, dermal, systemic			0.722
PROC10		longterm, combined, systemic			0.815
PROC15	ECETOC TRA 3	longterm,			< 0.01

		inhalative, systemic			
PROC15	ECETOC TRA 3	longterm, dermal, systemic			< 0.01
PROC15		longterm, combined, systemic			0.018

*Risk characterisation ratio

4. Guidance to Downstream User to evaluate whether he works inside the boundaries set by the Exposure Scenario

For scaling of worker exposure assessments performed with ECETOC TRA, please consult the Merck tool ScIDeEx® at www.merckmillipore.com/scideex.
Please refer to the following documents: ECHA Guidance on information requirements and chemical safety assessment Chapter R.12: Use descriptor system; ECHA Guidance for downstream users; ECHA Guidance on information requirements and chemical safety assessment Part D: Exposure Scenario Building, Part E: Risk Characterisation and Part G: Extending the SDS; VCI/Cefic REACH Practical Guides on Exposure Assessment and Communications in the Supply Chain; CEFIC Guidance Specific Environmental Release Categories (SPERCs).

1. Short title of Exposure Scenario: Professional use

Main User Groups : **SU 22**
 Sectors of end-use : **SU 22**
 Chemical product category : **PC21**
 Process categories : **PROC15**
 Environmental Release Categories : **ERC2, ERC6a, ERC6b:**

2.2 Contributing scenario controlling worker exposure for: PROC15

Product characteristics

Concentration of the Substance in Mixture/Article : Covers the percentage of the substance in the product up to 100 % (unless stated differently).
 Physical Form (at time of use) : Solid, medium dustiness
 Process Temperature : < 116 °C

Frequency and duration of use

Frequency of use : 8 hours/day
 Frequency of use : 5 days/week

Other operational conditions affecting workers exposure

Outdoor / Indoor : Indoor without local exhaust ventilation (LEV)

Conditions and measures related to personal protection, hygiene and health evaluation

Wear suitable gloves tested to EN374., Tightly fitting safety goggles

Additional good practice advice beyond the REACH Chemical Safety Assessment

Wear suitable coveralls to prevent exposure to the skin.

3. Exposure estimation and reference to its source

Environment

A chemical safety assessment was performed according REACH Article 14(3), Annex I, sections 3 (Environmental Hazard assessment) and 4 (PBT/vPvB Assessment). As no hazard was identified, an exposure assessment and risk characterisation is not necessary (REACH Annex I section 5.0).

Workers

Contributing Scenario	Exposure Assessment Method	Specific conditions	Value	Level of Exposure	RCR*
PROC15	ECETOC TRA 3	longterm, inhalative, systemic			< 0.01
PROC15	ECETOC TRA 3	longterm, dermal, systemic			< 0.01
PROC15		longterm, combined, systemic			0.01

*Risk characterisation ratio

4. Guidance to Downstream User to evaluate whether he works inside the boundaries set by the Exposure Scenario

For scaling of worker exposure assessments performed with ECETOC TRA, please consult the Merck tool ScIDeEx® at www.merckmillipore.com/scideex.

Please refer to the following documents: ECHA Guidance on information requirements and chemical safety assessment Chapter R.12: Use descriptor system; ECHA Guidance for downstream users; ECHA Guidance on information requirements and chemical safety assessment Part D: Exposure Scenario Building, Part E: Risk Characterisation and Part G: Extending the SDS; VCI/Cefic REACH Practical Guides on Exposure Assessment and Communications in the Supply Chain; CEFIC Guidance Specific Environmental Release Categories (SPERCs).