

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 7.0

Revision Date 14.08.2024

Print Date 20.08.2024

GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Methyl benzoate for synthesis

Product Number : 8.22330
Catalogue No. : 822330
Brand : Millipore
REACH No. : 01-2119969268-21-XXXX
CAS-No. : 93-58-3

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

Identified uses : Chemical for synthesis

1.3 Details of the supplier of the safety data sheet

Company : Merck KGaA
Frankfurter Str. 250
D-64271 DARMSTADT

Telephone : +49 (0)6151 72-0
Fax : +49 6151 727780
E-mail address : TechnicalService@merckgroup.com

1.4 Emergency telephone

Emergency Phone # : +(44)-870-8200418 (CHEMTREC (GB))
+(353)-19014670 (CHEMTREC Ireland)
001-803-017-9114 (CHEMTREC India)

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture**

Acute toxicity, (Category 4) H302: Harmful if swallowed.

Reproductive toxicity, (Category 2) H361d: Suspected of damaging the unborn child.

2.2 Label elements**Labelling according Regulation (EC) No 1272/2008**

Pictogram



Signal Word	Warning
Hazard Statements	
H302	Harmful if swallowed.
H361d	Suspected of damaging the unborn child.
Precautionary Statements	
P202	Do not handle until all safety precautions have been read and understood.
P264	Wash skin thoroughly after handling.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P405	Store locked up.
Supplemental Hazard Statements	none

Reduced Labeling (<= 125 ml)

Pictogram



Signal Word	Warning
Hazard Statements	
H361d	Suspected of damaging the unborn child.
Precautionary Statements	
P202	Do not handle until all safety precautions have been read and understood.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P405	Store locked up.
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.

Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula : C₈H₈O₂

Millipore- 8.22330

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The life science business of Merck operates as MilliporeSigma in the US and Canada



Molecular weight : 136,15 g/mol
CAS-No. : 93-58-3
EC-No. : 202-259-7

Component		Classification	Concentration
Methyl benzoate			
CAS-No.	93-58-3	Acute Tox. 4; Repr. 2; H302, H361d	<= 100 %
EC-No.	202-259-7		

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

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. Consult a physician.

In case of eye contact

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

If swallowed

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

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

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

Remove container from danger zone and cool with water. 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: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. 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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep locked up or in an area accessible only to qualified or authorized persons.

Recommended storage temperature see product label.

Storage class

Storage class (TRGS 510): 10: Combustible liquids

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

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). Safety glasses

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0,7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

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 EN 16523-1 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: 0,4 mm

Break through time: 10 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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) Physical state | liquid |
| b) Color | colorless |



c) Odor	characteristic odour
d) Melting point/freezing point	Melting point: -14,5 °C at 1.013,25 hPa - Regulation (EC) No. 440/2008, Annex, A.1
e) Initial boiling point and boiling range	199,5 °C at 1.013 hPa - OECD Test Guideline 103
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	Upper explosion limit: 20 %(V) Lower explosion limit: 8,6 %(V)
h) Flash point	77 °C - Pensky-Martens closed cup
i) Autoignition temperature	537 - 547 °C at 1.019 hPa
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: 1,94 mPa.s at 23 °C
m) Water solubility	2,1 g/l at 20 °C - soluble
n) Partition coefficient: n-octanol/water	log Pow: 2,1 - Bioaccumulation is not expected.
o) Vapor pressure	0,51 hPa at 25 °C
p) Density	1,088 g/cm ³
Relative density	1,08 at 20 °C - OECD Test Guideline 109
q) Relative vapor density	4,7 - (Air = 1.0)
r) Particle characteristics	No data available
s) Explosive properties	Not classified as explosive.
t) Oxidizing properties	none

9.2 Other safety information

Relative vapor density	4,7 - (Air = 1.0)
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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.

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 alkalis
rubber
various plastics

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

No data 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 toxicity

LD50 Oral - Rat - male - 1.625 mg/kg
(OECD Test Guideline 401)
Symptoms: Stomach/intestinal disorders, Nausea, Vomiting
Acute toxicity estimate Oral - 1.625 mg/kg
(ATE value derived from LD50/LC50 value)
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit
Result: No eye irritation - 72 h
(OECD Test Guideline 405)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse
Result: negative
(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Mutagenicity (mammal cell test): micronucleus.
Test system: Human lymphocytes
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 487
Result: negative
Test Type: In vitro mammalian cell gene mutation test
Test system: Chinese hamster lung cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative

Carcinogenicity

No data available

Reproductive toxicity



Suspected of damaging the unborn child.

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

Endocrine disrupting properties

Product:

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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

Systemic effects:

Headache
Dizziness

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	semi-static test LC50 - Danio rerio (zebra fish) - 23 mg/l - 96 h (Regulation (EC) No. 440/2008, Annex, C.1)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - 111,9 mg/l - 72 h (Directive 67/548/EEC, Annex V, C.3.)
Toxicity to bacteria	

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 29 d Result: 62 % - Readily biodegradable. (Regulation (EC) No. 440/2008, Annex, C.4-C) Remarks: The 10 day time window criterion is not fulfilled.
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12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available



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.

Product:

Assessment	: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.
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Discharge into the environment must be avoided.

No data available

ADR/RID: - IMDG: - IATA: -

ADR/RID: Not dangerous goods
IMDG: Not dangerous goods
IATA: Not dangerous goods

ADR/RID: - IMDG: - IATA: -

ADR/RID: - IMDG: - IATA: -

ADR/RID: no IMDG Marine pollutant: no IATA: no

No data available

Further information : No data available

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

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

H302	Harmful if swallowed.
H361d	Suspected of damaging the unborn child.

Relevant changes since previous version

2. Hazards identification

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative



Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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