

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 13.08.2018

Version 5.9

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

1.1 Product identifier

Catalogue No.	808333
Product name	Methyl-4-toluenesulfonate for synthesis
REACH Registration Number	01-2120752485-49-xxxx
CAS-No.	80-48-8

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.
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SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Acute toxicity, Category 4, Oral, H302

Skin corrosion, Category 1B, H314

Skin sensitisation, Category 1, H317

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

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Product name Methyl-4-toluenesulfonate for synthesis

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H317 May cause an allergic skin reaction.

Precautionary statements

Prevention

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

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.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

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Hazard statements

H314 Causes severe skin burns and eye damage.

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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.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

Contains: methyl 4-toluenesulphonate

CAS-No. 80-48-8

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	4-(CH ₃)C ₆ H ₄ SO ₃ CH ₃	C ₈ H ₁₀ O ₃ S (Hill)
EC-No.	201-283-5	
Molar mass	186,23 g/mol	

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

Chemical name (Concentration)

CAS-No.	Registration number	Classification
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methyl 4-toluenesulphonate (>= 80 % - <= 100 %)

80-48-8	01-2120752485-49-
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xxxx

Acute toxicity, Category 4, H302

Skin corrosion, Category 1B, H314

Skin sensitisation, Category 1, H317

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Toluene ($\geq 1\%$ - $< 3\%$)

108-88-3 01-2119471310-51-
xxxx

Flammable liquid, Category 2, H225
Skin irritation, Category 2, H315
Reproductive toxicity, Category 2, H361d
Specific target organ toxicity - single exposure, Category 3, H336
Specific target organ toxicity - repeated exposure, Category 2,
H373
Aspiration hazard, Category 1, H304

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. 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

irritant effects, Allergic reactions, Cough, Shortness of breath

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

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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

Combustible.

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

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

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.

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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

Storage conditions

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

Derived No Effect Level (DNEL)

Toluene (108-88-3)

Worker DNEL, acute	Systemic effects	inhalation	384 mg/m ³
Worker DNEL, acute	Local effects	inhalation	343 mg/m ³
Worker DNEL, longterm	Systemic effects	inhalation	192 mg/m ³

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Worker DNEL, longterm	Local effects	inhalation	192 mg/m ³
Worker DNEL, longterm	Systemic effects	dermal	384 mg/kg Body weight
Consumer DNEL, acute	Systemic effects	inhalation	226 mg/m ³
Consumer DNEL, acute	Local effects	inhalation	226 mg/m ³
Consumer DNEL, longterm	Systemic effects	inhalation	56,5 mg/m ³
Consumer DNEL, longterm	Systemic effects	oral	8,13 mg/kg Body weight
Consumer DNEL, longterm	Systemic effects	dermal	226 mg/kg Body weight

Predicted No Effect Concentration (PNEC)

Toluene (108-88-3)

PNEC Fresh water	0,68 mg/l
PNEC Fresh water sediment	16,39 mg/kg
PNEC Soil	2,89 mg/kg
PNEC Sewage treatment plant	13,61 mg/l

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

Safety glasses

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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

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/vapours/aerosols are generated.

Recommended Filter type: Filter P 2 (acc. to DIN 3181) for solid and liquid particles of harmful substances

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.

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SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	solid
Colour	colourless
Odour	like fruit
Odour Threshold	No information available.
pH	No information available.
Melting point	No information available.
Boiling point/boiling range	292 °C at 1.013 hPa
Flash point	130 °C Method: DIN 51758
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	0,13 kPa at 20 °C

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Relative vapour density	6,45 (Air = 1.0)
Density	ca. 1,23 g/cm ³ at 25 °C
Relative density	No information available.
Water solubility	at 20 °C insoluble
Partition coefficient: n-octanol/water	log Pow: 1,47 (calculated) Bioaccumulation is not expected. (External MSDS)
Auto-ignition temperature	No information available.
Decomposition temperature	> 292 °C
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

none

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.

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10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents, Strong acids, Bases

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

no information available

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: 341 mg/kg

(RTECS)

Acute inhalation toxicity

This information is not available.

Acute dermal toxicity

This information is not available.

Skin irritation

Result: Corrosive

Experience with human exposure

Causes burns.

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Eye irritation

Causes serious eye damage.

Risk of blindness!

Sensitisation

May cause an allergic skin reaction.

Germ cell mutagenicity

This information is not available.

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

After absorption:

We have no description of any symptoms of toxicity.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

No information available.

12.2 Persistence and degradability

No information available.

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12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 1,47

(calculated)

Bioaccumulation is not expected. (External MSDS)

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

Discharge into the environment must be avoided.

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. (METHYLTOLUENESULFONATE)
14.3 Class	8
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

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

Sea transport (IMDG)

14.1 UN number	UN 3261
14.2 Proper shipping name	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (METHYLTOLUENESULFONATE)
14.3 Class	8
14.4 Packing group	II
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. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.
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Product name	Methyl-4-toluenesulfonate for synthesis

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

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).
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National legislation

Storage class	8A
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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.

H225	Highly flammable liquid and vapour.
H302	Harmful if swallowed.
H304	May be fatal if swallowed and enters airways.
H314	Causes severe skin burns and eye damage.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H336	May cause drowsiness or dizziness.
H361d	Suspected of damaging the unborn child.
H373	May cause damage to organs through prolonged or repeated exposure.

Training advice

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Provide adequate information, instruction and training for operators.

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.